FINAL REPORT

TEXAS AIR QUALITY RESEARCH PROGRAM

April 30, 2010 through April 27, 2016

Texas Commission on Environmental Quality
Contract Number 582-10-94300
Awarded to The University of Texas at Austin

Submitted to

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Final Report

Executive Summary

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

The Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP for the 2010 – 2011 biennium beginning on April 30, 2010. That contract was renewed for the 2012 – 2013 and 2014 – 2015 biennia, and the end date was extended to April 27, 2016, to allow for final project close out and reporting. Over this period, the AQRP funded 52 air quality research projects for a total of $9,561,372.87. These projects contributed to the scientific understanding of air quality in Texas in a variety of areas including emissions, tropospheric chemistry, and atmospheric chemical processes, through field studies, data analysis, and modeling activities. A State of the Science Assessment was completed at the end of the first and third biennia, to summarize the findings of the AQRP research projects.

AQRP administrative activities focused primarily on proposal solicitation and review, contracting, financial oversight, and reporting to the TCEQ. Proposal solicitation and review included developing research priorities, issuing and publicizing the request for proposals, as well as, managing the proposal review process through the technical, relevancy, and funding assessments. Once individual proposals were selected for funding, the AQRP negotiated contracts with each entity involved in the research. This required close interaction with the project managers as the project work plans were developed and refined. Once a project became active, the AQRP administration provided close financial oversight throughout its life. These activities took place once per biennium, for a total of three rounds of research projects. Across the life of the AQRP, the administration worked closely with the TCEQ, providing detailed monthly financial reports, formal quarterly and annual reports, and frequent communication in the interim to facilitate the Program's success.

BACKGROUND

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

> Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.
>
> (b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.
>
> (c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.
>
> (d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.
>
> (e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.
>
> (f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010 for the 2010-2011 biennium, and was renewed in June 2011 for the 2012-2013 biennium and in June 2013 for the 2014-2015 biennium. The contract ended on April 27, 2016. Consistent with the provisions in HB 1796, 10% of the available funding was used for program administration; the remainder (90%) of the available funding was used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

For the 2010-2011 biennium, the AQRP had approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released its first request for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received. After review by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs, the results of the reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. A total of 15 proposals were selected for funding. All projects were completed as of November 30, 2011, and final reports have been posted to the AQRP website.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding of $1,000,000 for the FY 2012 period was awarded in February 2012. An additional $1,000,000 for the FY 2013 period was awarded in June 2012. At the same time an additional $160,000 was awarded for FY 2012, to support funding for two specific air quality projects recommended by the TCEQ. A call for proposals was released in May 2012. Thirty-two proposals, requesting $5 million in research funding were received. The proposals were reviewed by the ITAC and the TCEQ. The Advisory Council selected 14 projects for funding.

In June 2013, the TCEQ issued Amendment 9 to the AQRP grant. This amendment had two purposes, 1) it renewed the AQRP for the 2014-2015 biennium (but did not award any funding for that biennium), and 2) it awarded an additional $2,500,000 in FY 2013 funds. Ten percent (10%) of these funds were allocated for Project Administration, and the remaining funds were allocated to the Research program per the terms of the AQRP grant. A portion of the research funds were awarded to the 2012-2013 Discover-AQ Ground Sites Infrastructure Support project, in order to expand logistical support for the Discover-AQ study, at the request of TCEQ and with the Advisory Council's approval.

All 2012 – 2013 research projects were completed by November 30, 2013. The final reports for the projects have been posted to the AQRP website. All FY 2012 funds were fully expended and the remaining FY 2013 funds were held for use on future projects.

After the TCEQ issued Amendment 9 to renew the grant, the AQRP developed the FY 2014 - 2015 research priorities and submitted them to the ITAC for input and to the TCEQ for review. Funding of $1,000,000 for FY 2014 and $1,000,000 for FY 2015 was awarded via Amendment 10 in October 2013. A call for proposals was released and by the November 22, 2013 due date, 31 proposals requesting $5.8 million in research funding were received. In December and January the ITAC and the TCEQ reviewed the proposals. The Advisory Council selected 16 projects for funding. These projects were funded with a combination of FY 2013, 2014, and 2015 funds.

All 2014 – 2015 projects were completed by November 30, 2015 and the final reports were posted to the AQRP website. All FY 2013 and 2014 funds were fully expended. A total of $804.90 of FY 2015 funds were returned to the TCEQ.

RESEARCH PROJECT CYCLE

The Research Program was implemented through a 9 step cycle. The steps in the cycle are described below from project concept generation to final project evaluation for a single project cycle.

1.) The project cycle was initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and the TCEQ, developed research priorities; the research priorities were released together with a Request for Proposals.

2.) Project proposals relevant to the research priorities were solicited via the Request for Proposals (RFP). The RFP was posted on the AQRP website and an email notification went out to over 400 email addresses of individuals who have shown a past interest in air quality research in Texas.

3.) The Independent Technical Advisory Committee (ITAC) performed a scientific and technical evaluation of the proposals.

4.) The project proposals and ITAC recommendations were forwarded to the TCEQ. The TCEQ evaluated the project recommendations from the ITAC and commented on the relevancy of the projects to the State's air quality research needs.

5.) The recommendations from the ITAC and the TCEQ were presented to the Council and the Council selected the proposals to be funded. The Council also provided comments on the strategic research priorities.

6.) All Investigators were notified of the status of their proposals, either funded, not funded, or not funded at this time, but held for possible reconsideration if funding became available.

7.) Funded projects were assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin was responsible for ensuring that project objectives were achieved in a timely manner and that effective communication was maintained among investigators involved in multi-institution projects. The Project Manager had responsibility for documenting progress toward project measures of success for each project. The Project Manager worked with the researchers, and the TCEQ, to create an approved work plan for the project.

    The Project Manager also worked with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved Quality Assurance Project Plan (QAPP) for each project. The Project Manager reviewed monthly, annual and final reports from the researchers and worked with the researchers to address deficiencies.

8.) The AQRP Director and the Project Manager for each project described progress on the project in the ITAC and Council meetings dedicated to on-going project review.

9.) The project findings were communicated through multiple mechanisms. Final reports were posted to the Program web site; research briefings were developed for the public and air quality decision makers; and a bi-annual research conference/data workshop was held.

Independent Technical Advisory Committee (ITAC)

The AQRP funding was used primarily for research projects, and one of three groups responsible for selecting the projects was the Independent Technical Advisory Committee (ITAC). The ITAC, composed of up to 15 individuals with scientific expertise relevant to the Program, was charged with recommending technical approaches, and establishing research priorities. Initially, the ITAC was to meet at least twice per year at locations rotating between Austin, Dallas and Houston. As the Program proceeded, it was more efficient for the ITAC to meet once in Austin and as needed via conference call/webinar. Generally, the meetings in Austin were dedicated to new project review, reviewing progress on funded projects, and reviewing the Program's strategic plan.

Members of the ITAC consisted of the TCEQ Project Director (or designee), the AQRP Program Director, and representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC were drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas. The members of the ITAC are listed in Table 1.

As the ITAC membership was intentionally drawn from air quality researchers who had experience in Texas; many of these researchers and their colleagues had an interest in responding to the requests for research proposals issued by the AQRP. This raised potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas required that the AQRP maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members were required to certify:

> *Confidentiality:* As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)

Table 1: Members of the Independent Technical Advisory Committee

Name	Title	Organization
David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	University of Colorado - Boulder
Sarwar Golam	Research Physical Scientist, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Tho (Thomas) Ching Ho	Chairman, Dan F. Smith Dept. of Chemical Engineering	Lamar University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Associate Professor, Department of Earth and Atmospheric Sciences	The University of Houston
John Nielsen-Gammon	Professor and Texas State Climatologist Center for Atmospheric Chemistry and the Environment	Texas A&M University
David Parrish	Program Lead, Tropospheric Chemistry, NOAA/ESRL/Chemical Sciences Division	National Oceanic and Atmospheric Administration
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Associate Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ

Conflict of Interest: As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or the TCEQ Project Director. If there is a question of interpretation regarding whether a conflict of interest exists, I agree that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Most members of the ITAC were active participants throughout the Program period, attending both in person meetings and conference calls when requested, and responding in a timely manner to email requests for information or electronic voting when requested by the AQRP Administration. This allowed for a well-informed and effective committee to provide advice on technical matters.

TCEQ Relevancy Review

Once the ITAC reviewed and ranked research project proposals according to technical merit, they were submitted to the TCEQ for a relevancy review. The TCEQ reviewed proposals for relevancy to the State's air quality research needs. TCEQ approval was required for a project to receive funding from the Program.

Advisory Council

The final group responsible for selecting AQRP research projects was the Advisory Council. The Council consisted of up to 11 members, all residents of the State of Texas. Two Council members with relevant scientific expertise were nominated by the TCEQ. As defined in the AQRP contract, up to four members of the Council could be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. Additional members included government officials from Texas Near-Non-Attainment Areas active in air quality management. The purpose of the Council was to give final approval to projects recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. At least one meeting in Austin was dedicated to new project selection. Additional meetings, either in person or via webinar, and email updates were dedicated to providing summaries of on-going projects and review of the strategic plan.

The members of the Advisory Council all attempted to actively engage in the AQRP.

Table 2: Members of the Advisory Council

Name	Title	Organization
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

Administrative and Project Management Overview of the Research Projects

From an administrative and project management perspective, most of the research projects progressed with minimal problems. The challenges that did arise were primarily related to negotiating contracts and the timeliness of meeting reporting requirements. In the first biennium of the program, The University of Texas at Austin was unable to come to terms with entities such as the National Center for Atmospheric Research (NCAR) and the National Oceanic and Atmospheric Administration (NOAA), as well a Pennsylvania State University due to terms in the contract related to indemnity, insurance, and other similar issues. Discussions on these issues with TCEQ resulted in an amendment to the contract between UT Austin and the TCEQ. While the amendment did not provide the necessary changes to enable a contract with NOAA and NCAR, it did ease the negotiations with other out of state academic entities.

Once projects became active, most investigators met all reporting requirements in a timely manner. Delays in the submission of the final reports, or revisions to final reports did occur on a few projects, but active follow up by the Project Managers ensured that all reports were finalized before critical program deadlines passed.

Frequent communication between the AQRP administration and the TCEQ program manager enabled a smooth flow of information in both directions. Procedures and processes were developed to meet the needs of both agencies and potential issues were addressed quickly and efficiently.

FINANCIAL STATUS REPORT

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May 2010 an amendment was issued increasing the budget by $40,000. Funding for fiscal year 2011 was established at $2,106,071, for a total award of $4,878,142 for the FY 2010/2011 biennium. FY 2010 funds were fully expended in early 2012 and the FY 2011 funds expired on June 30, 2013 with a remaining balance of $0.11.

In February 2012, funding of $1,000,000 was awarded for FY 2012. In June 2012, an additional $160,000 was awarded in FY 2012 funds and $1,000,000 was awarded in FY 2013 funds, for a total of $2,160,000 in funding for the FY 2012/2013 biennium.

In April 2013, the grant was amended to reduce the FY 2012 funds by $133,693.60 and increase the FY 2011 funds by the same amount.

In June 2013, the grant was amended to increase the FY 2013 funds by $2,500,000.

In October 2013, the grant was amended to award FY 2014 funds of $1,000,000 and FY 2015 funds of $1,000,000. The budget for each fiscal year can be found in Appendix C.

FY 2012 funds were fully expended at the end of April 2014. FY 2013 funds were fully expended at the end of June 2015.

The program end date was April 27, 2016. As of that date, FY 2014 and FY 2015 funds were nearly fully expended, pending the final close-out of the accounts. At the end of May 2016, one project returned funds in the amount of $804.90 due to a prior rate adjustment that was not reflected in an earlier invoice. As these funds were returned after the end date of the AQRP, they will be returned to the TCEQ. Final close-out of the accounts will occur in July 2016. At that time an amount not to exceed $810.00 is expected to be returned to the AQRP.

For each biennium (and fiscal year) of the program the funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories were:

Program Administration – limited to 10% of the overall funding (per Fiscal Year)
This category included all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also included the costs for the Council meetings.

ITAC
These funds covered the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project was assigned a Project Manager to ensure that project objectives were achieved in a timely manner and that effective communication was maintained among investigators in multi-institution projects. These funds were to support the staffing and performance of project management.

Research Projects / Contractual
These were the funds available to support the research projects that were selected for funding.

Program Administration

Program Administration included salaries and fringe benefits for those overseeing the program as a whole, as well as materials and supplies, travel, equipment, and other expenses. This category allowed indirect costs in the amount of 10% of salaries and wages.

During the reporting period several staff members were involved, part time, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, was responsible for the overall administration of the AQRP. James Thomas, AQRP Manager, was responsible for assisting Dr. Allen in the program administration. Maria Stanzione, AQRP Grant Manager, with Rachael Bushn, Melanie Allbritton, and Susan McCoy each provided assistance with program organization and financial management. This included assisting with the contracting process. Denzil Smith was responsible for the AQRP Web Page development and for data management.

Fringe benefits for the administration of the AQRP were initially budgeted to be 22% of salaries and wages across the term of the project. It should be noted that this was an estimate, and actual fringe benefit expenses were reported for each month. The fringe benefit amount and percentage fluctuated each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. For example, the amount of fringe benefits was greater for a person with family medical insurance versus a person with individual medical insurance. Actual fringe benefit expenses to date are included in the spreadsheets provided in this report.

Research Projects

FY 2010-2011

The FY 2010 Research/Contractual budget was originally funded at $2,286,000. After all transfers, it was increased by $1,827.93. The FY 2011 Research/Contractual budget was originally funded at $1,736,063. After all transfers, it was increased by $377.62, plus an additional $116,000 from FY 2012 funds that were changed to FY 2011 funds. This was an overall net increase of $13,205.55 to the Research/Contractual funds (and net reduction in Project Management/ITAC funds). ($105,000 in FY 2012 research funds were transferred to FY 2011, the remaining $11,000 were transfers from Project Management funds.)

All FY 2010 Research Project funding was fully expensed before the expiration of FY 2010 funds in June 2012. The FY 2011 Research Project funding that remained after all FY 2011 research projects were completed was allocated to FY 2012-2013 projects. This included the funds that were reallocated from FY 2012 to FY 2011. The funds were allocated to project 13-016 Valparaiso and project 13-004 Discover AQ Infrastructure. Both projects utilized their FY 2011 funds (project 13-004 $116,000 and project 13-016 $20,168.90) by June 30, 2013. A remaining balance of $0.11 was returned to TCEQ.

Table 3 on the following pages illustrates the 2010-2011 Research Projects, including the funding awarded to each project and the total expenses reported on each project through the expiration of the FY 2011 funds on June 30, 2013.

FY 2012-2013

The FY 2012 Research/Contractual budget was originally funded at $815,000. Transfers increased the budget by $32,438.67. These funds were fully expended as of April 2014. The FY 2013 Research Contractual budget was originally funded at $835,000. In June 2013, Amendment 9 increased this budget by $2,100,000. (The remaining $400,000 was allocated to Admin and Project Management.) Transfers to date have increased that by an additional $55,026 for a total FY 2013 Research Contractual budget of $2,990,026. This includes funds transferred from the FY 13 Project Management budget to the Research Projects budget, in order to fund as many research projects as possible, and the return of $53,974 to FY 13 Project Management to cover the additional Project Manager needed for the additional 5 projects.

Funds that were not expended by the FY 2012 – 2013 research projects totaling $1,716,863.39 (including an April 2015 refund of $18.40 to a project that ended in March 2014) were allocated to projects from the FY 2014-2015 RFP, with $53,974 of the funds allocated to Project Management. Table 4 illustrates the 2012-2013 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of May 31, 2015.

Many of the projects from the FY 2014-2015 RFP were funded from a combination of FY 2013 funds and either FY 2014 or FY 2015 funds. In order to expend all FY 2013 funding by June 30, 2015, adjustments were made to the amount of FY 2013 funding allocated to specific projects, and project expenses that were originally charged to the FY 2014 or FY 2015 portion of the project funds were transferred to the FY 2013 portion.

FY 2014-2015

The FY 2014 and 2015 Research/Contractual budgets were originally funded at $825,000 each. This was increased by $7,500 each when the unused ITAC funds were transferred in June 2015. Research projects were awarded to FY 2013, 2014, and 2015 funds. As of June 2015, all FY 2013 funds were expended and all remaining expenditures on the Research Projects posted to FY 2014 or 2015 funds.

The State of the Science assessment project was funded from the remaining Research/Contractual funds and unspent funds that were returned from research projects as they were completed.

Several research projects requested an end date extension to November 30, 2015. Because this required additional Project Management time, $3006 in funds were transferred from the Research/Contractual category to Project Management in each fiscal year, in order to fund the extended effort of Project Management personnel. Project Management expenses are capped at 8.5% of the Research/Contractual budget. This cap was not exceeded. These funds also were made available from the research projects that did not fully expend their budgets.

Table 5 illustrates the portion of the Research Projects funded with FY 2014 – 2015 funds. This includes the funding awarded to each project (from this source of funding) and the total expenses reported on each project as of November 30, 2015.

The remaining Research/Contractual funds were spent on digital storage of the program information, including individual project data, through August 31, 2019, the time period specified in the agreement between UT and TCEQ. The remaining funds were utilized to extend the period of digital storage for an additional five years and six months per a request from TCEQ for a litigation hold.

Table 3: 2010/2011 Contractual Expenses

Contractual Expenses

FY 10 Contractual Funding	$2,286,000
FY 10 Contractual Funding Transfers	$1,827.93
FY 10 Total Contractual Funding	**$2,287,827.93**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-008	Rice University	$128,851	$126,622.32	$2,228.68
10-008	Environ International	$49,945	$49,944.78	$0.22
10-009	UT-Austin	$591,332	$591,306.66	$25.34
10-021	UT-Austin	$248,786	$248,786.41	-$0.41
10-022	Lamar University	$150,000	$132,790.80	$17,209.20
10-032	University of Houston	$176,314	$176,314	$0
10-032	University of New Hampshire	$23,054	$18,850.65	$4,203.35
10-032	UCLA	$49,284	$47,171.32	$2,112.68
10-034	University of Houston	$195,054	$186,657.54	$8,396.46
10-042	Environ International	$237,481	$237,479.31	$1.69
10-045	UCLA	$149,773	$142,930.28	$6,842.72
10-045	UNC - Chapel Hill	$33,281	$33,281	$0
10-045	Aerodyne Research Inc.	$164,988	$164,988.10	-$0.10
10-045	Washington State University	$50,000	$50,000	$0
10-DFW	UT-Austin	$37,857	$37,689.42	$167.58
FY 10 Total Contractual Funding Awarded		$2,286,000		
FY 10 Contractual Funding Expended (Init. Projects)			$2,244,812.59	
FY 10 Contractual Funds Remaining Unspent after Project Completion				$41,187.41
FY 10 Additional Projects				
	Data Storage	$7,015.34	$7,015.34	$0
10-SOS	State of the Science	$36,000.00	$36,000.00	$0
FY 10 Contractual Funds Expended to Date*			$2,287,827.93	
FY 10 Contractual Funds Remaining to be Spent				$0

FY 11 Contractual Funding		$1,736,063.00		
FY 11 Contractual Funding Transfers		$116,377.62		
FY 11 Total Contractual Funding		**$1,852,440.62**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179	$262,179	$0
10-006	University of Houston	$222,483	$217,949.11	$4,533.89
10-015	Environ International	$201,280	$201,278.63	$1.37
10-020	Environ International	$202,498	$202,493.48	$4.52
10-024	Rice University	$225,662	$223,769.99	$1,892.01
10-024	University of New Hampshire	$70,747	$70,719.78	$27.22
10-024	University of Michigan	$64,414	$60,597.51	$3,816.49
10-024	University of Houston	$98,134	$88,914.46	$9,219.54
10-029	Texas A&M University	$80,108	$78,276.97	$1,831.03
10-044	University of Houston	$279,642	$277,846.38	$1,795.62
11-DFW	UT-Austin	$50,952	$29,261.75	$21,690.25
FY 11 Total Contractual Funding Awarded		$1,758,099		
FY 11 Contractual Funds Expended (Init. Projects)			$1,713,287.06	
FY 11 Contractual Funds Remaining Unspent after Project Completion				$44,811.94
FY 11 Additional Projects				
	Data Storage	$2,984.66	$2,984.66	$0.00
	12-016 Valparaiso	$20,168.90	$20,168.90	$0.00
	12-004 Discover AQ Infrastructure	$116,000.00	$115,999.89	$0.11
FY 11 Contractual Funds Expended to Date*			$1,852,440.51	
FY 11 Contractual Funds Remaining to be Spent				$0.11
Total Contractual Funding		$4,022,063.00		
Total Contractual Funding Transfers		$118,205.55		
Total Contractual Funding Available		$4,140,268.55		
Total Contractual Funds Expended to Date			$4,140,268.44	
Total Contractual Funds Remaining				$0.11

Table 4. 2012/2013 Contractual Expenses

Contractual Expenses

FY 12 Contractual Funding	$815,000.00
FY 12 Contractual Funding Transfers	$32,438.67
FY 12 Total Contractual Funding	**$847,438.67**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
12-004	UT-Austin (Torres)	$20,174.10	$20,174.10	$0.00
12-006	UC-Riverside	$101,765.00	$101,765.00	$0.00
12-006	TAMU/TEES	$44,494.00	$42,134.22	$2,359.78
12-011	Environ International	$77,420.00	$77,410.16	$9.84
12-012	UT-Austin (Hildebrandt)	$79,463.00	$79,173.94	$289.06
12-012	Environ International	$69,374.00	$69,372.64	$1.36
12-013	Environ International	$59,974.00	$59,960.93	$13.07
12-018	UT-Austin (McDonald-Buller)	$85,282.00	$85,197.80	$84.20
12-018	Environ International	$21,688.00	$21,686.26	$1.74
12-028	University of Houston	$19,599.00	$16,586.51	$3,012.49
12-028	UCLA	$17,944.00	$17,709.51	$234.49
12-028	Environ International	$44,496.00	$44,496.00	$0.00
12-028	UNC - Chapel Hill	$35,230.00	$35,230.00	$0.00
12-032	Baylor	$45,972.00	$43,642.21	$2,329.79
12-TN1	Maryland	$64,994.00	$64,537.12	$456.88
12-TN2	Maryland	$69,985.00	$68,362.27	$1,622.73
FY 12 Total Contractual Funding Awarded		$847,438.67		
FY 12 Contractual Funds Expended to Date			$847,438.67	
FY 12 Contractual Funds Remaining to be Spent				$0.00

Note:
Project 12-004 on this page and Project 13-004 on the following page were the same project, with funding split across fiscal years. After all FY12 projects were completed and fully invoiced, the remaining FY12 funds were transferred to 12-004 and 13-004 was reduced by the same amount, so that the total project budget remained the same, but all FY12 funds could be expended.

FY 13 Contractual Funding		$835,000		
FY 13 Contractual Funding Transfers		$2,209,000		
FY 13 Total Contractual Funding		**$3,044,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
13-004	UT-Austin (Torres)	$1,555,770	$805,209.66	$750,560.24
13-005	Chalmers University of Tech	$129,047	$129,047.00	$0.00
13-005	University of Houston	$48,506	$44,928.24	$3,577.76
13-016	Valparaiso	$46,652	$46,652.10	$0.00
13-016	University of Houston	$19,846	$14,101.40	$5,744.60
13-022	Rice University	$89,912	$75,881.86	$14,030.14
13-022	University of Houston	$116,903	$116,122.47	$780.53
13-024	Maryland	$90,444	$89,658.88	$785.12
FY 13 Total Contractual Funding Awarded		$2,097,080		
FY 13 Contractual Funds Expended (Init. Projects)			$1,321,601.61	
FY 13 Contractual Funds Remaining Unspent				$1,722,398.39
FY 13 Additional Expenditures				
	DATA Storage	$5,535	$5,535	$0.00
FY 13 Contractual Funds Expended			$1,327,136.61	
FY 13 Contractual Funds Remaining Unspent				$1,716,863.39

Note:
After all FY13 projects were completed contractual funds in the amount of $1,716,844.99 remained. In April 2015, a refund of an expense totaling $18.40 was reimbursed to project 13-004, increasing the remaining funds to $1,716,863.39. The funds will be utilized for FY14 projects and will be accounted for on the following page.

FY 13 Remaining Contractual Funding		**$1,716,863.39**		
FY 13 Remaining Contractual Funding Transfers		**($53,974.00)**		
FY 13 Total Remaining Contractual Funding		**$1,662,889.39**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-002	University of CO - Boulder	$136,818.02	$136,818.02	$0.00
14-003	UNC Chapel Hill	$80,632.41	$80,632.41	$0.00
14-006	Sonoma Technology	$41,235.05	$41,235.05	$0.00
14-006	Valparaiso	$3,578.11	$3,578.11	$0.00
14-006	St. Edwards University	$0.00	$0.00	$0.00
14-007	Chalmers Univ.	$64,584.00	$64,548.00	$0.00
14-007	Univ. of Houston	$23,081.00	$23,081.00	$0.00
14-008	UT-Austin (McDonald-Buller)	$155,378.82	$155,378.82	$0.00
14-009	Rice University	$60,000.00	$60,000.00	$0.00
14-011	UT-Austin (McDonald-Buller)	$111,426.21	$111,426.21	$0.00
14-011	Environ	$6,000.00	$6,000.00	$0.00
14-016	Environ	$240,000.00	$240,000.00	$0.00
14-017	University of Alabama - Huntsville	$25,000.00	$25,000.00	$0.00
14-017	Rice University	$18,152.98	$18,152.98	$0.00
14-023	UT-Austin (Torres)	$25,874.37	$25,874.37	$0.00
14-023	Aerodyne	$10,712.74	$10,712.74	$0.00
14-024	UT-Austin (Hildebrandt Ruiz)	$138,585.78	$138,585.78	$0.00
14-024	Environ	$25,000.00	$25,000.00	$0.00
14-024	UC Riverside	$30,875.39	$30,875.39	$0.00
14-025	Environ	$89,000.00	$89,000.00	$0.00
14-025	TAMU	$47,970.84	$47,970.84	$0.00
14-029	Baylor University	$109,650.32	$109,650.32	$0.00
14-030	TEES	$112,056.23	$112,056.23	$0.00

FY 13 Total Remaining Contractual Funding Awarded	$1,662,889.39		
FY 13 Remaining Contractual Funds Expended		$1,662,889.39	
FY 13 Remaining Contractual Funds Remaining to be Spent			$0.00
Total Contractual Funding	$3,837,464.67		
Total Contractual Funding Awarded	$3,837,464.67		
Total Contractual Funding Remaining to be Awarded	$0		
Total Contractual Funds Expended to Date		$3,837,464.67	
Total Contractual Funds Remaining to be Spent			$0.00

Table 5. 2014/2015 Contractual Expenses

Contractual Expenses

FY 14 Contractual Funding	**$825,000**
FY 14 Contractual Funding Transfers	**$4,494**
FY 14 Total Contractual Funding	**$829,494**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-002	CU - Boulder	$13,689.98	$13,685.68	$4.30
14-002	Univ. of Maryland	$49,387.00	$49,386.97	$0.03
14-003	UNC Chapel Hill	$119,367.59	$119,279.00	$88.59
14-004	Univ. of Maryland	$55,056.00	$55,055.96	$0.04
14-004	Morgan State Univ.	$54,055.00	$53,899.53	$155.47
14-006	St. Edwards Univ.	$6,303.89	$3,506.72	$2,797.17
14-009	Rice Univ.	$49,867.00	$46,259.42	$3,607.58
14-009	Univ. of Houston	$109,635.00	$106,416.84	$3,218.16
14-014	Univ. of Houston	$84,927.00	$82,769.39	$2,157.61
14-022	Univ. of Alabama–Huntsville	$71,004.00	$71,004.00	$0.00
14-022	George Mason Univ.	$44,996.00	$44,719.46	$276.54
14-026	Environ	$58,284.88	$57,801.91	$482.97
14-030	TAMU/TEES	$64,052.77	$43,690.03	$20,362.74
FY 14 Total Contractual Funding Awarded		$780,626.11		
FY 14 Contractual Funds Expended to Date			$747,474.91	
FY 14 Contractual Funds Remaining Unspent				$33,151.20
FY 14 Additional Expenditures				
	State of the Science	$50,000.00	$50,000.00	$0.00
	Data Storage	$32,019.09	$32,019.09	$0.00
FY 14 Contractual Funds Expended			$829,494.00	
FY 14 Contractual Funds Remaining to be Spent				$0.00

FY 15 Contractual Funding		**$825,000**		
FY 15 Contractual Funding Transfers		**$4,494**		
FY 15 Total Contractual Funding		**$829,494**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-005	TAMU	$103,890.00	$84,373.04	$19,516.96
14-006	Sonoma Technology	$14,470.95	$14,468.72	$2.23
14-007	Chalmers University	$9,595.00	$9,595.00	$0.00
14-007	Univ. of Houston	$0.00	$0.00	$0.00
14-008	Univ. of Texas - Austin	$19,621.18	$17,406.12	$2,215.06
14-010	TAMU	$79,325.00	$78,456.53	$868.47
14-011	Univ. of Texas - Austin	$39,740.79	$39,655.48	$85.31
14-011	Environ	$22,419.00	$22,234.65	$184.35
14-016	Environ	$31,911.00	$29,354.48	$2,556.52
14-017	Univ. of Alabama - Huntsville	$112,003.00	$112,002.77	$0.23
14-017	Rice University	$44,826.02	$44,826.02	$0.00
14-020	Univ. of Maryland	$70,000.00	$69,996.13	$3.87
14-023	Aerodyne Research	$0.00	$0.00	$0.00
14-024	Univ. of Texas - Austin	$24,696.22	$24,696.22	$0.00
14-024	Environ	$76,404.00	$76,404.00	$0.00
14-025	Environ	$46,735.00	$46,603.98	$131.02
14-025	TAMU	$72,555.16	$67,819.58	$4,735.58
14-029	Baylor University	$69,028.68	$64,824.39	$4,204.29
FY 15 Total Contractual Funding Awarded		$837,221.00		
FY 15 Contractual Funds Expended (Init. Projects)			$802,717.11	
FY 15 Contractual Funds Remaining Unspent				$34,503.89

FY 15 Additional Expenditures			
Data Storage	$25,937.33	$25,937.33	$0.00
FY 15 Contractual Funds Expended to Date		$828,654.44	
FY 15 Contractual Funds Remaining to be Spent			$804.90
Total Contractual Funding	$1,658,953.34		
Total Contractual Funding Awarded	$1,658,953.34		
Total Contractual Funding Remaining to be Awarded	$0.00		
Total Contractual Funds Expended to Date		$1,658,148.44	
Total Contractual Funds Remaining to be Spent			$804.90

Financial Review

Over the past three biennia The University of Texas at Austin has administered a total of $11,537,337 for the Texas Air Quality Research Program. As stated earlier in this report, 10% of these funds were allocated for the administration of the program (including the Advisory Council costs), with the other 90% allocated to the research projects (including project, project management and ITAC costs). Much of the effort involved in the administration of the AQRP was focused on monitoring the use of funds by the research projects and providing detailed reports to the TCEQ on a monthly, quarterly, and annual basis.

Up to 8.5% of the research project funds were allowed for technical project management costs. Throughout the program, every effort was made to keep these costs as low as possible and maximize the funds available to the research projects. Final expenses for project management totaled $718,090 or just 7.45% of the research project funds (6.22% of total program funds).

Of the total program funds $9,635,882 (83.5%) was used to award a total of 54 projects that have provided new information from field studies, data analysis, and models to inform and improve upon air quality in Texas. Each research project was monitored closely by both the project manager and the AQRP administration to ensure that all project funds were used as affectively as possible towards meeting the project and program goals.

Some challenges arose in the monitoring of expenditures, most notably in the reimbursement of travel costs. The travel rules imposed by the TCEQ in the contract for the AQRP are uniformly more stringent than those imposed by the entities engaged in the research activities (as well as state of Texas and federal standards). This created confusion among the researchers and reporting problems from their various home institutions. It also created difficulties in the contracting process, with almost every entity requesting an exception to these provisions in its contract.

The most common issue was the requirement for actual receipts for meals, as opposed to allowing a standard charge for per diem. This was especially true of research projects that engaged in lengthy field studies. In these situations, researchers often had the ability to make their own meals at the lodging, and a daily trip to the grocery store was not an efficient use of time or resources. For these cases, the administration was able to work with TCEQ to allow for a per diem averaging across multiple days, as long as a receipt was also presented.

At the end of each research project cycle, the remaining funds from each project were released back to the AQRP. Most projects returned between 0% and 5% of the awarded funds. Three projects returned greater than 10% of the funds awarded. In at least one of these, the researcher was unable to complete all of the project tasks due to scheduling issues. Finally, one project was cancelled due to the partner providing site access backing out. This was early enough in the project cycle for the funds to be reallocated to a new project. The funds that were released back to the AQRP were either used to fund the State of the Science projects (see Appendix E) or to fund the storage of all program data at the Texas Advanced Computing Center, where it can be accessed for future use.

Appendix A

Research Projects

(Expenditures reported as of May 31, 2016)

FY 2010-2010 Funded Research Projects

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
10-006	**Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS**	**2/16/2011**	**11/30/2011**	**$484,662.00**	**$480,128.11**	**$4,533.89**
	*Chalmers University of Technology	Johan Mellqvist		$262,179.00	$262,179.00	$0.00
	University of Houston	Bernhard Rappenglüeck		$222,483.00	$217,949.11	$4,533.89
10-008	**Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling**	**10/21/2010**	**9/30/2011**	**$178,796.00**	**$176,567.10**	**$2,228.90**
	*Rice University	Daniel Cohan		$128,851.00	$126,622.32	$2,228.68
	ENVIRON International	Greg Yarwood		$49,945.00	$49,944.78	$0.00
10-009	**Additional Flare Test Days for TCEQ Comprehensive Flare Study**	**9/8/2010**	**11/30/2011**	**$591,332.00**	**$591,306.66**	**$25.34**
	*The University of Texas at Austin	Vincent Torres				
10-015	**An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-attainment areas in Texas**	**3/4/2011**	**11/30/2011**	**$201,280.00**	**$201,278.63**	**$1.37**
	*ENVIRON International	Greg Yarwood				
10-020	**NO_x Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone**	**3/5/2011**	**11/30/2011**	**$202,498.00**	**$202,493.48**	**$4.52**
	*ENVIRON International	Greg Yarwood				

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
10-021	**Dry Deposition of Ozone to Built Environment Surfaces**	**10/11/2010**	**8/31/2011**	**$248,786.00**	**$248,786.41**	**($0.41)**
	*The University of Texas at Austin	Richard Corsi				
10-022	**Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas**	**2/16/2011**	**11/30/2011**	**$150,000.00**	**$132,790.80**	**$17,209.20**
	*Lamar University	Daniel Chen				
10-024	**Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area**	**2/16/2011**	**9/30/2011**	**$458,957.00**	**$444,001.74**	**$14,955.26**
	*Rice University	Robert Griffin		$225,662.00	$223,769.99	$1,892.01
	University of Houston	Barry Lefer		$98,134.00	$88,914.46	$9,219.54
	University of New Hampshire	Jack Dibb		$70,747.00	$70,719.78	$27.22
	University of Michigan	Allison Steiner		$64,414.00	$60,597.51	$3,816.49
10-029	**Wind Modeling Improvements with the Ensemble Kalman Filter**	**12/1/2010**	**11/30/2011**	**$80,108.00**	**$78,276.97**	**$1,831.03**
	*Texas A & M University	John Neilson-Gammon				
10-032	**SHARP Data Analysis: Radical Budget and Ozone Production**	**2/9/2011**	**11/30/2011**	**$248,652.00**	**$242,335.97**	**$6,316.03**
	*University of Houston	Barry Lefer		$176,314.00	$176,314.00	$0.00
	University of California - Los Angeles	Jochen Stutz		$23,054.00	$18,850.65	$4,203.35
	University of New Hampshire	Jack Dibb		$49,284.00	$47,171.32	$2,112.68

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
10-034	**Dallas Measurements of Ozone Production**	**2/2/2011**	**11/30/2011**	**$195,054.00**	**$186,657.54**	**$8,396.46**
	*University of Houston	Barry Lefer				
10-042	**Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms**	**10/8/2010**	**11/30/2011**	**$237,481.00**	**$237,479.31**	**$1.69**
	*ENVIRON International	Greg Yarwood				
10-044	**Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season**	**3/25/2011**	**11/30/2011**	**$279,642.00**	**$277,846.38**	**$1,795.62**
	*University of Houston	Maxwell Shauck				
10-045	**Quantification of Hydrocarbon, NOx, and SO2 emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR dataset**	**1/22/2011**	**9/30/2011**	**$398,042.00**	**$391,199.38**	**$6,842.62**
	*University of California - Los Angeles	Jochen Stutz		$149,773.00	$142,930.28	$6,842.72
	University of North Carolina - Chapel Hill	William Vizeute		$33,281.00	$33,281.00	$0.00
	Aerodyne Research Inc.	Scott Herndon		$164,988.00	$164,988.10	($0.10)
	Washington State University	George Mount		$50,000.00	$50,000.00	$0.00
10-DFW	**Dallas - Fort Worth Field Study**	**2/1/2011**	**8/31/2011**	**$37,857.00**	**$37,689.42**	**$167.58**
	*The University of Texas at Austin	Vincent Torres				
11-DFW	**Dallas - Fort Worth Field Study**	**2/1/2011**	**8/31/2011**	**$50,952.00**	**$29,261.75**	**$21,690.25**
	*The University of Texas at Austin	Vincent Torres				

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
11-SOS	**State of the Science**	**2/8/2012**	**4/30/2012**	**$36,000.00**	**$36,000.00**	**$0.00**
	*The University of Texas at Austin	David Allen				
Notes:	The State of the Science project was funded from monies returned from the completed research projects. The Dallas - Fort Worth Field Study project was partially funded by a transfer of monies from the Project Management budget ($22,036). The full amount was returned to the Project Management budget at the conclusion of the Research Projects.					

FY 2012-2013 Funded Research Projects

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
12-004	**DISCOVER-AQ Ground Sites Infrastructure Support**	**3/1/2013**	**11/30/2013**	**$1,691,944**	**$941,383.65**	**$750,560.35**
	*The University of Texas at Austin	Vincent Torres				
13-005	**Quantification of industrial emissions of VOCs, NO2 and SO2 by SOF and mobile DOAS during DISCOVER AQ**	**1/15/2013**	**11/30/2013**	**$177,553.00**	**$173,975.24**	**$3,577.76**
	*Chalmers University of Technology	Johan Mellqvist		$129,047.00	$129,047.00	$0.00
	University of Houston	Barry Lefer		$48,506.00	$44,928.24	$3,577.76

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
12-006	**Environmental chamber experiments and CMAQ modeling to improve mechanisms to model ozone formation from HRVOCs**	**2/8/2013**	**11/30/2013**	**$146,259.00**	**$143,899.22**	**$2,359.78**
	*University of California - Riverside	Gookyoung Heo		$101,765.00	$101,765.00	$0.00
	Texas A&M University	Qi Ying		$44,494.00	$42,134.22	$2,359.78
12-011	**Investigation of Global Modeling and Lightning NOx Emissions as Sources of Regional Background Ozone in Texas**	**1/17/2013**	**11/30/2013**	**$77,420.00**	**$77,410.16**	**$9.84**
	*ENVIRON International	Chris Emery				
12-012	**Interactions Between Organic Aerosol and NOy: Influence on Oxidant Production**	**12/19/2012**	**11/30/2013**	**$148,837.00**	**$148,546.58**	**$290.42**
	*The University of Texas at Austin	Lea Hildebrandt Ruiz		$79,463.00	$79,173.94	$289.06
	ENVIRON International	Greg Yarwood		$69,374.00	$69,372.64	$1.36
12-013	**Development of Transformation Rate of SO2 to Sulfate for the Houston Ship Channel using the TexAQS 2006 Field Study Data**	**12/14/2012**	**11/30/2013**	**$59,974**	**$59,960.93**	**$13.07**
	* ENVIRON International	Ralph Morris				
13-016	**Ozonesonde launches from the University of Houston and Smith Point, Texas in Support of DISCOVER AQ**	**11/20/2012**	**11/30/2013**	**$86,667.00**	**$80,922.40**	**$5,744.60**
	*Valparaiso University	Gary Morris		$66,821.00	$66,821.00	$0.00
	University of Houston	Barry Lefer		$19,846.00	$14,101.40	$5,744.60

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
12-018	**The Effects of Uncertainties in Fire Emissions Estimates on Predictions of Texas Air Quality**	**1/8/2013**	**11/30/2013**	**$106,970.00**	**$106,884.06**	**$85.94**
	*The University of Texas at Austin	Elena McDonald-Buller		$85,282.00	$85,197.80	$84.20
	ENVIRON International	Chris Emery		$21,688.00	$21,686.26	$1.74
13-022	**Surface Measurements of PM, VOCs, and Photochemically Relevant Gases in Support of DISCOVER-AQ**	**1/29/2013**	**11/30/2013**	**$206,815.00**	**$192,004.33**	**$14,810.67**
	*Rice University	Robert Griffin		$89,912.00	$75,881.86	$14,030.14
	University of Houston	Barry Lefer		$116,903.00	$116,122.47	$780.53
13-024	**Surface Measurement of Trace Gases in Support of DISCOVER-AQ in Houston in Summer 2013**	**2/20/2013**	**11/30/2013**	**$90,444.00**	**$89,658.88**	**$785.12**
	*University of Maryland	Xinrong Ren				
12-028	**Implementation and evaluation of new HONO mechanisms in a 3-D Chemical Transport Model for Spring 2009 in Houston**	**1/29/2013**	**11/30/2013**	**$117,269.00**	**$114,022.02**	**$3,246.98**
	*University of Houston	Barry Lefer		$19,599.00	$16,586.51	$3,012.49
	University of California - Los Angeles	Jochen Stutz		$17,944.00	$17,709.51	$234.49
	ENVIRON International	Greg Yarwood		$44,496.00	$44,496.00	$0.00
	University of North Carolina – Chapel Hill	Will Vizuette		$35,230.00	$35,230.00	$0.00

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
12-032	**Collect, Analyze, and Archive Filters at two DISCOVER-AQ Houston Focus Areas: Initial Characterization of PM Formation and Emission Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms**	**1/25/2013**	**11/30/2013**	**$45,972.00**	**$43,642.21**	**$2,329.79**
	*Baylor University	Rebecca Sheesley				
12-TN1	**Investigation of surface layer parameterization of the WRF model and its impact on the observed nocturnal wind speed bias**	**2/21/2013**	**11/30/2013**	**$64,994.00**	**$64,537.12**	**$456.88**
	*University of Maryland	Daniel Tong / Pius Lee				
12-TN2	**Development of IDL-based geospatial data processing framework for meteorology and air quality modeling**	**2/21/2013**	**11/30/3013**	**$69,985.00**	**$68,362.27**	**$1,622.73**
	*University of Maryland	Daniel Tong / HyunCheol Kim				

FY 2014-2015 Funded Research Projects

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
14-002	**Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC4RS Campaigns**	**6/6/2014**	**11/30/2015**	**$199,895.00**	**$199,890.67**	**$4.33**
	*University of Colorado – Boulder	Alan Fried		$150,508.00	$150,503.70	$4.30
	University of Maryland	Christopher Loughner		$49,387.00	$49,386.97	$0.03
14-003	**Update and Evaluation of model algorithms needed to predict Particulate Matter from Isoprene**	**5/28/2014**	**6/30/2015**	**$200,000.00**	**$199,911.41**	**$88.59**
	*Univ. of North Carolina – Chapel Hill	William Vizuete		$200,000.00	$199,911.41	$88.59
14-004	**Emission Source region contributions to a high surface ozone episode during DISCOVER-AQ**	**6/20/2014**	**7/31/2015**	**$109,111.00**	**$108,955.49**	**$155.51**
	*University of Maryland	Christopher Loughner		$55,056.00	$55,055.96	$0.04
	Morgan State University	Melanie Follette-Cook		$54,055.00	$53,899.53	$155.47
14-005	**Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation**	**2/5/2015**	**9/30/2015**	**$103,890.00**	**$84,373.04**	**$19,516.96**
	*Texas A&M University	Sarah Brooks		$103,890.00	$84,373.04	$19,516.96

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
14-006	**Characterization of Boundary-Layer Meteorology during DISCOVER-AQ Using Radar Wind Profiler and Balloon Sounding Measurements**	**6/12/2014**	**10/31/2015**	**$65,588.00**	**$62,788.60**	**$2,799.40**
	*Sonoma Technology, Inc.			$55,706.00	$55,703.77	$2.23
	Valparaiso University			$3,578.11	$3,578.11	$0.00
	St. Edwards University			$6,303.89	$3,506.72	$2,797.17
14-007	**ImprovedAnalysis of VOC, NO2, SO2 and HCHO data from SOF, mobile DOAS and MW-DOAS during DISCOVER-AQ**	**6/23/2014**	**6/30/2015**	**$97,260.00**	**$97,260.00**	**$0.00**
	*Chalmers University			$74,179.00	$74,179.00	$0.00
	University of Houston			$23,081.00	$23,081.00	$0.00
14-008	**Investigation of Input Parameters for Biogenic Emissions Modeling in Texas during Drought Years**	**4/17/2014**	**7/31/2015**	**$175,000.00**	**$172,784.94**	**$2,215.06**
	*The University of Texas at Austin			$175,000.00	$172,784.94	$2,215.06
14-009	**Analysis of Surface Particulate Matter and Trace Gas Data Generated during the Houston Operations of DISCOVER-AQ**	**7/1/2014**	**6/30/2015**	**$219,502.00**	**$212,676.26**	**$6,825.74**
	*Rice University			$109,867.00	$106,259.42	$3,607.58
	University of Houston			$109,635.00	$106,416.84	$3,218.16

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
14-010	**Impact of large-scale circulation patterns on surface ozone concentrations in HGB**	**1/26/2015**	**11/30/2015**	**$79,325.00**	**$78,456.53**	**$868.47**
	*Texas A&M University – Galveston			$79,325.00	$78,456.53	$868.47
14-011	**Targeted Improvements in the Fire Inventory from NCAR (FINN) Model for Texas Air Quality Planning**	**6/23/2014**	**11/30/2015**	**$179,586.00**	**$179,316.34**	**$269.66**
	*The University of Texas at Austin			$151,167.00	$151,081.69	$85.31
	Environ			$28,419.00	$28,234.65	$184.35
14-014	**Constraining NOx Emissions Using Satellite NO2 and HCHO Column Measurements over the Southeast Texas**	**1/27/2015**	**11/30/2015**	**$84,927.00**	**$82,769.39**	**$2,157.61**
	*University of Houston			$84,927.00	$82,769.39	$2,157.61
14-016	**Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations**	**6/4/2014**	**6/30/2015**	**$271,911.00**	**$270,159.38**	**$1,571.62**
	*Environ			$271,911.00	$270,159.38	$1,571.62
14-017	**Incorporating Space-borne Observations to Improve Biogenic Emission Estimates in Texas**	**7/8/2014**	**11/30/2015**	**$199,982.00**	**$199,981.77**	**$0.23**
	*University of Alabama – Huntsville			$137,003.00	$137,002.77	$0.23
	Rice University			$62,979.00	$62,979.00	$0.00

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
14-020	**Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC4RS**	**2/2/2015**	**11/30/2015**	**$70,000.00**	**$69,996.13**	**$3.87**
	*University of Maryland			$70,000.00	$69,996.13	$3.87
14-022	**Use of satellite data to improve specifications of land surface parameters**	**2/19/2015**	**11/30/2015**	**$116,000.00**	**$114,687.90**	**$1,312.10**
	University of Alabama – Huntsville			$71,004.00	$69,968.44	$1,035.56
	George Mason University			$44,996.00	$44,716.46	$276.54
14-023	**Assessment of Two Remote Sensing Technologies to Control Flare Performance**	**5/23/2014**	**8/31/2014**	**$480,201.00**	**$36,587.11**	**$444,153.89**
	*The University of Texas at Austin			$239,773.00	$25,874.37	$213,898.63
	Aerodyne Research, Inc.			$157,066.00	$10,712.74	$146,353.26
	Leak Surveys, Inc.			$26,716.00	$0.00	$26,716
	Providence Photonics			$57,186.00	$0.00	$57,186
14-024	**Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ Data, Modeling and Experiments**	**6/18/2014**	**8/31/2015**	**$297,956.50**	**$295,561.39**	**$4,438.61**
	*The University of Texas at Austin			$163,282.00	$163,282.00	$0.00
	Environ			$101,404.00	$101,404.00	$0.00
	University of California – Riverside			$33,270.50	$30,875.39	$4,438.61

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
14-025	**Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model**	**5/21/2014**	**7/31/2015**	**$256,261.00**	**$251,394.40**	**$4,866.60**
	*Environ			$135,735.00	$135,603.98	$131.02
	Texas A&M University			$120,526.00	$115,790.42	$4,735.58
14-026	**Quantifying ozone production from light alkenes using novel measurements of Hydroxynitrate reaction products in Houston during the NASA SEAC4RS project**	**5/21/2014**	**09/30/2015**	**$165,562.00**	**$165,079.03**	**$482.97**
	*Environ			$165,562.00	$165,079.03	$482.97
14-029	**Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ**	**7/10/2014**	**6/30/2015**	**$178,679.00**	**$174,474.71**	**$4,204.29**
	*Baylor University			$178,679.00	$174,474.71	$4,204.29
14-030	**Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation**	**6/25/2014**	**11/30/2015**	**$176,109.00**	**$155,746.26**	**$20,362.74**
	*Texas A&M University			$176,109.00	$155,746.26	$20,362.74
14-SOS	**AQRP State of the Science Assessment**	**7/1/2015**	**12/31/2015**	**$50,000.00**	**$50,000.00**	**$0.00**
	*The University of Texas at Austin			$50,000.00	$50,000.00	$0.00

Appendix B

Publications and Presentations

FY 10-11

10-006

Johansson, J., Johan Mellqvist, Jerker Samuelsson, Brian Offerle, Jana Moldanova , Bernhard Rappenglück, Barry Lefer, and James Flynn (2014) , Formaldehyde Quantitative Measurements and Modeling of Industrial Formaldehyde Emissions in the Greater Houston Area during Campaigns in 2009 and 2011, Journal of Geophysical Research: Atmospheres, 119, DOI: 10.1002/2013JD020159

Johansson, J. K. E., J. Mellqvist, J. Samuelsson, B. Offerle, B. Lefer, B. Rappenglück, J. Flynn, and G. Yarwood(2014), Emission measurements of alkenes, alkanes, SO2, and NO2 from stationary sources in Southeast Texas over a 5 year period using SOF and mobile DOAS, J. Geophys. Res. Atmos., 119, doi:10.1002/2013JD020485.

10-008

Digar, A., D.S. Cohan, X. Xiao, K.M. Foley, B. Koo, and G. Yarwood (2013). Constraining ozone-precursor responsiveness using ambient measurements. *Journal of Geophysical Research*, 118(2), 1005-1019, doi:10.1029/2012JD018100.

Daniel S. Cohan and Antara Digar, "Observation-constrained probabilistic evaluation of modeled concentrations and sensitivities." CMAS Annual Conference, Chapel Hill, NC, October 2012.

10-009

The following papers were published in the journal Industrial & Engineering Chemistry Research in a Special Issue on Industrial Flaring:

Torres, V.M., Herndon, S., Wood, E., Al-Fadhli, F.M., Allen, D.T., Emissions of Nitrogen Oxides from Flares Operating at Low Flow Conditions, *Industrial & Engineering Chemistry Research,* 51, 12600-12605, DOI: 10.1021/ie300179x (2012)

Pavlovic, R.T., Al-Fadhli, Kimura, Y., Allen, D.T., and McDonald-Buller, E.C. Impacts of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area, *Industrial & Engineering Chemistry Research,* 51, 12593-12599, DOI: 10.1021/ie203052w (2012).

Knighton, W.B., Herndon, S.C., Franklin, J.F., Wood, E.C., Wormhoudt, J., Brooks, W., Fortner, E.C., and Allen, D.T. Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy, *Industrial & Engineering Chemistry Research,* 51, 12674-12684, DOI: 10.1021/ie202695v (2012)

Torres, V.M., Herndon, S., Kodesh, Z., Nettles, R., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research,* 51, 12559-12568, DOI: 10.1021/ie202674t (2012).

Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research,* 51, 12569-12576, DOI: 10.1021/ie202675f (2012)

Herndon, S.C., Nelson, D.D., Wood, E.C., Knighton, W.B., Kolb, C.E., Kodesh, Z., Torres, V.M., and Allen, D.T., Application of the carbon balance method to flare emissions characteristics, *Industrial & Engineering Chemistry Research,* 51, 12577-12585, DOI: 10.1021/ie202676b (2012)

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research,* 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

The following presentations were given at the Air& Waste Management Association June 2012 Conference, and papers were published in the Conference Proceedings:

Torres, V.M., Allen, D.T., Herndon, S. and Kodesh, Z., Overview of the Texas Commission on Environmental Quality 2010 Flare Study, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-437-AWMA, San Antonio, June, 2012.

Torres, V.M., Al-Fadhli, F.M., Allen, D.T., Herndon, S., and Wood, E., NOx Emissions from Industrial Flaring, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-315-AWMA, San Antonio, June, 2012.

10-015
The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models
J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride
J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

10-020
Brown, S. S., et al. (2012), Effects of NO_xcontrol and plume mixing on nighttime chemical processing of plumes from coal-fired power plants, J. Geophys. Res., 117, D07304, doi:10.1029/2011JD016954.

Brown, S. S., Dubé, W. P., Bahreini, R., Middlebrook, A. M., Brock, C. A., Warneke, C., de Gouw, J. A., Washenfelder, R. A., Atlas, E., Peischl, J., Ryerson, T. B., Holloway, J. S., Schwarz, J. P., Spackman, R., Trainer, M., Parrish, D. D., Fehshenfeld, F. C., and Ravishankara, A. R.: Biogenic VOC oxidation and organic aerosol formation in an urban nocturnal boundary layer: aircraft vertical profiles in Houston, TX, Atmos. Chem. Phys., 13, 11317-11337, doi:10.5194/acp-13-11317-2013, 2013.

In preparation for Atmosphere:
Reactive Plume Modeling to Investigate NOx Reactions and Transport at Night
Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:
Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique
Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021
The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the submitted abstract was *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022
Kanwar Devesh Singh, Tanaji Dabade, Hitesh Vaid, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, Kuyen Li, and Christopher B. Martin "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Model," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12611-12620

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, " Parametric Study of Ethylene Flare Operations and Validation of a Reduced Combustion Mechanism," Engineering Applications of Computational Fluid Mechanics, Vol. 8, No. 2, pp. 211–228 (2014).

Hitesh S. Vaid, Kanwar Devesh Singh, Helen H. Lou, Daniel Chen, Peyton Richmond, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale CFD Simulations," International Journal of Numerical Methods for Heat and Fluid Flow, Vol. 24 No. 1, 2014, pp. 21-35.

K. Singh, T. Dabade, H. Vaid, P. Gangadharan, D. Chen, H. Lou, X. Li, K. Li, C. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Ind. & Eng. Chem. Research, 51 (39), 12611-12620, October, 2012.

H. Lou, D. Chen, C. Martin, X. Li, K. Li, H. Vaid, K. Singh, P. Gangadharan, "Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, " Industrial &

Engineering Chemistry Research, Industrial flares special issue, 51 (39), 12697-12705, October, 2012.

H. Lou, C. Martin, D. Chen, X. Li, K. Li, H. Vaid, A. Tula, K. Singh,"Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, Volume 14, Issue 4, pp 737-748, August 2012, DOI 10.1007/s10098-011-0441-6.

Helen H. Lou, Christopher B. Martin, Daniel Chen, Xianchang Li, Kyuen Li, Hitesh Vaid, Anjan Tula Kumar, Kanwar Devesh Singh, & Doyle P. Bean, "A reduced reaction mechanism for the simulation in ethylene flare combustion," Clean Technologies and Environmental Policy, Volume 14, Issue 2, pp 229-239, April 2012, doi:10.1007/s10098-011-0394-9.

10-024

E.T. Gall, R.J. Griffin, A.M. Steiner, J.E. Dibb, E. Scheuer, L. Gong, A.P. Rutter, B.K. Cevik, S. Kim, B. (2016) Lefer, and J. Flynn, Evaluation of nitrous acid sources and sinks in urban outflow, *Atmos. Environ.*, *127*, 272-282.

B. Karakurt Cevik, A.P. Rutter, L. Gong, R.J. Griffin, J.H. Flynn, B.L. Lefer, and S. Kim (2016), Estimates of airmass aging using particle and other measurements near Fort Worth, *Atmos. Environ.*, *126*, 45-54.

A.P. Rutter, R.J. Griffin, B. Karakurt Cevik, K.M. Shakya, L. Gong, S. Kim, J.H. Flynn, and B.L. Lefer (2015), Sources of air pollution in a region of oil and gas development downwind of a large city, *Atmos. Environ.*, *120*, 89-99.

S. Kim, A.B. Guenther, B. Lefer, J. Flynn, R. Griffin, A.P. Rutter, L. Gong, and B.Karakurt Cevik (2015), Field observations of the role of stabilized Criegee radicals in sulfuric acid production in a high biogenic VOC environment, *Environ. Sci. Technol.*, *49*, 3383-3391.

L. Gong, R. Lewicki, R.J. Griffin, A. Rutter, F.K. Tittel, B.L. Lefer, J.H. Flynn, J.E. Dibb, and E. Scheuer (2012), Gas-particle partitioning of ammonia in the Fort Worth, TX area, *American Association for Aerosol Research Annual Conference*, Minneapolis, MN, October 2012. (poster)

B. Karakurt Cevik, L. Gong, R. Lewicki, R.J. Griffin, A. Rutter, F.K. Tittel, B.L. Lefer, J.H. Flynn, J.E. Dibb, and E. Scheuer 2012), Comparison of estimates of airmass aging using particle and other measurements near Fort Worth, TX, *American Association for Aerosol Research Annual Conference*, Minneapolis, MN.

A. P. Rutter, B. Karakurt Cevik, K.M. Shakya, L. Gong, C. Gutierrez, M. Calzada, S. Kim, R.J. Griffin, J.H. Flynn, and B.L. Lefer, Source apportionment of organic aerosols and VOCs near Fort Worth, TX (2012), *American Association for Aerosol Research Annual Conference*, Minneapolis, MN.

S. Kim, A.B. Guenther, T. Karl, B.L. Lefer, J.H. Flynn, R.J. Griffin, and A.P. Rutter, Sub-urban OH response to isoprene chemistry: A case study in the Dallas Fort-Worth area (2012), *American Geophysical Union Winter Meeting,* San Francisco, CA, December 2012. (poster)

10-032
Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhan, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappengluck, K. W. Wong. C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke and P. Kelley (2013), Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *Journal of Geophysical Research-Atmospheres,118*,5770-5780,doi:10.1002/jgrd.50342.

10-042
Heo, G., McDonald-Buller, E.C., Carter, W.P.L., Yarwood, G., Whitten, G.Z. and Allen, D.T. "Modeling Ozone Formation from Alkene Reactions using the Carbon Bond Chemical Mechanism, *Atmospheric Environment*, 59, 141-150, DOI: 10.1016/j.atmosenv.2012.05.042 (2012).

Heo, G. Y. Kimura, E. McDonald-Buller, D. T. Allen, G. Yarwood, G. Z. Whitten Evaluation of a New Toluene Mechanism For Carbon Bond 05 Using Environmental Chamber Data and Ambient Data, Air and Waste Management Association Annual Meeting, Paper #154, Detroit, June 2009

In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate NOx removal and recycling represented in atmospheric mechanisms for air quality modeling* Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen

In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial NOx* Gookyoung Heo, William Carter, Greg Yarwood

10-045
Olga Pikelnaya, James H. Flynn, Catalina Tsai, and Jochen Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, Journal of Geophysical Reserch, Volume 118, Issue 15, pages 8716–8728, 16 August 2013, DOI: 10.1002/jgrd.50643

The following papers were published in Industrial & Engineering Chemistry Research Special Issue on Industrial Flaring. The paper edition of this special edition came out in Fall 2012.

W. Berk Knighton, Scott C. Herndon, Ezra C. Wood, Edward C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Detecting Fugitive Emissions of 1,3-Butadiene and Styrene from a Petrochemical Facility: An Application of a Mobile Laboratory and a Modified Proton Transfer Reaction Mass Spectrometer," *Industrial & Engineering Chemistry Research* **2012** *51* (39), 12706-12711

Ezra C. Wood, Scott C. Herndon, Ed C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, W. Berk Knighton, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Combustion and Destruction/Removal Efficiencies of In-Use Chemical Flares in the

Greater Houston Area," *Industrial & Engineering Chemistry Research* **2012** *51* (39), 12685-12696

Pikelnaya, O., J. H. Flynn, C. Tsai, and J. Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, J. Geophys. Res. Atmos., 118,8716–8728, doi:10.1002/jgrd.50643.

This project has also resulted in the following publications:
Olga Pikelnaya, Jochen Stutz, Scott Herndon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuete, Evan Couzo, "*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview",* in preparation for Journal of Geophysical Research

Olga Pikelnaya, Scott Herndon, Ezra Wood, and Jochen Stutz, "*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign,"* under development.

Presentation
Stutz, Jochen; 2011, Aerosols in Urban and Rural Environments: Sources, Transformations, Properties, and Atmospheric Effects, presented at 2011 Fall Meeting, AGU, San Francisco, CA 5-9 Dec.

FY 12-13

13-005

Publications:

Johansson, J. K. E., J. Mellqvist, B. Lefer and L. Judd (2016), *Mobile MAX-DOAS measurements of NO2 and HCHO during the 2013 DISCOVER-AQ campaign in Houston*, paper in manuscript.

Johansson, J. K. E. (2016), *Optical remote sensing of industrial gas emission fluxes*, Doctoral thesis, 162 pp, ISBN 978-81-7597-316-6, Chalmers University of Technology, Gothenburg.

Presentations:

Johansson, J. K. E., J. Mellqvist, J. Samuelsson, B. Offerle and P. Andersson (2014), *Preliminary results from the SOF mobile lab - Summary and outlook*, presentation at DISCOVER-AQ science meeting, February 28, Hampton, Virginia

Johansson, J. K. E., J. Mellqvist, B. Lefer and L. Judd (2015), *Improved Analysis of VOC, NO2, SO2 and HCHO Data from SOF, Mobile DOAS and MW-DOAS during DISCOVER-AQ*, presentation at AQRP workshop, June 18, Austin, Texas

Johansson, J. K. E. (2016), *Optical remote sensing of industrial gas emission fluxes*, presentation of Doctoral thesis, February 4, Gothenburg, Sweden

Johansson, J. K. E. (2016), *Mobile DOAS measurements of NO2 and HCHO during DISCOVER-AQ*, presentation at Gothenburg Atmospheric Science Centre Conference, April 27, Gothenburg, Sweden

12-006

Journal Papers:

Gookyoung Heo, Peng Wang, Qi Ying, Ron Thomas, William P.L. Carter. Using chemically detailed emissions data to test assumptions used in developing chemical mechanisms: a case study for southeast Texas, USA. [To be submitted to Atmospheric Environment in Summer 2015]

Peng Wang, Gookyoung Heo, William P.L. Carter, Qi Ying. Comparison of a detailed and a lumped version of SAPRC-11 photochemical mechanism during a summer ozone episode. [To be submitted to Atmospheric Environment in Summer 2015]

Gookyoung Heo, Chia-Li Chen, Ping Tang, William P.L. Carter. Evaluation of mechanisms for major terminal and internal alkenes with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2015]

Gookyoung Heo, Shunsuke Nakao, William P.L. Carter. Evaluation of mechanisms for 1,3-butadiene with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2015]

Conference Paper:
Heo, G., Carter, W.P.L., Wang, P., Ying, Q., Thomas, R. (2013). Evaluating and improving atmospheric chemical mechanisms used for modeling ozone formation from alkenes. Presented at the 12th Annual CMAS Conference, Chapel Hill, NC, October 28-30, 2013.

12-012
Conference presentations:
C. Faxon, J. Bean, L. Hildebrandt Ruiz. Evidence of atmospheric chlorine chemistry in Conroe, TX: Regional implications. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

J. Bean, C. Faxon, L. Hildebrandt Ruiz. Atmospheric processing of pollutants in the Houston Region: First insights from DISCOVER-AQ. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

L. Hildebrandt Ruiz, J. Bean, G. Yarwood, B. Koo, U. Nopmongcol. Formation and Gas-Particle Partitioning of Organic Nitrates: Influence on Ozone Production. American Association for Aerosol Research Annual Meeting, October 2013, Portland, OR.

J. Bean and L. Hildebrandt Ruiz. Hydrolysis and gas-particle partitioning of organic nitrates formed in environmental chamber experiments. American Association for Aerosol Research Annual Meeting, October 2014, Orlando, FL.

Submitted publications:
J.K. Bean and L. Hildebrandt Ruiz. Hydrolysis and Gas-particle Partitioning of Organic Nitrates Formed from the Oxidation of α-Pinene in Environmental Chamber Experiments. *Atmospheric Chemistry and Physics Discussions*, in press, 2015.

Planned publications:
C. Faxon, J. Bean and L. Hildebrandt Ruiz. Preliminary title "Significant Inland Concentrations of ClNO2 Detected in Conroe TX during DISCOVER-AQ 2013". Submission planned for August 2014.

J. Bean, C. Faxon and L. Hildebrandt Ruiz. Manuscript summarizing particle-phase measurements from DISCOVER-AQ. Submission planned for late 2014.

Planned Presentations:
J. Bean and L. Hildebrandt Ruiz. Sources and composition of aerosol measured near Houston, TX: anthropogenic-biogenic interactions. American Association for Aerosol Research Annual Meeting, October 2015, Minneapolis, MN.

D. Wang, Surya V. Dhulipala and L. Hildebrandt Ruiz. Secondary Organic Aerosol from Chlorine-Radical Initiated Oxidation of Volatile Organic Compounds: Organic Aerosol Mass Yields, Composition, and Gas-Phase Products. American Association for Aerosol Research Annual Meeting, October 2015, Minneapolis, MN.

B. Koo, L. Hildebrandt Ruiz, R. Sheesley and G. Yarwood. Evaluation of Modeled Organic Aerosol Formation in the Houston Region Using Measurements from the 2013 DISCOVER-AQ

Campaign. American Association for Aerosol Research Annual Meeting, October 2015, Minneapolis, MN.

13-016

Gary Morris presented a poster entitled "Tropospheric Ozone Pollution Project (TOPP) Overview: A Context for DISCOVER-AQ Houston 2013" at the DISCOVER-AQ Science Team Meeting on February 27, 2014.

Morris, G.A., B.L. Lefer, A.M. Thompson, A.J. Weinheimer, H.B. Selkirk, D.K. Martins, and A. Kotsakis, Urban-scale boundary layer and lower free tropospheric ozone variability in Houston during DISCOVER-AQ (September 2013), 2014 Fall Meeting, AGU, San Francisco, CA, 15 – 19 December 2014.

Kotsakis, A., B.L. Lefer, G.A. Morris, A.M. Thompson, D.K. Martins, A.J. Weinheimer, and R.E. Orville, Sources of Ozone in the Free Troposphere in Houston During DISCOVER-AQ 2013, 2014 Fall Meeting, AGU, San Francisco, CA, 15 – 19 December 2014.

12-018

Posters:

Kimura, Y., C. Wiedinmyer, J. Zheng, E. McDonald-Buller, The Influence of Land Cover Characterization on Emission Estimates from the Fire INventory from NCAR (FINN), American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014 (poster).

13-022

Publications

J. Bean, C. Faxon, Y.J. Leong, H.W. Wallace IV, B. Karakurt Cevik, S. Ortiz, M. Canagaratna, S. Usenko, R. Sheesley, R.J. Griffin, and L. Hildebrandt Ruiz, Composition and sources of particulate matter measured near Houston, TX: Anthropogenic-biogenic interactions, *Atmosphere*, *7*, 73, doi: 10.3390/atmos7050073, 2016.

M. Jahjah, W. Jiang, N. Sanchez, W. Ren, P. Patimisco, V. Spagnolo, S. Herndon, R.J. Griffin, and F.K. Tittel, Atmospheric CH_4 and N_2O measurements near greater Houston area landfills using a QCL-based QEPAS sensor system during DISCOVER-AQ 2013, *Opt. Lett., 39*, 957-960, 2014.

Y.J. Leong, N.P. Sanchez, H.W. Wallace, B. Karakurt Cevik, C.S. Hernandez, Y. Han, J.H. Flynn, B. Lefer, and R.J. Griffin, Overview of surface measurements and spatial characterization of submicron particulate matter during the DISCOVER-AQ 2013 campaign in Houston, TX, to be submitted to *Atmos. Chem. Phys.*, expected submission June 2016.

K. Sun, L. Tao, D.J. Miller, D. Pan, L.M. Golston, M.A. Zondlo, R.J. Griffin, H.W. Wallace, Y.J. Leong, M.M. Yang, Y. Zhang, D.L. Mauzerall, and T. Zhu, Vehicle emissions as an important urban ammonia source in the United States and China, for submission to *Environ. Sci. Technol.*, expected submission June 2016.

Presentations:

Y.J. Leong, N. Sanchez, H.W. Wallace, B. Karakurt Cevik, J. Flynn, Y. Han, P. Massoli, C. Floerchinger, E. Fortner, S. Herndon, B. Lefer, and R. Griffin, Overview of surface measurements of submicron particulate matter in the greater Houston area during the DISCOVER-AQ 2013 field campaign, American Association for Aerosol Research Annual Meeting, Minneapolis, MN, October 2015.

N. Sanchez, Y.J. Leong, H.W. Wallace, B. Karakurt Cevik, J. Flynn, B. Lefer, and R. Griffin, Understanding the character and dynamics of organic aerosol in the Houston area using multi-way factor analysis, American Association for Aerosol Research Annual Meeting, Minneapolis, MN, October 2015.

R.J. Griffin, Measurements and modeling of NO_3-BVOC reactions in Houston, Workshop on NO_3-BVOC Reactions, Georgia Institute of Technology, Atlanta, GA, June 2015. (keynote)

R.J. Griffin, Houston Aerosol Characterization and Health Experiment (HACHE), Health: Global Lens, Local Focus Conference, Houston, TX, May 2015.

B. Lefer, J. Flynn, L. Judd, X. Ren, M. Estes, and R. Griffin, The spatial and temporal variability of ozone in the Houston metropolitan area during DISCOVER-AQ and its relation to meteorological conditions, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014.

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

R. Ferrare, J. Crawford, R. Griffin, C.Hostetler, B. Anderson, B. Holben, R. Hoff, A. Beyersdorf, and L. Ziemba, DISCOVER-AQ investigation of aerosol impacts on air quality over Houston, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

H.W. Wallace, Y.J. Leong, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, and R.J. Griffin, Characterization of aerosol organic nitrate in the outflow from Houston, TX, during the DISCOVER-AQ campaign, *American Chemical Society Annual Meeting*, San Francisco, CA, August 2014.

R.J. Griffin, Houston Aerosol Characterization and Health Experiment (HACHE), University of Texas at Houston, School of Public Health, Houston, TX, January 2014.

R.J. Griffin, Houston Aerosol Characterization and Health Experiment (HACHE), *Houston Regional Air Quality Planning Advisory Committee Meeting*, Houston, TX, January 2014.

H.W. Wallace, Chemical characterization of submicron aerosol emissions in the greater Houston area using an aerosol mass spectrometer on a mobile platform, *American Chemical Society Southwestern Regional Meeting*, Waco, TX, November 2013.

Posters:

A. Bui, Y.J. Leong, N. Sanchez, H.W. Wallace, and R. Griffin, Distribution, influential factors, and sources of aerosol liquid water during the DISCOVER-AQ 2013 campaign in Houston, TX, American Association for Aerosol Research Annual Meeting, Minneapolis, MN, October 2015. (poster)

H.W. Wallace, Y.J. Leong, N. Sanchez, B. Schulze, J. Flynn, B. Lefer, and R. Griffin, Houston Aerosol Characterization and Health Experiment: A two-year health impacts survey of chemically resolved, non-refractory PM_1 in the Houston, TX metropolitan area, American Association for Aerosol Research Annual Meeting, Minneapolis, MN, October 2015. (poster)

Y.J. Leong, N.P. Sanchez, H.W. Wallace IV, A.T Bui, C.S. Hernandez, B. Karakurt Cevik, J.H. Flynn, B. Lefer, and R.J. Griffin, Overview of surface PM_1 measurements during DISCOVER-AQ Houston 2013, Atmospheric Chemistry Gordon Research Conference, Waterville Valley, NH, August 2015.

R. Sheesley, T. Barrett, S. Yoon, A. Clark, L. Hildebrandt-Ruiz, R. Griffin, B. Karakurt Cevik, R. Long, R. Duvall, and S. Usenko, Spatial trends in surface-based carbonaceous aerosol, including organic, water-soluble, and elemental carbon, during DISCOVER-AQ in Houston, TX, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014.

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *International Global Atmospheric Chemistry Quadrennial Meeting*, Natal, Brazil, September 2014

Y.J. Leong, H.W. Wallace, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, R.J. Griffin, Chemical characterization of submicron aerosol emissions in the greater Houston area using an aerosol mass spectrometer on a mobile platform, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2013. (poster)

13-024

Publications:

Nowlan, C. R., X. Liu, J. Leitch, K. Chance, G. González Abad, C. Liu, P. Zoogman, J. Cole, T. Delker, W. Good, F. Murcray, L. Ruppert, D. Soo, M. B. Follette-Cook, S. Janz, M. Kowalewski, C. Loughner, K. Pickering, J. Herman, M. Beaver, R. Long, J. Szykman, L. Judd, X. Ren, W. Luke, P. Kelly, and J. Al-Saadi, Nitrogen dioxide observations from the Geostationary Trace gas and Aerosol Sensor Optimization airborne instrument: Retrieval algorithm and measurements during DISCOVER-AQ Texas 2013, *Atmos. Meas. Tech. Discuss.*, 8, 13,099–13,155, doi:10.5194/amtd-8-13099-2015, 2016.

Presentations:
Ren, X., P. Kelley, and W. Luke, Measurements of Trace Gases at the Manvel Croix and Galveston Sites during DISCOVER-AQ, the 6th NASA AQAST meeting at Rice University, Houston, TX, January 15-17, 2014

Luke, W., X. Ren, and P. Kelley, NOAA/Air Resources Laboratory Surface Observations at Galveston and Manvel-Croix: Summary and Comparison with Aircraft Data, NASA DISCOVER-AQ Science Meeting, Hampton, VA, February 24-28, 2014

Judd, L., B. Lefer, J. Herman, N. Abuhassan, A. Cede, S. Janz, J. H. Crawford, A. Weinheimer, R. Cohen, X. Ren, W. Luke, H. C. Kim, R. Long, Comparison of Pandora spectrometer NO2 measurements to aircraft, satellite, and ground measurements during the DISCOVER-AQ Texas campaign, Abstract #: A33I-3318, AGU Fall Meeting,, San Francisco, CA, December 15-19, 2014.

12-028
Implementation and Refinement of a Surface Model for HONO formation in a 3-D Chemical Transport Model. Prakash Karamchandani[1], Chris Emery[1], Greg Yarwood[1], Barry Lefer[2], Jochen Stutz[3], Evan Couzo[4], and William Vizuete[5]. ([1]ENVIRON, [2]University of Houston, [3]University of California-Los Angeles, [4]University of North Carolina-Asheville, and [5]University of North Carolina-Chapel Hill.)

Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas. Evan Couzo[1], Barry Lefer[2], Jochen Stutz[3], Greg Yarwood[4], Prakash Karamchandani[4], Barron Henderson[5], and William Vizuete[1]. ([1]University of North Carolina-Asheville, [2]University of Houston, [3]University of California-Los Angeles, [4]ENVIRON, [5]University of Florida.)

Heterogeneous HONO sources and ozone chemistry in Houston, Texas" W. Vizuete*, E. Couzo, P. Karamchandani, G. Yarwood, J. Stutz, and B. Lefer presented at the Annual Community Modeling and Analysis System (CMAS) Conference, (October 2014).

Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas. E. Couzo, P. Karamchandani, G. Yarwood, J. Stutz, and B. Lefer presented at the 96th annual AMS conference New Orleans, LA. January 2016

12-032
Publication
Clark, A. E.; Yoon, S.; Sheesley, R. J.; Usenko, S., Pressurized liquid extraction technique for the analysis of pesticides, PCBs, PBDEs, OPEs, PAHs, alkanes, hopanes, and steranes in atmospheric particulate matter. *Chemosphere* 2015, *137*, 33-44.

Manuscript in preparation. Submission planned to Atmospheric Environment in summer 2014. Draft title: "*Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX*."

Poster
Poster at the American Geophysical Union national meeting (Dec 2013) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Poster at the DISCOVER-AQ Science Working Group meeting (Feb 2014) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Clark, A. E.; Yoon, S.; Sheesley, R. J.; Usenko, S., Pressurized liquid extraction technique for the analysis of pesticides, PCBs, PBDEs, OPEs, PAHs, alkanes, hopanes, and steranes in atmospheric particulate matter. *Chemosphere* 2015, *137*, 33-44.

Manuscript in preparation. Submission planned to Atmospheric Environment in summer 2014. Draft title: "*Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX*."

12-TN1
Presentation
"A regional chemical reanalysis prototype" Pius Lee , Greg Carmichael, Tianfeng Chai, Rick Saylor, Li Pan, Hyuncheol Kim, Daniel Tong, and Ariel Stein

Poster
"Preliminary analyses of flight measurements and CMAQ simulation during Southeast Nexus (SENEX) field experiment" Li Pan, Pius Lee , Hyun Cheol Kim, Daniel Tong ,Rick Saylor and Tianfeng Chai

Publication
Pius Lee, Fantine Ngan, Hang Lei, Barry Baker, Bright Dornblaser, Gary McGauhey,and Daniel Tong. An Application for Improving Air Quality: a Houston Case Study, Earthzine 2014 [available at: http://www.earthzine.org/2014/03/29/an-application-for-improving-air-quality-a-houston-case-study/?shareadraft=baba698217_53330c8eab882]

12-TN2
The project team presented at the Community Modeling and Analysis System (CMAS) Conference in October 2013.

Presentation
"HCHO and NO2 column comparisons between OMI, GOME-2 and CMAQ during 2013 SENEX campaign (21 slides)" Hyun Cheol Kim, Li Pan, Pius Lee, Rick Saylor, and Daniel Tong

Poster
Fine-scale comparison of GOME-2, OMI and CMAQ NO2 columns over Southern California in 2008" Hyun Cheol Kim, Sang-Mi Lee, Fong Ngan, and Pius Lee

FY 14- 15

14-003

Chen, Y.Z., et al., Assessment of SAPRC07 with updated isoprene chemistry against outdoor chamber experiments. *Atmospheric Environment*, 2015. 105: p. 109-120.

Riedel, T.P., et al., Heterogeneous Reactions of Isoprene-Derived Epoxides: Reaction Probabilities and Molar Secondary Organic Aerosol Yield Estimates. *Environmental Science & Technology Letters*, 2015. 2(2): p. 38-42.

Riedel, T. P., Z. Zhang, K. Chu, J. Thornton, W. Vizuete, A. Gold and j. d. Surratt, Constraining Condensed-Phase Formation Kinetics of Secondary Organic Aerosol Components from Isoprene Epoxydiols. *Atmospheric Chemistry and Physics*, in preparation 2015.

Surratt, J. D.* (2016) Secondary Organic Aerosol Formation from the Atmospheric Oxidation of Isoprene: Implications for Air Quality, Climate and Public Health in the Southeastern US. UNC's Ruth and Philip Hettleman Lecture for Artistic and Scholarly Achievement. Chapel Hill, NC USA. May 18.

Surratt, J. D.* (2016) *Multiphase Chemistry Promotes Isoprene-Derived Secondary Organic Aerosol Formation: Implications for Air Quality, Climate and Public Health in the Southeastern USA*. Invited Plenary Lecture. Nordic Society for Aerosol Research (NOSA) Symposium. Aarhus University, Aarhus, Denmark. April 5.

Surratt, J. D.* (2016) *Multiphase Chemistry Promotes Isoprene-Derived Secondary Organic Aerosol Formation in the Southeastern USA*. ES&T @ 50: Award Winning Researchers, Past, Present and Future Session. James J. Morgan Early Career Award Lectureship. American Chemical Society (ACS), San Diego, CA USA. March 16.

Surratt, J. D.* (2016) *Secondary Organic Aerosol Formation from the Atmospheric Oxidation of Isoprene: Implications for Air Quality, Climate and Public Health in the Southeastern U.S.* Engineering and Applied Sciences, Harvard University, Boston, MA USA. January 29.

Surratt, J. D.* (2015) *Multiphase Chemistry Promotes Isoprene-Derived Secondary Organic Aerosol Formation in the Southeastern United States.* Department of Chemistry, University of Toronto, Toronto, Canada. November 12.

Riedel, T. P.; Chu, K.; Cui, T.; Lin, Y.-H.; Budisulistiorini, S. H.; Zhang, Z.; Thornton, J. A.; Gold, A.; Vizuete, W.; Surratt, J. D.* (2015) *Constraining Condensed-Phase Kinetics of Secondary Organic Aerosol Components from Isoprene Epoxydiols.* American Association for Aerosol Research (AAAR) Annual Meeting. Minneapolis, MN USA. October 13.

Surratt, J. D.* (2015) *Multiphase Chemistry Promotes Isoprene-Derived Secondary Organic Aerosol Formation.* Gordon Research Conference on Atmospheric Chemistry. Invited Speaker for the Organic Chemistry in the Particle Phase Session. Waterville Valley, NH USA. August 4.

Chen, Yuzhi, Roger Jerry, Kenneth Sexton, Jason Surratt, William Vizuete. Assessment of SAPRC07 with Updated Isoprene Chemistry against Outdoor Chamber Experiments; 13th Annual CMAS Conference, Chapel Hill, NC, Oct 27, 2014

14-004

Follette-Cook, M. B., et al., Evaluation of high-resolution WRF and CMAQ simulations of the Houston, TX DISCOVER-AQ campaign period, Community Modeling and Analysis (CMAS) conference, Chapel Hill, NC, Oct 2015.

Follette-Cook, M. B., et al., Regional Model Evaluation During the NASA DISCOVER-AQ Campaigns, Meteorology And Climate – Modeling for Air Quality (MAC-MAQ) conference, Sacramento, CA, Sep 2015.

Follette-Cook, M. B., et al., Evaluation of a high resolution Houston, TX WRF/CMAQ Simulation, oral presentation at the DISCOVER-AQ Science Team Meeting, Boulder, CO, May 2015.

Follette-Cook, M. B., et al., Preliminary comparisons between WRF/CMAQ and in-situ trace gas observations during the Houston, TX deployment of DISCOVER-AQ, Community Modeling and Analysis (CMAS) conference, Chapel Hill, NC, Oct 2014.

Loughner, C.P., M.B. Follette-Cook, A. Fried, and K.E. Pickering (2015), The role of bay breezes and a large petrochemical emissions event on a high surface ozone episode during the Houston, Texas DISCOVER-AQ field campaign, AGU Fall Meeting, San Francisco, CA.

Loughner, C.P., M.B. Follette-Cook, A. Fried, K.E. Pickering, R. Gilliam, and J. MacKay (2015), The role of bay breezes on a high surface ozone episode during the Houston, Texas DISCOVER-AQ field campaign, 7th International Workshop on Air Quality Forecasting Research, College Park, MD.

Loughner, C.P. M.B. Follette-Cook, and A. Fried (2015), Emission source region contributions to a high surface ozone episode during DISCOVER-AQ, Texas Air Quality Research Program Workshop, Austin, TX.

Loughner, C.P., M. Follette-Cook, K.E. Pickering, A. Fried, and M. Estes (2015), High resolution WRF/CMAQ simulation of bay and sea breeze circulations leading to enhanced ozone on September 25, FRAPPE/DISCOVER-AQ Science Team Meeting, Boulder, CO.

Loughner, C.P., M. Follette-Cook, K.E. Pickering, and M. Estes (2014), The role of bay breezes and regional transport on a high surface ozone episode during the Houston, Texas DISCOVER-AQ field campaign, AGU Fall Meeting, San Francisco, CA.

Loughner, C.P., M. Follette-Cook, K.E. Pickering, and M. Estes (2014), Bay breeze enhanced air pollution event in Houston, Texas during the DISCOVER-AQ field campaign, 13th Annual CMAS Conference, Chapel Hill, NC.

14-008

Posters:

McGaughey, G., Y. Sun, L. Huang, Y. Kimura, R. Fu, E. McDonald-Buller, Soil Moisture Characterization for Biogenic Emissions Modeling in Texas, American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014 (poster).

14-009

J. Bean, C. Faxon, Y.J. Leong, H.W. Wallace IV, B. Karakurt Cevik, S. Ortiz, M. Canagaratna, S. Usenko, R. Sheesley, R.J. Griffin, and L. Hildebrandt Ruiz, Composition and sources of particulate matter measured near Houston, TX: Anthropogenic-biogenic interactions, *Atmosphere*, *7*, 73, doi: 10.3390/atmos7050073, 2016.

M. Jahjah, W. Jiang, N. Sanchez, W. Ren, P. Patimisco, V. Spagnolo, S. Herndon, R.J. Griffin, and F.K. Tittel, Atmospheric CH_4 and N_2O measurements near greater Houston area landfills using a QCL-based QEPAS sensor system during DISCOVER-AQ 2013, *Opt. Lett., 39*, 957-960, 2014.

Y.J. Leong, N.P. Sanchez, H.W. Wallace, B. Karakurt Cevik, C.S. Hernandez, Y. Han, J.H. Flynn, B. Lefer, and R.J. Griffin, Overview of surface measurements and spatial characterization of submicron particulate matter during the DISCOVER-AQ 2013 campaign in Houston, TX, to be submitted to *Atmos. Chem. Phys.*, expected submission June 2016.

K. Sun, L. Tao, D.J. Miller, D. Pan, L.M. Golston, M.A. Zondlo, R.J. Griffin, H.W. Wallace, Y.J. Leong, M.M. Yang, Y. Zhang, D.L. Mauzerall, and T. Zhu, Vehicle emissions as an important urban ammonia source in the United States and China, for submission to *Environ. Sci. Technol.*, expected submission June 2016.

Presentations:

Y.J. Leong, N. Sanchez, H.W. Wallace, B. Karakurt Cevik, J. Flynn, Y. Han, P. Massoli, C. Floerchinger, E. Fortner, S. Herndon, B. Lefer, and R. Griffin, Overview of surface measurements of submicron particulate matter in the greater Houston area during the DISCOVER-AQ 2013 field campaign, *American Association for Aerosol Research Annual Meeting*, Minneapolis, MN, October 2015.

N. Sanchez, Y.J. Leong, H.W. Wallace, B. Karakurt Cevik, J. Flynn, B. Lefer, and R. Griffin, Understanding the character and dynamics of organic aerosol in the Houston area using multi-way factor analysis, *American Association for Aerosol Research Annual Meeting*, Minneapolis, MN, October 2015.

R.J. Griffin, Measurements and modeling of NO_3-BVOC reactions in Houston, Workshop on NO_3-BVOC Reactions, Goergia Institute of Technology, Atlanta, GA, June 2015. (keynote)
R.J. Griffin, Houston Aerosol Characterization and Health Experiment (HACHE), Health: Global Lens, Local Focus Conference, Houston, TX, May 2015.

B. Lefer, J. Flynn, L. Judd, X. Ren, M. Estes, and R. Griffin, The spatial and temporal variability of ozone in the Houston metropolitan area during DISCOVER-AQ and its relation to meteorological conditions, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014.

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

R. Ferrare, J. Crawford, R. Griffin, C.Hostetler, B. Anderson, B. Holben, R. Hoff, A. Beyersdorf, and L. Ziemba, DISCOVER-AQ investigation of aerosol impacts on air quality over Houston, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

H.W. Wallace, Y.J. Leong, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, and R.J. Griffin, Characterization of aerosol organic nitrate in the outflow from Houston, TX, during the DISCOVER-AQ campaign, *American Chemical Society Annual Meeting*, San Francisco, CA, August 2014.

R.J. Griffin, Houston Aerosol Characterization and Health Experiment (HACHE), University of Texas at Houston, School of Public Health, Houston, TX, January 2014.

R.J. Griffin, Houston Aerosol Characterization and Health Experiment (HACHE), Houston Regional Air Quality Planning Advisory Committee Meeting, Houston, TX, January 2014.

H.W. Wallace, Chemical characterization of submicron aerosol emissions in the greater Houston area using an aerosol mass spectrometer on a mobile platform, American Chemical Society Southwestern Regional Meeting, Waco, TX, November 2013.

Posters:

A. Bui, Y.J. Leong, N. Sanchez, H.W. Wallace, and R. Griffin, Distribution, influential factors, and sources of aerosol liquid water during the DISCOVER-AQ 2013 campaign in Houston, TX, American Association for Aerosol Research Annual Meeting, Minneapolis, MN, October 2015. (poster)

H.W. Wallace, Y.J. Leong, N. Sanchez, B. Schulze, J. Flynn, B. Lefer, and R. Griffin, Houston Aerosol Characterization and Health Experiment: A two-year health impacts survey of chemically resolved, non-refractory PM_1 in the Houston, TX metropolitan area, American Association for Aerosol Research Annual Meeting, Minneapolis, MN, October 2015. (poster)

Y.J. Leong, N.P. Sanchez, H.W. Wallace IV, A.T Bui, C.S. Hernandez, B. Karakurt Cevik, J.H. Flynn, B. Lefer, and R.J. Griffin, Overview of surface PM_1 measurements during DISCOVER-AQ Houston 2013, Atmospheric Chemistry Gordon Research Conference, Waterville Valley, NH, August 2015.

R. Sheesley, T. Barrett, S. Yoon, A. Clark, L. Hildebrandt-Ruiz, R. Griffin, B. Karakurt Cevik, R. Long, R. Duvall, and S. Usenko, Spatial trends in surface-based carbonaceous aerosol, including organic, water-soluble, and elemental carbon, during DISCOVER-AQ in Houston, TX, American Geophysical Union Winter Meeting, San Francisco, CA, December 2014.

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, International Global Atmospheric Chemistry Quadrennial Meeting, Natal, Brazil, September 2014

Y.J. Leong, H.W. Wallace, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, R.J. Griffin, Chemical characterization of submicron aerosol emissions in the greater Houston area using an aerosol mass spectrometer on a mobile platform, American Geophysical Union Winter Meeting, San Francisco, CA, December 2013. (poster)

14-010

Publications:

Wang Yuxuan, et al., Influence of the Bermuda High on interannual variability of summertime ozone in the Houston-Galveston-Brazoria region, manuscript to be submitted to Atmospheric Chemistry and Physics.

Presentations:

Wang Yuxuan, Understanding the relationship between HGB ozone and large-scale circulation, Texas Air Quality Symposium, UT Austin, April, 2015

Wang Yuxuan, Impact of Large-Scale Circulation on Air Pollution, NASA Jet Propulsion Laboratory, Pasadena, CA, Aug 2015 (invited seminar)

Posters:

Wang Yuxuan et al., Impact of large-scale circulation patterns on surface ozone concentrations in Houston-Galveston-Brazoria (HGB), AGU Fall Meeting, San Francisco, CA, Dec 2015

14-011

Kimura, Y., C. Wiedinmyer, J. Zheng, E. McDonald-Buller, The Influence of Land Cover Characterization on Emission Estimates from the Fire INventory from NCAR (FINN), American Geophysical Union Fall Meeting, San Francisco, CA, December 15-19, 2014 (poster).

14-014

Publications:

Souri, A.H., Choi, Y., Jeon, W., Li, X., Pan, S., Diao, L., and Westenbarger, D.A., Constraining NOx emissions using satellite NO2 measurements during 2013 DISCOVER-AQ Texas campaign, 2016, Atmospheric Environment., 131,371-381

Pan, S., Choi, Y., Roy, A., Li, X., Jeon, W., and Souri A.H., Modeling the uncertainty of several VOC and its impact on simulated VOC and ozone in Houston, Texas, 2015, Atmospheric Environment, 120, 404-416

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Jeon, W., Choi, Y., Lee, H-W., Lee, S-H., Yoo, J-W., Park, J., and Lee H-J., A quantitative analysis of grid nudging effect on each process of PM2.5 production in Korean Peninsula, 2015, Atmospheric Environment, 122, 763-774

14-016

Presentations:

Southeast Atmosphere Studies Workshop: Intensive Observation Period Modeling to Improve Mechanistic Representation of Trends. NOAA Geophysical Fluid Dynamics Laboratory (GFDL), Princeton, NJ. June 8-10, 2015

“Isoprene emissions from measurements and inventories” Carsten Warneke (NOAA ESRL & CIRES)

“Revised MEGAN emission factors based on high-resolution land cover and aircraft flux data” Haofei Yu & Alex Guenther (PNNL) ACS meeting, Boston, August 16-20, 2015

"Characterizing regional OH with airborne measurements of isoprene and its products" Alex Guenther, Dasa Gu, Haofei Yu, John Shilling, Manish Shrivastava (PNNL), Saewung Kim, Roger Seco (UC Irvine), Paulo Artaxo (USP), Fernando Cavalcante, Karla Longo (INPE), Rodrigo Souza (UEA), Julio Tota (UFOPA), Scot Martin (Harvard), Thomas Karl (U. Innsbruck), Lisa Kaser (NCAR), Bin Yuan (NOAA), Chris Cantrell, Lee Mauldin (U. Colorado)

14-020

Publications:

Gina M. Mazzuca, Xinrong Ren, Christopher P. Loughner, Mark Estes, James H. Crawford, Kenneth E. Pickering, and Russell R. Dickerson, Ozone Production and Its Sensitivity to NOx and VOCs: Results from DISCOVER-AQ in Houston in 2013, Atmos. Chem. Phys. Discuss., doi:10.5194/acp-2016-215, 2016

14-022

Publications:

Huang, M., Lee, P., McNider, R., Crawford, J., Buzay, E., Barrick, J., Liu, Y. and Krishnan, P., 2016. Temporal and spatial variability of daytime land surface temperature in Houston: Comparing DISCOVER-AQ aircraft observations with the WRF model and satellites. *Journal of Geophysical Research: Atmospheres.* Published online: 14 JAN 2016 DOI: 10.1002/2015JD023996

Presentations:

McNider, Richard T., K. Doty, Y. Wu, A. Pour-Biazar, P. Lee, M. Huang, B. Dornblaser, and C. Hain, 2016: Use of Satellite Skin Temperatures to Improve Surface Evapotranspiration Performance in WRF, Advances in Evaporation and Evaporative Demand, 30th Conference on Hydrology. American Meteorological Society, Annual Meeting, Jan.11-14, 2016, New Orleans, LA

McNider, Richard T., K. Doty, Y. Wu, A. Pour-Biazar, 2016: Initial tests of satellite skin temperature moisture nudging in the WRF Pleim-Xiu scheme, Air Quality Applied Science Team Annual meeting, Tenth Semi-annual Meeting, Research Triangle Park, NC January 4-6, 2016

McNider, R.T. Kevin Doty ,Yu Ling Wu, Min Huang, Pius Lee: Use of Satellite Data to Improve Specifications of Land Surface Parameters. Second Meteorology And Climate - Modeling for Air Quality (MAC-MAC) , September 16-18 , Sacramento, CA

17th GEIA Conference, November 18-20, 2015, Beijing China. "Top down emission analyses theme" presented by Alex Guenther (UC Irvine)

14-029

Publications:

Bean J, Faxon C, Leong YJ, Wallace HW, Cevik BK, Ortiz S, Canagaratna M, Usenko S, Sheesley RJ, Griffin RJ, Hildebrandt Ruiz L. (2016) Composition and Sources of Particulate Matter Measured near Houston, TX: Anthropogenic-Biogenic Interactions. *Atmosphere*. (5), 73; doi:10.3390/atmos7050073

Adelaide E. Clark, Subin Yoon, Rebecca J. Sheesley, Sascha Usenko. (2016) Spatial and Temporal Distribution of Current-Use Pesticides in Houston, Texas. Submitted to Bulletin of Environmental Contamination and Toxicology.

Presentations:
Oral Presentation at the American Geophysical Union national meeting; Dec 2015. *Radiocarbon Source Apportionment of Fossil and Modern Atmospheric Carbon from DISCOVER-AQ Houston*. Stephanie Ortiz*, Tate E. Barrett, Subin Yoon, Adelaide Clark, Sascha Usenko, and Rebecca J. Sheesley.

Posters:
Poster at the American Geophysical Union national meeting; Dec 2015. *Source Apportionment of Organic Aerosols across Houston, TX during NASA's DISCOVER-AQ* Subin Yoon*, Adelaide Clark, Stephanie Ortiz*, Sascha Usenko, and Rebecca J. Sheesley.

Poster at American Geophysical Union (AGU) 47th Annual Fall Meeting; Dec 2015. *Spatial and Temporal Distributions of Mosquito Adulticides in Houston during Spraying Season* Adelaide E. Clark, Subin Yoon, Rebecca J. Sheesley, and Sascha Usenko.

Poster at 36th Annual Society for Environmental Toxicology and Chemistry (SETAC) North American Meeting; Nov 2015. *Assessment of Spatial and Temporal Distribution of Current-Use Organophosphate Esters in Houston, Texas* Adelaide E. Clark, Subin Yoon, Rebecca J. Sheesley, and Sascha Usenko.

Poster at 36th Annual Society for Environmental Toxicology and Chemistry (SETAC) North American Meeting; Nov 2015. *Spatial and Temporal Distributions of Mosquito Adulticides in Houston during Spraying Season* Adelaide E. Clark, Subin Yoon, Rebecca J. Sheesley, and Sascha Usenko.

Poster at the American Association for Aerosol Research (AAAR); Oct 2015. *Evaluation of Modeled OA Formation in the Houston Region Using Measurements from the 2013 DISCOVER-AQ Campaign.* Bonyoung Koo, Lea Hildebrandt Ruiz, Rebecca J. Sheesley, Sascha Usenko, and Greg Yarwood.

Poster at the Annual Society for Environmental Toxicology and Chemistry (SETAC) South-Central Regional Chapter Meeting; May 2015. *Spatial trends in surface-based atmospheric particulate matter composition during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark, Stephanie Ortiz, Lea Hildebrandt Ruiz, and Sascha Usenko.

Poster at the Annual Society for Environmental Toxicology and Chemistry (SETAC) South-Central Regional Chapter Meeting; May 2015. *Spatial trends in surface-based carbonaceous aerosols measurements during DISCOVER-AQ in Houston, TX* Stephanie Ortiz, Tate E. Barrett, Subin Yoon, Adelaide Clark, Lea Hildebrandt Ruiz, Robert Griffin, Russell Long, Rachelle Duvall, Sascha Usenko, and Rebecca J. Sheesley.

Poster at the European Geophysical Union (EGU) General Assembly; Apr 2015. *A Pressurized Liquid Extraction Technique for the Analysis of Pesticides, PCBs, PBDEs, OPFRs, PAHs, Alkanes, Hopanes, and Steranes from Airborne Particulate Matter.* Adelaide Clark, Subin Yoon, Rebecca J. Sheesley, and Sascha Usenko.

Poster presented at the 1st Annual Texas Air Quality Symposium; Apr 2015. *Spatial Trends in Surface-based Carbonaceous Aerosols, including organic, water-soluble and elemental carbon, during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark, Lea Hildebrandt Ruiz, Robert Griffin, Russell Long, Rachelle Duvall, Sascha Usenko.

Poster presented at the 1st Annual Texas Air Quality Symposium; Apr 2015. *A Pressurized Liquid Extraction Technique for the Analysis of Pesticides, PCBs, PBDEs, OPFRs, PAHs, Alkanes, Hopanes, and Steranes from Airborne Particulate Matter*. Adelaide Clark, Subin Yoon, Rebecca J. Sheesley, and Sascha Usenko.

Poster at the American Geophysical Union national meeting Dec 2014 *Spatial trends in surface-based carbonaceous aerosol, including organic, water-soluble and elemental carbon, during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley*, Tate E. Barrett, Subin Yoon, Adelaide Clark, Lea Hildebrandt Ruiz, Robert Griffin, Russell Long, Rachelle Duvall and Sascha Usenko

Poster at the American Geophysical Union national meeting Dec 2014 *A Pressurized Liquid Extraction Technique for the Analysis of Pesticides, PCBs, PBDEs, OPEs, PAHs, Alkanes, Hopanes, and Steranes from Atmospheric Particulate Matter* Clark, A.E*; Yoon, S.; Sheesley, R.J., Usenko, S.

Poster at the SETAC North America 35th Annual Meeting in Vancouver Nov 2014. A Pressurized Liquid Extraction Technique for the Analysis of PAHs, Hopanes, Pesticides, PCBs and PBDEs from Air Filter Samples. Clark, A.E*., Barrett, T.E., Dev Nallathamby, P., Sheesley, R.J., Usenko, S.

Poster at the ACS 247th National Meeting in Dallas March 2014. A Pressurized Liquid Extraction Technique for the Analysis of PAHs, Hopanes, Pesticides, PCBs and PBDEs from Air Filter Samples. Clark, A.E.*, Barrett, T.E., Dev Nallathamby, P., Sheesley, R.J., Usenko, S.

14-025
"Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model." Chris Emery, Jeremiah Johnson, DJ Rasmussen, Wei Chun Hsieh, Greg Yarwood (Ramboll Environ) John Nielsen-Gammon, Ken Bowman, Renyi Zhang, Yun Lin, Leong Siu (Texas A&M University). Presented at the 14th Annual CMAS Conference, University of North Carolina, Chapel Hill, NC, October 5-7, 2015

14-030
"Improved MEGAN Predictions of Biogenic Isoprene in the Continental United States", Peng Wang; Gunnar W Schade; Mark Estes; Qi Ying. Atmospheric Environment. Under Review.

Appendix C

Financial Reports by Fiscal Year

(Expenditures reported as of May 31, 2016)

FY 10 and 11

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67		$0
Fringe Benefits		$38,665.65	$38,665.65		$0
Travel		$346.85	$346.85		$0
Supplies		$15,096.14	$15,096.14		$0
Equipment		$0.00			$0
Other					
Contractual					
Total Direct Costs		$256,925.31	$256,925.31		$0
Authorized Indirect Costs		$20,281.69	$20,281.69		$0
10% of Salaries and Wages					
Total Costs		**$277,207.00**	**$277,207.00**	**$0**	**$0**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00		$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment					
Other		$0.00			$0.00
Contractual					
Total Direct Costs		$206,706.26	$206,706.26	$0.00	$0.00
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$223,976.46**	**$223,976.46**	**0.00**	**$0.00**

ITAC Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,378.86	$16,378.86	$0	$0
Supplies		$1039.95	$1,039.95		$0
Equipment					
Other					
Total Direct Costs		$17,418.81	$17,418.81	$0	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$17,418.81**	**$17,418.81**	**$0**	**$0**

ITAC Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$6,292.97	$6,292.97	$0.00	$0
Supplies		$284.67	$284.67	$0.00	$0
Equipment					
Other					
Total Direct Costs		$6,577.64	$6,577.64	$0.00	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$6,577.64**	**$6,577.64**	**$0.00**	**$0**

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$145,337.70	$145,337.70		$0
Fringe Benefits		$28,967.49	$28,967.49		$0
Travel		$0	$0		$0
Supplies		$778.30	$778.30		$0
Equipment					
Other					
Total Direct Costs		$175,083.49	$175,083.49	$0	$0
Authorized Indirect Costs		$14,533.77	$14,533.77		$0
10% of Salaries and Wages					
Total Costs		**$189,617.26**	**$189,617.26**	**$0**	**$0**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$121,326.64	$121,326.64	$0	$0
Fringe Benefits		$23,102.60	$23,102.77	$0	($0.17)
Travel		$0			$0
Supplies		$207.98	$207.92	$0	$0.06
Equipment					
Other					
Total Direct Costs		$144,637.22	$144,637.33	$0	($0.11)
Authorized Indirect Costs		$12,132.66	$12,132.55	$0	$0.11
10% of Salaries and Wages					
Total Costs		**$156,769.88**	**$156,769.88**	**$0**	**$0.00**

AQRP Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67	$0.00	$0.00
Fringe Benefits		$38,665.65	$38,665.65	$0.00	$0.00
Travel		$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$15,096.14	$0.00	$0.00
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,287,827.93	$2,287,827.93	$0.00	$0.00
ITAC		$17,418.81	$17,418.81	$0.00	$0.00
Project Management		$189,617.26	$189,617.26	$0.00	$0.00
Total Direct Costs		$2,751,789.31	$2,751,789.31	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$20,281.69	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,772,071.00**	**$2,772,071.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$1,852,440.62	$1,852,440.51	$0.00	$0.11
ITAC		$6,577.64	$6,577.64	$0.00	$0.00
Project Management		$156,769.88	$156,769.88	$0.00	$0.00
Total Direct Costs		$2,222,494.40	$2,222,494.29	$0.00	$0.11
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,239,764.60**	**$2,239,764.49**	**$0.00**	**$0.11**

FY 12 and 13

Administration Budget (includes Council Expenses)

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$74,238.65	$74,238.65	$0.00	$0.00
Fringe Benefits		$17,068.38	$17,068.38	$0.00	$0.00
Travel		$339.13	$339.13		$0.00
Supplies		$3,560.62	$3,560.62	$0.00	$0.00
Equipment		$0.00			$0.00
Other					
Total Direct Costs		$95,206.78	$95,206.78	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$7,423.86	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$102,630.64**	**$102,630.64**	**$0.00**	**$0.00**

Administration Budget (includes Council Expenses)

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$256,154.46	$256,154.46		$0.00
Fringe Benefits		$59,405.87	$59,405.87		$0.00
Travel		$0.00	$0.00		$0.00
Supplies		$8,824.23	$8,824.23		$0.00
Equipment					
Other		$0.00			
Total Direct Costs		$324,384.56	$324,384.56	$0.00	$0.00
Authorized Indirect Costs		$25,615.44	$25,615.44		$0.00
10% of Salaries and Wages					
Total Costs		**$350,000.00**	**$350,000.00**	**$0.00**	**$0.00**

ITAC Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$5,323.31	$5,323.31		$0.00
Supplies		$231.86	$231.86		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$5,555.17	$5,555.17	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$5,555.17**	**$5,555.17**	**$0.00**	**$0.00**

ITAC Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00		$0.00
Supplies		$0.00	$0.00		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$53,384.46	$53,384.46	$0.00	$0.00
Fringe Benefits		$10,991.04	$10,991.04	$0.00	$0.00
Travel		$0.00	$0.00		$0.00
Supplies		$967.98	$967.98		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$65,343.48	$65,343.48	$0.00	$0.00
Authorized Indirect Costs		$5,338.44	$5,338.44	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$70,681.92**	**$70,681.92**	**$0.00**	**$0.00**

Project Management Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$123,279.85	$123,279.85		$0.00
Fringe Benefits		$23,666.75	$23,666.75		$0.00
Travel					
Supplies		$699.40	$699.40		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$147,646.00	$147,646.00	$0	$0.00
Authorized Indirect Costs		$12,328.00	$12,328.00		$0.00
10% of Salaries and Wages					
Total Costs		**$159,974.00**	**$159,974.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$74,238.65	$74,238.65	$0.00	$0.00
Fringe Benefits		$17,068.38	$17,068.38	$0.00	$0.00
Travel		$339.13	$339.13	$0.00	$0.00
Supplies		$3,560.62	$3,560.62	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$847,438.67	$847,438.67	$0.00	$0.00
ITAC		$5,555.17	$5,555.17	$0.00	$0.00
Project Management		$70,681.92	$70,681.92	$0.00	$0.00
Total Direct Costs		$1,018,882.54	$1,018,882.54	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$7,423.86	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$1,026,306.40**	**$1,026,306.40**	**$0.00**	**$0.00**

AQRP Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$256,154.46	$256,154.46	$0.00	$0.00
Fringe Benefits		$59,405.87	$59,405.87	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$8,824.23	$8,824.23	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$2,990,026.00	$2,990,026.00	$0.00	$0.00
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$159,974.00	$159,974.00	$0.00	$0.00
Total Direct Costs		$3,474,384.56	$3,474,384.56	$0.00	$0.00
Authorized Indirect Costs		$25,615.44	$25,615.44	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$3,500,000.00**	**$3,500,000.00**	**$0.00**	**$0.00**

FY 14 and 15

Administration Budget (includes Council Expenses)

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$72,835.93	$72,835.93	$0.00	$0.00
Fringe Benefits		$17,865.93	$17,865.93	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$2,014.54	$2,014.54	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$92,716.40	$92,716.40	$0.00	$0.00
Authorized Indirect Costs		$7,283.60	$7,283.60	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$100,000.00**	**$0.00**	**$0.00**

Administration Budget (includes Council Expenses)

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$72,127.87	$72,127.87	$0.00	$0.00
Fringe Benefits		$18,448.69	$18,448.69	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$2,210.63	$2,210.63	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$92,787.19	$92,787.19	$0.00	$0.00
Authorized Indirect Costs		$7,212.81	$7,212.81	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$100,000.00**	**$0.00**	**$0.00**

ITAC Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$0.00	$0.00	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

ITAC Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$0.00	$0.00	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$53,932.44	$53,932.44	$0.00	$0.00
Fringe Benefits		$11,011.39	$11,011.39	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$168.93	$168.93	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$65,112.76	$65,112.76	$0.00	$0.00
Authorized Indirect Costs		$5,393.24	$5,393.24	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$70,506.00**	**$70,506.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$54,059.53	$54,059.53	$0.00	$0.00
Fringe Benefits		$10,537.20	$10,537.20	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$537.98	$537.98	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$65,134.71	$65,134.71	$0.00	$0.00
Authorized Indirect Costs		$5,405.95	$5,405.95	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$70,540.66**	**$70,540.66**	**$0.00**	**$0.00**

AQRP Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$72,835.93	$72,835.93	$0.00	$0.00
Fringe Benefits		$17,865.93	$17,865.93	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$2,014.54	$2,014.54	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$829,494.00	$829,494.00	$0.00	$0.00
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$70,506.00	$70,506.00	$0.00	$0.00
Total Direct Costs		$992,716.40	$992,716.40	$0.00	$0.00
Authorized Indirect Costs		$7,283.60	$7,283.60	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$1,000,000.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$72,127.87	$72,127.87	$0.00	$0.00
Fringe Benefits		$18,448.69	$18,448.69	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$2,210.63	$2,210.62	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$829,459.34	$829,459.34	($804.90)	$804.90
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$70,540.66	$70,540.66	$0.00	$0.00
Total Direct Costs		$992,787.19	$992,787.19	($804.90)	$804.90
Authorized Indirect Costs		$7,212.81	$7,212.81	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$1,000,000.00**	**($804.90)**	**$804.90**

Appendix D

Texas AQRP Annual Reports

FY 2010 – 2011 through FY 2014 - 2015

AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-10-94300
awarded to The University of Texas at Austin

Annual Report

Fiscal Year 2010

May 1, 2010 through August 31, 2010

Submitted to

David Brymer
Texas Commission on Environmental Quality
12100 Park 35 Circle
Austin, TX 78753

Prepared by

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September 30, 2010

The preparation of this report was financed through a grant from the Texas Commission on Environmental Quality (TCEQ), administered by The University of Texas at Austin through the Air Quality Research Program (AQRP). The contents, findings, opinions, and conclusions are the work of the author(s) and do not necessarily represent findings, opinions, or conclusions of the TCEQ.

Texas Air Quality Research Program

Annual Progress Report

September 30, 2010

Overview

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the FY 2010-2011 biennium, the AQRP has approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released a call for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received by the due date of June 25, 2010. These proposals were reviewed by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs. The results of these reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. Successful proposers were notified, and subcontracts are currently being initiated. At the end of the fiscal year, no sub-contracts were in place, however, several of the subcontracts should be in place in early September, 2010.

Background

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

> Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.
>
> (b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.
>
> (c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.
>
> (d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.
>
> (e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.
>
> (f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC). The research projects are selected after a three stage review process. In the first stage, an Independent Technical Advisory Committee (ITAC, up to 15 members) reviews research proposals based on technical merit. In a second stage of review, the TCEQ reviews the projects for relevancy to the State's air quality research needs. In a final stage of review, an Advisory Council approves projects.

During the first four months of operation, the University of Texas established the Independent Advisory Committee (ITAC) and the Advisory Council (Council). A program web site was established, and a request for proposals was released; proposals were reviewed and an initial

group of proposals was approved for funding. This first annual report describes the AQRP's activities in these areas.

Independent Technical Advisory Committee (ITAC)

The AQRP funding is to be used primarily for research projects, and one of three groups responsible for selecting the projects is the Independent Technical Advisory Committee (ITAC). The ITAC is composed of up to 15 individuals with scientific expertise relevant to the Program. The ITAC is charged with recommending technical approaches, and establishing research priorities. The ITAC meets at least twice per year at locations rotating between Austin, Dallas and Houston. One of the meetings each year is dedicated to new project review. A second meeting each year is dedicated to reviewing progress on funded projects and review of the Program's strategic plan. Members of the ITAC consist of the TCEQ Project Director (or designee), representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC are listed in Table 1. The members of the ITAC are drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas.

The ITAC membership is intentionally drawn from air quality researchers who have experience in Texas; these researchers and their colleagues will likely have interest in responding to the requests for research proposals issued by the AQRP. This raises potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas requires that the AQRP shall maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members are required to certify:

Confidentiality: As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)

Conflict of Interest: As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or the TCEQ Project Director If there is a question of interpretation regarding whether a conflict of interest exists, I agree

that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Table 1. Members of the Independent Technical Advisory Committee

Name	Title	Organization
David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	Colorado University
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Assistant Professor, Department of Earth and Atmospheric Sciences	The University of Houston
Jim Meagher	Deputy Director, Chemical Science Division, Earth Systems Research Laboratory	National Oceanic and Atmospheric Administration
J. David Mobley	Deputy Director, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
John Nielsen-Gammon	Professor and Texas State Climatologist The Center for Atmospheric Chemistry and the Environment	Texas A&M University
George O. Talbert	Director, Texas Air Research Center	Lamar University
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Assistant Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ

On July 19 and July 22, 2010, the Independent Technical Advisory Committee met to evaluate proposals submitted to the Air Quality Research Program. The meeting on July 19 was a 3-hour conference call and the meeting on July 22 was a full day meeting held at the University of Texas Pickle Research Campus. Attendees at the meetings were limited to ITAC members and AQRP staff. All ITAC members (or in two cases, approved substitutes) participated in both meetings.

In these meetings, the ITAC ranked all 45 proposals that were submitted to the AQRP by the deadline of June 25 at 5PM Central Time. Each proposal was assigned three ITAC members who served as lead reviewers. As each proposal was considered by the full ITAC, these lead reviewers summarized the proposal, along with its strengths and weaknesses. The full ITAC then discussed the proposal and all ITAC members who did not have conflicts of interest provided two assessments of the proposal – a numerical score (ranging from 0-100) and a letter score (A=high technical merit, high priority for funding; B=technically meritorious, but with some limitations, fund if resources are available; C=serious technical or other flaws, not recommended for funding).

The proposals were ranked according to both numerical score and technical score. The 12 most highly rated proposals based on numerical score were the same as the 12 most highly rated proposals based on letter score. The results of the ITAC meeting were sent to the TCEQ with proposals grouped into 3 categories:

1. Highly recommended (12 proposals, $3,688,445 in funding requested).
2. Recommended (12 proposals, $3,438,480 in funding requested).
3. Not recommended (21 proposals).

TCEQ Relevancy Review

Once the ITAC reviewed and ranked the research project proposals according to technical merit, they were submitted to the TCEQ for a relevancy review. The TCEQ reviews proposals for relevancy to the State's air quality research needs. TCEQ approval is required for a project to receive funding from the Program.

TCEQ reviewed the top 24 proposals and provided comments on several of the projects to enhance their relevancy to the state's air quality research goals. In addition, the TCEQ provided a ranking of the proposals as a product of their relevancy review.

Stakeholder Meeting

On August 9 the AQRP held an open forum meeting to discuss the air quality research needs of the State of Texas. Seven individuals representing the environmental community, the regulated community, and the near non-attainment Council of Governments attended. The information gathered in this meeting was presented to the Advisory Council. Recommendations for future research priorities fell in to 2 categories, 1) future solicitations should promote a better understanding of emissions from mobile sources and 2) characterization of the long range transport of air pollutants into and within the state of Texas should be emphasized.

Advisory Council

The group responsible for selecting AQRP research projects is the Advisory Council. The Council serves as a Board of Directors for the Program and consists of up to 11 members, all residents of the State of Texas. As defined in the AQRP contract, two Council members with relevant scientific expertise are nominated by the TCEQ, and up to four members of the Council can be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. The purpose of the Council is to give final approval to projects

recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. The Council meets twice per year. One meeting is dedicated to new project selection. A second meeting each year will be dedicated to providing summaries of on-going projects and review of the strategic plan. The members of the Advisory Council and their affiliations are listed in Table 2.

Table 2. Members of the Advisory Council

Name	**Title**	**Organization**
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge Elect	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

The Council met on August 16 and approved fourteen proposals for funding by the AQRP. Two additional proposals were designated as alternates. The approved proposals are listed in Table 3 and the alternate proposals are listed in Table 4.

Principal Investigator's have been notified that their projects are approved for funding and the contracting process has begun.

Table 3. Awarded Projects

AQRP Project Number	Title	Principal Investigator	Institutions Represented	Funding Awarded	Project Managers
6	Quantification of Industrial Emisions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS	Johan Mellqvist	Chalmers Univ. of Technology & Univ. of Houston	$498,644	David Sullivan
8	Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling	Daniel Cohan	Rice, & Environ	$190,966	Elena McDonald-Buller
9	Additional Flare Test Days for TCEQ Comprehensive Flare Study	Vincent Torres	UT-Austin	$591,332	Cyril Durrenberger
14	Quantifying Emission Estimates from Biogenic and Oil and Gas Production Sources in Texas	Christine Wiedinmyer	UCAR/NCAR	$595,173	Elena McDonald-Buller
15	An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-attainment areas in Texas	James Roberts	NOAA, Environ	$201,306	Elena McDonald-Buller
20	NO_x Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone	Steven Brown	NOAA, Environ	$202,498	Elena McDonald-Buller
21	Dry Deposition of Ozone to Built Environment Surfaces	Richard Corsi	UT-Austin	$248,830	Elena McDonald-Buller
22	Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas	Daniel Chen	Lamar Univ.	$150,000	Vincent Torres
26	Biogenic VOC Flux Measurements in East Texas	Gunnar Schade	Texas A&M	$200,000	Elena McDonald-Buller
29	Wind Modeling Improvements with the Ensemble Kalman Filter	John Neilson-Gammon	Texas A & M	$80,108	Gary McGaughey

32	SHARP Data Analysis: Radical Budget and Ozone Production	Barry Lefer	Univ. of Houston, Penn State, Univ. of New Hampshire, Univ. of Miami, & UCLA	$248,652	Cindy Murphy
34	Dallas Measurements of Ozone Production	Barry Lefer	Univ. of Houston & Penn State	$195,054	David Sullivan
42	Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms	Greg Yarwood	Environ, UC-Riverside, & Smog Reyes	$237,481	Elena McDonald-Buller
45	Quantification of Hydrocarbon, NOx, and SO2 emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR dataset	Jochen Stutz	UCLA, UNC, Aerodyne, & Washington State	$398,401	Cindy Murphy

Table 4. Alternate Projects

AQRP Project Number	Title	Principal Investigator	Institutions represented	Funding Awarded
24	Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area	Robert Griffin	Rice, Univ. of New Hampshire, NCAR, Univ. of Michigan, & Univ. of Houston	To Be Determined up to $511,878 if funding available
44	Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season	Maxwell Shauck	Univ. of Houston	$380,261

Research Project Cycle

The research program is being implemented through an 8 step cycle. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle. During the first 4 months of AQRP operation, steps 1-5 were completed for the first project cycle. The projected timeline for the remainder of the biennium is also outlined below.

1.) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and the TCEQ developed initial research priorities; the research priorities were released along with the initial Request for Proposals in May, 2010. An initial Strategic Plan was released in July, 2010. The Request for Proposals and the Strategic Plan are available at http://aqrp.ceer.utexas.edu/

2.) Project proposals relevant to the research priorities are solicited. The initial Request for Proposals was released on May 25, 2010. Proposals were due by June 25, 2010. Forty-five proposals, requesting $12.9 million in funding, were received by the deadline.

3.) The Independent Technical Advisory Committee (ITAC) performs a scientific and technical evaluation of the proposals. For the initial round of proposals, the ITAC reviewed the proposals in conference calls and in a meeting held in Austin, Texas. The reviews were completed on July 22, 2010. Twelve proposals were highly recommended for funding; twelve proposals were recommended for funding, and 21 proposals were not recommended for funding.

4.) The project proposals and ITAC recommendations will be forwarded to the TCEQ. The TCEQ will evaluate the project recommendations from the ITAC, comment on the relevancy of the projects to the State's air quality research needs. For the first round of proposals, the TCEQ rated, as highly recommended, the same 12 research projects that were highly recommended by the ITAC. The TCEQ also recommended for funding the same 12 proposals that the ITAC recommended, however, the rank ordering of these 12 recommended proposals differed between the two groups.

5.) The recommendations from the ITAC and the TCEQ will be presented to the Council for their approval. The Council will also provide comments on the strategic research priorities. For the first group of proposals, the Council approved for funding all of the projects that were highly recommended by both the ITAC and TCEQ (12 projects). In addition, the Council approved for funding several projects in the recommended category, which were highly ranked within the recommended category by both the ITAC and TCEQ.

6.) Funded projects will be assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin will be responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The Project Manager will have responsibility for documenting progress toward project measures of success for each project. The Project Manager will work with the researchers, and the TCEQ to create an approved work plan for the project. The Project Manager will also

work with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved QAPP for each project. The Project Manager will review monthly, annual and final reports from the researchers and work with the researchers to address deficiencies. For the first round of proposals all respondents to the RFP have been notified of their award status. For those projects that will be funded, a Project Manager has been assigned and they have made initial contact with their PIs. TCEQ has been given a list of projects that will be funded, and is currently assigning TCEQ Project Liaisons.

7.) The AQRP Director and the Project Manager for each project will describe progress on the project in the ITAC and Council meetings dedicated to on-going project review. The AQRP Director will ensure that at least 10% of project funds are available at the time of these presentations so that recommendations can be incorporated into final project deliverables.

8.) The project findings will be communicated through multiple mechanisms. Final reports will be posted to the Program web site; research briefings will be developed for the public and air quality decision makers; an annual research conference will be held.

Program Timeline, May 1, 2010-August 31, 2011

May 2010: Finalize membership in Council and ITAC; solicit project proposals

June 2010: Proposals due; send proposals to ITAC for review.

July 2010: ITAC conducts review and ranking of proposals; TCEQ to review immediately after ITAC ratings are complete, Council to meet to approve projects immediately after TCEQ work is complete.

August 2010: Council to meet to approve projects immediately after TCEQ work is complete; issue contracts for approved projects

September 2010-April 2011: Project reports and deliverables completed on an on-going basis

September 2010: Program quarterly report due to TCEQ

December 2010: Program quarterly report due to TCEQ

March 2010: Program quarterly report due to TCEQ

April 2011: Project progress report to ITAC and TCEQ; strategic plan review.

May 2011: Project progress reports to Council; strategic plan review. Program quarterly report due to TCEQ.

May 2011-August 2011: Projects continue with ITAC, TCEQ, and Council input; project reports and deliverables completed on an on-going basis

August 2011: Project completion; Program final report completed.

Financial Status Report

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May an amendment was issued increasing the budget by $40,000. The entirety of these funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

Program Administration – limited to 10% of the overall funding
This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC
These funds are to cover the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project will be assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual
These are the funds available to support the research projects that are selected for funding.

At this time it is anticipated that all of the contractual funds will be dispersed to the research projects, and the Program Administration, ITAC, and Project Management funds will be spent by August 31, 2011.

Program Administration

Program Administration includes salaries and fringe benefits for those overseeing the program as a whole, as well as, materials and supplies, travel, equipment, and other expenses. This category allows indirect costs in the amount of 10% of salaries and wages.

During the reporting period nine staff members were involved in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. James Thomas, AQRP Manager, is responsible for assisting Dr. Allen in the program administration. His primary responsibilities during this reporting period involved working with the ITAC members and organizing the Council membership. Ms. Maria Stanzione, AQRP Grant Manager, assisted with proposal management, development of the Sub-award document for the research projects, and communication with the ITAC members.

Table 5. AQRP Administration Budget (FY 10)

Administration Budget (includes Council Expenses)

Budget Category		FY10 Budget	Invoiced Expenses*	Pending Expenses	Remaining Balance
Personnel/Salary		$173,100	$65,155		$107,945
Fringe Benefits		$38,082	$10,110		$27,972
Travel		$8,500			$8,500
Supplies		$34,215	$1,056	$2,169	$30,990
Equipment		$6,000			$6,000
Other					
Total Direct Costs		$259,897	$76,321	$2,169	$181,407
Authorized Indirect Costs		$17,310	$6,516		$10,794
10% of Salaries and Wages					
Total Costs		**$277,207**	**$82,837**	**$2,169**	**$192,201**
Fringe Rate		22%			

*Includes actual invoices from April 30, 2010 to July 31, 2010, and the projected invoice for August 1, 2010 – August 31, 2010.

Ms. MaryAnn Foran assisted with the development of the Sub-award document and provided input on program organization. Ms. Rachael Bushn assists with administrative functions. Her initial responsibilities have included working with the ITAC and Council, and providing notification of funding decisions to those who submitted proposals to the AQRP RFP. Mr. Denzil Smith is responsible for the AQRP Web Page development and for data management.

A graduate student and post-doctoral associate, Cameron Faxon and Mariana Dionisio, respectively, are working on the development of a state of the science document. This is an extension of the initial research priorities and Strategic Plan, and will be used to assess project objectives.

Mr. Cyril Durrenberger, a Project Manager, is providing assistance with the development and review of the Quality Assurance Project Plans for all research projects.

Not all Council Meeting expenses have posted as of the writing of this report. These are included in the supplies category.

ITAC

The ITAC met in Austin, Texas, on July 22, 2010, to complete their review and ranking of the proposals. The total amount charged to the ITAC account as of August 31, 2010, is $9,053.49, though not all ITAC meeting expenses have posted as of that date.

Table 6. ITAC Budget (FY 10)

ITAC Budget

Budget Category		FY10 Budget	Invoiced Expenses*	Pending Expenses	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,500	$8,894	$2,298	$5,308
Supplies		$2,364	$160		$2,204
Equipment					
Total Direct Costs		$18,864	$9,054	$2,298	$7,512
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$18,864**	**$9,054**	**$2,298**	**$7,512**

*Includes actual invoices from April 30, 2010 to July 31, 2010, and the projected invoice for August 1, 2010 – August 31, 2010.

Project Management

No expenses have been charged to the Project Management account as of the writing of this report.

Table 7: Project Management Budget (FY 10)

Project Management Budget

Budget Category		FY10 Budget	Invoiced Expenses*	Pending Expenses	Remaining Balance
Personnel/Salary		$139,653			$139,653
Fringe Benefits		$30,725			$30,725
Travel		$4,000			$4,000
Supplies		$1,657			$1,657
Equipment					
Other					
Total Direct Costs		$176,035	$0	$0	$176,035
Authorized Indirect Costs		$13,965			
10% of Salaries and Wages					
Total Costs		**$190,000**	**$0**	**$0**	**$190,000**
Fringe Rate		22%			

*Includes actual invoices from April 30, 2010 to July 31, 2010, and the projected invoice for August 1, 2010 – August 31, 2010.

Research Projects

As of August 31, 2010, no sub-awards (contracts) have been issued for the Research Projects, so no expenditures have been incurred.

Appendix A

Cumulative Financial Report

Fiscal Year 2010

For the period

May 1, 2010 through August 31, 2010

Air Quality Research Program
Cumulative Financial Report
Fiscal Year 2010

Budget Category	AQRP Administration Budget	ITAC Budget	Project Management Budget	Research Projects Budget	Total Budget FY 10	Total Invoiced Expenses FY 10*	Total Pending Expenses FY 10	Remaining Balance
Personnel/Salary	$173,100		$139,653		$312,753	$65,155.00	$0.00	$247,598.00
Fringe Benefits	$38,082		$30,725		$68,807	$10,110.10	$0.00	$58,696.90
Travel	$8,500	$16,500	$4,000		$29,000	$8,893.65	$2,298.00	$17,808.35
Supplies	$34,215	$2,364	$1,657		$38,236	$1,215.67	$2,169.11	$34,851.22
Equipment	$6,000				$6,000	$0.00	$0.00	$6,000.00
Other								
Contractual				$2,286,000	$2,286,000	$0.00	$0.00	$2,286,000.00
Total Direct Costs	$259,897	$18,864	$176,035	$2,286,000	$2,740,796	$85,374.42	$4,467.11	$2,650,954.47
Authorized Indirect Costs	$17,310		$13,965		$31,275	$6,515.50	$0.00	$24,759.50
10% of Salaries and Wages								
Total Costs	**$277,207**	**$18,864**	**$190,000**	**$2,286,000**	**$2,772,071**	**$91,889.92**	**$4,467.11**	**$2,675,713.97**
Fringe Rate	22%							

*Includes actual invoices from April 30, 2010 to July 31, 2010, and the projected invoice for August 1, 2010 – August 31, 2010.

AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-10-94300
Awarded to The University of Texas at Austin

Annual Report

September 1, 2010 through August 31, 2011

Submitted to

David Brymer
Texas Commission on Environmental Quality
12100 Park 35 Circle
Austin, TX 78753

Prepared by

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October 5, 2011

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Texas Air Quality Research Program

Annual Report

October 5, 2011

OVERVIEW

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the 2010-2011 biennium, the AQRP had approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released a call for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received by the due date of June 25, 2010. These proposals were reviewed by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs. The results of these reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. Successful proposers were notified, and subcontracts were initiated. The subcontracting involved two phases. First, a sub-agreement was established with each institution specifying terms and conditions. Second, once a sub-agreement was in place and a project Work Plan was approved, a Task Order was issued authorizing work to commence. A description of project activities is described in this progress report.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding for this period has yet to be determined.

BACKGROUND

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

> Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.
>
> (b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.
>
> (c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.
>
> (d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.
>
> (e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.
>
> (f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

Research Project Cycle

The research Program was implemented through an 8 step cycle. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle. During the first quarter of AQRP operation, steps 1-5 were completed for the first project cycle. During the second quarter, sub-agreements for most projects were established and Task Orders began to be initiated (step 6 and parts of step 7). In the third quarter, the final sub-agreements were executed and Task Orders were initiated for the majority of the projects. In the fourth quarter, Task Orders were finalized for the remaining Projects and work was in progress on every Project. During the fifth quarter, work progressed on all projects, including the DFW Field Study. On August 31, 2011, six (6) projects were completed and the remaining projects were issued a 90-day contract extension.

1.) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and the TCEQ developed initial research priorities; the research priorities were released along with the initial Request for Proposals in May, 2010. An initial Strategic Plan was released in July, 2010. The Request for Proposals and the Strategic Plan are available at http://aqrp.ceer.utexas.edu/

2.) Project proposals relevant to the research priorities are solicited. The initial Request for Proposals was released on May 25, 2010. Proposals were due by June 25, 2010. Forty-five proposals, requesting $12.9 million in funding, were received by the deadline.

3.) The Independent Technical Advisory Committee (ITAC) performs a scientific and technical evaluation of the proposals. For the initial round of proposals, the ITAC reviewed the proposals in conference calls and in a meeting held in Austin, Texas. The reviews were completed on July 22, 2010. Twelve proposals were highly recommended for funding; twelve proposals were recommended for funding, and 21 proposals were not recommended for funding.

4.) The project proposals and ITAC recommendations are forwarded to the TCEQ. The TCEQ evaluates the project recommendations from the ITAC and comments on the relevancy of the projects to the State's air quality research needs. For the first round of proposals, the TCEQ rated, as highly recommended, the same 12 research projects that were highly recommended by the ITAC. The TCEQ also recommended for funding the same 12 proposals that the ITAC recommended, however, the rank ordering of these 12 recommended proposals differed between the two groups.

5.) The recommendations from the ITAC and the TCEQ are presented to the Council for their approval. The Council also provides comments on the strategic research priorities. For the first group of proposals, the Council approved for funding all of the projects that were highly recommended by both the ITAC and TCEQ (12 projects). In addition, the Council approved for funding several projects in the recommended category, which were highly ranked within the recommended category by both the ITAC and TCEQ. Two

projects were selected as recommended for funding in the event that funding later became available.

6.) All Investigators are notified of the status of their proposals, funded, not funded, or not funded at this time, but being held for possible reconsideration if funding becomes available.

7.) Funded projects are assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin is responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The Project Manager has responsibility for documenting progress toward project measures of success for each project. The Project Manager works with the researchers, and the TCEQ to create an approved work plan for the project. The Project Manager also works with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved QAPP for each project. The Project Manager reviews monthly, annual and final reports from the researchers and works with the researchers to address deficiencies. All respondents to the RFP have been notified of their award status. A Project Manager has been assigned to each project and s/he continues to have ongoing contact with his/her PIs. TCEQ has assigned a TCEQ Project Liaison to each project.

8.) The AQRP Director and the Project Manager for each project describes progress on the project in the ITAC and Council meetings dedicated to on-going project review. Six projects have been completed, having met project objectives, as of August 31, 2011. All projects were reviewed by the ITAC at a meeting held in Austin on September 27 and 28, 2011. The AQRP Director will ensure that any comments made by the ITAC in the September 2011 meeting are responded to in the final project deliverables of the remaining active projects.

9.) The project findings will be communicated through multiple mechanisms. Final reports will be posted to the Program web site; research briefings will be developed for the public and air quality decision makers.

Program Timeline, May 1, 2010-August 31, 2011

May 2010: Finalize membership in Council and ITAC; solicit project proposals

June 2010: Proposals due; send proposals to ITAC for review.

July 2010: ITAC conducts review and ranking of proposals; TCEQ to review immediately after ITAC ratings are complete.

August 2010: Council to meet to approve projects immediately after TCEQ work is complete.

September 2010 – February 2011: Issue contracts and Task Orders for approved projects

September 2010-April 2011: Project reports and deliverables completed on an on-going basis

September 2010: Program quarterly report due to TCEQ

December 2010: Program quarterly report due to TCEQ

March 2010: Program quarterly report due to TCEQ

April 2011: Project progress report to ITAC and TCEQ; strategic plan review.

May 2011: Project progress reports to Council; strategic plan review. Program quarterly report due to TCEQ.

May 2011-November 2011: Projects continue with ITAC, TCEQ, and Council input; project reports and deliverables completed on an on-going basis

August 2011-November 2011: Project completion; Project final report completed. Contract Extensions granted, if needed.

September 27 & 28, 2011: AQRP Data Workshop

November 30, 2011: Project completion date for all extended projects.

Independent Technical Advisory Committee (ITAC)

The AQRP funding is used primarily for research projects, and one of three groups responsible for selecting the projects is the Independent Technical Advisory Committee (ITAC). The ITAC, composed of up to 15 individuals with scientific expertise relevant to the Program, is charged with recommending technical approaches, and establishing research priorities. Initially, the ITAC was to meet at least twice per year at locations rotating between Austin, Dallas and Houston. As the Program proceeded, it was more efficient for the ITAC to meet once in Austin and as needed via conference call/webinar. One of the meetings each year is dedicated to new project review. A second meeting each year is dedicated to reviewing progress on funded projects and review of the Program's strategic plan.

Members of the ITAC consist of the TCEQ Project Director (or designee), representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC are drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas. The members of the ITAC are listed in Table 1. Dr. Thomas Ho, of Lamar University was selected to fill the position left by the death of George Talbert in February 2011.

As the ITAC membership is intentionally drawn from air quality researchers who have experience in Texas; these researchers and their colleagues will likely have interest in responding to the requests for research proposals issued by the AQRP. This raises potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas requires that the AQRP shall maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members are required to certify:

> *Confidentiality:* As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)
> *Conflict of Interest:* As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or

the TCEQ Project Director. If there is a question of interpretation regarding whether a conflict of interest exists, I agree that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Table 1: Members of the Independent Technical Advisory Committee

Name	**Title**	**Organization**
David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	Colorado University
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Assistant Professor, Department of Earth and Atmospheric Sciences	The University of Houston
Jim Meagher	Deputy Director, Chemical Science Division, Earth Systems Research Laboratory	National Oceanic and Atmospheric Administration
J. David Mobley	Deputy Director, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
John Nielsen-Gammon	Professor and Texas State Climatologist The Center for Atmospheric Chemistry and the Environment	Texas A&M University
Tho (Thomas) Ching Ho	Chairman, Dan F. Smith Department of Chemical Engineering	Lamar University
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Assistant Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ

TCEQ Relevancy Review

Once the ITAC has reviewed and ranked research project proposals according to technical merit, they are submitted to the TCEQ for a relevancy review. The TCEQ reviews proposals for relevancy to the State's air quality research needs. TCEQ approval is required for a project to receive funding from the Program.

Advisory Council

The final group responsible for selecting AQRP research projects is the Advisory Council. The Council serves as a Board of Directors for the Program and consists of up to 11 members, all residents of the State of Texas. Two Council members with relevant scientific expertise are nominated by the TCEQ. As defined in the AQRP contract, up to four members of the Council can be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. Additional members include government officials from Texas Near-Non-Attainment Areas active in air quality management. The purpose of the Council is to give final approval to projects recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. The Council meets twice per year. One meeting is dedicated to new project selection. A second meeting each year will be dedicated to providing summaries of on-going projects and review of the strategic plan.

Table 2: Members of the Advisory Council

Name	Title	Organization
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

Table 3 below provides a list of the top two-thirds of the projects that were recommended by the ITAC and forwarded to the TCEQ and Advisory Council for review. The column titled Funding Awarded by Council shows the amounts approved; changes are shown in the notes. Some projects were able to reduce their budget slightly as the Scopes of Work and QAPPs were refined.

Table 3: Project Selection

AQRP Project Number	Title	Principal Investigator	Institutions represented	ITAC 1st Tier	ITAC 2nd Tier	Funding Awarded by Council	Notes
6	Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS	Johan Mellqvist	Chalmers Univ. of Technology & Univ. of Houston	x		$498,644	Actually funded at $484,662.
8	Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling	Daniel Cohan	Rice, & Environ	x		$190,966	Actually funded at $178,796.
9	Additional Flare Test Days for TCEQ Comprehensive Flare Study	Vincent Torres	UT-Austin	x		$591,332	
14	Quantifying Emission Estimates from Biogenic and Oil and Gas Production Sources in Texas	Christine Wiedinmyer	UCAR/NCAR	x		$595,173	Unable to agree to contractual terms – Project not awarded.
15	An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-attainment areas in Texas	James Roberts	NOAA, Environ	x		$201,306	Unable to agree to contractual terms with NOAA as PI. Changed Environ to Lead PI and reduced NOAA's Scope to specific task deliverables. Actually funded at $201,280.
20	NO_x Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone	Steven Brown	NOAA, Environ	x		$202,498	Unable to agree to contractual terms with NOAA as PI. Changed Environ to Lead PI and reduced NOAA's Scope to specific task deliverables.
21	Dry Deposition of Ozone to Built Environment Surfaces	Richard Corsi	UT-Austin	x		$248,830	Actually funded at $248,786.
22	Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas	Daniel Chen	Lamar Univ.		x	$150,000	

26	Biogenic VOC Flux Measurements in East Texas	Gunnar Schade	Texas A&M		x	$200,000	After funding was announced PI withdrew, during Work Plan development.
29	Wind Modeling Improvements with the Ensemble Kalman Filter	John Neilson-Gammon	Texas A & M	x		$80,108	
32	SHARP Data Analysis: Radical Budget and Ozone Production	Barry Lefer	Univ. of Houston, Penn State, Univ. of New Hampshire, Univ. of Miami, & UCLA	x		$248,652	
34	Dallas Measurements of Ozone Production	Barry Lefer	Univ. of Houston & Penn State	x		$195,054	
42	Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms	Greg Yarwood	Environ, UC-Riverside, & Smog Reyes	x		$237,481	
45	Quantification of Hydrocarbon, NOx, and SO2 emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR dataset	Jochen Stutz	UCLA, UNC, Aerodyne, & Washington State	x		$398,401	Actually funded at $398,042
Contingency Projects							
24	Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area	Robert Griffin	Rice, Univ. of New Hampshire, NCAR, Univ. of Michigan, & Univ. of Houston		x	To Be Determined up to $511,878 if funding available	Funding awarded at $458,957. NCAR's portion of the project had to be removed due to contractual issues.
44	Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season	Maxwell Shauck	Univ. of Houston		x	Up to $380,261, depending on funding available	Funding Awarded at $279,642.

Not Selected for Funding by Council						Funding Requested	
2	Measurement of Atmospheric Nitrophenols in the HGA and DFW Areas	Purnendu Dasgupta	UT-Arlington & Univ. of Houston		x	$270,798	
12	Attribution of Ozone and Ozone Precursors in Texas based Upstream Source regions and Emission Control Regulations using a Source-Oriented Air Quality Model	Qi Ying	Texas A&M & Molina Center for Strategic Studies in Energy and the Environment		x	$94,411	
18	Evaluating Texas Emissions and Land Use with Models and Observations	Michael Trainer	NOAA		x	$200,555	
19	Impact of aerosol-activated chlorine on tropospheric ozone production	Alexei Khalizov	Texas A&M		x	$226,261	
23	Investigation of the Importance of Heterogeneous Reactions of Nitric Acid as a Source of Radical Precursor Nitrous Acid	Robert Griffin	Rice, Aerodyne, & Univ. of New Hampshire		x	$174,982	
31	Evaluating and Improving Transport Algorithms in the CAMx Grid Model	Chris Emery	Environ		x	$149,881	
36	Tropospheric Ozone Pollution Project's Ozonesonde Network in Texas (TOPP's ON IT)	Gary Morris	Valparaiso & Univ. of Houston		x	$273,746	
40	Assessment of Estimates of Radical Sources from Recent Field Measurements in a Box Model and Regulatory Air Quality Model	William Vizuete	UNC-Chapel Hill & UCLA		x	$389,283	

PROGRAM ADMINISTRATION

This Section summarizes activities performed during the current Program year, beginning in September 2010.

During September through November 2010, Program Administration was focused on establishing the systems and procedures that would be required to manage the Program once the Research Projects were underway. The contracting mechanism, which was implemented in two parts, was completed. PIs were notified of their project award status, and Project Managers were assigned to funded projects. Work began on the Project Work Plans (Scope of work, Budget, and QAPP).

In order to maintain more direct control of the expenditures of all of the research partners in any given project, it was decided that UT would strictly limit the number of subcontracts that it would allow. Instead of having a single prime contract and multiple sub-contracts issued by the prime contractor, each entity that made up a component of a project contracted individually with UT for their portion of the Work Plan. Because of the array of projects that were awarded, this meant that some institutions would be awarded multiple contracts. To deal with this most efficiently, the first part of the contracting mechanism was a blanket agreement with each institution that defined basic terms and conditions.

These were issued to the institutions in September and October, and required significant negotiation. UT was unable to agree to terms with Federal agencies and Federally Funded Research Centers, due to the indemnity and insurance language required in the contract. Because of this, the projects with NCAR had to be dropped and the NOAA projects were reorganized so that they no longer led the project and a much larger role was played by their partner, Environ International, Inc. Many of the other institutions also took issue with the indemnity and insurance clauses, and well as with the Warranty, Publication, and Intellectual Property clauses. One PI decided not to continue with the research project, but this was unrelated to the contract negotiations.

By the end of October, the umbrella portion of the contract had been agreed to by most institutions, and Work Plan development began. As the Work Plans were approved by the Project Managers and the TCEQ Liaisons, often after multiple revisions, Task Orders, the second part of the contract mechanism, were issued to each separate entity taking part in the Project. This process took several months and was the primary activity through February.

In December, when it was determined that two of the projects would not have Task Orders issued, UT contacted the Council and began negotiations with the lead PIs of the two (2) projects that had been selected as contingency projects. Because of the timing of the notifications, these projects were the last to begin.

The individual contracting entities for each Project executed the Task Orders, work began and Program Administration efforts turned to the review and payment of invoices. Monthly invoices were carefully reviewed to ensure that all charges were allowable and allocable. This effort was especially time consuming when the institutions involved in the DFW Field Study began submitting invoices and often required working directly with the PIs and institutional accounting offices to produce payable invoices.

In early spring, the AQRP website was modified to reflect the Research Projects and provide information for those interested in learning more about the Program. A page was set up for each Project providing project information, an executive summary, and monthly technical reports.

In April and May, the Program Administration worked with the PI of the DFW Site Set-up Committee to ensure that all permissions were in place for the field study teams to use the Eagle Mountain Lake site (Site). This included working with the property owner to secure site access, and putting a site access agreement in place with each institution that would be operating at the Site.

In June, the Flair Project, under the direction of Jochen Stutz, held a data workshop at the Pickle Research Campus of UT. The Program Administration assisted with the logistical arrangements for this meeting, including securing a location for the meeting, securing a block of hotel rooms at the state rate, and ensuring that TCEQ personnel were informed of and invited to the Workshop.

In this same month, UT-Austin received a Contract Extension for the AQRP. This extension continues the program through the end of the 2012/2013 biennium, and allows the AQRP to utilize the FY 10 funds through April 30, 2012, and the FY 11 funds through April 30, 2013. The extension enabled the AQRP to allow the Research Projects to request contract extensions and part of August was spent providing amendments to those who requested them. More details on this are provided under the Research Project section of this report.

Each month a Financial Status Report/Invoice from UT to TCEQ has been produced. As the projects began, these invoices became much more complex. In an effort to meet the requirements of the TCEQ and to make the invoices easier to review, UT has developed an organized system for reporting Program activities and Project progress as it relates to expenditures.

Throughout the entire Program, UT and the TCEQ have communicated frequently on a variety of topics including notification of research project activities, program activities, preferences for reporting information, and other topics, as needed. In a continuing effort to transmit information from the Program and Projects, a Data Workshop and ITAC meeting will be held September 27 and 28, 2011, at the UT Pickle Research Campus. All research projects will be required to present at the Workshop which is being organized by the AQRP Program Administration. TCEQ personnel will be notified of and invited to the event.

Program Administration Financial Information

The Program Administration budget includes salaries and fringe benefits for those overseeing the program as a whole, as well as, materials and supplies, travel, equipment, and other expenses, including those related to the Advisory Council. This category allows indirect costs in the amount of 10% of salaries and wages.

Fringe benefits for the Administration of the AQRP are budgeted to be 22% of salaries and wages across the term of the project. It should be noted that this is an estimate, and actual fringe benefit expenses are reported for each month. The fringe benefit amount and percentage will fluctuate each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. At the end of the project, the

overall total of fringe benefit expensed is expected to be at or below 22% of the total salaries and wages. Actual fringe benefit expenses through August 31, 2011 are included in the spreadsheet below.

The AQRP Administration requested and received permission to utilize the FY 10 funds during FY 11. This is for all classes of funds including Administration, ITAC, Project Management, and Contractual. The intent is to fully expend (or encumber, in the case of the contractual funds) the FY 10 funds, and then begin spending the FY 11 funds.

The AQRP also requested and was granted a rebudget of the FY 10 Administration funds, to better reflect the expenditures of this portion of the program.

Table 4: AQRP Administration Budget

Administration Budget (includes Council Expenses)

Budget Category		FY10	FY11	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$195,100	$148,755	$343,855	$281,894.52		$61,960.48
Fringe Benefits		$38,082	$32,726	$70,808	$51,271.43		$19,536.57
Travel		$500	$7,500	$8,000	$346.85		$7,653.15
Supplies		$24,015	$2,744	$26,759	$12,802.66		$13,956.34
Equipment		$0	$0	$0			$0
Other			$4,007	$4,007			$4,007.00
Total Direct Costs		$257,697	$195,732	$453,429	$346,315.46	$0	$107,113.54
Authorized Indirect Costs		$19,510	$14,876	$34,386	$28,189.46		$6,196.54
10% of Salaries and Wages							
Total Costs		**$277,207**	**$210,608**	**$487,815**	**$374,504.92**	**$0**	**$113,310.08**
Fringe Rate		22%	22%		18%		

PROJECT MANAGEMENT

Once the awards were announced, each Research Project was assigned a Project Manager (PM). The PM worked with the PIs to accomplish project goals and ensure that all reporting requirements were met. Initially, this focused on the development of the Project Work Plan and a detailed QAPP (Quality Assurance Project Plan). The amount of effort required on the part of the PM depended on the Project requirements, as well as the PI's prior experience developing a Work Plan and QAPP. Two PMs were assigned to review the QAPP for all Projects to ensure a consistent level of detail and rigor.

Once Task Orders were issued, the PM ensured that all reporting requirements were met, and acted as a liaison between the PI and TCEQ for any issues requiring special attention. This included getting permission for the purchase of equipment, budget amendments, and other procedural matters. The PM also reviewed each invoice to ensure the level of effort matched the activities described in the Monthly Technical Report, and that all purchases were allocable to the project. Finally, the PMs acted as a liaison between the Program Administration and the PIs.

Project Management Financial Information

As none of the Research Projects were approved for funding until the end of FY 10, as with the Project Administration funds, the intent is to utilize the FY 10 and FY 11 funds during FY 11 to cover costs associated with project management. As with the Administration funds, the contract extension will allow the AQRP to utilize the FY 10 funds through April 30, 2012, and the FY 11 funds through April 30, 2013. All funds are expected to be fully expended.

Initially, all of the expenses relating to the DFW Field Study Site preparation (discussed in more detail in the Research Projects section of this report) were allocated to the Project Management account. Per direction from the TCEQ, in June the AQRP established two separate Research Projects for the DFW Field Study Site. The first account was established utilizing the remainder of the FY 10 Research Project funds (10-DFW). The second account utilized the remainder of the FY 11 Research Project funds, and a portion of the FY 11 Project Management funds (11-DFW). Thus a request was submitted to rebudget funds from the Project Management pool to the Research Project pool. This was done because there were not enough funds remaining in the Research Project pool to cover the expenses anticipated for the DFW Site.

The expenses associated with the DFW site preparation initially charged to Project Management have been moved to the new accounts. It is anticipated that the expenses related to the DFW Field Study Site will fully utilize the previously unallocated Research Project funds in FY 10 and FY 11. Any funds remaining unspent in the 11-DFW account will be returned to the Project Management pool.

Table 5: Project Management Budget

Project Management Budget

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$144,380	$83,434	$227,814	$161,593.46	$0	$66,220.54
Fringe Benefits		$30,724	$17,764	$48,488	$32,178.45	$0	$16,309.55
Travel		$0	$5,200	$5,200	$0		$5,200.00
Supplies		$458	$1,465	$1,923	$267.44		$1,655.56
Equipment							
Other							
Contractual							
Total Direct Costs		$175,562	$107,863	$283,425	$194,039.35	$0	$89,385.65
Authorized Indirect Costs		$14,438	$10,101	$24,539	$16,159.34		$8,379.66
10% of Salaries and Wages							
Total Costs		**$190,000**	**$117,964**	**$307,964**	**$210,198.69**	**$0**	**$97,765.31**

RESEARCH PROJECTS

After projects were selected by the Council in August, 2010, (see Table 3 for a list of funded projects) Project Managers and TCEQ Project Liaisons were assigned to each of the projects and the Principal Investigators (PIs) began putting together project Work Plans, which include the Statement of Work, a detailed budget, and a Quality Assurance Project Plan (QAPP). Work on the Research Projects began after Agreements were put in place, Work Plans were approved, and Task Orders were issued.

Due to the fact that there were 4 projects dealing with issues in the DFW area the AQRP wanted to actively promote integration of the measurements and ensure the projects worked cohesively. In cooperation with TCEQ Field Operations and TCEQ Region 4, the DFW Field Study Committee was formed.

The projects that made-up the DFW Field Study were:

- 10-006 – Quantification of Industrial Emissions of VOCs, NO2, and SO2 by SOF and Mobile DOAS (PI – John Mellqvist, Chalmers University)
- 10-024 – Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area (PI – Robert Griffin, Rice University)
- 10-034 – Dallas Measurements of Ozone Production (PI – Barry Lefer, University of Houston)
- 10-044 - Airborn Measurements to Investigate Ozone Production and Transport in the Dallas Fort Worth (DFW) Area During the 2011 Ozone Season (PI – Max Schauk, University of Houston)

The funding for the DFW Field Study was discussed in the Project Management section of this report. A summary of the activities for this, and all other Projects, can be found in the Appendix.

As of August 31, 2011, six projects were complete and the others remained active. Table 6 on the following 2 pages illustrates the funding awarded to each project and the total expenses reported on each project as of August 31, 2011. Please note that this reflects expenses that have posted to the UT-Austin accounting system as of August 31, 2011. There may be additional expenses pending that will not post until the following month.

At this time, all funding for research projects has been allocated to the projects or to the DFW Field Study. As discussed earlier in this report, projects 10-021, 10-DFW, and 11-DFW are complete, though a final invoice has not yet been received for any of the projects; 30-day contract extensions have been granted to projects 10-008, 10-024, and 10-045, to allow travel expenses associated with the AQRP Data Workshop to be charged; and 90-day contract extensions have been granted to all remaining projects.

Table 7 shows the funds that are estimated to be returned to the AQRP from each project upon completion. At this time, it is estimated that $38,200 of FY10 funds will be returned, and $7,954 of FY 11 funds will be returned. Also, all of the funds that were moved from Project Management to Project 11-DFW will be returned.

Per the agreement with TCEQ, FY 10 funds must be fully expended from the categories as budgeted by April 30, 2012. As such, UT has developed a plan for expending the $38,200 of FY 10 funds. The first step will be to increase the budget for the 10-DFW project and move all expenditures out of the 11-DFW project to the 10-DFW project. This will move expenditures totaling $29,262 from FY 11 to FY 10. The remainder of the funds will be used to fulfill a contractual requirement that all project data be stored in an accessible, yet protected location for 3 years after the project ends. The AQRP has contracted with the Texas Advanced Computing Center (TACC) for that data storage at a cost of $10,000. This will fully expend the FY 10 funds and leave approximately $35,000 in FY 11 funds. The AQRP will have until April 2013 to fully expend those funds.

At this time, the AQRP, with input from the TCEQ, is considering using the remaining FY 11 funds for the development of a State of the Science Assessment. The purpose of this Assessment will be to provide a summary of prior air quality research activities and their results, and provide a roadmap for the direction of future air quality research activities.

Table 6: Contractual Expenses

Contractual Expenses

FY 10 Contractual Funding		**$2,286,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-008	Rice University	$128,851	$96,765	$32,086
10-008	Environ International	$49,945	$46,670	$3,275
10-009	UT-Austin	$591,332	$590,747	$585
10-021	UT-Austin	$248,786	$244,068	$4,718
10-022	Lamar University	$150,000	$9,631	$140,369
10-032	University of Houston	$176,314	$2,589	$173,725
10-032	University of New Hampshire	$23,054	$0	$23,054
10-032	UCLA	$49,284	$14,195	$35,089
10-034	University of Houston	$195,054	$34,913	$160,141
10-042	Environ International	$237,481	$156,574	$80,907
10-045	UCLA	$149,773	$65,026	$84,747
10-045	UNC - Chapel Hill	$33,281	$28,711	$4,570
10-045	Aerodyne Research Inc.	$164,988	$88,707	$76,281
10-045	Washington State University	$50,000	$31,591	$18,409
10-DFW	UT-Austin	$37,857	$37,857	$0
FY 10 Total Contractual Funding Awarded		$2,286,000		
FY 10 Contractual Funding Remaining to be Awarded		$0		
FY 10 Contractual Funds Expended to Date*			$1,448,044	
FY 10 Contractual Funds Remaining to be Spent				$837,956

FY 11 Contractual Funding		**$1,736,063**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179	$118,651	$143,528
10-006	University of Houston	$222,483	$146,892	$75,591
10-015	Environ International	$201,280	$107,044	$94,236
10-020	Environ International	$202,498	$130,290	$72,208
10-024	Rice University	$225,662	$50,855	$174,807
10-024	University of New Hampshire	$70,747	$37,779	$32,968
10-024	University of Houston	$64,414	$19,212	$45,202
10-024	University of Michigan	$98,134	$16,477	$81,657
10-029	Texas A&M University	$80,108	$54,136	$25,972
10-044	University of Houston	$279,642	$12,973	$266,669
11-DFW	UT-Austin	$50,952	$29,262	$21,690
FY 11 Total Contractual Funding Awarded		$1,758,099		
FY 11 Contractual Funding Remaining to be Awarded		-($22,036)		
FY 11 Contractual Funds Expended to Date*			$723,571	
FY 11 Contractual Funds Remaining to be Spent				$1,034,528
Total Contractual Funding		$4,022,063		
Total Contractual Funding Awarded		$4,044,099		
Total Contractual Funding Remaining to be Awarded		-($22,036)		
Total Contractual Funds Expended to Date*			$2,171,615	
Total Contractual Funds Remaining to be Spent				$1,872,484

*(Expenditures Reported as of August 31, 2011.)

Table 7: Research Funds Estimated to be Returned to AQRP (Estimates as of September 30, 2011)

Funds Estimated to be Returned			
FY 10 Contractual Funding		**$2,286,000**	
Project Number		Amount Awarded (Budget)	Amount Estimated to be Returned
10-008	Rice University	$128,851	$3,200
10-008	Environ International	$49,945	$0
10-009	UT-Austin	$591,332	$0
10-021	UT-Austin	$248,786	$0
10-022	Lamar University	$150,000	$22,000
10-032	University of Houston	$176,314	$6,000
10-032	University of New Hampshire	$23,054	$1,000
10-032	UCLA	$49,284	$0
10-034	University of Houston	$195,054	$1,000
10-042	Environ International	$237,481	$0
10-045	UCLA	$149,773	$5,000
10-045	UNC - Chapel Hill	$33,281	$0
10-045	Aerodyne Research Inc.	$164,988	$0
10-045	Washington State University	$50,000	$0
10-DFW	UT-Austin	$37,857	$0
FY 10 Contractual Funds Estimated to be Returned			$38,200
FY 11 Contractual Funding		**$1,736,063**	
Project Number		Amount Awarded (Budget)	Amount Estimated to be Returned
10-006	Chalmers University of Tech	$262,179	$0
10-006	University of Houston	$222,483	$0
10-015	Environ International	$201,280	$0
10-020	Environ International	$202,498	$0
10-024	Rice University	$225,662	$0
10-024	University of New Hampshire	$70,747	$0
10-024	University of Houston	$64,414	$3,000
10-024	University of Michigan	$98,134	$3,800
10-029	Texas A&M University	$80,108	$1,500
10-044	University of Houston	$279,642	$0
11-DFW	UT-Austin	$28,916	($346)
FY 11 Contractual Funds Estimated to be Returned			$7,954
Total Contractual Funds Estimated to be Returned			$46,154

FINANCIAL STATUS REPORT

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May 2010 an amendment was issued increasing the budget by $40,000. Funding for fiscal year 2011 was established at $2,106,071, for a total project award of $4,878,142. These funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

Program Administration – limited to 10% of the overall funding
This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC
These funds are to cover the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project was assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual
These are the funds available to support the research projects that are selected for funding.

The following tables show the budget and cumulative expenditures for each piece of the AQRP for FY 10 and FY 11, as well as a total Financial Status Report by fiscal year. Expenditures are reported as of August 31, 2011.

Table 8: Program Administration Financial Summary

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$195,100	$195,028.64		$71.36
Fringe Benefits		$38,082	$36,849.42		$1,232.58
Travel		$500	$346.85		$153.15
Supplies		$24,015	$12,802.66		$11,212.34
Equipment		$0			$0
Other					
Contractual					
Total Direct Costs		$257,697	$245,027.57	$0	$12,669.43
Authorized Indirect Costs		$19,510	$19,502.88		$7.12
10% of Salaries and Wages					
Total Costs		**$277,207**	**$264,530.45**	**$0**	**$12,676.55**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$148,755	$86,865.88		$61,889.12
Fringe Benefits		$32,726	$14,422.01		$18,303.99
Travel		$7,500			$7,500.00
Supplies		$2,744			$2,744.00
Equipment					
Other		$4,007			$4,007.00
Contractual					
Total Direct Costs		$195,732	$101,287.89	$0	$94,444.11
Authorized Indirect Costs		$14,876	$8,686.58		$6,189.42
10% of Salaries and Wages					
Total Costs		**$210,608**	**$109,974.47**	**$0**	**$100,633.53**

Table 9: ITAC Financial Summary

ITAC Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,500	$8,990.45		$7,509.55
Supplies		$2,364	$249.38		$2,114.62
Equipment					
Other					
Total Direct Costs		$18,864	$9,239.83	$0.00	$9,624.17
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$18,864**	**$9,239.83**	**$0.00**	**$9,624.17**

ITAC Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,600			$16,600.00
Supplies		$2,800			$2,800.00
Equipment					
Other					
Total Direct Costs		$19,400			$19,400.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$19,400**	**$0.00**	**$0.00**	**$19,400.00**

Table 10: Project Management Financial Summary

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$14,380	$138,706.71		$5,673.29
Fringe Benefits		$30,724	$27,899.29		$2,824.71
Travel		$0	$0		$0
Supplies		$458	$7.44		$450.56
Equipment					
Other					
Total Direct Costs		$175,562	$166,613.44	$0	$8,948.56
Authorized Indirect Costs		$14,438	$13,870.67		$567.33
10% of Salaries and Wages					
Total Costs		**$190,000**	**$180,484.11**	**$0**	**$9,515.89**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$83,434	$22,886.75		$60,547.25
Fringe Benefits		$17,764	$4,279.16		$13,484.84
Travel		$5,200			$5,200.00
Supplies		$1,465	$260.00		$1,205.00
Equipment					
Other					
Total Direct Costs		$107,863	$27,425.91	$0	$80,437.09
Authorized Indirect Costs		$10,101	$2,288.67		$7,812.33
10% of Salaries and Wages					
Total Costs		**$117,964**	**$29,714.58**	**$0**	**$88,249.42**

Table 11: AQRP Financial Summary – FY 10

AQRP Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$195,100	$195,028.64	$0.00	$71.36
Fringe Benefits		$38,082	$36,849.42	$0.00	$1,232.58
Travel		$500	$346.85	$0.00	$153.15
Supplies		$24,015	$12,802.66	$0.00	$11,212.34
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,286,000	$1,448,044.00	$0.00	$837,956.00
ITAC		$18,864	$9,239.83	$0.00	$9,624.17
Project Management		$190,000	$180,484.11	$0.00	$9,515.89
Total Direct Costs		$2,754,761	$1,882,795.51	$0.00	$869,765.49
Authorized Indirect Costs		$19,510	$19,502.88	$0.00	$7.12
10% of Salaries and Wages					
Total Costs		**$2,772,071**	**$1,902,298.39**	**$0.00**	**$869,772.61**

Table 12: AQRP Financial Summary – FY 11

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$148,755	$86,865.88	$0.00	$61,889.12
Fringe Benefits		$32,726	$14,422.01	$0.00	$18,303.99
Travel		$7,500	$0.00	$0.00	$7,500.00
Supplies		$2,744	$0.00	$0.00	$2,744.00
Equipment		$0	$0.00	$0.00	$0.00
Other		$4,007	$0.00	$0.00	$4,007.00
Contractual		$1,758,099	$723,571.00	$0.00	$1,034,528.00
ITAC		$19,400	$0.00	$0.00	$19,400.00
Project Management		$117,964	$29,714.58	$0.00	$88,249.42
Total Direct Costs		$2,091,195	$854,573.47	$0.00	$1,236,621.53
Authorized Indirect Costs		$14,876	$8,686.58	$0.00	$6,189.42
10% of Salaries and Wages					
Total Costs		**$2,106,071**	**$863,260.05**	**$0.00**	**$1,242,810.95**

Appendix

Research Project Summaries

Project 10-006 **STATUS: Active – February 16, 2011**
End Date Extended to November 30, 2011

Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS

Chalmers University – Johan Mellqvist
University of Houston – Bernhard Rappenglüeck
AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – John Jolly

Funding Awarded: $484,662
($262,179 Chalmers, $222,483 UH)

Annual Project Update:
A measurement study was performed from April 6 – June 18, 2011, in southeast Texas, with the aim to study direct emission of volatile organic compounds (VOCs), sulfur dioxide (SO_2), nitrogen dioxide (NO_2), and formaldehyde from refineries and petrochemical industries. The substances above are key species for the formation of photochemical smog. Several techniques were used, i.e. Solar Occultation Flux (SOF), mobile Differential Optic Absorption Spectrometry (DOAS) and thermal Fourier Transform Infrared (FTIR) and canister sampling.

In addition, measurements of methane, ethane, propane, carbon monoxide (CO), nitric oxide (NO) and other VOCs were made in the Fort Worth area, to study emission from natural gas production. The techniques used here were mobile extractive FTIR and tracer correlation combined with canister sampling. In addition, SOF measurements were carried out.

In the sites surveyed with SOF and mobile DOAS in previous studies i.e. Houston Ship Channel (HSC), Mt Belvieu and Texas City we have measured emissions of alkanes, alkenes, SO_2, NO_2 and formaldehyde. The general emission patterns are the same in 2011 as in previous campaigns in 2006 and 2009, although there are differences.

The Beaumont and Port Arthur area was surveyed for the first time with SOF in this campaign. Alkane emissions as summed from seven individual plant areas, averaged about 6700 kg/h. This is slightly more than half of the alkane emissions measured from the HSC area in 2011. In terms of alkenes four plants in the Beaumont Port Arthur area contributed with 148 kg/h of ethene emissions on average, whereas no major propene emissions were observed. At one plant also emissions of 1,3 butadiene and 1-butene was observed. The adjacent petrochemical site in Orange was measured to have ethene emissions of on average 197 kg/h. A major alkene source was found in Longview, also surveyed for the first time with SOF. The site showed an ethene emission of 452 kg/h and a propene emission 282 kg/h.

In the Fort Worth study we find that the largest continuous sources are the treatment facilities and the large compressor stations emitting up to 100 kg/h of methane, 5 kg/h of ethane and other species. Another source is well pads emitting about 1 kg/h of methane and about 2-5% by mass of ethane. Due to the large amount of well pads, this constitutes a major source. There are reports in the literature claiming that regeneration of drying liquid from well pads may constitute a large source. It is believed that this occurred during one of our measurements from a well pad. Here emissions of 2 kg/h of ethane and 0.4 kg/h of ethene was measured by meFTIR and canister sampling; noteworthy is the importance of the latter species for ozone formation.

Project 10-008 **STATUS: Active – October 21, 2010**
End Date Extended to September 30, 2011

Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling

Rice University – Daniel Cohan
ENVIRON International – Greg Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Jim Smith

Funding Awarded: $178,796
($128,851 Rice, $49,945 ENVIRON)

Annual Project Update:

"Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling," investigated the influence of input uncertainties on model predictions of pollutant responsiveness to emission controls. Models used to inform air quality decision-making are known to be uncertain, but they are usually applied deterministically with whatever are thought to be the best available model formulations and inputs. This project characterized how various alternate choices for model formulations (structural uncertainty) and input parameters (parametric uncertainty) influence predictions of ozone-precursor response in Texas State Implementation Plan (SIP) modeling episodes. Both Bayesian and non-Bayesian approaches were applied to compute probabilistic representations of the sensitivity of ozone to changes in precursor emissions.

Base case modeling was taken from TCEQ's CAMx simulations of ozone during two month-long episodes in 2006. Structural scenarios were then developed by applying alternate options for the biogenic emissions model, the deposition scheme, the chemical mechanism, the global model for deriving boundary conditions, and satellite-based photolysis rates. Screening analysis of the impacts of these options on ozone concentrations and sensitivities led to a focus on scenarios involving alternate choices for biogenic emissions model and chemical mechanism. The base model achieved very low bias during the June 2006 episode (NMB = -1.0% relative to ozone monitors in the 12-km domain), so the structural scenarios provide plausible alternatives but could not dramatically improve model performance.

For parametric uncertainties, screening analysis identified the specific emission rates, reaction rate constants, and boundary conditions that most influence ozone concentrations and their sensitivities to nitrogen oxide (NO_x) and volatile organic compound (VOC) emissions. Some parameters such as ozone boundary conditions were found to impact concentrations far more strongly than sensitivities, whereas the converse was true for some other parameters such as anthropogenic VOC emissions.

Bayesian Monte Carlo analysis was then applied to weight the relative likelihood of alternate structural and parametric scenarios, based on model performance in simulating observed concentrations within the Dallas-Fort Worth (DFW) region during the June 2006 episode. Metric 1 evaluated model performance on high-ozone days at three DFW monitors, while Metric 2 considered average 8-hour ozone concentrations across all DFW monitors on each episode day.

A non-Bayesian metric for assigning weights based on standard model performance statistics (Metric 3) was also developed and was applied to produce alternative weightings of the Monte Carlo scenarios.

The Bayesian and non-Bayesian analyses generated probabilistic representations of ozone responses to changes in precursor emissions and of model input parameters. All of the results confirmed the findings of the base model that 8-hour ozone in the DFW region during the June 2006 episode was predominately NO_x-limited. However, the three metrics yielded conflicting shifts in the probability distributions of ozone sensitivities. For example, results from Metric 1 tended to increase the predicted sensitivity of ozone to NO_x, whereas Metric 2 indicated slightly greater sensitivity to VOC than originally modeled. Non-Bayesian Metric 3 yielded a slight shift toward greater sensitivity to VOCs, but retained the primarily NO_x-limited conditions of the base model. Further work is needed to refine the metrics and incorporate consideration of other measurements beyond ozone for evaluating model performance. Nevertheless, the project has demonstrated how probabilistic analyses via an ensemble approach can supplement deterministic estimates of ozone response and characterize the uncertainty of those results.

Project 10-009 **STATUS: Active – September 8, 2010**
End Date Extended to November 30, 2011

Additional Flare Test Days for TCEQ Comprehensive Flare Study

University of Texas at Austin – Vincent Torres

AQRP Project Manager – Cyril Durrenberger
TCEQ Project Liaison – Russell Nettles

Funding Awarded: $591,332

Annual Project Update:

Task 1 - In May 2009, the TCEQ contracted with The University of Texas at Austin (UT Austin) to conduct the Comprehensive Flare Study Project (Tracking Number 2010-04) (TCEQ, 2009). In August 2010, the Air Quality Research Program (TCEQ Grant No. 582-10-94300) provided supplemental funding for this project. The purpose of this project was to conduct field tests to measure flare emissions and collect process and operational data in a semi-controlled environment to determine the relationship between flare design, operation, vent gas lower heating value (LHV) and flow rate, destruction and removal efficiency (DRE), and combustion efficiency (CE). The TCEQ's primary study objectives for this project in order of decreasing priority are:

- Assess the potential impact of vent gas flow rate turndown on flare CE and VOC DRE;
- Assess the potential impact of steam/air assist on flare CE and VOC DRE at various operating conditions, including low vent gas flow rates;
- Determine whether flares operating over the range of requirements stated in 40 Code of Federal Regulations (CFR) § 60.18 achieve the assumed hydrocarbon DRE of 98 percent at varying waste gas flow rate turndown, assist ratios and waste stream heat content; and
- Identify and quantify the hydrocarbon species in flare plumes currently visualized with passive infrared cameras.

The field tests were conducted in September 2010 on a steam-assisted flare (nominal 36-inch diameter, rated at 937,000 lbs/hr) and on an air-assisted flare (nominal 24-inch in diameter, rated at 144,000 lbs/hr) at the John Zink Company, LLC flare test facility in Tulsa, Oklahoma. The test plan consisted of a matrix of flare operating conditions designed to provide data that would be the basis to address as many of the study objectives as possible. This matrix of operating conditions included two low vent gas flow rates for the steam flare (937 and 2,342 lbs/hr) and two low LHVs (300 and 600 Btu/scf). For the air-assisted flare, 359 and 937 lbs/hr vent gas flow rates and the same two low LHVs used for the steam flare were used. The vent gas composition used was a 1:4 ratio of Tulsa Natural Gas to propylene diluted to achieve the desired LHV. Air and steam assist rates used varied from the amount used to achieve the incipient smoke point to an amount near the snuff point. All of the tests in this study were conducted under conditions that are in compliance with all criteria of 40 CFR § 60.18.

All operating parameters for the flare were measured and monitored during each test run. The CE and DRE of the flare for each test point were determined by continuously extracting a sample from the flared gas beyond the point in the plume where all combustion had ceased and then

analyzing the sample at a rate of 1 Hz using a suite of analytical instruments operated by Aerodyne Research Incorporated. A carbon balance was performed on the constituents in the sample as compared to the constituents in the vent gas flow and the appropriate quantities were used to calculate DRE and CE. Two remote-sensing technologies were also employed in the study and were compared to the extractive measurement results. A final report (*TCEQ 2010 Flare Study Final Report)* for this task is now posted on the TCEQ website at http://www.tceq.texas.gov/airquality/stationary-rules/flare_stakeholder.html

Task 2 - The goal of the modeling project (Task 2) is to be able to assess the relative impact on combustion efficiency by operating variables such as vent gas flow, steam or air assist, flame temperature, and the presence of certain volatile organic compounds. Two types of models were used to better understand the performance data obtained in Task 1 and the effect of such parameters as wind, vent gas flow rate and composition, and air and steam assist at operating points that were not run in Task 1. One modeling approach (Multivariate Image Analysis or MIA) uses feature variables extracted from the spectral information of the flare images on the video recordings from the tests. This complements the predictive capability of the computational fluid dynamics (CFD) model, which uses first principles to model the full-scale flares used in the Task 1 tests. The CFD model will predict flare performance, i.e., combustion efficiency and destruction and removal efficiency, while at the same time predicting emissions produced at different operating conditions.

In the MIA approach (Task 2.1) for the steam-assisted flare, 8 tests were usable (the flame was visible), while there were 13 usable tests for the air-assisted flare. Different training/validation approaches were examined:

(1) Use half the images from each test as a training set, and the other half to validate the model.

(2) Use data from some of the tests as a training set, and use all the sets to validate.

Other variables recorded for each test included lower heating value of fuel stream, assist gas flow rate, air to fuel ratio in combined assist/fuel stream, and crosswind velocity. These variables were used along with the feature variables in the regression. The best results were obtained when odd-numbered images were used to train the model and even-numbered images were used as the validation set. When building a model with the goal of making predictions about previously unseen flares, a wide range of training data is required. In this case, combustion efficiency from analytical equipment such as FTIR will be needed to train the image analysis model. Then the MIA model could be used for real-time adjustment of steam flow to a flare.

In Task 2.2, a CFD model was used to model a flare and calculate the combustion efficiency for use in MIA. However, It takes a long time (hours) to obtain a result from CFD, so this approach could not be used to analyze on-line measurements. Fitting of the CFD model to the data was needed due to the uncertainty of the reaction kinetics mechanism for propylene combustion, so one parameter is adjusted to match the field data, which provides a reasonably accurate fit for both steam and air-assisted flare tests. In Task 2.3, the Combustion Zone Heating Value (CZHV), or the heating value of the combined assist gas and fuel stream, is related to the combustion efficiency. We have concluded that the correlation is not strong enough to make accurate predictions (± 20% in some cases).

Project 10-015 **STATUS: Active – March 4, 2011**
End Date Extended to November 30, 2011

An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-attainment areas in Texas

ENVIRON International – Greg Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Awarded: $201,280

Annual Project Update:
The primary goals of this project are to analyze nitryl chloride formation in urban areas utilizing the existing field campaign data sets and to implement this chemistry in photochemical grid models to aid the Texas SIP development.

Background
Results from the 2006 TexAQS-II/Gulf of Mexico Atmospheric Composition and Climate Study (TexAQS-II for short) in Houston showed that reactions at night between ozone (O_3), nitrogen oxides (NOx), hydrogen chloride (HCl) and particulate matter (PM) gave rise to nitryl chloride ($ClNO_2$). This finding was confirmed by other studies and is significant because $ClNO_2$ undergoes rapid photolysis in the morning and can influence photochemistry and O_3 formation at the start of the day. Sea salt PM is an important source of chloride in coastal regions but $ClNO_2$ also has been observed far from the ocean (in Boulder, Colorado) indicating that other sources of chloride can give rise to $ClNO_2$ and that its influence on photochemistry may not be limited to coastal regions.

This study analyzed the ambient measurements made during TexAQS-II, along with the other ambient measurement and laboratory chemistry studies pertinent to the Texas non-attainment areas, to provide the sound technical basis needed for the inclusion of this important chemistry in air quality models. This new chemistry was included in the Comprehensive Air-quality Model with Extensions (CAMx) photochemical grid model that is used by the TCEQ for SIP modeling. The CAMx model was applied using a national modeling database that includes all of the field study locations. The emission inventories for the national database were reviewed and expanded to include as many sources of chloride as possible, including sea salt, HCl, molecular Cl_2 and PM chloride. Performance of the national CAMx model was assessed to evaluate the chemistry included for $ClNO_2$ and the completeness of the chloride emission inventory.

Assessment of Nitryl Chloride Formation in Urban Areas
Observations during the 2006 TexAQS-II study brought up a number of questions about whether or not the $ClNO_2$ chemistry was self-consistent, how the chemistry depended on N_2O_5 uptake, and aerosol chloride concentration, if there was enough soluble chloride to produce the observed $ClNO_2$, and how these aspects of the chemistry could be incorporated into regional air quality models that describe ozone production in non-attainment areas. To answer these questions, the

project team further examined the ambient data set acquired during the TexAQS-II study and assessed the data sets from the Study of Houston Atmospheric Radical Precursors (SHARP) in 2009, and the CalNex study conducted in the Los Angeles area in May and June of 2010. Several approaches were used to estimate N_2O_5 uptake rate and $ClNO_2$ conversion efficiencies from ambient measurements: the odd-nitrogen budget of isolated nighttime plumes, and box modeling of the few reactions that govern N_2O_5 formation and N_2O_5 to $ClNO_2$ conversion. In addition, gas phase HCl, HNO_3 and particle nitrate and chloride measurements for these three studies were analyzed to assess the importance of sea salt acidification as a source of soluble aerosol chloride, and the adequacy of aerosol measurements in providing the information necessary to model $ClNO_2$ formation.

Three-Dimensional Photochemical Grid Modeling

The CAMx photochemical grid model was updated to include a parameterization of the ClNO2 chemistry and applied to a summer 2006 ozone and PM modeling episode using the EPA's nationwide 12-km grid modeling database. The reactive chlorine and particle chloride emission inventories in the EPA's modeling database were extended to include additional chlorine/chloride emission sources, e.g., swimming pools, sea salt and wildfires.

The simulation results were compared with two ground site measurement datasets, the CalNex 2010 LA site at Pasadena and the SHARP 2009 Moody Tower site near downtown Houston. At the Pasadena site, CAMx significantly underestimates HCl and PCl while overestimating HNO_3 which may indicate a shortfall in the amount of chloride in the emission inventory. The missing chloride could be sea salt or additional chlorine and/or chloride emission categories that are missing in the current emission inventory. At this site, almost all of the total chloride resides in the gas phase, which could also result in less chloride available to form $ClNO_2$ because HCl is efficiently removed from atmosphere by deposition process. Another possible explanation for the discrepancy between the model and observation is that there exist abundant sea salts deposited on the surface which release HCl by acid displacement following HNO_3 deposition. CAMx underpredicts HCl and N_2O_5 at the Moody Tower site, but predicts similar to or higher $ClNO_2$ concentrations than the measurements. The observed $ClNO_2$ concentrations at this site are quite low compared to measurements made on board the NOAA R/V Ron Brown during the TexAQS-II 2006 campaign. On average, the Pasadena site observed lower HCl + PCl concentrations but higher $ClNO_2$ than the Houston site.

Conclusions

The results of ambient data analyses have illustrated several key features of the $ClNO_2$ chemistry. The highest $ClNO_2$ concentrations were observed when N_2O_5 uptake coefficient was high but N_2O_5 to $ClNO_2$ conversion efficiencies were fairly modest. Episodes when high N_2O_5 was observed, but $ClNO_2$ was very low corresponded to low N_2O_5 uptake and there was very low conversion. Relative humidity appears to be one of the more important parameters controlling N_2O_5 uptake, but high aerosol organic fraction may also suppress uptake.

Photochemical grid modeling showed that the model significantly underpredicted HCl and PCl. Several hypotheses were proposed and tested to explain the discrepancies between the model and observations. The test results are expected to provide valuable insights to improve our understanding of nitryl chloride formation in the region.

Project 10-020 **STATUS: Active – March 5, 2011**

End Date Extended to November 30, 2011

NO_x Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone

ENVIRON International – Greg Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Dick Karp

Funding Awarded: $202,498

Annual Project Update:

Background

Understanding atmospheric chemical transformations and pollutant transport are critical to assessing the impacts of emissions sources on formation of ozone (O_3). Chemical transformations of nitrogen oxides (NO_x) emissions that occur at night will influence their availability to participate in next day O_3 formation. During the second Texas Air Quality Study in 2006 (TexAQS II), the NOAA P-3 aircraft measured a wide suite of atmospheric species at high temporal resolution during a series of nighttime flights, including flights downwind of several Texas power plants. The primary objective of AQRP Project 10-020 was to take advantage of the P-3 data collected during the nighttime plume intercepts of two power plants to understand and simulate the fate of emissions from these plants during the night and the implications for next-day ozone formation. The two plants are the Oklaunion plant in north Texas, near the Oklahoma border and the city of Wichita Falls, TX, and the W.A. Parish plant, located on the southwest side of the city of Houston.

The AQRP project consists of three main components:

- Data analysis and empirical modeling analysis of night-time chemistry and mixing in NO_x plumes from power plants
- Deterministic modeling of night-time power plant plumes using a reactive plume model (SCICHEM) and a three-dimensional chemical transport model (CAMx)
- Data analysis of night-time vertical profiles in the Houston boundary layer

Analysis of Chemistry and Mixing in NO_x Plumes from Large Point Sources

The aim of the analyses was to understand: 1) nighttime NO_x plume widths and depths in order to characterize nighttime plume mixing; 2) the mass balance of ozone and total nighttime odd oxygen to measure the conversion of nitrogen oxides into both reservoir and reactive compounds; and 3) direct measurement and/or estimates of nighttime nitrogen containing species that result from heterogeneous N_2O_5 reactions, such as HNO_3. An assessment of the impact of NO_x emission control technology on nighttime NO_x transport and loss was also conducted.

The analysis showed that mixing of intense point source NO_x plumes with background air is inefficient at night, and the chemistry within these plumes is spatially confined. The plume NO_x has the potential to completely consume the background O_3, effectively shutting off further NO_x oxidation through the formation of NO_3 and N_2O_5 since these species cannot co-exist with the excess NO present in a fully O_3-titrated plume. Overnight NO_x transport without oxidation or conversion to soluble species such as HNO_3 is more efficient if full titration of background O_3 occurs. The hypothetical control analysis showed that plumes with selective catalytic reduction control (SCR) are more likely to have insufficient NO_x to titrate background O_3 and thus undergo rapid oxidation, while those without such controls transport non-oxidized NO_x overnight.

A draft manuscript detailing this analysis is currently under review by co-investigators at both NOAA and ENVIRON. The draft manuscript has also been submitted to AQRP for review. The manuscript will be submitted to a peer-reviewed journal after incorporating revisions arising from the reviews.

SCICHEM and CAMx Modeling of the Oklaunion Night-time Plume

The reactive plume model, SCICHEM (Second-order Closure Integrated puff model with CHEMistry), and the Comprehensive Air quality Model with extensions (CAMx) were used to simulate the Oklaunion power plant plume during the night of October 10, 2006. SCICHEM was able to capture many of the observed features of the aircraft plume measurements by restricting horizontal and vertical plume growth, increasing puff resolution (in time and space) and using aircraft measurements of wind speed, direction, and temperature.

The CAMx simulations were conducted with two configurations to simulate the Oklaunion plume: a Plume-in-Grid (PiG) configuration with five reactors in each PiG puff to capture the chemical inhomogeneity across the plume; and a high-resolution flexi-nest with 200 m grid spacing downwind of the power plant. The results with the latter approach were in better agreement with the aircraft measurements than those from the PiG approach. With the PiG approach, the modeled plume was significantly wider than the observed plume. The wider modeled puffs were attributed to the large shear in the model wind fields, and a sensitivity study in which shear-induced growth was set to zero resulted in narrower plumes. The PiG approach also could not capture the variations in chemistry across the plume as well as the flexi-nest approach.

Analysis of Night-time P-3 Profiles of the Houston Urban Boundary Layer

This analysis is still ongoing.

Project 10-021 **STATUS: Active – October 11, 2010**

Project Complete: August 31, 2011

Dry Deposition of Ozone to Built Environment Surfaces

University of Texas at Austin – Richard Corsi

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Jim Smith

Funding Awarded: $248,786

Annual Project Update:

Photochemical grid models, such as the Comprehensive Air Quality Model with extensions (CAMx) that is used by the State of Texas, have a central role in the design of emission control strategies for attainment demonstrations and air quality planning. Dry deposition is an important physical removal mechanism for ozone in Texas. Consequently, it is critical that related model algorithms be as accurate as possible in order to reduce uncertainties in predictions that will be used to implement ozone reduction strategies. Currently, national default values for dry deposition resistances are used in CAMx. Improvements in the dry deposition algorithms in CAMx are particularly important given the rapidly changing nature of urban landscapes, including increases in built environment surfaces (BES) such as roofing, building façades, and roadways, and changes in urban vegetative cover. In this study we assessed whether built environment surfaces can appreciably affect the dry deposition of ozone in urban settings. The research included two major phases. Phase 1 involved extensive experiments to determine the reactivity, or inversely the surface resistance, of large built environment surface materials with ozone. Phase 2 involved applications of CAMx with a more refined urban deposition calculation to account for variations in built environment surfaces and updated surface resistances.

Experiments to determine surface resistances involved eighteen different materials. Materials were placed in electro-polished stainless-steel chambers and exposed to ozone in a laboratory setting. Built environment surface materials were also placed outdoors and allowed to weather in order to explore temporal changes in surface resistances.

Geospatial data were collected for three broad types of built environment surfaces in areas classified as urban in Travis County, including the transportation network, residential properties, and commercial and tax-exempt properties. Among the primary data sources utilized for the project were the Texas Department of Transportation's (TxDOT's) Pavement Management Information System (PMIS), the City of Austin's 2003 ArcGIS transportation and building footprint files, the Travis County Appraisal District (TCAD) database, Google Earth, and field surveys conducted by our team. These data were matched with surface resistances for fresh and weathered materials, respectively, determined from the experiments to obtain new estimates of dry deposition velocities and ozone concentrations using CAMx.

Major findings from the experimental phase of the study are listed below:

1. Initial (Day 0) surface resistances associated with ozone removal to test materials ranged over a factor of 30, from a low (most reactive) of 150 seconds/meter (s/m) for limestone to a high (least reactive) of 4,300 s/m for painted concrete.

2. Painted materials (brick, concrete, Hardie Board, wood siding) had initial surface resistances that were approximately an order of magnitude greater than most unpainted materials.

3. Other than limestone, unpainted materials exhibited a relatively narrow range (370 to 670 s/m) of initial surface resistances.

4. Weathering of test materials for two months on the top of an office building generally led to an increase in surface resistance to ozone removal. This was true for all materials except for limestone, one concrete specimen, and painted brick; each of these exhibited a slight reduction in surface resistance after two months of weathering.

Major findings from the characterization of the built environment and air quality modeling are listed below:

5. Improved characterization of the urban environment resulted in decreases in predicted daily maximum 8-hour average ozone concentrations of 0.2 to 1.3 ppb in the Austin area relative to a 2007 CAMx Base Case.

6. The maximum decreases in predicted 8-hour ozone concentrations regardless of time of day or grid cell location across the Austin area ranged from 1.2 to 1.6 ppb.

7. The results indicated the large contribution of vegetation in comparison to built surfaces to the dry deposition of ozone, suggesting the need for better characterization of urban vegetation and future changes due to urban growth and building practices.

8. Decreases in 8-hour average ozone concentrations could primarily be attributed to urban vegetation with the built environment moderating the impacts of ozone removal by dry deposition in Travis County.

9. The framework for characterizing the urban built environment and experimental results for material surface resistances are applicable to other regions of Texas.

Project 10-022 **STATUS: Active – February 16, 2011**

End Date Extended to November 30, 2011

Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas

Lamar University – Daniel Chen

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Jim MacKay

Funding Awarded: $150,000

Annual Project Update:

In this project, computational fluid dynamics (CFD) methods based on CHEMKIN-CFD and FLUENT are used to model low-Btu, low-flow rate propylene/TNG/nitrogen flare tests conducted during September 2010 in the John Zink test facility, Tulsa, Oklahoma. The flare test campaign was the focus of the TCEQ Comprehensive Flare Study Project (PGA No. 582-8-862-45-FY09-04) in which plume measurements using both remote sensing and direct extraction were carried out to determine flare efficiencies and emissions of regulated and photo-chemically important pollution species for air-assisted and steam-assisted flares under open-air conditions. This project (1) predicts the performance of Tulsa testing flares by using CFD modeling, and (2) further compares with the measured flare performance data and speciated volatile organic compound (VOC) concentrations. This modeling tool has the potential to help TCEQ's on-going evaluation on flare emissions and to serve as a basis for a future State Implementation Plan (SIP) revision.

The 50-species combustion mechanism is reduced from the combined GRI and USC mechanisms with the goal of allowing NOx formation and handling light hydrocarbon combustion. This optimized Lamar mechanism has been validated against methane, ethylene, and propylene experimental data. Further, NO_2 is added to the existing mechanism and is shown in good agreement with the full mechanism. FLUENT models (Species, Turbulence-Chemistry, Viscous, and Numerical Solution), model parameters, and boundary conditions have been selected.

The main operating, design, and meteorological data of the flare test campaign were provided by the University of Texas (UT) including Combustion Efficiency (CE), Destruction & Removal Efficiencies (DRE). Both Probability Density Function (PDF) and Eddy Dissipation Concept (EDC) turbulence-chemistry interaction approaches have been adopted to run Tulsa flare test cases. Two air-assisted flare test cases and one steam-assisted flare test case have been run and compared with the measured DRE/CE data. Even though the PDF approach was verified with University of Alberta wind tunnel data and was shown in good agreement; the more simplistic PDF model tends to predict somewhat higher flare efficiencies than the measured ones. The more rigorous EDC model, however, tends to give low DRE/CE due to the low fuel flow rates and low fuel heating values. The EDC approach is also sensitive to the inclusion of the pilot flame. More time is needed to resolve the aforementioned CFD simulation issues; consequently, no-cost contract extension to November 30, 2011 has been requested and approved for the project.

Project 10-024 **STATUS: Active – February 16, 2011**

End Date Extended to September 30, 2011

Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area

Rice University – Robert Griffin
University of Houston – Barry Lefer
University of New Hampshire – Jack Dibb
University of Michigan – Allison Steiner
NCAR – Withdrawn

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Doug Boyer

Funding Awarded: $458,957
($225,662 Rice, $98,134 Houston, $70,747 New Hampshire $64,414 Michigan)

Annual Project Update:

Ozone (O_3) in the part of the atmosphere closest to the Earth's surface is an air pollutant that is a respiratory irritant and that causes damage to plant leaves and human-made structures. It is important to note that O_3 is not emitted directly from pollution sources but rather forms in the atmosphere when oxides of nitrogen (NO_x) and volatile organic compounds (VOCs) mix in the presence of sunlight. While some amount of O_3 in the lower atmosphere is formed naturally, the amount of O_3 in the atmosphere of the Dallas-Fort Worth (DFW) region exceeds that which is allowable by the National Ambient Air Quality Standards established by the Environmental Protection Agency.

In the DFW area, the most prevalent local emission sources of NO_x and VOCs are automobiles and other motor vehicles and a number of large point sources, specifically electric power plants and cement kilns. However, O_3 levels have not decreased significantly in recent years despite gradual decreases in NO_x and VOC emissions from automobiles. It is theorized that the dramatic increase in both the number of natural gas wells and the production of natural gas in the DFW region are contributing to additional VOC and NO_x sources, leading to the hypothesis that there is a relationship between O_3 levels and natural gas activities. A team from Rice University, the University of Houston (UH), and the University of New Hampshire (UNH) are investigating this hypothesis through performance of an air quality sampling campaign and subsequent data analyses.

The Rice, UH, and UNH team installed several additional pieces of air quality monitoring equipment at the Eagle Mountain Lake Texas Commission on Environmental Quality monitoring site for a one-month period from May 30 to June 30, 2011. Eagle Mountain Lake is located approximately 40 kilometers to the northwest of downtown Forth Worth. This location was chosen for several reasons: a wealth of natural gas activity, wind that predominantly blows from the direction of the DFW metropolitan area, and monitoring that has noted the high levels of O_3 in the northwest corner of the DFW region. The timing of the campaign was selected to optimize likely O_3 formation (due to favorable meteorological conditions), staff availability, and duration of the project.

Relevant measurements included not only the concentrations of O_3, NO_x, and VOCs but also values for other relevant chemical and physical variables, including meteorological parameters. In addition, a group from the University of Michigan conducted computational modeling used in conjunction with the data generated from these measurements to determine the VOC emissions, atmospheric reactions, and meteorological conditions that lead to O_3 formation in the DFW region.

The first round of data analyses indicate that the air quality at the Eagle Mountain Lake site is determined by being a receptor of aged and processed air from the DFW metropolitan area. However, there are strong indications that intermittent local sources influence air quality at the site. Future analyses will focus on deconvolving the relative influences of local and distal sources and on determining how the mixing of aged air and fresh emissions affects pollutant concentrations at Eagle Mountain Lake.

Project 10-029 **STATUS: Active – December 1, 2010**
End Date Extended to November 30, 2011

Wind Modeling Improvements with the Ensemble Kalman Filter

Texas A&M University – John Nielsen-Gammon AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Bright Dornblaser

Funding Awarded: $80,108

Annual Project Update:
Introduction

Computer-based simulations of the atmosphere are a vital component of a comprehensive air quality research program. Scientists and regulators use simulations to help understand the causes and sources of high levels of air pollution and to test various strategies for reducing air pollution levels. The Environmental Protection Agency requires that State Implementation Plans to reduce air pollution include computer simulations demonstrating that the proposed strategy will actually do the job.

It is essential that the simulation be accurate, that it not only reproduce the observed pattern of air pollution during a given episode (to within specified tolerances) but also correctly simulate the processes leading to the particular observed pattern. Otherwise, regulations might be proposed to reduce emissions from one set of sources when the pollution is actually being caused by a different set of sources.

Most air pollution modeling systems consist of three essential components:

- the emission inventory and models, which specify which pollutants enter the atmosphere where, as a function of time of day, day of week, and meteorological conditions;
- the meteorological model, which simulates the wind, temperature, moisture, cloud, and rainfall; and
- the photochemical model, which uses the output from the emission inventory and meteorological model to simulate the transport and mixing of pollutants and the chemical reactions that take place among them.

Errors in the meteorological model output, or met model output for short, harm the air pollution simulation in several ways. For example, winds that are too strong will produce pollution concentrations that are too weak and in the wrong place. Winds that are from the wrong direction will produce pollution concentrations in the wrong place. Too much cloud cover or precipitation will reduce pollution concentrations. Too much vertical mixing of pollutants will reduce pollution concentrations and allow them to be more easily dispersed at night.

Many of these errors can be reduced or eliminated by incorporating available data into the met model simulation. Wind observations, for example, can be "assimilated" into the met model so that the simulation closely matches the observations. For other errors, the best solution is to improve the model itself.

This is especially true for vertical mixing. Vertical mixing is important because it affects horizontal wind speeds as well as vertical dispersion of pollutants. Direct observations of vertical mixing are rare and are difficult to incorporate into a met model. Furthermore, met models do not directly simulate vertical mixing. Instead, they estimate it on the basis of the simulated vertical profiles of wind and temperature. The estimation scheme, called a "parameterization", is based on measurements of the atmosphere in very simple situations that may not directly apply to a particular urban area.

Observations during field programs show that met models handle vertical mixing poorly, and that these errors can lead to a factor of two difference in surface concentrations of various pollutants. Thus, it is important to reduce these parameterization errors.

Project Overview

The purpose of this project is to improve and refine a vertical mixing parameterization scheme used by a standard met model known as WRF. The idea behind the project is to combine two sources of information to accomplish this task. The first set of information is the set of differences between the met model output and observations. The second set of information is a set of differences between met model outputs from models whose parameterizations have been altered slightly. This latter set of met model output contains information on which changes to the parameterization produce which changes in the output. By combining the two sources of information, it is possible to determine which changes to the parameterization would help the model reduce the differences between the met model output and observations.

The basic technique used for this task is called the Ensemble Kalman Filter (EnKF). Earlier work has demonstrated that this particular use of the EnKF can improve the accuracy of met simulations and forecasts, but the testing was conducted on a single ozone episode. This project is designed to obtain firmer conclusions regarding improved model performance by testing the procedure on other ozone episodes, examining how many different aspects of the parameterization should be changed at one time, and determining whether the parameterization gets modified in the same way in different simulations.

Summary of Progress and Results

Because the EnKF system had been designed for older versions of the WRF model, the focus of the project so far has been to lay the groundwork for future simulations and ultimate adoption by TCEQ. The EnKF software system has been documented and a description of scientific papers describing the evolution and testing of the EnKF has been prepared. Because the EnKF system has been written by several different individuals over the course of several years, part of the project has been devoted to refining the system and making it more robust. Meanwhile, the WRF modeling system has been upgraded to the current version (version 3.3), and testing is underway to work through any issues with compatibility with the computer system used for this project.

To date, the preparation work is nearing completion, and future work during the next few months will focus on running the test cases and analyzing the results.

Project 10-032	**STATUS: Active - February 9, 2011** **End Date Extended to November 30, 2011**

SHARP Data Analysis: Radical Budget and Ozone Production

University of Houston – Barry Lefer
UCLA – Jochen Stutz
University of New Hampshire -

AQRP Project Manager – Cindy Murphy
TCEQ Project Liaison – John Jolly

Funding Awarded: $248,652
($176,314 UH, $23,054 New Hampshire, $49,284 UCLA)

Annual Project Update:

The chemistry of atmospheric radicals, especially the hydroxyl radical (OH) and hydroperoxyl radical (HO_2), together called HO_x, is deeply involved in the formation of secondary pollutants ozone and fine particles. Radical precursors, such as nitrous acid (HONO) and formaldehyde (HCHO), significantly affect the HO_x budget in urban environments such as Houston. These chemical processes connect surface emissions, both human and natural, to local and regional pollution, and climate change. This project will evaluate the radical budget and ozone production using the data collected during the Study of Houston Atmospheric Radical Precursors (SHARP) on the campus of the University of Houston in the spring of 2009.

The purpose of this work is to inform policy decisions related to the development of ozone control strategies for State Implementation Plans in Texas; particularly those that rely on the use of appropriately represented chemical reactions in photochemical modeling. This project will directly support these goals by using statistical methods to analyze the observations related to ozone formation, and also using numeric zero-dimensional models with five different chemical mechanisms to simulate the oxidation processes during this study. Using the model results, the radical budget will be calculated and the sensitivity of ozone production to oxides of nitrogen (NO_x) and volatile organic compounds (VOCs) will be analyzed. The model results also allow the comparison of the observed OH reactivity and ozone production rate to the model calculations. The models used in this project have been previously used for similar studies (Shuang et al., 2010; Flynn et al., 2010; Bais et al., 2003, Wong and Stutz, 2010).

The primary objectives of this project include:

- Identify the variation of measured HO_x and HO_2/OH with NO_x and VOCs and compare to the model prediction.
- Quantify OH reactivity and compare observed and calculated OH reactivity to examine any missing OH sink species.
- Examine the significance of nighttime OH and determine the importance of both the reaction of O_3 + alkenes and NO_3 chemistry as nighttime OH sources.

- Compare and contrast the HO_x levels in Houston to those in Mexico, Nashville and New York City.
- Investigate the instantaneous O_3 production and deviations of the NO_x photostationary state due to clouds and aerosols. This analysis will also include comparison of observed and calculated $HO_2 + RO_2$ mixing ratios and net O_3 production.
- Study the sensitivity of O_3 production to NO_x and VOCs.
- Investigate the potential of HONO as a daytime precursor of OH.
- Evaluate the role of nitryl chloride ($ClNO_2$) as an early morning radical source and its' contribution to ozone production.
- Investigate the processes creating strong correlations between HNO_3 and gas phase chloride, and their implications for coupled Cl and NOx chemistry in Houston.

Project Update by Objective:
The PI team has been working on the preparation of the mechanism schemes (RACM2, CB05, MCM, SAPRC07, and LaRC) for the SHARP data analysis. Input files for these mechanisms have been created and the model mechanisms have been updated to the available constrained chemical and meteorological parameters. Almost all model simulation runs have been run, and the analysis of the SHARP data and the various 0-D and 1-D box modeling simulations is underway. The preliminary model results have been shared with all members of the PI team to help their data analyses. Initial results for each of the project objectives are summarized below:

Objective 1. Identify the variation of measured HOx and HO_2/OH with NOx and VOCs and compare to the model prediction. (UMiami and Penn State)

Objective 1A: Comparison of observed and modeled HOx

The measured and modeled OH and HO_2 exhibit similar diurnal and day-to-day variations, with maxima in the early afternoon and minima at night. The median daytime observed-to-modeled OH ratio is 1.08 with a correlation coefficient, r, of 0.68. The median daytime observed-to-modeled HO_2 ratio is 1.34 with a correlation coefficient, r, of 0.87.

Two oxidation pathways can contribute to nighttime HOx in the planetary boundary layer: (1) O_3 can react with alkenes to produce a significant amount of OH and HO_2, and (2) NO_3 can produce HOx directly via reaction with HCHO or indirectly after conversion of the RO_2 that is initially produced by VOCs+NO_3. These processes become more important for the nighttime HOx production because daytime HOx photolytic sources vanish at night. At night, the modeled HO_2 agrees reasonably well with the measurements during nighttime, with a median measured-to-modeled ratio of 1.41, which is within the combined uncertainties of measured and modeled HO_2. However, nighttime OH is significantly under-predicted, with a median measured-to-modeled ratio of 6.2. This difference indicates that the RACM mechanism fails to capture the processes that create nighttime OH in this urban environment.

Objective 1B: Observed-to-modeled ratios as a function of NO

The observed-to-modeled OH and HO_2 ratios can test our understanding of the HOx photochemistry because the cycling between OH and HO2 is very fast and the photochemical equilibrium among OH and HO_2 is closely tied to the interconversion of NO to NO_2 in the troposphere. Both the measured and modeled HO2/OH ratios decrease with increasing NO. This decrease occurs because NO shifts HOx into OH by reacting with HO_2. However, when NO is lower than a few hundred pptv, the modeled HO_2/OH ratios are significantly higher than the measured. The agreement of measured and modeled HO_2 to OH ratios is good when NO is around a few hundred pptv. The slope of measured HO_2/OH as a function of NO is significantly less than the modeled slope. This difference is consistent with measured OH being greater than modeled OH at low NO, while measured HO_2 is much greater than modeled HO_2 at high NO.

Objective 2. Quantify OH reactivity and compare observed and calculated OH reactivity to examine any missing OH sink species. Examine HOx Budget. (Penn State and UMiami)

Calculated HOx production is dominated by photolysis of HONO in the early morning and by O_3 photolysis in the midday, and is mainly from O_3 reactions with alkenes a night. On average, the daily HOx production rate was 23.8 ppbv day^{-1}, of which 31% is from O_3 photolysis, 23% from HONO photolysis, 12% from HCHO photolysis, and 14% from O_3 reactions with alkenes. For HOx loss, the clearly dominant process was the OH reaction with NO_2, while the self-reactions between OH, HO_2, RO_2 become important in the afternoon when their concentrations are the highest.

Objective 3. Examine the significance of nighttime OH and to determine the importance of both the reaction of O_3 + alkenes and NO_3 chemistry as nighttime OH sources. (UMiami)

Objective 3A. Nighttime OH

The median measured nighttime OH concentration is 0.038 pptv or $9.4x10^5$ molecules cm^{-3}, while the modeled nighttime OH concentration is 0.009 pptv or $2.1x10^5$ molecules cm^{-3}. The median measured nighttime HO_2 on is 5.9 pptv, while the modeled nighttime HO_2 concentration is 3.9 pptv. This indicates that OH and HO_2 may also play important roles in the nighttime oxidation chemistry. The model underpredicts both nighttime OH and HO_2. The median measured-to-modeled HO_2 ratio at night is 1.54, which is within the combined uncertainty of measured and modeled HO_2. The median measured-to-modeled OH ratio at night is 6.2, which is significantly beyond the combined uncertainty of the measured and modeled OH. This difference indicates that the RACM2 mechanism fails to capture the processes that create nighttime OH in this urban environment.

Objective 3B. Importance of the O_3 + alkene reactions and NO_3 chemistry as nighttime HOx sources

Modeling results show that typical diurnal variations of HOx production from these two pathways were calculated. HOx production from O_3 + alkene reactions peaks in the midday when O_3 concentration reaches highest, while HOx production from NO_3 chemistry peaks at night because of low NO_3 concentration during the day due to its fast photolysis. In general, NO_3 chemistry contributes less HOx production than O_3 + alkene reaction, except for a few

nights (e.g., the night of May 20 and 21) when NOx concentrations were high and NO titrated O_3 to very low levels while the reaction of NO_2 with O_3 produced high concentrations of NO_3 on these nights. Modeled NO_3 concentrations are used in the calculation due to the low data coverage in the DOAS NO_3 measurements. In general the modeled NO_3 is in good agreement with observed NO_3, with the modeled NO_3 lower than the observed NO_3, but within the uncertainty of the observed NO_3. On average, O_3 + alkene reactions contribute about two thirds (~68%) of nighttime HOx production while the other one third comes from NO_3 chemistry.

Objective 4. Compare and contrast the HOx levels in Houston to those in Mexico, Nashville and New York City. (UH, UMiami & Penn State)

Compared to the OH and HO_2 measurements in other two cities in Mexico City and New York City, the measured OH concentrations in Houston during SHARP are comparable to the OH measurements in the other two cities. However, the peak HO_2 concentration in Mexico City is the highest, while the HO_2 concentrations in New York City are the lowest, simply because of the high NOx concentrations in New York City throughout the day.

Objective 5. Investigate the instantaneous O_3 production and deviations of the NOx photostationary state due to clouds and aerosols. This analysis will also include comparison of observed and calculated $HO_2 + RO_2$ mixing ratios and net O_3 production. (UH).

To assess the impacts of changes in actinic flux on ozone production and loss rates, the LaRC 0-D photochemical box model was run with photolysis rates from both measured and modeled actinic fluxes. The reduction in measured photolysis rates relative to modeled rates are quantified by taking the ratio of SAFS derived photolysis rates to the CFM rates generated by TUV, defined as the j-value impact factor (JIF). The median JIF for 6 cloud free days was 0.98, while the median JIF for the remaining 42 days was 0.83. For JIFs of 1 ± 0.15, O_3 production can reach instantaneous rates greater than 50 ppbv/hour. While other factors besides j-values were also regulating ozone production during SHARP (wind speed & direction, boundary layer height, emissions, etc.), reductions in $j(NO_2)$ correspond to reduced net O_3 production rates with a nearly one-to-one relationship, albeit of much smaller net O_3 production rates below JIFs of 0.85.

For all days of the SHARP, the median O_3 destruction terms are nearly an order of magnitude smaller than the formation rates. During the SHARP campaign, clouds and aerosols reduced the net O_3 production during the campaign by an average of ~3.1 ppbv/hour out of 10.4 ppbv/hour. On high ozone days there was a 9% reduction in ozone production (average of 1.3 out of 14.3 ppbv) ozone per hour which was primarily due to aerosol reductions in solar UV radiation.

Objective 6. Study the sensitivity of O_3 production to NOx and VOCs. (UMiami)

The ozone production sensitivity to NOx or VOCs has a similar behavior for TexAQS2000, TRAMP2006 and SHARP2009; it is VOC sensitive in the early morning and late afternoon but NOx-sensitive throughout the afternoon. This behavior is typical of US urban areas. These results are independent of the differences between the measured and modeled OH and HO_2. Note that in the afternoon the ozone sensitivity in SHARP2009 has a longer NOx-sensitive period than TexAQS2000 and TRAMP2006, indicating that NOx control is an efficient approach for the O_3 control in springtime.

Objective 7. Investigate the potential of HONO as a daytime precursor of OH. (UCLA)

Initial results indicate that the reaction of OH + NO is unimportant as a source of HONO in this campaign, and thus the PI team did not correct the OH formation from HONO photolysis by the rate of this back-reaction. These calculations were based on UCLA's LP-DOAS observations of O_3, HCHO, and HONO mixing ratios at three light paths nominally at 40-70 m, and 70-150 m and 150-300 m above ground. In general, HONO photolysis dominates in the lowest and middle light path in the morning. Morning HONO photolysis in the upper height interval is about equally important as HCHO, and sometimes O_3, photolysis. At around 10:00 CST ozone photolysis becomes the most important OH source. However, both HCHO and HONO photolysis remain important. It is interesting to note that OH formation from ozone and HCHO photolysis show little altitude dependence, although it appears that O_3 photolysis is slightly higher aloft. In contrast, OH formation through HONO photolysis shows very distinct gradients, with higher rates near the surface. In the lower two height intervals HONO photolysis is the second most important OH source after 10:00 CST. In the upper interval HCHO photolysis is equally or even more important than HONO photolysis. In the later afternoon HONO photolysis again becomes the dominant OH source in the lowest two height intervals.

Objective 9. Investigate the processes creating strong correlations between HNO_3 and gas phase chloride, and their implications for coupled Cl and NOx chemistry in Houston. (UNH).

Gaseous nitric acid (HNO_3) and gas phase soluble chloride (Cl^-) were highly correlated on short (minutes to hours) time scales throughout the SHARP campaign. This correlation between soluble Cl^- and HNO_3 was discovered during the early days of SHARP campaign and re-analysis of the 2006 TRAMP data revealed that is also phenomenon also occurred during that project. Peak mixing ratios of soluble Cl^- occurred during transport from south (i.e., clean conditions) with lower mixing ratios occurring in polluted from the north and east. Overall the opposite conditions resulted in peak HNO_3 mixing ratios yet there is a remarkably strong correlation between HNO_3 and soluble Cl^- from sample to sample and diurnally were observed regardless of wind direction. During intervals with sustained northerly flow (relatively low Cl^-) daytime maxima routinely exceeded 1 ppbv. Similar observations made during TexAQS 2006 on the Moody Tower and the NOAA vessel Ronald H. Brown indicate that abundant soluble Cl^-, linked with HNO_3 by processes not yet understood, is characteristic of the Houston-Galveston Bay region during both spring and summer.

Project 10-034 **STATUS: Active – February 2, 2011**

End Date Extended to November 30, 2011

Dallas Measurements of Ozone Production

University of Houston – Barry Lefer

AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Doug Boyer

Funding Awarded: $195,054

Annual Project Update:

The Dallas-Fort Worth-Arlington Metroplex (DFW) includes approximately 6.5 million people, making it the largest metropolitan area in Texas and the 4th largest in the United States. Given that the DFW area does not include large petrochemical facilities, the primary source of the anthropogenic ozone precursor NOx and VOCs emissions are the significant mobile source emissions and a number of large point sources, specifically electric power plants and cement kilns. While the ozone design value for DFW is very close to being in compliance with NAAQS 8-hr ozone standard of 84 ppbv it is interesting to note that ozone levels have not decreased significantly in recent years (Allen and Olaguer, 2004). In addition, improvements in the production of natural gas from a combination of horizontal drilling and hydraulic fracturing of the Fort Worth Basin of the Barnett Shale formation have resulted in a dramatic increase in both number natural gas wells and production of natural gas in the DFW region. The network of 18 TCEQ ozone monitoring sites in the DFW area is designed to capture both upwind and downwind ozone mixing ratios; the peak ozone values are frequently observed along the northwestern border of the network. This may be due to the prevailing southeast winds transporting polluted air from the urban areas, the recent increase in energy industry activities in the area, or some combination of the two.

The understanding of photochemical ozone production in the Dallas – Fort Worth (DFW) Metroplex is still incomplete (AQRP, 2010). Central to gaining a better understanding of the DFW ozone issue is providing chemical measurements that can directly be compared to the SIP chemical transport models. Measurements of the ozone production rates would quickly and significantly help constrain the degree to which the TCEQ chemical transport models are performing in a realistic way and improve the understanding of how these models can be employed for policy recommendations. Direct measurements of the ozone production rate can be used to determine not only if the measured ozone is similar to the forecasted but if the ozone measured at a site was produced locally or transported from somewhere else. As the NAAQS for ozone decreases, the distinction between transported (or background) ozone and locally produced ozone is critical. To help provide the measurements to reduce the uncertainty in our understanding of the conditions contributing to photochemical ozone in the Dallas area, two of the new Pennsylvania State University Measurements of Ozone Production Sensors (MOPS) are being deployed to continuously measure ozone production rates in the DFW region, beginning with the TCEQ Eagle Mountain Lake site (CAMS 75), and additional locations to be determined with the guidance of the AQRP and TCEQ.

The data will show the temporal and spatial variability of *in situ* net ozone production rates in the DFW area, as well as potential NO_x sensitivity. This data will enable determination of the fraction of the ozone is produced locally compared to the transported or background ozone. Coupling this data with speciated auto-GC data and other measurements (i.e. meteorological, ozone, NO, NO_x, etc.) from the TCEQ CAMS sites where the instruments will be located will help determine how ozone production changes with varying air composition. This information will be useful in developing ozone control strategies and determining whether local or regional controls may be best suited for this area in the State Implementation Plan.

Project Update (February 2001 – August 2011):

Task 1 was to purchase and fabricate the various components of the MOPS instruments. A new design adds a bit more complexity to the instrument, but this new method is significantly faster and more importantly provides a better measure of the "background" ozone production for the MOPS system.

Task 2 was to identify CAMS sites with help of AQRP and TCEQ for MOPS instrument deployments. The PI team selected and received permission from the City of Fort Worth and TCEQ to setup MOPS instruments at the Eagle Mountain Lake (C75) and Fort Worth Northwest (C13) sites for summer and fall of 2011.

Task 3 was to deploy two MOPS instruments for an extended period of time in the DFW area. The MOPS team installed the 1st MOPS instrument at the Eagle Mountain Lake (C75) site during the first week of August 2011. The second MOPS system was installed at the Fort Worth Northwest (C13) site during the 3rd week of August

During the last two weeks of August the MOPS instruments have been working consistently; with intermittent problems. The MOPS PI team is currently evaluating the August MOPS data, a month with a number of DFW ozone exceedances. Specifically for the month of August, the MOPS System at Eagle Mountain Lake (MOPS-C75) has deployed for a total of 26 days, with the cover working for 9.5 days (36%); the cover was open for 3 days (11%); and offline for 13.5 days (52%). The (MOPS-C13) was deployed for the last 17 days of the month with the cover working for 4 days (23%); the cover open for 2.5 days (18%); cover closed for 1 day (7%); and instrument off-line for 7.5 days (53%). With fixes to the communication string that UH has made the last week of August the time off-line has shrunk to less than 4%.

Data collection will continue in September and October.

Project 10-042 **STATUS: Active – October 8, 2010**

End Date Extended to November 30, 2011

Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms

ENVIRON International – Greg Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Awarded: $237,481

Annual Project Update:

Introduction

Formation of ground level ozone requires both NOx and VOCs and air quality management planning seeks the combination of NOx and VOC emission reductions that will most effectively reduce ozone. When VOCs undergo chemical reactions in the atmosphere they can reduce the availability of NOx by converting it to un-reactive compounds which we call NOx-sinks. However, some of these "NOx-sink" compounds can react further in the atmosphere and may return the NOx to an active form, which we refer to as NOx-sources. The chemical reactions of VOCs with NOx can be characterized by environmental chamber experiments which expose controlled amounts of VOC and NOx to light and measure the products (e.g., ozone) that are formed. This project performed new environmental chamber experiments to characterize NOx sinks and sources for VOCs that are poorly understood. New experiments were performed using the aromatic hydrocarbon toluene and its degradation products, the biogenic hydrocarbon isoprene, and several nitrogen-containing organic compounds that are prototypical of compounds found in the atmosphere. In addition, data were obtained from chamber experiments performed in Europe that have not been utilized in the US for developing chemical mechanisms. The data obtained have been used to improve the chemical reaction mechanisms that are used in the TCEQ's State Implementation Plan (SIP) ozone modeling and control strategy development. The project benefit will be more accurate modeling of the ozone benefits of emission control strategies in Texas and elsewhere.

Experiments Performed

A total of 33 dual reactor environmental chamber experiments were performed for this AQRP project at the University of California at Riverside (UCR). Because of the dual reactor design, each successful experiment provides data for two separate reactor irradiations, each of which can be treated as a separate experiment for modeling purposes. Modeling input and experimental output data were obtained for a total of 55 such reactor irradiations (runs). The experiments may be divided into 3 groups: NOx sink experiments, NOx source experiment and chamber characterization experiments needed to support interpretation of the former.

NOx sink experiments added a test compound to an alkene-NOx mixture and measured the resulting change in ozone and other compounds. Because alkene-NOx experiments inherently have strong radical production and weak NOx sinks they are sensitive to NOx sinks introduced by the test compound. Experiments were carried out for toluene, o-cresol, furan (a precursor to the aromatic fragmentation product 2-butene-1,4-dial), and isoprene. Several isoprene-NOx experiments with low initial NOx concentrations were also performed to support interpretation of the NOx sink experiments for isoprene. The NOx sink experiments demonstrated that all of the compounds tested inhibited ozone formation by mixtures of ethene and NOx because the test compounds have strong NOx sinks that convert NOx to inactive forms.

NOx source experiments were carried out using two different methods with the test compounds isopropyl nitrate, isobutyl nitrate and 2-nitrophenol. Experiments mixed the test compound with hydrogen peroxide and acetaldehyde or CO. The purpose of adding hydrogen peroxide was to produce OH radicals that can react with the test compound. The additions of acetaldehyde or CO are two different approaches to preserving NOx released by the test compound for quantification. In all cases, release of NOx from the test compound was observed with consequent ozone formation providing firm evidence for NOx recycling from NOx source compounds. These experiments have been used by SmogReyes and ENVIRON to improve the CB6 mechanisms for aromatic hydrocarbons (i.e., for nitrophenol type compounds formed from benzene, toluene, xylene, etc.) and alkanes (i.e., for alkyl nitrates from propane, butane, etc).

Chemical Mechanism Development

The TCEQ is using the CB6 mechanism for ozone SIP modeling and mechanism improvements will benefit the reliability of SIP planning. The new experiments conducted at UCR, combined with experiments retrieved from the European EUPHORE chamber for this project, have been used to improve the Carbon Bond 6 (CB6) mechanism. The revised mechanism is to be called CB6r1.

The results of NOx sink experiments conducted with toluene, o-cresol, furan (a precursor to 2-butenedial) and isoprene are shown in Figure 1. The effect on ozone and NO_2 of adding the test compound was simulated very well for o-cresol and isoprene and fairly well for toluene and furan. These results suggest that CB6r1 is performing well in representing the strengths of the NOx-sinks present for toluene, o-cresol, and isoprene. The results for furan are complicated by the fact that furan is not the compound of interest but rather was used as a precursor to make 2-butenedial (the compound of interest) during the chamber experiment. Results from a EUPHORE experiment (not shown) that was performed using 2-butenedial directly are being used to complement results from the experiment with furan shown in Figure 1.

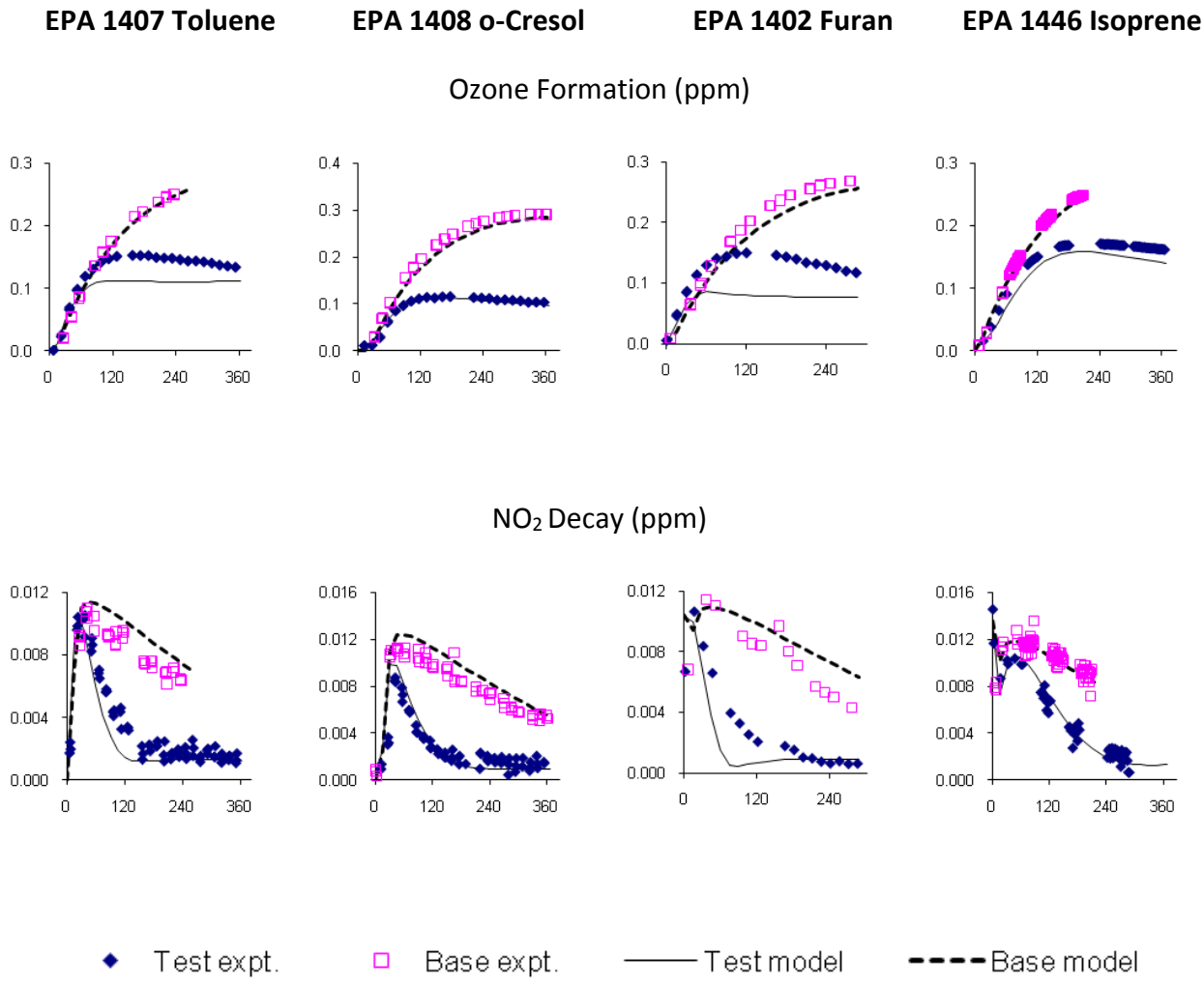

Figure 1. Model simulations with CB6r1 of NOx sink experiments with toluene, o-cresol, furan and isoprene added to a base mixture of ethene and NOx .

The NOx source experiments with alkyl nitrates (isopropyl nitrate and isobutyl nitrate) demonstrate formation of NOx when organic nitrates undergo photolysis and reaction with OH. The evidence is stronger for photolysis than OH reaction because photolysis dominated the decay of the organic nitrates in the experiments performed. Figure 2 shows results of NOx source experiments and simulations with CB6r1. The yields of NO_2 (and O_3) are simulated very well by CB6r1 for experiments with isopropyl nitrate and isobutyl nitrate.

Simulations of experiments with 2-nitrophenol are shown in Figure 2. Simulations using several test mechanisms confirm that 2-nitrophenol decayed rapidly by photolysis and this reaction needed to be added to CB6r1. Formation of NO_2 from 2-nitrophenol was observed and CB6r1 simulates the NO_2 formation fairly well. Formation of O_3 was observed although the

measurement suffers from strong interference (i.e., UV absorption) by 2-nitrophenol and the apparent good agreement for the final O_3 may be misleading. The NOx source experiments for 2-nitrophenol provided important evidence for photolysis of nitrophenols accompanied by formation of NOx and this process has been included in CB6r1 for nitrophenols and nitrocresols formed from aromatic hydrocarbons.

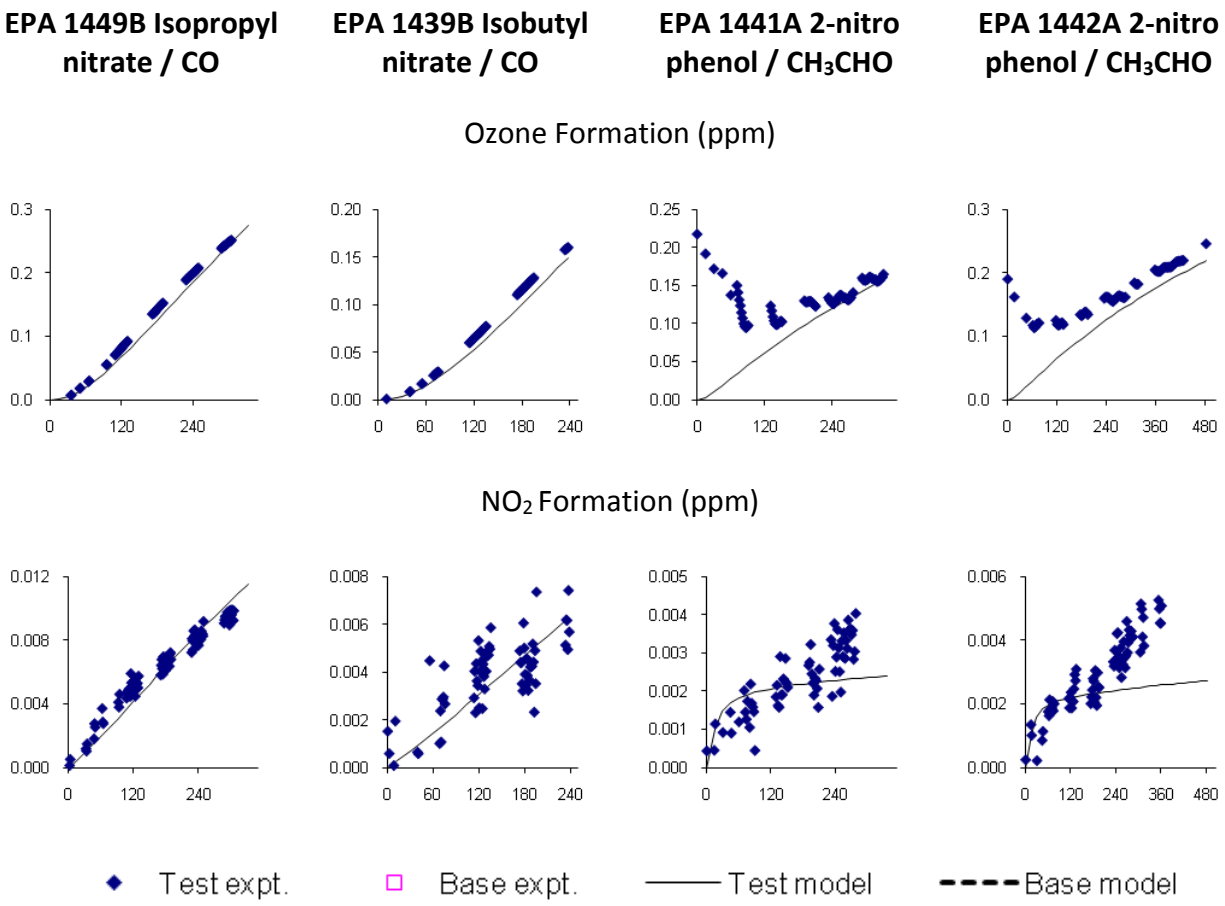

Figure 2. Model simulations with CB6r1 of NOx source experiments with organic nitrates added to mixtures of CO and H_2O_2 or CH_3CHO and H_2O_2.

Project 10-044 **STATUS: Active – March 25, 2011**

End Date Extended to November 30, 2011

Airborne Measurements to Investigate Ozone Production and Transport in the Dallas-Fort Worth (DFW) Area during the 2011 Ozone Season

University of Houston – Maxwell Shauck

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Erik Gribbin

Funding Awarded: $279,642

Annual Project Update:
The University of Houston (UH) aircraft-based Air Quality Monitoring Team participated in an air quality field study in the Dallas Fort Worth (DFW) area during the 2011 ozone season. This study, administered by the Air Quality Research Program (AQRP), was conducted in coordination with ground based air quality measurements performed by UH and other institutions.

Airborne air quality measurements enable investigators to better understand the mechanisms associated with the transport of precursors and their contribution to ozone formation under specific meteorological conditions.

A twin-engine Piper Aztec aircraft equipped with a full complement of instrumentation was utilized. Both aircraft and instruments were extensively modified for the purpose of air quality monitoring.

The aircraft sampling data complemented the ground based measurements to enhance the understanding of atmospheric chemistry processes, meteorology, spatial distribution and transport of pollutants of interest in and around the DFW area. The campaign included 50 flight hours flown during the latter part of June and early part of July. The primary objectives of the program addressed the characterization of the air quality, the transport of ozone and ozone precursors and the potential contribution of emissions associated with natural gas production in the vicinity of gas wells and compressor stations located in the Barnett Shale region.

Detailed flight plans were developed in coordination with AQRP that provided identification of emission sources and objectives for each measurement flight. The UH Aztec collected airborne samples on five science flights measuring ozone (O_3), nitrogen oxides (NOx), sulfur dioxide (SO_2), formaldehyde (HCHO), reactive alkenes, volatile organic compounds (VOC), and meteorological parameters.

The meteorological conditions were quite consistent during the measurement period with steady southerly synoptic flows, sunny and hot conditions. Thus, it was possible to collect data under very similar conditions. The study focused on Barnett Shale and the DFW downwind conditions during photochemically active daytime periods.

Major results of the project include the following observations:

Regional DFW Metroplex: Upwind ozone levels (i.e. in this case south of the DFW Metroplex) typically range between 30-50 ppbv and largely agree with ozone background levels determined in other studies in Texas. Highest secondary pollutants occur in the downwind area of the urban DFW Metroplex. Typically, maximum ozone values may be enhanced by a factor 2-2.5 compared with the values obtained in the upwind area on the same day.

Urban DFW area: the urban plume is characterized by enhanced NOy and CO. Levels of NO, NO_2 and reactive alkenes remain modest in the downwind area of the DFW Metroplex indicating photochemically aged air masses.

Barnett Shale area: at times HCHO and reactive alkenes correlate in the Barnett Shale area, while ozone and NOy are not that well correlated with reactive alkenes.

Project 10-045 **STATUS: Active - January 22, 2011**

End Date Extended to September 30, 2011

Quantification of Hydrocarbon, NOx, and SO2 emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR dataset

UCLA – Jochen Stutz
UNC - Chapel Hill – William Vizuete
Aerodyne – Scott Herndon
Washington State University – George Mount

AQRP Project Manager – Cindy Murphy
TCEQ Project Liaison – Marvin Jones

Funding Awarded: $398,401
($150,132 UCLA, $33,281 UNC, $164,988 Aerodyne, $50,000 Washington State)

Annual Project Update:

In the spring of 2009 a multi-institutional and multi-platform field experiment to understand and classify industrial sources of ozone-forming chemicals took place in Houston, TX. During the "Formaldehyde and Olefin from Large Industrial Sources" (FLAIR) project the Aerodyne Research Inc. (ARI) mobile laboratory performed in-situ measurements of VOCs, NO_x and HCHO. At the same time an Imaging Differential Optical Absorption Spectrometer (I-DOAS) developed by the University of California Los Angeles (UCLA) sampled flares and other individual sources for emissions of HCHO, SO_2 and NO_2. Two Multi-Axis Differential Optical Absorption Spectrometers (MAX-DOAS) operated by UCLA and Washington State University (WSU) sampled air masses upwind and downwind of a large petrochemical complex to determine facility-wide emissions of HCHO and NO_2. As a result of all these efforts, a unique observational dataset of VOCs, HCHO, and NO_x observations was created.

Here we report our findings from a follow-up project to interpret this observational data-set with the goal of determining emission rates of ozone precursors, such as VOCs, HCHO, SO_2, and NO_2, for the specific times and locations of the observation. The project was a collaborative effort between the University of California Los Angeles (UCLA), Aerodyne Research Inc. (ARI), Washington State University (WSU), and the University of North Carolina Chapel Hill (UNC).

In general we found that HCHO is not directly emitted by un-ignited flare stacks, while burning flares clearly emit HCHO at the flare tip. This is based on observations of flares in the Houston area from the different measurement platforms. Direct HCHO emission rates of burning flares observed during FLAIR varied between 0.3-2.5 kg/h. Direct emissions of HCHO from burning flares are currently not considered in emission inventories. We also observed emissions of SO_2 (up to 2-5kg/h) and NO_2 (up to 0.3 kg/hr) from certain flares, but many other burning flares did not emit these compounds above the average detection limit of 0.7 kg/hr for SO_2 and 0.1 kg/hr for NO_2.

The destruction removal efficiency, DRE, and combustion efficiencies, CE, from in-use flares were also quantified using ground-based in situ measurements. Uncertainty in knowledge of the vent gas leads to uncertainties in the DRE but not the CE values. A range of DRE and CE values were observed for in-use flares – ranging from 0 (unlit) to 0.7 (steaming) to 0.999 (presumably operating as intended).

One of the surprises in the FLAIR data was the observation of a large source of HCHO in the Texas City refinery complex. This source was observed from all platforms in this project as well as from the SOF van from Chalmers University, Sweden. The estimates of the strength of this source of 18 ± 5 kg/h during one of the events on May 13, 2009 agreed remarkably well between the different platforms. Our analysis suggests that this is a direct primary source of HCHO. Analysis of the HCHO/SO_2 ratio revealed that during most of the time this source(s) co-emitted both species with ratios of 0.06 (MAX-DOAS) or 0.07-0.16 (in-situ), with an in-situ average of 0.12. However, all systems also found HCHO emission that showed no correlation with SO_2. We conclude that separate HCHO and SO_2 sources are co-located within ~300 ft and that emissions of HCHO and SO_2 are either not simultaneous, or that sometimes there is another strong unrelated HCHO source. Area averaged HCHO fluxes were also determined. A facility-averaged HCHO flux of ~45 kg/h was determined. Using the reported SO_2 fluxes and the average HCHO/SO_2 ratio the flux of HCHO co-emitted with SO_2 is 20 - 25 kg/h, in good agreement with the other observations.

Analysis of the emission inventory in Texas City, as well as triangulation and wind field analysis revealed that the most likely source of HCHO is a FCCU regeneration unit. The 2006 ozone non-acid rain inventory reports 2.6 kg/h of HCHO emissions from this FCCU unit. The 2006 base case reg 10 emission inventories shows that the area around this unit emits 3.3 – 4.3 kg/h of formaldehyde-like compounds (designated in inventory as FORM). All reported HCHO emission rates are considerably smaller than those found in our observations. It is not clear at this point if units of this type in other refineries would also emit HCHO.

Average SO_2 fluxes from Texas City industrial complex during FLAIR were determined to be 510 kg/h, with average flux from the eastern part of the facility of 360 kg/h. For 2006, the non-acid rain data base lists the SO_2 emission for the FCCU unit, which is by far the largest SO_2 source in Texas City, located east to the WSU MAX-DOAS instrument, as 453 kg/h. The observed flux and the emission inventory agree well. The average NO_2 flux from the Texas City industrial complex was determined to be ~100 kg/h.

Ethylene and propylene chemical plants did not show direct emissions of HCHO, but HCHO was observed both downwind and above these facilities. This HCHO is most likely of secondary nature, i.e. it is chemically formed from the oxidation of hydrocarbons emitted at the facilities.

An important finding was that emissions of highly reactive VOCs are important for ozone production because they serve as the “fuel” for ozone production, and also because their reaction with O_3 increases the flux of OH radicals through the radical cycling. These factors result in enhanced rates of HRVOC oxidation and ozone formation in freshly emitted HRVOC plumes. This finding is supported by an analysis of the impact of the ozonolysis of HRVOCs in freshly emitted plumes (from flares and/or fugitive emissions) showing a great enhancement of the radical production rates. Even during the night this can lead to production rates approaching

typical daytime values of 0.3 to 1.5 ppt/s. The total OH loss rate in a fresh alkene plume was calculated as 47 s^{-1}, mostly due to high concentrations of ethylene and propylene.

Using the Aerodyne Inverse Modeling System (AIMS), we have computed emission rates from data obtained at Mt. Belvieu (ethene and propene), Texas City (benzene), Ship Channel (butadiene) and the Texas City Courthouse (SO_2). Computed ethene and propene emission rates significantly exceed the levels reported in emission inventories (by over 2 orders of magnitude in some cases) and support the values of Mellqvist et al (2010) that were derived from the Solar Occultation Flux (SOF) method. Computed benzene emission rates in Texas City were also found to be much greater than the inventory values, with episodes of up to two to three orders of magnitude higher. Computed butadiene emission rates in the Ship Channel area were found to vary widely over time and were in some cases over four times the reported inventory rates. Inverse modeling of the Texas City courthouse in-situ observations yielded SO_2 emission rates between 100-500 kg/h, confirming the observations by the other FLAIR participants and matching the reported inventory values. While not the main purpose of this project, observations of ship plumes were also analyzed. This analysis revealed that the NO_2/NO_X emission ratio in the observed vessels in the Houston ship channel was between 6% and 12%. The thus far unreported $HONO/NO_X$ emission ratio of ships was between 0.7% and 1.4%, similar to that observed for diesel vehicles.

Project 10-DFW & 11-DFW **STATUS: Active - February 1, 2011**

Project Complete: August 31, 2011

Dallas – Fort Worth Field Study

UT-Austin – Vincent Torres

AQRP Project Manager – Jim Thomas
TCEQ Project Liaison – Raj Nadkarni

Funding Awarded: $88,809
($37,857 10-DFW (FY 10 Funds) $50,952 11-DFW (FY 11 Funds))

Executive Summary:
Due to the fact that there are 4 projects dealing with issues in the DFW area the AQRP wanted to actively promote integration of the measurements and ensure the projects worked cohesively. In cooperation with TCEQ Field Operations and TCEQ Region 4, the DFW Field Study Committee was formed.

The Committee consists of the AQRP Project Management (David Allen, Jim Thomas, and Maria Stanzione), the PIs of each of the projects being performed in the DFW area (Johan Mellqvist, Robert Griffin, Barry Lefer and Maxwell Shauck), the AQRP Project Managers for those projects (David Sullivan, Vincent Torres, and Gary McGaughey), the TCEQ Project Liaisons for those projects (John Jolly, Doug Boyer, and Erik Gribbin), TCEQ management representing the Chief Engineer, the Air Quality Division, Field Operations, and Region 4 (Mark Estes, Keith Sheedy, Raj Nadkarni, Ejaz Baig, Patricia De La Cruz, and Alyssa Taylor), and other interested parties (Kuruvilla John and John Nielson-Gammon). Expenditures for the project were dedicated to making the DFW field site ready for the measurement teams, including arranging access agreements, preparing the site, and arranging for power, communications and site security.

Project Update:
Observations and data collection at the DFW Site at Eagle Mountain Lake began on May 30, 2011 and ended on June 30, 2011. Regular conference calls were held throughout the month to facilitate operations at the Site.

All projects completed their activities and vacated the Site by July 2, 2011. The following week work began to decommission the Site and restore it to pre-operations conditions. As of July 31, 2011, all activities were complete and the Texas Adjutant General's Office, the property manager, was notified that we no longer were utilizing the Site.

AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-10-94300
Awarded to The University of Texas at Austin

Annual Report

September 1, 2011 through August 31, 2012

Submitted to

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Texas Commission on Environmental Quality
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October 1, 2012

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Texas Air Quality Research Program

Annual Report

October 1, 2012

OVERVIEW

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the 2010-2011 biennium, the AQRP had approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released a call for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received by the due date of June 25, 2010. These proposals were reviewed by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs. The results of these reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. Projects commenced shortly thereafter, and as of November 30, 2011, all projects have been completed. Final reports on all but one project have been posted to the AQRP website.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding of $1,000,000 for the FY 2012 period was awarded in February 2012. An additional $1,000,000 for the FY 2013 period was awarded in June 2012. At the same time an additional $160,000 was awarded for FY 2012, to support funding for additional air quality projects recommended by the TCEQ. A call for proposals was released in May 2012. Thirty-two proposals, requesting $5 million in research funding were received. The proposals were reviewed by the ITAC and the TCEQ. The Advisory Council selected 14 projects for funding. Investigators have been notified of their funding status and the contracting process has commenced.

BACKGROUND

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

> Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.
>
> (b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.
>
> (c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.
>
> (d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.
>
> (e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.
>
> (f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010 for the 2010-2011 biennium, and was renewed in June 2011 for the 2012-2013 biennium. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

RESEARCH PROJECT CYCLE

The Research Program is being implemented through a 9 step cycle. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle.

1.) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and the TCEQ develop research priorities; the research priorities are released along with a Request for Proposals.

2.) Project proposals relevant to the research priorities are solicited. The Request for Proposals can be found at http://aqrp.ceer.utexas.edu/ .

3.) The Independent Technical Advisory Committee (ITAC) performs a scientific and technical evaluation of the proposals. (More information on the ITAC is provided below.)

4.) The project proposals and ITAC recommendations are forwarded to the TCEQ. The TCEQ evaluates the project recommendations from the ITAC and comments on the relevancy of the projects to the State's air quality research needs. (More information on the TCEQ relevancy review is provided below.)

5.) The recommendations from the ITAC and the TCEQ are presented to the Council and the Council selects the proposals to be funded. The Council also provides comments on the strategic research priorities. (More information on the Council is provided below.)

6.) All Investigators are notified of the status of their proposals, either funded, not funded, or not funded at this time, but being held for possible reconsideration if funding becomes available.

7.) Funded projects are assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin is responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The Project Manager has responsibility for documenting progress toward project measures of success for each project. The Project Manager works with the researchers, and the TCEQ to create an approved work plan for the project. The Project Manager also works with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved QAPP for each project. The Project Manager reviews monthly, annual and final reports from the researchers and works with the researchers to address deficiencies.

8.) The AQRP Director and the Project Manager for each project describe progress on the project in the ITAC and Council meetings dedicated to on-going project review.

9.) The project findings are communicated through multiple mechanisms. Final reports are posted to the Program web site; research briefings are developed for the public and air quality decision makers; and a bi-annual research conference/data workshop is held.

Independent Technical Advisory Committee (ITAC)

The AQRP funding is used primarily for research projects, and one of three groups responsible for selecting the projects is the Independent Technical Advisory Committee (ITAC). The ITAC, composed of up to 15 individuals and an alternate with scientific expertise relevant to the Program, is charged with recommending technical approaches, and establishing research priorities. Initially, the ITAC was to meet at least twice per year at locations rotating between Austin, Dallas and Houston. As the Program proceeded, it was more efficient for the ITAC to meet once in Austin and as needed via conference call/webinar. Generally, the meetings in Austin are dedicated to new project review, reviewing progress on funded projects, and reviewing the Program's strategic plan.

Members of the ITAC consist of the TCEQ Project Director (or designee), representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC are drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas. The members of the ITAC are listed in Table 1.

As the ITAC membership is intentionally drawn from air quality researchers who have experience in Texas; these researchers and their colleagues will likely have interest in responding to the requests for research proposals issued by the AQRP. This raises potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas requires that the AQRP shall maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members are required to certify:

> *Confidentiality:* As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)
>
> *Conflict of Interest:* As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or the TCEQ Project Director. If there is a question of interpretation regarding whether a conflict of interest exists, I agree

that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Table 1: Members of the Independent Technical Advisory Committee

Name	**Title**	**Organization**
David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	University of Colorado - Boulder
Sarwar Golam	Research Physical Scientist, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Tho (Thomas) Ching Ho	Chairman, Dan F. Smith Dept. of Chemical Engineering	Lamar University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Associate Professor, Department of Earth and Atmospheric Sciences	The University of Houston
John Nielsen-Gammon	Professor and Texas State Climatologist Center for Atmospheric Chemistry and the Environment	Texas A&M University
David Parrish	Program Lead, Tropospheric Chemistry, NOAA/ESRL/Chemical Sciences Division	National Oceanic and Atmospheric Administration
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Associate Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ

TCEQ Relevancy Review

Once the ITAC has reviewed and ranked research project proposals according to technical merit, they are submitted to the TCEQ for a relevancy review. The TCEQ reviews proposals for relevancy to the State's air quality research needs. TCEQ approval is required for a project to receive funding from the Program.

Advisory Council

The final group responsible for selecting AQRP research projects is the Advisory Council. The Council serves as a Board of Directors for the Program and consists of up to 11 members, all residents of the State of Texas. Two Council members with relevant scientific expertise are nominated by the TCEQ. As defined in the AQRP contract, up to four members of the Council can be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. Additional members include government officials from Texas Near-Non-Attainment Areas active in air quality management. The purpose of the Council is to give final approval to projects recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. At least one meeting in Austin is dedicated to new project selection. Additional meetings, either in person or via webinar, and email updates are dedicated to providing summaries of on-going projects and review of the strategic plan.

Table 2: Members of the Advisory Council

Name	Title	Organization
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

PROJECT TIMELINE

This section will discuss the activities that took place in support of the AQRP. In the period covered by this report, four primary activities took place:

- FY 2010 – 2011 Projects completed
- Data Workshop
- State of the Science – Strategic planning document completed
- New funding for FY 2012 – 2013 – decisions on new projects

September – November 2011

The primary activities during the first quarter of FY 2011 – 2012 were the completion of the remaining research projects and the Data Workshop.

On September 27 and 28, 2011, the AQRP hosted a Data Workshop and ITAC meeting at The University of Texas at Austin's Pickle Research Campus. During the first day and a half, a representative from each project presented a report on project results and recommendations. The ITAC meeting was held during the last half of the second day. Topics of discussion included the upcoming NASA Discovery AQ project, procedures for possible future requests for proposals (RFPs), and the development of a State of the Science document to provide background information for establishing future research priorities.

All of the FY 2010 - 2011 Research Projects initially had an end date of August 30, 2011; however, eight Principal Investigators requested a 90 day contract extension. Project Managers reviewed final reports for those projects that were completed on August 30, and worked with the PIs of the extended Projects to ensure their timely completion. As of November 30, 2012, all Projects were completed, and draft final reports were submitted to the Project Managers and TCEQ Liaisons for review.

Program Administration during this period focused on the payment of monthly invoices for projects, reporting activities, and the planning and execution of the Data Workshop.

Table 3 on the following page, is a list of all FY 2010-2011 Research Projects, the amount they were funded, the amount they expended, and the amount they returned to the AQRP.

Table 3: FY 2010-2011 Funded Research Projects

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
10-006	**Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS**	**2/16/2011**	**11/30/2011**	**$484,662.00**	**$480,128.11**	**$4,533.89**
	*Chalmers University of Technology	Johan Mellqvist		$262,179.00	$262,179.00	$0.00
	University of Houston	Bernhard Rappenglüeck		$222,483.00	$217,949.11	$4,533.89
10-008	**Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling**	**10/21/2010**	**9/30/2011**	**$178,796.00**	**$176,567.10**	**$2,228.90**
	*Rice University	Daniel Cohan		$128,851.00	$126,622.32	$2,228.68
	ENVIRON International	Greg Yarwood		$49,945.00	$49,944.78	$0.00
10-009	**Additional Flare Test Days for TCEQ Comprehensive Flare Study**	**9/8/2010**	**11/30/2011**	**$591,332.00**	**$591,306.66**	**$25.34**
	*The University of Texas at Austin	Vincent Torres				
10-015	**An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-attainment areas in Texas**	**3/4/2011**	**11/30/2011**	**$201,280.00**	**$201,278.63**	**$1.37**
	*ENVIRON International	Greg Yarwood				
10-020	**NO_x Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone**	**3/5/2011**	**11/30/2011**	**$202,498.00**	**$202,493.48**	**$4.52**
	*ENVIRON International	Greg Yarwood				

10-021	**Dry Deposition of Ozone to Built Environment Surfaces**	**10/11/2010**	**8/31/2011**	**$248,786.00**	**$248,786.41**	**($0.41)**
	*The University of Texas at Austin	Richard Corsi				
10-022	**Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas**	**2/16/2011**	**11/30/2011**	**$150,000.00**	**$132,790.80**	**$17,209.20**
	*Lamar University	Daniel Chen				
10-024	**Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area**	**2/16/2011**	**9/30/2011**	**$458,957.00**	**$444,001.74**	**$14,955.26**
	*Rice University	Robert Griffin		$225,662.00	$223,769.99	$1,892.01
	University of Houston	Barry Lefer		$98,134.00	$88,914.46	$9,219.54
	University of New Hampshire	Jack Dibb		$70,747.00	$70,719.78	$27.22
	University of Michigan	Allison Steiner		$64,414.00	$60,597.51	$3,816.49
10-029	**Wind Modeling Improvements with the Ensemble Kalman Filter**	**12/1/2010**	**11/30/2011**	**$80,108.00**	**$78,276.97**	**$1,831.03**
	*Texas A & M University	John Neilson-Gammon				
10-032	**SHARP Data Analysis: Radical Budget and Ozone Production**	**2/9/2011**	**11/30/2011**	**$248,652.00**	**$242,335.97**	**$6,316.03**
	*University of Houston	Barry Lefer		$176,314.00	$176,314.00	$0.00
	University of California - Los Angeles	Jochen Stutz		$23,054.00	$18,850.65	$4,203.35
	University of New Hampshire	Jack Dibb		$49,284.00	$47,171.32	$2,112.68
10-034	**Dallas Measurements of Ozone Production**	**2/2/2011**	**11/30/2011**	**$195,054.00**	**$186,657.54**	**$8,396.46**
	*University of Houston	Barry Lefer				
10-042	**Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms**	**10/8/2010**	**11/30/2011**	**$237,481.00**	**$237,479.31**	**$1.69**
	*ENVIRON International	Greg Yarwood				

10-044	**Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season**	**3/25/2011**	**11/30/2011**	**$279,642.00**	**$277,846.38**	**$1,795.62**
	*University of Houston	Maxwell Shauck				
10-045	**Quantification of Hydrocarbon, NOx, and SO2 emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR dataset**	**1/22/2011**	**9/30/2011**	**$398,042.00**	**$391,199.38**	**$6,842.62**
	*University of California - Los Angeles	Jochen Stutz		$149,773.00	$142,930.28	$6,842.72
	University of North Carolina - Chapel Hill	William Vizeute		$33,281.00	$33,281.00	$0.00
	Aerodyne Research Inc.	Scott Herndon		$164,988.00	$164,988.10	($0.10)
	Washington State University	George Mount		$50,000.00	$50,000.00	$0.00
10-DFW	**Dallas - Fort Worth Field Study**	**2/1/2011**	**8/31/2011**	**$37,857.00**	**$37,689.42**	**$167.58**
	*The University of Texas at Austin	Vincent Torres				
11-DFW	**Dallas - Fort Worth Field Study**	**2/1/2011**	**8/31/2011**	**$50,952.00**	**$29,261.75**	**$21,690.25**
	*The University of Texas at Austin	Vincent Torres				
11-SOS	**State of the Science**	**2/8/2012**	**4/30/2012**	**$36,000.00**	**$36,000.00**	**$0.00**
	*The University of Texas at Austin	David Allen				
Notes:	The State of the Science project was funded from monies returned from the completed research projects. The Dallas - Fort Worth Field Study project was partially funded by a transfer of monies from the Project Management budget ($22,036). The full amount was returned to the Project Management budget at the conclusion of the Research Projects.					

December 2011 – Feb 2012

During the second quarter of FY 2011-2012, Program Administration focused on the close-out and final payment of invoices for projects, as well as the completion of reporting activities. Project Managers and TCEQ Liaisons completed the review of the Final Reports.

Once all reviews were completed, the Final Report for each project was posted on the AQRP website at http://aqrp.ceer.utexas.edu/projects.cfm. All Final Reports, with the exception of one have been posted to the website.

Principal Investigators notified Project Managers and TCEQ Liaisons of impending publications developed from the AQRP Projects. A reference list of the publications for each project can be found in Appendix C.

The State of the Science project was initiated in February to help determine the high priority scientific and technical issues to be addressed in the 2012-2013 biennium.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding of $1,000,000 for the FY 2012 period was awarded in February 2012.

March 2012 – May 2012

State of the Science Assessment

The State of the Science project was completed in April. The primary product of the project was a State of the Science Assessment that was released and posted on the AQRP website (http://aqrp.ceer.utexas.edu). The Assessment provided an overview of the current understanding of key scientific and technical issues, relevant to Texas, in emissions inventory development, atmospheric chemistry, meteorology and air quality modeling. The Assessment also summarized key findings from AQRP research projects and defined the research priorities for the 2012-2013 biennium.

The findings from the fourteen (14) research projects, organized by research topic, are briefly described below:

Emissions:
Despite improvements in inventory estimates over the past decade, significant discrepancies are still observed between annual average reported emissions and instantaneous emission estimates inferred from observed concentrations. Some of these discrepancies can be resolved through refinement of the temporal resolution of emissions; other discrepancies may be due to missing or under-estimated sources.

The AQRP projects related to industrial flaring have provided information about both temporal variability and potential underestimation of emissions. The studies of flares under controlled operating conditions demonstrated that at low flow rates, and with low heating value gases, standard emission estimation methods may understate emissions if excess steam or air-assist is used. Subsequent air quality modeling demonstrated that these emissions, coupled with the temporal variability in the emissions, can lead to additional ozone formation both locally and

over large spatial scales. Field observations in the FLAIR project support these findings. Specifically:

- Field tests in a semi-controlled environment indicate that the most efficient industrial flare operation, as measured by the destruction and removal efficiency and combustion efficiency, are achieved at or near the incipient smoke point. Minimum levels of steam or air assist that comply with the flare manufacturer's recommendations should be used when possible.
- Further development of remote sensing technologies, such as Passive and Active Fourier Transform Infrared Spectroscopy, and modeling techniques, such as Multivariate Image Analysis, may offer approaches for improving the detection, monitoring, and evaluation of flare operational conditions in the future.

A variety of additional studies have involved field measurements to resolve emission inventories. A particular focus has been on alkenes and aldehydes.

- Remote sensing measurements in the Houston Ship Channel and Texas City indicated that alkane and ethene emissions were similar in 2006, 2009, and 2011, while propene emissions decreased. Formaldehyde emissions in the Houston Ship Channel and Texas City were similar between 2009 and 2011, and many sources were associated with industries also emitting alkenes. In the Houston Ship Channel, Beaumont/Port Arthur, and Longview areas, comparison of the 2011 measurements with the 2009 TCEQ inventory showed primarily good agreement for NO_x and SO_2 but large discrepancies in VOC with observations at certain locations, such as Mont Belvieu, exceeding reported emissions by 400-1500% for alkanes, 300-1500% for ethene, and 170-800% for alkenes.
- The strength of industrial emissions sources of formaldehyde and olefins were assessed in Texas City and the Houston Ship Channel region during the 2009 FLAIR study. Consistent with previous studies, computed ethene, propene, benzene, and 1,3-butadiene emission rates significantly exceeded levels reported in emissions inventories (by more than 2 orders of magnitude in some cases). Ignited flares emitted formaldehyde at the tip at rates between 0.3-2.5 kg/h. Combustion efficiencies were found to vary from 0 (unlit) to 0.7 (steaming) to 0.999. A large source of primary formaldehyde emissions was identified in a Texas City refinery complex with a strength of 18 ± 5 kg/h, which may be associated with a FCCU regeneration unit.

Chemistry:

Atmospheric chemistry in Texas has a number of unique features. The combinations of industrial and urban emissions, and forested and coastal environments lead certain chemical pathways to become more significant in Texas than in other regions. Specific findings arising from the AQRP program that address ozone and radical formation under Texas conditions include:

- Nitryl chloride can affect tropospheric oxidation capacity and ozone formation in coastal and inland regions. Representation of the chemistry of nitryl chloride formation in CAMx has been implemented and chlorine/chloride sources have been characterized for Texas emissions inventories.
- Volatile organic compounds can remove NO_x by forming NO_x sink compounds that reduce the availability of NO_x for ozone formation. These NO_x sink species may eventually react to return NO_x back to the atmosphere, known as NO_x recycling,

potentially causing additional ozone production in NO_x-limited regions. Novel experimental data, describing the NO_x sinks for aromatics and isoprene and NO_x-recycling from photolysis of alkyl nitrates and nitrocresols, have been obtained and used to develop a revised version of the Carbon Bond mechanism (CB6) known as CB6r1.

- Calculated HO_x production during the SHARP campaign in Houston was dominated by the photolysis of HONO in the early morning and by photolysis of O_3 in the midday; at night, OH production occurred mainly via O_3 reactions with alkenes. On average, the daily HO_x production rate was 23.8 ppbv day^{-1} in the region, of which 31% was from O_3 photolysis, 23% from HONO photolysis, 12% from HCHO photolysis, and 14% from O_3 reactions with alkenes.
- Recent measurements have indicated that daytime observed HONO mixing ratios are often far larger than the expected photostationary state with OH and NO in Houston and other locations throughout the world. Statistically significant vertical gradients of HONO throughout the day, with smaller mixing ratios aloft, have suggested that a likely source of daytime HONO could be photocatalytic conversion of NO_2 on the ground in Houston. Although daytime mechanisms for HONO formation have been a subject of exploration, it is evident that uncertainty remains and further studies are needed. As further progress is made, incorporation into air quality models will be important.

Transport/Modeling:

One of the ways in which air quality models are improved is by collecting detailed field measurements that can be used to evaluate the performance of the air quality models. Previous field measurement campaigns in the state were primarily focused on southeast Texas. In 2010-2012, a field measurement program in the Dallas-Fort Worth area was funded by AQRP. The measurements led to a number of significant findings and future comparisons with modeling results are expected to lead to additional insights.

- Aircraft measurements downwind of the Dallas-Fort Worth area indicated enhancements in maximum ozone concentrations by factors ranging from 1.5-2.5 relative to upwind concentrations. Downwind concentrations of NO, NO_2, and reactive alkenes were modest indicating a photochemically aged air mass.
- Aircraft flights over portions of the Barnett Shale did not find enhancements in ozone concentrations clearly associated with oil and gas emissions, but persistent southerly winds (~10 mph) may not have favored mixing of urban DFW and Barnett Shale emissions that would change the VOC/NOx ratio towards a regime favoring ozone production. On some occasions, elevated concentrations of reactive alkenes (up to 10 ppbv) and formaldehyde (4-6 ppbv compared to background concentrations of 2-3 ppbv) were measured over the Barnett Shale, such as immediately downwind of a large compressor station in the Eagle Mountain Lake area.
- Preliminary results from deployment of the Measurement of Ozone Production Sensor (MOPS) during August – October 2011 at the Meacham site near Dallas-Fort Worth showed that ozone production on sunny days peaked at 40-60 ppbv/h in the mid-mornings, which suggested that Meacham may be an ozone source region. Preliminary ozone production rates at Eagle Mountain Lake were generally lower, with peak ozone productivities of 40 ppbv/h in the late mornings on only a few days.

- Preliminary analyses of surface measurements during May 30 – June 30, 2011 indicated that Eagle Mountain Lake was most often affected by aged and processed air from the Dallas-Fort Worth metropolitan area and intermittently by emissions from nearby oil and gas operations in the Barnett Shale.
- The largest sources of methane and other hydrocarbon species at oil and gas locations near Fort Worth were gas treatment facilities combined with large compressor stations. Emissions were an order of magnitude lower from smaller compressor stations and well pads; however, flashing emissions on one occasion from a condensate tank were estimated at 140 kg/h methane and 10 kg/h ethane (and other species) suggesting further study for this potentially important intermittent source.

In addition to the field measurement program, AQRP projects also included data analysis of previously conducted field programs. Among these were flights examining the long range transport, overnight, of urban, industrial and power plant plumes. Results from laboratory and field studies of pollutant loss mechanisms (dry deposition) were also incorporated into air quality models.

- Overnight transport of plumes from urban, petrochemical, and coal-fired power plant plumes can affect regional air quality the following day. Aircraft flights in the Houston area have shown NO_3 to be 3 to 5 times more important than O_3 as a nighttime oxidant of VOCs. Net NO_3 radical productions rates can be large (1–2 ppbv h^{-1}) within NO_x-containing plumes of industrial origin from Houston. Nighttime NO_x loss through N_2O_5 heterogeneous uptake is modest, but should be an area of continued study.
- Analysis of nighttime aircraft intercepts from two different Texas power plants resulted in improvements to the plume-in-grid formulation in CAMx version 5.40, released in October 2011. Plume-in-grid puff growth rates were modified to ignore growth contributions from horizontal and vertical shear during stable/nighttime conditions. Shear effects remain during neutral/unstable/daytime conditions. Minimum limits on vertical diffusivity, turbulent flux moments, and nighttime planetary boundary layer depths were reduced. With these improvements, plume-in-grid puff behavior will change potentially significantly at night and above the boundary layer, usually leading to longer lifetime.
- The heterogeneity of the urban environment is typically not represented in the dry deposition algorithms used for photochemical modeling. Refined characterization of the urban built environment on the dry deposition of ozone in Austin, Texas resulted in decreases in predicted daily maximum 8-hour average ozone concentrations of 0.2 to 1.3 ppb. The results were primarily attributed to deposition to urban vegetation and highlighted the importance of characterizing Texas urban landscapes undergoing rapid development.

Investigators planning to respond to AQRP requests for proposals during the 2012-2013 biennium were directed to the Assessment for guidance in identifying research areas in which proposals are sought.

For the 2012-2013 biennium, the targeted areas for AQRP research are:

- Analysis of data collected in the Dallas-Fort Worth (Barnett Shale) field campaign
- Analysis of flare operating regimes that provide both high combustion efficiency and minimal smoke formation
- Deployment of supplementary measurements in a large field measurement campaign planned by NASA for the summer of 2013
- Analysis of prior Texas field study data and modeling tools to investigate transformation of gas-phase pollutants to aerosol phase
- Investigation of how the temporal resolution of meso-scale meteorology and photochemical grid models must be altered for high spatial resolution modeling; investigation of mesoscale modeling of cloud formation and the effects of clouds upon ozone and PM chemistry;
- Analysis of radical chemistry in Texas cities, especially HONO formation, ozone removal and production by halogen chemistry, and atmospheric chemistry within industrial plumes.
- Analysis of the impact of global and regional transport of air pollutants on Texas.

RFP Released

In May 2012, a Request for Proposals (RFP) for 2012-2013 funding was released. Potential responders were notified via email and the RFP was posted on the AQRP website, along with instructions for applying. The submission deadline for proposals was June 15, 2012 at 5pm Central Time.

June 2012

The AQRP received thirty-two (32) proposal submissions, requesting $5 million in funding, by the due date of June 15, 2012. The ITAC conducted the scientific and technical review of the proposals via a conference call on June 26, 2012 and in a meeting held in Austin, Texas, on June 29, 2012. Ten proposals were highly recommended for funding; five proposals were recommended for funding; and seventeen proposals were not recommended for funding.

July 2012

On July 4, 2012, the project proposals and ITAC recommendations were forwarded to TCEQ. The TCEQ evaluated the project recommendations from the ITAC and provided comment on the relevancy of the projects to the State's air quality research needs. The TCEQ recommended for funding twelve (12) of the fifteen (15) proposals that the ITAC recommended.

Several of the highly recommended and recommended proposals were projects associated with the NASA DISCOVER-AQ field campaign. Dr. James Crawford of NASA provided additional input on whether any of the proposed projects were duplicative of projects already funded. His

assessment determined that none of the projects recommended for funding would be duplicative of NASA-funded activities.

Prior to the issuance of the RFP, two proposals were submitted to the AQRP for consideration in the FY 2012-2013 funding cycle. The TCEQ supported these proposals and indicated they would provide additional funding to the AQRP to support these proposals. Because these proposals were not a direct response to the RFP, and were not competing for the same funding, they were not included in the proposals discussed above. They were, however, reviewed independently by the ITAC and the TCEQ, both of which recommended the proposals be funded.

August 2012

On August 2, 2012, the recommendations from the ITAC and the TCEQ were presented to the Advisory Council, as well as an overview of the strategic research priorities developed as part of the State of the Science project. The Council members expressed concern about the large number of projects associated with the DISCOVER-AQ field campaign and the geographic distribution of the funding, however, they also recognized that the DISCOVER-AQ campaign offered an opportunity to make measurements of great interest to the State at a time when many complementary measurements would be made, thus leveraging the State's investments in research. They felt that the highly recommended and recommended projects represented good science, but recommended considering additional projects that address mobile source (vehicular) emissions, and that address air quality issues relevant to regions that have not been as extensively studied as southeast Texas (e.g. central Texas).

The Council recommended that the twelve (12) proposals recommended by both the ITAC and the TCEQ be funded, as well as the two (2) additional proposals. They also recommended that a targeted RFP be published for the distribution of any remaining 2012-2013 funding. The Council members agreed to solicit and provide input regarding high priority needs for various areas within the state of Texas. This process is currently ongoing.

At this time, all principal investigators have been notified of the status of their proposals. Those that were selected for funding have been assigned an AQRP Project Manager and a TCEQ Liaison. The contracting process has begun. An amended Master Agreement will be issued to those entities which had projects funded in FY 2010-2011. A new Master Agreement will be issued to those entities newly funded by the AQRP

The proposals that were recommended for funded are listed in Table 4.

Table 4: FY 2012-3012 AQRP Proposals Selected for Funding

Proposal Number		Proposal Title	PI	Lead Institution	Collaborating Institutions	Funding Awarded by Council
12-004		DISCOVER-AQ Ground Sites Infrastructure Support	Vincent Torres	The University of Texas at Austin	None	$289,200
12-005		Quantification of industrial emissions of VOCs, NO2 and SO2 by SOF and mobile DOAS during DISCOVER AQ	Johan Mellqvist	Chalmers University of Technology	University of Houston	$177,652
12-006		Environmental chamber experiments and CMAQ modeling to improve mechanisms to model ozone formation from HRVOCs	Gookyoung Heo	University of California, Riverside	TAMU	$146,259
12-011		Investigation of Global Modeling and Lightning NOx Emissions as Sources of Regional Background Ozone in Texas	Chris Emery	Environ	Princeton University	$72,856
12-012		Interactions Between Organic Aerosol and Noy: Influence on Oxidant Production	Lea Hildebrandt	The University of Texas at Austin	Environ	$148,837
12-013		Development of Transformation Rate of SO2 to Sulfate for the Houston Ship Channel using the TexAQS 2006 Field Study Data	Ralph Morris	Environ	None	$59,974
12-016		Ozonesonde launches from the University of Houston and Smith Point, Texas in Support of DISCOVER AQ	Gary Morris	Valparaiso University	University of Houston	$86,666

12-018		The Effects of Uncertainties in Fire Emissions Estimates on Predictions of Texas Air Quality	Elena McDonald-Buller	The University of Texas at Austin	ENVIRON	$112,864
12-022		Surface Measurements of PM, VOCs, and Photochemically Relevant Gases in Support of DISCOVER-AQ	Robert Griffin	Rice University	University of Houston	$206,815
12-024		Surface Measurement of Trace Gases in Support of DISCOVER-AQ in Houston in Summer 2013	Xinrong Ren	University of Maryland	NOAA	$90,444
12-028		Implementation and evaluation of new HONO mechanisms in a 3-D Chemical Transport Model for Spring 2009 in Houston	Barry Lefer	University of Houston	University of California - Los Angeles, ENVIRON, University of North Carolina - Chapel Hill	$117,446
12-032		Collect, Analyze, and Archive Filters at two DISCOVER-AQ Houston Focus Areas: Initial Characterization of PM Formation and Emission	Rebecca Sheesley	Baylor University	None	$45,972
12-TN1		Investigation of surface layer parameterization of the WRF model and its impact on the observed nocturnal wind speed bias	Pius Lee	NOAA	None	$65,000
12-TN2		Development of IDL-based geospatial data processing framework for meteorology and air quality modeling	HyunCheol Kim	NOAA	None	$70,000

FINANCIAL STATUS REPORT

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May 2010 an amendment was issued increasing the budget by $40,000. Funding for fiscal year 2011 was established at $2,106,071, for a total award of $4,878,142 for the FY 2010/2011 biennium. As of August 31, 2012, $59,410.76 remains unspent. These funds will be used in conjunction with the FY 2012 and 2013 funds and will be fully expended by March 2013.

In February 2012, funding of $1,000,000 was awarded for FY 2012. In June 2012, an additional $160,000 was awarded in FY 2012 funds and $1,000,000 was awarded in FY 2013 funds, for a total of $2,160,000 in funding for the FY 2012/2013 biennium.

All of these funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

Program Administration – limited to 10% of the overall funding (per Fiscal Year)
This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC
These funds are to cover the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project will be assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual
These are the funds available to support the research projects that are selected for funding.

Program Administration

Program Administration includes salaries and fringe benefits for those overseeing the program as a whole, as well as, materials and supplies, travel, equipment, and other expenses. This category allows indirect costs in the amount of 10% of salaries and wages.

During the reporting period six staff members were involved, part time, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. James Thomas, AQRP Manager, is responsible for assisting Dr. Allen in the program administration. Maria Stanzione, AQRP Grant Manager, with assistance from Rachael Bushn and Melanie Allbritton assisted with program organization and financial management. This included assisting with the issuance of the RFP, the proposal review process, the contracting process, invoice review and payment, and other invoicing functions. Denzil Smith is responsible for the AQRP Web Page development and for data management.

Table 2: AQRP Administration Budget

Administration Budget (includes Council Expenses)
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$202,816.67	$163,120.24	$365,936.91	$365,936.91	$0	$0
Fringe Benefits		$38,665.65	$31,173.03	$69,838.68	$69,838.68	$0	$0
Travel		$346.85	$0	$346.85	$346.85		$0
Supplies		$15,096.14	$4.51	$15,100.65	$15,096.14		$4.51
Equipment		$0	$0	$0			$0
Total Direct Costs		$256,925.31	$194,297.78	$451,223.09	$451,218.58	$0	$4.51
Authorized Indirect Costs		$20,281.69	$16,310.22	$36,591.91	$36,591.91		$0
10% of Salaries and Wages							
Total Costs		**$277,207**	**$210,608**	**$487,815**	**$487,810.49**	**$0**	**$4.51**
Fringe Rate		22%	22%		19%		

Administration Budget (includes Council Expenses)
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$80,440	$70,040	$150,480	$28,220.55	$0	122,259.45
Fringe Benefits		$14,666	$12,606	$27,272	$6,182.19	$0	$21,089.81
Travel		$350	$350	$700	$0		$700.00
Supplies		$10,000	$10,000	$20,000	$275.10		$19,724.90
Equipment		$0	$0	$0			$0
Total Direct Costs		$105,456	$92,996	$198,452	$34,677.84	$0	$163,774.16
Authorized Indirect Costs		$8,044	$7,004	$15,048	$2822.05		$12,225.95
10% of Salaries and Wages							
Total Costs		**$113,500**	**$100,000**	**$213,500**	**$37,499.89**	**$0**	**$176,000.11**
Fringe Rate		22%	22%		17%		

Fringe benefits for the administration of the AQRP were initially budgeted to be 22% of salaries and wages across the term of the project. It should be noted that this was an estimate, and actual fringe benefit expenses have been reported. The fringe benefit amount and percentage fluctuate each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. For example, the amount of fringe benefits are greater for a person with family medical insurance versus a person with individual medical insurance. At the end of the project, the overall total of fringe benefit expensed is expected to be at or below 22% of the total salaries and wages. Actual fringe benefit expenses through July 2012 are included in the spreadsheets above. The amount for August is estimated.

Actual indirect costs for the months through July 2012 are included in Table 2. The amount for August is estimated. The accounting records for the month of August do not close until after the due date of this report, thereby requiring the estimate.

As discussed in previous Quarterly Reports, the AQRP Administration requested and received permission to utilize funds in future fiscal years. This is for all classes of funds including Administration, ITAC, Project Management, and Contractual. As of the writing of this report, the FY 10 funds have been fully expended. The intent is to fully expend the FY 11 funds, by March 2013. This same procedure will be followed for the FY 12 funds.

In June 2011, UT-Austin received a Contract Extension for the AQRP. This extension will continue the program through the end of the 2012/2013 biennium.

ITAC

The ITAC had two meetings in Austin and one conference call during this reporting period.

A half-day meeting was held following the Data Workshop on September 28, 2011. The purpose of the meeting was to discuss the upcoming NASA Discovery AQ project, procedures for possible future requests for proposals (RFPs), and the development of a State of the Science document to provide background information for establishing future research priorities. ITAC expenses incurred included lodging and travel to Austin for those ITAC members who did not have active research projects.

The ITAC met in Austin, Texas, on June 29, 2012, to complete their review and ranking of the proposals. ITAC expenses incurred include lodging and travel costs for members to travel to Austin, Texas, for the meeting. As the meeting was a full day meeting, a working lunch was provided to the meeting participants.

Table 3: ITAC Budget

ITAC Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$16,378.86	$16,714.53	$33,093.39	$22,312.76	$1,759.00	$9,021.63
Supplies		$1,039.95	$4,130.66	$5,170.61	$1,324.62		$3,845.99
Total Direct Costs		$17,418.81	$20,845.19	$38,264	$23,637.38	$1,759.00	$12,867.62
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$17,418.81**	**$20,845.19**	**$38,264**	**$23,637.38**	**$1,759.00**	**$12,867.62**

ITAC Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$10,000	$0	$10,000	$0	$0	$10,000
Supplies		$500	$0	$500	$0		$500
Total Direct Costs		$10,500	$0	$10,500	$0	$0	$10,500
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$10,500**	**$0**	**$10,500**	**$0**	**$0**	**$10,500**

Project Management

Project management activities from September through January focused on the completion of the research projects, the review and approvals of the final reports, and the reviews of any publications. From February through July, there were minimal project management activities other than for the State of the Science project. In August 2012, Project Managers were assigned to the FY 2012-2013 Research Projects and they began working with the PIs to begin the Work Plans.

A transfer of funds from the FY 11 Project Management account to the FY 11 Contractual account was approved and processed in February 2011 in order to fully fund the DFW Field Study Logistics project (FY 11). Once all expenses had posted for that project, there were enough funds remaining to return the full amount of the transferred funds to the Project Management account. During the grant period ending May 31, 2012, $345.75 of the FY 11 Contractual funds were returned to the FY 11 Project Management account. The remaining $21,690.25 was returned in June 2012.

Table 4: Project Management Budget

Project Management Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$145,337.70	$106,907.22	$252,244.92	$233,254.14		$18,990.78
Fringe Benefits		$28,967.49	$22,142.56	$51,110.05	$45,692.19		$5,417.86
Travel		$0	$0	$0	$0		$0
Supplies		$778.30	$260.00	$1,038.30	$911.98		$126.32
Total Direct Costs		$175,083.49	$129,309.78	$304,393.27	$279,858.31	$0.00	$24,534.96
Authorized Indirect Costs		$14,533.77	$10,690.22	$25,223.99	$23,325.41		$1,898.58
10% of Salaries and Wages							
Total Costs		**$189,617.26**	**$140,000.00**	**$329,617.26**	**$303,183.72**	**$0.00**	**$26,433.54**

Project Management Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$60,700	$46,000	$106,700	$0		$106,700
Fringe Benefits		$11,230	$8,400	$19,630	$0		$19,630
Travel		$500	$0	$500	$0		$500
Supplies		$7,500	$6,000	$13,500	$0		$13,500
Total Direct Costs		$79,930	$60,400	$140,330	$0	$0	$140,330
Authorized Indirect Costs		$6,070	$4,600	$10,670	$0		$10,670
10% of Salaries and Wages							
Total Costs		**$86,000**	**$65,000**	**$151,000**	**$0**	**$0**	**$151,000**

Research Projects

Table 5 on the following 2 pages lists the 2010-2011 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of August 31, 2012.

As of the end of August there was $18,346.09 of FY 2011 funding available in Research Projects. The FY 10 Research/Contractual budget was originally funded at $2,286,000. After all transfers, it has been increased by $1,827.93. The FY 11 Research/Contractual budget was originally funded at $1,736,063. After all transfers, it has been decreased by $1,445,19 (the amount transferred to Project Management). This is an overall net increase of $382.74 to the Research/Contractual funds (and an equal net reduction in Project Management funds).

The remaining FY 2011 Research/Contractual funds will be awarded to one of the 2012-2013 Research Projects, and will be fully expended by March 2013.

A spreadsheet is not included in this report for FY 2012 and 2013 funds, as the projects have not yet been assigned to a particular fiscal year of funding (this happens later in the contracting process), and no expenditures have yet occurred. FY 2012 funds in the amount of $950,000 and FY 2013 funds in the amount of $835,000 are budgeted for Research Projects.

Table 5: Contractual Expenses

Contractual Expenses

FY 10 Contractual Funding	$2,286,000
FY 10 Contractual Funding Transfers	$1,827.93
FY 10 Total Contractual Funding	**$2,287,827.93**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-008	Rice University	$128,851	$126,622.32	$2,228.68
10-008	Environ International	$49,945	$49,944.78	$0.22
10-009	UT-Austin	$591,332	$591,306.66	$25.34
10-021	UT-Austin	$248,786	$248,786.41	-$0.41
10-022	Lamar University	$150,000	$132,790.80	$17,209.20
10-032	University of Houston	$176,314	$176,314	$0
10-032	University of New Hampshire	$23,054	$18,850.65	$4,203.35
10-032	UCLA	$49,284	$47,171.32	$2,112.68
10-034	University of Houston	$195,054	$186,657.54	$8,396.46
10-042	Environ International	$237,481	$237,479.31	$1.69
10-045	UCLA	$149,773	$142,930.28	$6,842.72
10-045	UNC - Chapel Hill	$33,281	$33,281	$0
10-045	Aerodyne Research Inc.	$164,988	$164,988.10	-$0.10
10-045	Washington State University	$50,000	$50,000	$0
10-DFW	UT-Austin	$37,857	$37,689.42	$167.58
FY 10 Total Contractual Funding Awarded		$2,286,000		
FY 10 Contractual Funding Expended (Init. Projects)			$2,244,812.59	
FY 10 Contractual Funds Remaining Unspent after Project Completion				$41,187.41
FY 10 Additional Projects				
	Data Storage	$7,015.34	$7,015.34	$0
10-SOS	State of the Science	$36,000.00	$36,000.00	$0
FY 10 Contractual Funds Expended to Date*			$2,287,827.93	
FY 10 Contractual Funds Remaining to be Spent				$0

FY 11 Contractual Funding		**$1,736,063**		
FY 11 Contractual Funding Transfers		-$1,445.19		
FY 11 Total Contractual Funding		$1,734,617.81		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179	$262,179	$0
10-006	University of Houston	$222,483	$217,949.11	$4,533.89
10-015	Environ International	$201,280	$201,278.63	$1.37
10-020	Environ International	$202,498	$202,493.48	$4.52
10-024	Rice University	$225,662	$223,769.99	$1,892.01
10-024	University of New Hampshire	$70,747	$70,719.78	$27.22
10-024	University of Michigan	$64,414	$60,597.51	$3,816.49
10-024	University of Houston	$98,134	$88,914.46	$9,219.54
10-029	Texas A&M University	$80,108	$78,276.97	$1,831.03
10-044	University of Houston	$279,642	$277,846.38	$1,795.62
11-DFW	UT-Austin	$50,952	$29,261.75	$21,690.25
FY 11 Total Contractual Funding Awarded		$1,758,099		
FY 11 Contractual Funds Expended (Init. Projects)			$1,713,287.06	
FY 11 Contractual Funds Remaining Unspent after Project Completion				$44,811.94
FY 11 Additional Projects				
	Data Storage	$2,984.66	$2,984.66	$0.00
FY 11 Contractual Funds Expended to Date*			$1,716,271.72	
FY 11 Contractual Funds Remaining to be Spent				$18,346.09
Total Contractual Funding		$4,022,063.00		
Total Contractual Funding Transfers		$382.74		
Total Contractual Funding Available		$4,022,445.74		
Total Contractual Funds Expended to Date*			$4,004,099.65	
Total Contractual Funds Remaining				$18,346.09

*(Expenditures Reported as of August 31, 2012.)

Conclusion

The ITAC FY 2011 budget has $12,867.62 remaining. These funds will be utilized for the remaining ITAC expenses for the meeting held in June 2012. It is anticipated that some or all of the remaining funds may be moved to support research projects in the 2012-2013 biennium. The amount will be determined during the next quarter.

The Project Management FY 2011 budget has $26,433.54 remaining after all August expenses are posted. These funds will be used to cover Project Management expenses until the funds are fully expended. Use of these funds may allow the release of FY 12 Project Management funds to be used for Research projects. This will be assessed during the next quarter.

The Research/Contractual category has $18,346.09 remaining. These funds will be used to fund research projects in the FY 2012-13 biennium (though they will be fully expended by March 31, 2013.) It should be noted that all FY 10-11 Research funds were allocated to projects, and an additional $22,036 was moved from Project Management to Research to cover additional expenses related to the DFW Field Study. Several projects returned funds to the AQRP when they concluded, thus the remaining balance. As these funds were committed to Research projects until the projects ended, the AQRP was unable to utilize the funds for any other purpose.

In summary, the remaining FY 2011 funds of $57,651.76 are expected to be fully expensed by March 31, 2013.

Each 2012-2013 Research Project will be funded from a specific fiscal year. The assignments will be made during the next quarter. Once all budgets have been approved and assignments made the program managers will assess whether any Research Project funds remain available, and will contact the ITAC, TCEQ, and Council to determine how to proceed in the allocation of those funds.

Appendix A

Financial Reports by Fiscal Year

FY 10 and 11

(Expenditures reported as of August 31, 2012.)

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67		$0
Fringe Benefits		$38,665.65	$38,665.65		$0
Travel		$346.85	$346.85		$0
Supplies		$15,096.14	$15,096.14		$0
Equipment		$0			$0
Other					
Contractual					
Total Direct Costs		$256,925.31	$256,925.31		$0
Authorized Indirect Costs		$20,281.69	$20,281.69		$0
10% of Salaries and Wages					
Total Costs		**$277,207**	**$277,207.00**	**$0**	**$0**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$163,120.24	$163,120.24	$0	$0
Fringe Benefits		$31,173.03	$31,173.03	$0	$0
Travel		$0			$0
Supplies		$4.51			$4.51
Equipment					
Other		$0			$0
Contractual					
Total Direct Costs		$194,297.78	$194,293.27	$0	$4.51
Authorized Indirect Costs		$16,310.22	$16,310.22		$0
10% of Salaries and Wages					
Total Costs		**$210,608**	**$210,603.49**	**$0**	**$4.51**

ITAC Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,378.86	$16,378.86	$0	$0
Supplies		$1039.95	$1,039.95		$0
Equipment					
Other					
Total Direct Costs		$17,418.81	$17,418.81	$0	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$17,418.81**	**$17,418.81**	**$0**	**$0**

ITAC Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,714.53	$5,933.90	$1,759.00	$9,021.63
Supplies		$4,130.66	$284.67		$3,845.99
Equipment					
Other					
Total Direct Costs		$20,845.19	$6,218.57	$1,759.00	$12,867.62
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$20,845.19**	**$6,218.57**	**$1,759.00**	**$12,867.62**

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$145,337.70	$145,337.70		$0
Fringe Benefits		$28,967.49	$28,967.49		$0
Travel		$0	$0		$0
Supplies		$778.30	$778.30		$0
Equipment					
Other					
Total Direct Costs		$175,083.49	$175,083.49	$0	$0
Authorized Indirect Costs		$14,533.77	$14,533.77		$0
10% of Salaries and Wages					
Total Costs		**$189,617.26**	**$189,617.26**	**$0**	**$0**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$106,907.22	$87,916.44	$0	$18,990.78
Fringe Benefits		$22,142.56	$16,724.70	$0	$5,417.86
Travel		$0			$0
Supplies		$260.00	$133.68		$126.32
Equipment					
Other					
Total Direct Costs		$129,309.78	$104,774.82	$0	$24,534.96
Authorized Indirect Costs		$10,690.22	$8,719.64		$1,898.58
10% of Salaries and Wages					
Total Costs		**$140,000.00**	**$113,566.46**	**$0**	**$26,433.54**

AQRP Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67	$0.00	$0.00
Fringe Benefits		$38,665.65	$38,665.65	$0.00	$0.00
Travel		$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$15,096.14	$0.00	$0.00
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,287,827.93	$2,287,827.93	$0.00	$0.00
ITAC		$17,418.81	$17,418.81	$0.00	$0.00
Project Management		$189,617.26	$189,617.26	$0.00	$0.00
Total Direct Costs		$2,751,789.31	$2,751,789.31	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$20,281.69	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,772,071.00**	**$2,772,071.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$163,120.24	$163,120.24	$0.00	$0.00
Fringe Benefits		$31,173.03	$31,173.03	$0.00	$0.00
Travel		$0	$0.00	$0.00	$0.00
Supplies		$4.51	$0.00	$0.00	$4.51
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$1,734,617.81	$1,716,271.72	$0.00	$18,346.09
ITAC		$20,845.19	$6,218.57	1,759.00	$12,867.62
Project Management		$140,000.00	$113,566.46	$0.00	$26,433.54
Total Direct Costs		$2,089,760.78	$2,030,350.02	$1,759.00	$57,651.76
Authorized Indirect Costs		$16,310.22	$16,310.22	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,106,071.00**	**$2,046,660.24**	**$1,759.00**	**$57,651.76**

Appendix B

Financial Reports by Fiscal Year

FY 12 and 13

(Expenditures reported as of August 31, 2012.)

Administration Budget (includes Council Expenses)

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$80,440.00	$28,220.55	$0	$52,219.45
Fringe Benefits		$14,666.00	$6,182.19	$0	$8,483.81
Travel		$350.00	$0.00		$350.00
Supplies		$10,000.00	$275.10	$0	$9,724.90
Equipment		$0.00			$0.00
Other					
Contractual					
Total Direct Costs		$105,456.00	$34,677.84	$0	$70,778.16
Authorized Indirect Costs		$8,044.00	$2,822.05		$5,221.95
10% of Salaries and Wages					
Total Costs		**$113,500.00**	**$37,499.89**	**$0**	**$76,000.11**

Administration Budget (includes Council Expenses)

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,040.00	$0.00		$70,040.00
Fringe Benefits		$12,606.00	$0.00		$12,606.00
Travel		$350.00	$0.00		$350.00
Supplies		$10,000.00	$0.00		$10,000.00
Equipment					
Other		$0.00	$0.00		$0.00
Contractual					
Total Direct Costs		$92,996.00	$0.00	$0.00	$92,996.00
Authorized Indirect Costs		$7,004.00	$0.00		$7,004.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$0.00**	**$0.00**	**$100,000.00**

ITAC Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$10,000.00			$10,000.00
Supplies		$500.00			$500.00
Equipment					
Other					
Contractual					
Total Direct Costs		$10,500.00	$0.00	$0.00	$10,500.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$10,500.00**	**0.00**	**$0.00**	**$10,500.00**

ITAC Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00		$0.00
Supplies		$0.00	$0.00		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$60,700.00			$60,700.00
Fringe Benefits		$11,230.00			$11,230.00
Travel		$500.00			$500.00
Supplies		$7,500.00			$7,500.00
Equipment					
Other					
Contractual					
Total Direct Costs		$79,930.00	$0.00	$0.00	$79,930.00
Authorized Indirect Costs		$6,070.00			$6,070.00
10% of Salaries and Wages					
Total Costs		**$86,000.00**	**0.00**	**$0.00**	**$86,000.00**

Project Management Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$46,000.00			$46,000.00
Fringe Benefits		$8,400.00			$8,400.00
Travel		$0.00			$0.00
Supplies		$6,000.00			$6,000.00
Equipment					
Other					
Contractual					
Total Direct Costs		$60,400.00	$0.00	$0	$60,400.00
Authorized Indirect Costs		$4,600.00			$4,600.00
10% of Salaries and Wages					
Total Costs		**$65,000.00**	**0.00**	**$0.00**	**$65,000.00**

AQRP Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$80,440.00	$28,220.55	$0.00	$52,219.45
Fringe Benefits		$14,666.00	$6,182.19	$0.00	$8,483.81
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$10,000.00	$275.10	$0.00	$9,724.90
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$950,000.00	$0.00	$0.00	$950,000.00
ITAC		$10,500.00	$0.00	$0.00	$10,500.00
Project Management		$86,000.00	$0.00	$0.00	$86,000.00
Total Direct Costs		$1,151,956.00	$34,677.84	$0.00	$1,117,278.16
Authorized Indirect Costs		$8,044.00	$2,822.05	$0.00	$5,221.95
10% of Salaries and Wages					
Total Costs		**$1,160,000.00**	**$37,499.89**	**$0.00**	**$1,122,500.11**

AQRP Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,040.00	$0.00	$0.00	$70,040.00
Fringe Benefits		$12,606.00	$0.00	$0.00	$12,606.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$10,000.00	$0.00	$0.00	$10,000.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$835,000.00	$0.00	$0.00	$835,000.00
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$65,000.00	$0.00	$0.00	$65,000.00
Total Direct Costs		$992,996.00	$0.00	$0.00	$992,996.00
Authorized Indirect Costs		$7,004.00	$0.00	$0.00	$7,004.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$0.00**	**$0.00**	**$1,000,000.00**

Appendix C

Publications

(Listed by Project Number)

10-008

Constraining ozone-precursor responsiveness using ambient measurements
A. Digar, D.S. Cohan, X. Xiao, K.M. Foley, B. Koo, G. Yarwood
Submitted to Journal of Geophysical Research, May 2012

D.S. Cohan and A. Digar, Observation-constrained probabilistic evaluation of modeled concentrations and sensitivities.
To be presented at CMAS Annual Conference, October 2012.

10-009

The following papers have been accepted in a Special Issue of the journal Industrial & Engineering Chemistry Research dedicated to Industrial Flaring. The paper edition of this special edition will come out in Fall 2012, but the online versions are available now.

Emissions of Nitrogen Oxides from Flares Operating at Low Flow Conditions
Torres, Vince; Herndon, Scott; Wood, Ezra; Al-Fadhli, Fahad; Allen, David
Industrial & Engineering Chemistry Research
Status: Published Online March 21, 2012
DOI: 10.1021/ie300179x

Impacts Of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area
Pavlovic, Radovan; Al-Fadhli, Fahad; Kimura, Yosuke; Allen, David; McDonald-Buller, Elena
Industrial & Engineering Chemistry Research
Status: Published Online

Comparison of remote sensing and extractive sampling measurements of flare combustion efficiency
Wormhoudt, Joda; Herndon, Scott; Franklin, Jonathan; Wood, Ezra; Knighton, W.; Evans, Scott; Laush, Curtis; Sloss, Mark; Spellicy, Robert
Status: Published Online

Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy.
Knighton, W.; Herndon, Scott; Franklin, Jon; Wood, Ezra; Wormhoudt, Joda; Brooks, William; Fortner, Edward; Allen, David
Industrial & Engineering Chemistry Research
Status: Published Online March 22, 2012
DOI: 10.1021/ie202695v

Particulate Emissions Measured During the TCEQ Comprehensive Flare Emission Study
Fortner, Edward; Brooks, William; Onasch, Timothy; Canagaratna, Manjula; Massoli, Paola; Jayne, John; Franklin, Jon; Knighton, W.; Wormhoudt, Joda; Worsnop, Douglas; Kolb, Charles; Herndon, Scott
Industrial & Engineering Chemistry Research
Status: Published Online

Industrial flare performance at low flow conditions: Part 1. Study Overview
Torres, Vince; Herndon, Scott; Kodesh, Zach; Allen, David
Industrial & Engineering Chemistry Research
Status: Published Online February 27, 2012
DOI: 10.1021/ie202674t

Industrial flare performance at low flow conditions: Part 2. Steam- and Air-Assisted Flares
Torres, Vince; Herndon, Scott; Allen, David
Industrial & Engineering Chemistry Research
Status: Published Online February 27, 2012
DOI: 10.1021/ie202675f

Application of the carbon balance method to flare emissions characteristics
Herndon, Scott; Nelson, David; Wood, Ezra; Knighton, W.; Kolb, Charles; Kodesh, Zach; Torres, Vince; Allen, David
Industrial & Engineering Chemistry Research
Status: Published Online April 6, 2012
DOI: 10.1021/ie202676b

Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas
Al-Fadhli, Fahad; Kimura, Yosuke; McDonald-Buller, Elena; Allen, David
Industrial & Engineering Chemistry Research
Status: Published Online

Multivariate Image Analysis (MIA) for Industrial Flare Combustion Control
Castineira, David; Rawlings, Blake; Edgar, Thomas
Industrial & Engineering Chemistry Research
Status: Published Online

The following presentations were given at the Air & Waste Management Association June 2012 Conference, and papers have been published in the Conference Proceedings:

Overview of the Texas Commission on Environmental Quality 2010 Flare Study
Torres, Allen, Herndon, Kodesh

NOx Emissions from Industrial Flaring
Torres, Fahad M. Al-Fadhli, Allen, Herndon, Ezra Wood

10-015

The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models
J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride
J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

10-020

The Effects of NOx Control and Plume Mixing on Nighttime Chemical Processing of Plumes from Coal-Fired Power Plants.
Steven S. Brown, William P. Dubé, Prakash Karamchandani, Greg Yarwood, Jeff Peischl, Thomas B. Ryerson, J. Andrew Neuman, John B. Nowak, John S. Holloway, Rebecca A. Washenfelder, Charles A. Brock, Gregory J. Frost, Michael, Trainer, David D. Parrish, Frederick C. Fehsenfeld and A. R. Ravishankara
Journal of Geophysical Researech, VOL. 117, D07304, doi:10.1029/2011JD016954, 2012

In preparation for Journal of Geophysical Research:
Biogenic VOC Oxidation and Organic Aerosol Formation within an Urban Nocturnal Boundary Layer – Aircraft Vertical Profiles in Houston, TX.
Steven S. Brown, William P. Dubé, Roya Bahreini, Ann M. Middlebrook, Charles A. Brock, Carsten Warneke, Joost A. de Gouw, Rebecca A. Washenfelder, Elliot Atlas, Jeff Peischl, Thomas B. Ryerson, J. Andrew Neuman, Jonathan B. Nowak, Michael Trainer, David D. Parrish, Frederick C. Feshenfeld and A. R. Ravishankara

In preparation for Atmosphere:
Reactive Plume Modeling to Investigate NOx Reactions and Transport at Night
Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:
Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique. Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021

The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the abstract is *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022

Kanwar Devesh Singh, Tanaji Dabade, Hitesh Vaid, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, Kuyen Li, Christopher B. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Industrial & Engineering Chemistry Research, DOI: 10.1021/ie300639f, Publication Date (Web): July 9, 2012.

Helen H. Lou, Daniel Chen, Peyton Richmond, Hitesh Vaid, Kanwar Devesh Singh, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale CFD Simulations," International Journal of Numerical Methods for Heat and Fluid Flow, 2012.

Helen H. Lou, Daniel Chen, Christopher B. Martin, Xianchang Li, Kuyen Li, Hitesh Vaid, Kanwar Devesh Singh, Preeti Gangadharan, "Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, "Publication Date (Web): February 13, 2012, *Industrial & Engineering Chemistry Research*, Industrial flares special issue, DOI: 10.1021/ie2027684.

H. Lou, C. Martin, D. Chen, X. Li, K. Li, H. Vaid, A. Tula, K. Singh, "Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, 14(1) 1-12, 2012. Published online Dec 27, 2011. DOI 10.1007/s10098-011-0441-6.
Helen H. Lou, Christopher B. Martin, Daniel Chen, Xianchang Li, Kyuen Li, Hitesh Vaid, Anjan Tula Kumar, Kanwar Devesh Singh, & Doyle P. Bean, "A reduced reaction mechanism for the simulation in ethylene flare combustion," Clean Technologies and Environmental Policy, published on line, June 14, 2011. doi:10.1007/s10098-011-0394-9

10-032

The following article is currently undergoing review in Atmospheric Environment:
Atmospheric Oxidation Chemistry and Ozone Production: Results from SHARP 2009 in Houston, Texas
Xinrong Ren, Diana van Duin, Maria Cazorla, Shuang Chen, Jingqiu Mao, William H. Brune, James H. Flynn, Nicole Grossberg, Barry L. Lefer, Bernhard Rappenglück, Kam W. Wong, Catalina Tsai, Jochen Stutz, Jack E. Dibb, B. Thomas Jobson, Winston T. Luke, and Paul Kelley

10-042

The following articles are in progress:

In preparation for Atmospheric Environment: *Development of version 6 of the carbon bond (CB6) chemical mechanism*
Greg Yarwood, Gookyoung Heo, Elena C. McDonald-Buller, David T. Allen, Gary Z. Whitten

In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate NOx removal and recycling represented in atmospheric mechanisms for air quality modeling*
Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen

In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial NOx*
Gookyoung Heo, William Carter, Greg Yarwood

In preparation for Atmospheric Environment: *Evaluation of CB05, CB6 and SAPRC-07 using EUPHORE chamber data: evaluation of mechanisms for modeling ozone formation from toluene*
Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten

10-045

The following papers have been published in Industrial & Engineering Chemistry Research in a Special Issue on Industrial Flaring. The paper edition of this special edition will come out in Fall 2012, but the online versions are available now.

Knighton, W.; Herndon, Scott; Wood, Ezra; Fortner, Edward; Onasch, Timothy; Wormhoudt, Joda; Kolb, Charles; Lee, Ben; Zavala, Miguel; Molina, Luisa; Jones, Marvin, "*Detecting fugitive emissions of 1,3-butadiene and styrene from a petrochemical facility: An application of a mobile laboratory and a modified proton transfer reaction mass spectrometer - NO+ PTR-MS"*
Status: Published Online

Wood, E.; Herndon, S.; Fortner, E. C.; Onasch, T.; Wormhoudt, J.; Kolb, C. E.; Knighton, W. B.; Lee, B.; Zavala, M.; Molina, L.; Jones, M., "*Combustion and Destruction/Removal efficiencies of in-use chemical flares in the greater Houston area*".
Status: Published Online

This project has also resulted in the following publications:

Olga Pikelnaya, Catalina Tsai, Barry Lefer, James H. Flynn, Dejian Fu, and Jochen Stutz,"*Imaging DOAS: a tool for monitoring of emission fluxes from small individual sources*", in preparation for Journal of Geophysical Research

Olga Pikelnaya, Jochen Stutz, Scott Herdon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuette, Evan Causo, "*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview*", in preparation for Journal of Geophysical Research

Olga Pikelnaya, George Mount, Elena Spinei, and Jochen Stutz, "*Dual MAX-DOAS approach to determine facility-averaged emissions of pollutants from petrochemical facilities*", under development.

Olga Pikelnaya, Scott Herrdon, Ezra Wood, and Jochen Stutz, "*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign*," under development.

AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-10-94300
Awarded to The University of Texas at Austin

Annual Report

September 1, 2012 through August 31, 2013

Submitted to

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Texas Air Quality Research Program

Annual Report

September 1, 2012 – August 31, 2013

Overview

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the 2010-2011 biennium, the AQRP had approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released its first request for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received. These proposals were reviewed by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs. The results of these reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. As of November 30, 2011, all projects have been completed. Final reports on all but one project have been posted to the AQRP website.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding of $1,000,000 for the FY 2012 period was awarded in February 2012. An additional $1,000,000 for the FY 2013 period was awarded in June 2012. At the same time an additional $160,000 was awarded for FY 2012, to support funding for two specific air quality projects recommended by the TCEQ. A call for proposals was released in May 2012. Thirty-two proposals, requesting $5 million in research funding were received. The proposals were reviewed by the ITAC and the TCEQ. The Advisory Council selected 14 projects for funding. Contracts have been signed with each organization and work plans have been approved, Task Orders are in place and work has begun on all projects.

In June 2013, the TCEQ renewed the AQRP for the 2014-2015 biennium via Amendment 9 of the Grant. At this time the TCEQ also awarded an additional $2,500,000 in FY 2013 funds to the AQRP. 10 % of these funds were allocated for Project Administration, and the remaining funds were allocated to the Research program. Initiated by the renewal, the AQRP developed the FY 2014/2015 research priorities and submitted them to the ITAC for input and to the TCEQ for review. A RFP is planned to be released in October 2013.

BACKGROUND

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

> Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.
>
> (b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.
>
> (c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.
>
> (d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.
>
> (e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.
>
> (f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010 for the 2010-2011 biennium, and was renewed

in June 2011 for the 2012-2013 biennium. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

RESEARCH PROJECT CYCLE

The Research Program is being implemented through a 9 step cycle. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle.

1.) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and the TCEQ, develop research priorities; the research priorities are released along with a Request for Proposals.

2.) Project proposals relevant to the research priorities are solicited. The Request for Proposals can be found at http://aqrp.ceer.utexas.edu/ .

3.) The Independent Technical Advisory Committee (ITAC) performs a scientific and technical evaluation of the proposals.

4.) The project proposals and ITAC recommendations are forwarded to the TCEQ. The TCEQ evaluates the project recommendations from the ITAC and comments on the relevancy of the projects to the State's air quality research needs.

5.) The recommendations from the ITAC and the TCEQ are presented to the Council and the Council selects the proposals to be funded. The Council also provides comments on the strategic research priorities.

6.) All Investigators are notified of the status of their proposals, either funded, not funded, or not funded at this time, but being held for possible reconsideration if funding becomes available.

7.) Funded projects are assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin is responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The Project Manager has responsibility for documenting progress toward project measures of success for each project. The Project Manager works with the researchers, and the TCEQ, to create an approved work plan for the project.

   The Project Manager also works with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved Quality Assurance Project Plan (QAPP) for each project. The Project Manager reviews monthly, annual and final reports from the researchers and works with the researchers to address deficiencies.

8.) The AQRP Director and the Project Manager for each project describe progress on the project in the ITAC and Council meetings dedicated to on-going project review.

9.) The project findings are communicated through multiple mechanisms. Final reports are posted to the Program web site; research briefings are developed for the public and air quality decision makers; and a bi-annual research conference/data workshop is held.

Steps 1 – 9 have all been completed for the initial (2010-2011) biennium. Steps 1 – 6 have been completed for the 2012 – 2013 biennium, and steps 7 and 8 are in progress. A summary of the 2012-2013 activities is described in the Project Timeline section of this report.

Independent Technical Advisory Committee (ITAC)

The AQRP funding is used primarily for research projects, and one of three groups responsible for selecting the projects is the Independent Technical Advisory Committee (ITAC). The ITAC, composed of up to 15 individuals and alternates with scientific expertise relevant to the Program, is charged with recommending technical approaches, and establishing research priorities. Initially, the ITAC was to meet at least twice per year at locations rotating between Austin, Dallas and Houston. As the Program proceeded, it was more efficient for the ITAC to meet once in Austin and as needed via conference call/webinar. Generally, the meetings in Austin are dedicated to new project review, reviewing progress on funded projects, and reviewing the Program's strategic plan.

Members of the ITAC consist of the TCEQ Project Director (or designee), representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC are drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas. The members of the ITAC are listed in Table 1.

As the ITAC membership is intentionally drawn from air quality researchers who have experience in Texas; these researchers and their colleagues will likely have interest in responding to the requests for research proposals issued by the AQRP. This raises potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas requires that the AQRP shall maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members are required to certify:

> *Confidentiality:* As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)
>
> *Conflict of Interest:* As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or the TCEQ Project Director. If there is a question of interpretation regarding whether a conflict of interest exists, I agree that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Table 1: Members of the Independent Technical Advisory Committee

Name	**Title**	**Organization**
David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	University of Colorado - Boulder
Sarwar Golam	Research Physical Scientist, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Tho (Thomas) Ching Ho	Chairman, Dan F. Smith Dept. of Chemical Engineering	Lamar University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Associate Professor, Department of Earth and Atmospheric Sciences	The University of Houston
John Nielsen-Gammon	Professor and Texas State Climatologist Center for Atmospheric Chemistry and the Environment	Texas A&M University
David Parrish	Program Lead, Tropospheric Chemistry, NOAA/ESRL/Chemical Sciences Division	National Oceanic and Atmospheric Administration
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Associate Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ
Dan Cohan (Alternate)	Assistant Professor, Civil and Environmental Engineering	Rice University

TCEQ Relevancy Review

Once the ITAC has reviewed and ranked research project proposals according to technical merit, they are submitted to the TCEQ for a relevancy review. The TCEQ reviews proposals for relevancy to the State's air quality research needs. TCEQ approval is required for a project to receive funding from the Program.

Advisory Council

The final group responsible for selecting AQRP research projects is the Advisory Council. The Council consists of up to 11 members, all residents of the State of Texas. Two Council members with relevant scientific expertise are nominated by the TCEQ. As defined in the AQRP contract, up to four members of the Council can be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. Additional members include government officials from Texas Near-Non-Attainment Areas active in air quality management. The purpose of the Council is to give final approval to projects recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. At least one meeting in Austin is dedicated to new project selection. Additional meetings, either in person or via webinar, and email updates are dedicated to providing summaries of on-going projects and review of the strategic plan.

Table 2: Members of the Advisory Council

Name	Title	Organization
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

PROJECT TIMELINE

This section will discuss the activities that took place in support of the AQRP. In the period covered by this report, two primary activities took place:

- FY 2012 – 2013 Projects begun
- Additional funding for FY 2013

September 2012 – November 2012

At the end of fiscal year 2012 a new set of proposals had been reviewed and selected for funding. Activities during the first quarter of fiscal year 2013 focused on contracting with the institutions where the research projects would be performed and working with investigators to develop the project Work Plans. Several of the proposals that were selected for funding came from institutions that had received AQRP funding in the prior biennium. Because Master Agreements were already in place with these organizations, the AQRP was able to issue amendments, decreasing the amount of time spent on contract negotiations. For those organizations that were new to the AQRP, new Master Agreements were negotiated. At the end of this quarter, all but one of these organizations (the home institution for 3 of the research projects) had completed the Master Agreement contracting process. Also, all but 3 of the projects had submitted Work Plans for review. (The Work Plan consists of the Project Plan, Budget and Justification, and Quality Assurance Project Plan (QAPP).)

December 2012 – Feb 2013

During this period the remaining contract completed negotiation and 13 of 14 work plans had been approved, with work starting on 10 projects. Projects were assigned funding from either fiscal year 2012 or 2013, with one project assigned partial funding from fiscal year 2011. This allowed the AQRP to fully expend all FY 2011 Research funds.

March 2013 – May 2013

The third quarter of the year saw the full execution of the final contract and all work plans fully approved with work started. Project managers continued to work with principal investigators to ensure that all project goals are met, as well as all reporting and invoicing requirements.

June 2013 – August 2013

The fourth quarter of the year saw the continuation of research project activities. As this period was in the middle of the research project cycle, ensuring that all reporting and invoicing requirements were met was the primary focus. With the renewal of the program for FY 2014 and 2015, Project Administration developed research priorities for the next RFP. The ITAC provided input into these priorities and they were submitted to the TCEQ for review.

Discover AQ

In September of 2013, the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program deployed NASA aircraft to make a series of flights with scientific instruments on board to measure gaseous and particulate pollution in the Houston, Texas area. The purpose, for NASA, of this campaign was to better understand how satellites could be used to monitor air quality for public health and environmental benefit.

To complement the NASA flight-based measurements, and to leverage the extensive measurements being funded by NASA to better understand factors that control air quality in Texas, ground-based air quality measurements were made simultaneously by researchers from collaborating organizations, including research scientists and engineers funded wholly or in part by the AQRP and the TCEQ. Because of the opportunity to leverage NASA measurements, projects related to DISCOVER-AQ were a high priority for the 2012-2013 biennium.

RESEARCH PROJECTS

Research Projects for FY 2010-2011 are now completed. All projects have submitted final invoices and those invoices have been paid. The Final Report for each project, with the exception of one, is posted on the AQRP website at http://aqrp.ceer.utexas.edu/projects.cfm.

A summary of the projects approved for funding for FY 2012-2013 follows.

Project 12-004 **STATUS: Active - March 1, 2013**

DISCOVER-AQ Ground Sites Infrastructure Support

University of Texas at Austin – Vincent Torres

AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Erik Gribbon

Funding Amount: $1,691,944

Executive Summary

In the summer of 2013, the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program deployed NASA aircraft to make a series of flights with scientific instruments on board to measure gaseous and particulate pollution in the Houston, Texas area. The purpose of this campaign, for NASA, was to improve the use of satellites to monitor air quality for public health and environmental benefit.

To complement the NASA flight-based measurements, and to leverage the extensive measurements being funded by NASA to better understand factors that control air quality in Texas, ground-based air quality measurements were made simultaneously by researchers from collaborating organizations, including research scientists and engineers funded wholly or in part by the AQRP and the TCEQ. Multiple ground sites were expanded or established to accommodate the instrumentation brought to Houston by research collaborators. This project centralized and coordinated the site infrastructure preparation for the ground sites identified for expansion to support DISCOVER-AQ Houston 2013.

The scope of work for this project began with meeting with and/or contacting appropriate DISCOVER-AQ and TCEQ personnel and determining how many and which ground sites will be used for the study. Once sites were determined, assignment of instrumentation to each site followed. Next, to accommodate the instrumentation and the associated support equipment and supplies that were located at the selected ground sites, site improvements were made; site access/use agreements, ground (site pad) preparation, installation of utilities (electrical and communication) and security fencing, and rental of temporary buildings to accommodate instrumentation that must be located in conditioned space were all performed. During the intensive measurements period of the campaign, some limited support was required by the

ground-based researchers should problems arise with the site accommodations. At the end of the campaign, each of these sites will be decommissioned and restored to their original condition or a condition required by the property owner.

Project Update

Throughout the year, the logistics team continued obtaining cost information for proposed site improvements, primarily electric utility modifications/upgrades, fencing modifications, and the addition of scaffolding to accommodate instrumentation that were added for DISCOVER-AQ, and supporting the TCEQ in obtaining site access agreements for the ground sites selected. As site access was obtained for each of the sites, purchase orders for site modifications that were required were submitted and issued. Additionally, TCEQ reassigned the responsibility for obtaining site access agreements for the four met profiler sites (Fayette County, Texas A&M, Smith Point and Danciger) to this project. The Danciger site was later changed to the Wharton Airport site. UT obtained site access agreements for these sites also. Approval and funding was obtained to issue a purchase order for the four met profilers that were used during the study at these four sites.

Site preparations were completed at all sites and then the logistics team ensured that as research teams installed equipment at a site, the site logistics were as planned and that all utilities were operating as requested.

The Aeronet and Pandora instruments began collecting data in late July and the four profiler sites (Smith Point, Texas A&M, Fayette County, and Wharton) were all operational and collecting data effective August 26. As of the end of the quarter, all research teams had installed their equipment and were ready for the start of the study.

Work to be performed in the next quarter will focus on providing support as needed for logistics in September during the measurement campaign phase of the study and decommissioning of the sites in October and November.

Project 13-005 **STATUS: Active – January 15, 2013**

Quantification of industrial emissions of VOCs, NO_2 and SO_2 by SOF and mobile DOAS during DISCOVER AQ

Chalmers University – Johan Mellqvist
University of Houston – Barry Lefer
AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – John Jolly

Funding Amount: $177,553
($129,047 Chalmers, $48,506 UH)

Executive Summary

Mobile remote sensing by SOF and mobile DOAS will be carried out in the Houston ship channel (HSC) area during September 2013. In this manner vertical columns will be obtained of VOCs (alkanes, alkenes), NH_3, NO_2, SO_2, HCHO and particles as inferred from aerosol optical depth. The optical remote data will be complemented by wind profile measurements. The data collected will have great value of its own to be applied for future ozone modeling since a good understanding of the emission variability and changes in the total emissions in the HSC will be obtained by comparison to similar studies in 2006, 2009 and 2011 [Mellqvist 2007; 2009; 2010 and Rivera 2010]. The emission data will be compared to available emission inventories and categorized in various industrial types.

Equally important, the measurements will complement the NASA Discover AQ campaign which will run in the HSC area during the targeted month. NASA will then fly a high altitude aircraft (B200) equipped with optical sensors measuring columns of SO_2, NO_2, HCHO and aerosol profiles (LIDAR). They will utilize a low flying airplane (P-3) that will make spirals in the vicinity of two ground stations in the HSC, to validate the high altitude measurements.

The spatial column data of NO_2, SO_2, and HCHO from the mobile DOAS will be directly comparable to the column data measured by the high altitude NASA aircraft, hence providing a performance evaluation data set across the whole ship channel. Secondly, by carrying out emission measurements of VOCs, NO_2, SO_2 and HCHO around the HSC, especially upwind the two sites, it will be possible to interpret the spiral measurements by the NASA P-3 and the high altitude measurements by the B200 more comprehensively. The combined airborne and ground based data set has potential to be used for modeling of the ozone in the HSC area. This project will support the AQRP priority research area: Improving the understanding of ozone and PM formation and emission characteristics in the Houston area through supplementary measurements to the NASA Discover-AQ campaign September 2013.

Project Update

During the period June 1 to August 31 the study team has carried out logistical and scientific planning of the campaign together with the University of Houston and participation in web meetings about NASA DISCOVER-AQ.

The SOF instrument was rebuilt by extending the solar tracker and it was fitted into a custom made cooled Zarges box. The mobile DOAS was improved by adding a scanner, making it possible to measure multiple angles while driving.

The SOF and mobile DOAS system was shipped to Houston in mid August and then it was installed in a Toyota Tundra at the University of Houston together with other equipment.

Figure 1. SOF and mobile DOAS system installed in a Toyota Tundra, here parked outside the Ellington field on Media day. Sep 2.

Project 12-006 **STATUS: Active – February 8, 2013**

Environmental chamber experiments and CMAQ modeling to improve mechanisms to model ozone formation from HRVOCs

University of California - Riverside – Gookyoung Heo
Texas A&M University – Qi Ying

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Ron Thomas

Funding Amount: $146,259
($101,765 UC-R, $44,494 TAMU)

Executive Summary

Using reliable atmospheric chemical mechanisms in regulatory models is necessary to formulate effective air quality policies for controls of secondary air pollutants such as ozone (O_3). It is well known that alkenes are a major contributor to radical and O_3 formation in Southeast Texas due to their high emissions and their high reactivities. Particularly, in Harris County, Texas, seven alkenes (ethene, propene, 1,3-butadiene, 1-butene, isobutene, trans-2-butene, and cis-2-butene) are classified as Highly Reactive Volatile Organic Compounds (HRVOCs), and HRVOC emissions have been regulated by Texas Administrative Code, Title 30, Part 1, Chapter 115 (TCEQ, 2102). However, condensed chemical mechanisms commonly used for air quality modeling in the U.S. are designed to model O_3 formation from typical urban ambient volatile organic compound (VOC) mixtures but are not designed to model O_3 formation under atmospheric conditions significantly influenced by highly variable HRVOC emissions that are dominated by a small number of VOC species. Therefore, a chemical mechanism that can be used to simulate O_3 formation from both urban emissions and industrial HRVOC emissions needs to be developed to accurately assess the impact on O_3 formation of regular and episodic HRVOC emissions from industrial sources in Southeast Texas. However, lack of environmental chamber data useful for mechanism evaluation is a critical obstacle to developing reliable mechanisms for the HRVOCs. Among the 7 alkenes regulated as HRVOCs in Southeast Texas, robust chamber data for mechanism evaluation are available only for ethene and propene. The situation is even worse for the higher molecular weight non-HRVOC alkenes. Thus, this study will develop more robust chemical mechanisms for the HRVOCs and non-HRVOC alkenes that are better suited for use under atmospheric conditions influenced by HRVOC emissions, and evaluate and update the initially proposed mechanisms by designing and carrying out environmental chamber experiments for the HRVOCs and non-HRVOC alkenes for which existing data are inadequate. The effect of the mechanism modifications on air quality predictions in Southeast Texas will be evaluated by carrying out 3-dimensional air quality modeling with the Community Multiscale Air Quality modeling system (CMAQ), using both existing mechanisms and the updated and more explicit mechanisms developed in this work.

Project Update

During June 1, 2013 to August 31, 2013, this project carried out 6 additional environmental chamber experiments using a large indoor environmental chamber at the University of California at Riverside to produce experimental data useful to improve atmospheric reaction mechanisms leading to ozone formation for five Highly Reactive Volatile Organic Compounds (HRVOCs; 1,3-butadiene, 1-butene, isobutene, trans-2-butene, and cis-2-butene) and five non-HRVOC alkenes (1-pentene, 1-hexene, trans-2-pentene, cis-2-pentene, and 2-methyl-2-butene). After analysis of experimental data of the 25 experiments (50 reactor runs) carried out for this project, relatively reliable experimental data (36 reactor runs in total) were selected and used for evaluating and improving mechanisms for the 10 alkenes. These newly obtained chamber experimental data as well as the information on kinetic and mechanistic reaction parameters for the 10 alkenes gathered by literature review was used to develop improved reaction mechanisms that can be used in CMAQ modeling by researchers at Texas A&M University. We developed and implemented emission speciation rules (i.e., rules to map emissions into model species in the chemical mechanism) to prepare emissions data to carry out 3-dimentional air quality modeling with the Community Multiscale Air Quality Modeling (CMAQ) system and carried out preliminary CMAQ simulations for this project with two versions: a relatively detailed version (SAPRC-11D) and a relatively compact version (SAPRC-11L). In September and October, 2013, we will further improve and test mechanisms using chamber experimental data and the improved mechanisms will be used for CMAQ modeling after implementation into CMAQ.

All funds allocated to the project will be used upon the project completion.

Project 12-011 **STATUS: Active – January 17, 2013**

Investigation of Global Modeling and Lightning NOx Emissions as Sources of Regional Background Ozone in Texas

ENVIRON International – Chris Emery

AQRP Project Manager – Elena McDonald- Buller
TCEQ Project Liaison – Jim Smith

Funding Amount: $77,420

Executive Summary

The production, transport, and fate of tropospheric ozone are highly dynamic processes with contributions from a multitude of anthropogenic and natural sources spanning spatial scales from local to global. The US Environmental Protection Agency (EPA) requires the use of regional photochemical models to demonstrate that local emission control plans will achieve the federal standard for ground-level ozone. As the ozone standard is lowered, sources contributing to uncontrollable "background" ozone become more significant and must be more accurately accounted. In response, regulatory modeling applications have employed continuously larger domains to explicitly include sources over broader portions of the continent. Regional models now include worldwide contributions by deriving boundary conditions from global models. As global models continue to emerge and improve, their contributions to background ozone as represented in regional models need to be evaluated.

The Texas Commission on Environmental Quality (TCEQ) uses the Comprehensive Air quality Model with extensions (CAMx) for research and regulatory photochemical modeling. Two popular global models have been routinely coupled to CAMx: the Goddard Earth Observing System - Chemistry model (GEOS-Chem), developed and distributed by Harvard University, and the Model for OZone and Related chemical Tracers (MOZART), developed and distributed by the National Center for Atmospheric Research (NCAR). A newer global model called AM3, which is the atmospheric component of the CM3 global coupled atmosphere-oceans-land-sea ice model, is developed by Princeton University and the National Oceanic and Atmospheric Administration's Geophysical Fluid Dynamics Laboratory (GFDL).

In this project, ENVIRON International Corporation will develop boundary condition inputs for CAMx utilizing output from all three global models (GEOS-Chem, MOZART, and AM3). The sensitivity of simulated ozone to regional boundary conditions will be investigated. We will develop quantitative comparisons of these global models with respect to their ability to provide accurate and reasonable boundary conditions for regional downscaling, particularly as it applies to regulatory ozone modeling.

Project Update

Task 1: Evaluation of Global Modeling Products Over North America

All work under this task was completed in June-July. Output from the AM3, GEOS-Chem, and AM3 global models were processed to supply boundary conditions for the CAMx regional model. ENVIRON completed an evaluation of global model performance against rural CASTNET surface ozone measurements, with a focus on the south-central US. All global models performed similarly, exhibiting large over predictions of surface ozone in the summer and early fall months.

We also developed new software to compare ozone sounding measurements from the NOAA ozonesonde network and from the Houston 2008 Tropospheric Ozone Pollution Project to the global and regional model ozone profiles. Comparisons of monthly-mean observed and modeled profiles were completed at four ozonesonde locations: Houston, Huntsville (Alabama), Boulder (Colorado), and Trinidad Head (California). All models performed well in simulating the monthly-mean tropospheric ozone profiles, but differed in their characterization of ozone at stratospheric altitudes.

Task 2: Global-Regional Model Coupling and Performance Comparison

CAMx modeling was performed for the period April through October 2008 on a continental-scale domain with 36 km grid spacing and a regional domain covering the south-central US with 12 km grid spacing. Details of the modeling configuration are described in the project Work Plan. CAMx was run with boundary conditions developed from the output of all three global models and results were inter-compared and evaluated against the same surface CASTNET data and ozonesonde profiles as was performed for the global models.

CAMx ozone performance at the rural CASTNET sites paralleled the global model results in that all model runs tended to over predict ozone in the summer and early fall months, but with less bias than the global models (Figure 1). Little difference in ozone performance resulted from use of the three different sets of boundary conditions. This suggests that for this specific modeling dataset, the CAMx model performance is more sensitive to the characterization of regional emissions and meteorology within the domain and is not particularly sensitive to boundary conditions. More detailed analyses of these CAMx results are on-going and will be documented in the project final report.

No technical issues have been encountered during the course of this project. Most technical work has been completed and the final project report is in preparation. We expect to deliver a first draft of the report to the AQRP in October. The project remains on schedule for completion by November 30.

All funds allocated to the project are intended to be used by 11/30/2013.

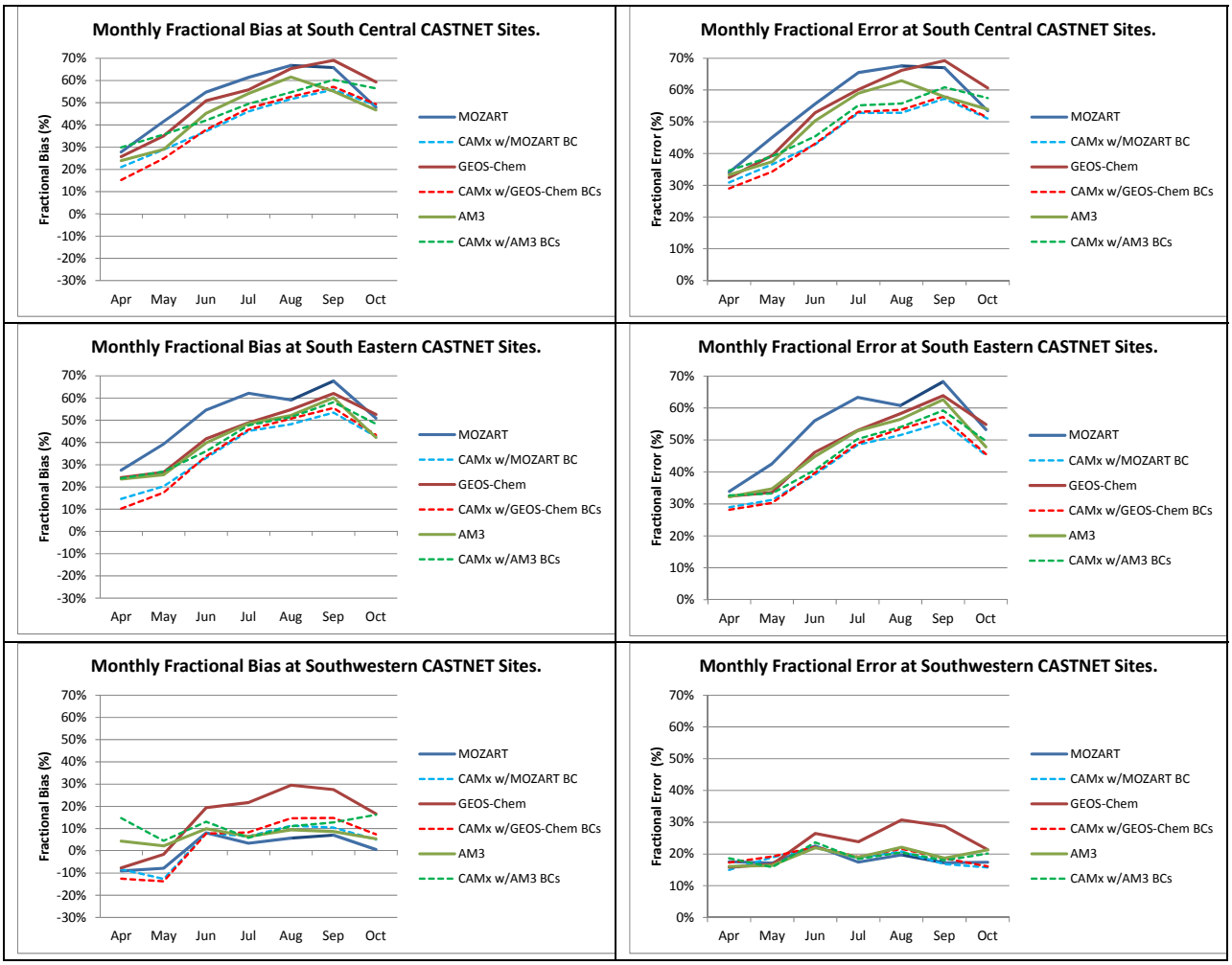

Figure 1. Monthly fractional bias (left) and error (right) for three global models (solid lines) and three corresponding CAMx runs (dashed lines) against 6-hourly CASTNET ozone data in the south-center (top), south-east (center), and south-west (bottom) US.

Project 12-012 **STATUS: Active - December 19, 2012**

Interactions Between Organic Aerosol and NOy: Influence on Oxidant Production

University of Texas at Austin – Lea H. Ruiz
ENVIRON International – Greg Yarwood
AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Mark Estes

Funding Amount: $148,835
($79,461 UT Austin, $69,374 Environ)

Executive Summary

In rural areas where emission rates of NO_x ($NO + NO_2$) are relatively low, ozone formation can be sensitive to secondary NO_x sources such as decomposition of organic nitrates ($R\text{-}ONO_2$). AQRP project 10-042 provided experimental evidence for NO_x production when organic nitrates degrade by OH reaction and photolysis. Implementing NO_x production from OH reaction with organic nitrates causes regional ozone increases that are large enough to affect model agreement with ozone observations. This implies that organic nitrates are less available to NO_x recycling than previous experiments suggested. We are investigating the hypothesis that uptake of organic nitrates into secondary organic aerosol (SOA) reduces the amount of NO_x recycled by organic nitrate photolysis and OH reaction.

The first task in this project is to add the uptake of organic nitrates by SOA to the Comprehensive Air quality Model with extensions (CAMx). The conceptual model of Perraud et al. (2012) is followed, in which organic nitrate molecules stick to aerosol surfaces and become irreversibly buried by accretion of SOA. Results of this initial modeling work is then used to design laboratory chamber experiments in which organic nitrates are formed from the oxidation of VOCs in the presence of NO_x and the distribution of organic nitrates between the gas and particle phases is observed. New chemistries and mechanisms inferred from the experimental data are then tested by including them in a box model of the chamber experiments before they are implemented in CAMx. Finally, the partitioning of organic nitrates between the gas- and particle phase is observed in natural aerosol by conducting ambient measurements near Houston.

Project Update

In this quarter we conducted CAMx simulations to test updates to the CB6r1 (Carbon Bond 6 revision 1) chemical mechanism using a box model version of CAMx which we developed last quarter. We compared simulations using the latest update to the CB6 chemical mechanism to ambient data collected at ground level (by TCEQ) and aloft (during INTEX-A). In order to obtain reasonable agreement between measured and observed concentrations of ozone it is necessary to assume that multifunctional nitrates are not available for NOx recycling. This could indicate that the organic nitrates are irreversibly incorporated in aerosol.

With our instrumentation now complete, we conducted experiments on the photolysis of organic nitrates and on their rate of reaction with the hydroxyl radical (OH). We also conducted experiments on the formation of organic nitrogen compounds in the gas and particle phases when VOCs are oxidized by OH in the presence of NOx. In all experiments we detected organic nitrogen compounds in the gas and particle phases.

We have started the ambient measurement campaign in Conroe. We arrived in Conroe on Aug. 22 and had enough time to set up and calibrate instrumentation before the initial start of the campaign on September 1. Since then we have been collecting data almost continuously, and we have detected organic nitrogen compounds in the gas and particle phases.

All funds allocated to the project are expected to be used by 11/30/2013.

Project 12-013 **STATUS: Active – December 14, 2012**

Development of Transformation Rate of SO_2 to Sulfate for the Houston Ship Channel using the TexAQS 2006 Field Study Data

ENVIRON International – Ralph Morris

AQRP Project Manager – Elena McDonald - Buller
TCEQ Project Liaison – Jim Price

Funding Amount: $59,974

Executive Summary

On June 2, 2010, EPA promulgated a new 1-hour SO_2 primary NAAQS with a threshold of 75 ppb. The 1-hour SO_2 NAAQS is much more stringent and replaces the old 24-hour (140 ppb) and annual (30 ppb) SO_2 NAAQS. States are required to submit 1-hour SO_2 State Implementation Plans (SIPs) by February 2014 that demonstrates compliance with the NAAQS by August 2017. Preliminary modeling indicates that SO_2 emissions for numerous sources will result in near-by exceedances of the 1-hour SO_2 NAAQS. Fossil-fueled power plants (73%) and industrial facilities (20%) are the main sources of SO_2 emissions in the U.S. Photochemical oxidants will convert some SO_2 to sulfate thereby reducing SO_2 concentrations. However, the EPA-recommended model for near-source 1-hour SO_2 modeling is the AERMOD steady-state Gaussian plume model that does not treat photochemical oxidants and has a very simple treatment of chemistry (exponential decay). EPA recommends that AERMOD be run with no SO_2 conversion for addressing 1-hour SO_2 NAAQS issues. This assumption may be appropriate for fossil-fueled power plants where the high NO_X concentrations inhibit photochemistry and consequently SO_2 oxidation near the source, but it may not be appropriate for the Houston Ship Channel where the atmosphere can be very reactive (due to HRVOC emissions) resulting in faster SO_2 to sulfate conversion rates.

The goal of this project is to develop a representative SO_2 transformation rate for the Houston Ship Channel area using measurements from the NOAA P-3 aircraft collected during the 2006 Texas Air Quality Study (TexAQS) that can be used with the AERMOD model to simulate 1-hour SO_2 concentrations. The proposed approach uses a grid model to simulate first-order transformation of SO_2 to sulfate for sources in the Houston Ship Channel. The model results with varying transformation rate are evaluated against the 2006 TexAQS P-3 aircraft measurement data to find what transformation rate best fits the observations and to determine whether one hypothetical transformation rate results in statistically better model performance than the other rates used.

Project Update

Task 3: Determine Transformation Rate of SO_2 to sulfate

We conducted a preliminary CAMx simulation for the September 19 flight transects with multiple model output reporting frequencies. The model predicted slightly lower peak SO_2 and sulfate concentrations with 1-hour output frequency than with 15- and 6-minute frequencies at the transects closer to the Houston Ship Channel while showing slightly higher peaks with 1-hour frequency at further downwind. As the model results with 15- and 6-minute frequencies do not show any significant differences in the model results, we selected the 15-minute output frequency for the subsequent model evaluation runs.

The model results showed that observed and modeled plumes were not exactly aligned because the meteorological model inputs were not sufficiently accurate to describe the actual wind direction at the time/height of the P-3 flights. Simply shifting the model plume direction would not help because multiple peaks were misaligned by different distances. Also, the modeled background sulfate concentrations appeared too high compared to those estimated by the observations. While the goal of this study is not directly related to accurate modeling of meteorology or background contributions, these factors made a conventional model evaluation methodology (i.e., biases and errors calculated from individual data points) less useful. Therefore, we devised an alternate model evaluation methodology that employs an aggregated quantity to represent the whole plume segment crossing a transect. An "average excess above background" concentration is defined as follows:

$$\frac{\int (C - C_B)dt}{\int dt}$$

where C and C_B are the total and background concentrations, respectively. The integration is limited to a transect segment identified as the Ship Channel plume (i.e., a segment dominated by the Ship Channel plume). The excess concentration is normalized by plume width (represented by flight time) so that uncertainties in the plume dispersion do not affect the model evaluation. For the modeled SO_2 and sulfate, the "excess above background" is simply the Ship Channel contribution as the model separately tracks SO_2 and sulfate from the Ship Channel sources. For the observed data, the background concentration is defined as the minimum concentration within the transect segment attributed to the Ship Channel plume. Model evaluation was performed over the ratios of sulfate to SO_2 average excess concentrations because our goal is to find the transformation rate of SO_2 to sulfate that best fits the aircraft measurement data. Figure 1 presents the root mean square error (RMSE) of the modeled ratio for each flight as well as the overall RMSE for SO_2-to-sulfate conversion rates from 0.01 to 0.1 hr-1. The result suggests the conversion rate of 0.04 hr^{-1} would best describe the transformation of SO_2 to sulfate in the Houston Ship Channel plumes.

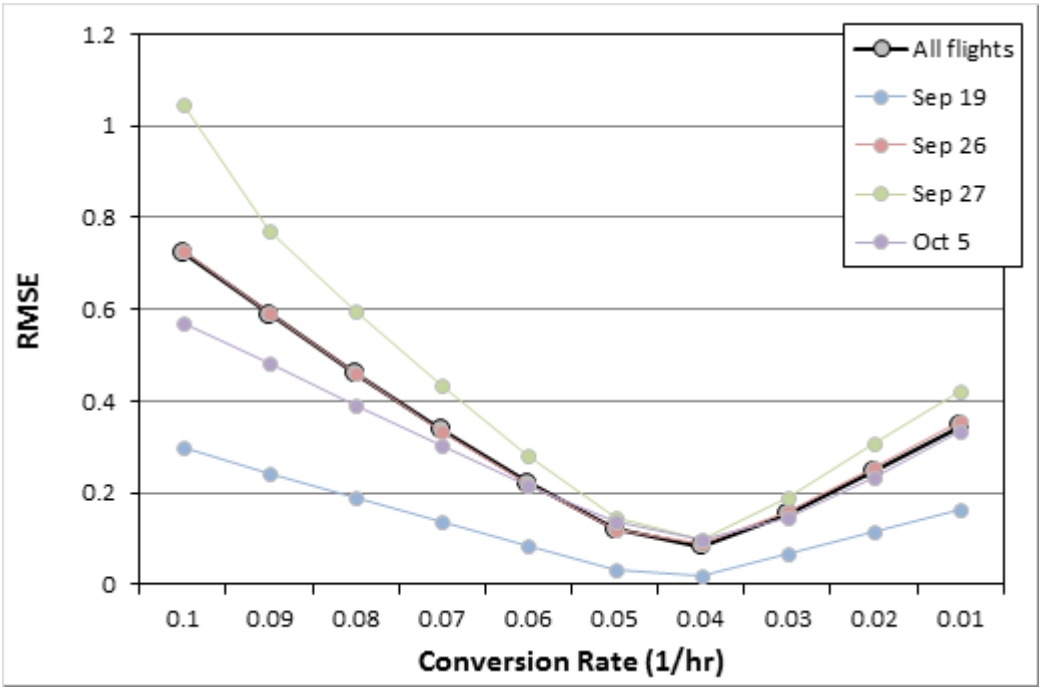

Figure 1. Root mean square errors of the modeled average excess SO_4 to SO_2 ratios.

An error was discovered in the emission input processing after the modeling analysis had been completed. The problem was fixed, and the grid model simulations and evaluation had to be re-done with the corrected emissions. It turned out that the error had only a small effect on the model results. However, it delayed the project schedule by about a month.

All funds allocated to the project will be used upon the project completion.

Project 13-016 **STATUS: Active – November 20, 2012**

Ozonesonde launches from the University of Houston and Smith Point, Texas in Support of DISCOVER AQ

Valparaiso University – Gary Morris
University of Houston – Barry Lefer
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Dave Westenbarger

Funding Amount: $86,667
($66,821 Valparaiso, $19,846 UH)

Executive Summary

An intensive series of ozonesonde launches during DISCOVER AQ (September 2013) provides insight into the recirculation of ozone over Galveston and Trinity Bays. With potential operational launch sites at LaPorte, the University of Houston Main Campus, and Smith Point, the coordinated set of ozone profiles will permit us further insights into the importance of re-circulated ozone on exceedence events during the late Summer high ozone season in Houston, Texas.

Project Update

This report summarizes our work on this project during the period 1 June through 31 August 2013. The investigators on this team prepared, revised, and submitted monthly reports for May, June, and July as well as a quarterly report for the period from the inception of the grant through 31 May 2013.

The investigators attended phone conferences led by Jim Crawford on DISCOVER-AQ planning.

The investigators worked with Anne Thompson (Penn State University, NASA Goddard Space Flight Center), Rich Clark (Millersville University), Henry Selkirk (USRA/GESTAR, NASA Goddard Space Flight Center), and Barry Lefer (University of Houston) to coordinate balloon activities in the Houston area during the DISCOVER-AQ period.

Dr. Morris also worked with the FAA to secure launch protocols for all of the various free release balloon sites that have been identified as possible launch locations for DISCOVER-AQ, including Galveston Island, the University of Houston Coastal Center, Ellington Field, the University of Houston Main Campus, the University of Houston Sugar Land Campus, Jones Forest, and Smith Point.

At present, the Penn State NATIVE trailer will be stationed at Smith Point, providing on ground, in situ observations that will be valuable for identifying diurnal variations in ozone and ozone

precursors as well as validation of the pre-launch ozonesonde data from Smith Point. The Penn State team will be responsible for Smith Point launches during DISCOVER-AQ.

Our team will launch at locations around Houston most favorable to the science of understanding the ozone distribution across Houston and the partitioning of sources.

Dr. Morris has also spent time developing an automated data processing system that will take the raw flight data, perform an initial quality check, correct pressure offsets when detected, and create the standard suite of plots to be posted on the project website: www.valpo.edu/ozone. The system has been tested with data from Houston and another site and is working well. Launch teams simply post the data to a Dropbox folder, and with a single command, the data are processed, quality checked, and archived. We are still developing the script that will automatically update the website. At present, that work still needs to be performed manually.

Project 12-018 **STATUS: Active – January 8, 2013**

The Effects of Uncertainties in Fire Emissions Estimates on Predictions of Texas Air Quality

University of Texas at Austin – Elena McDonald-Buller
ENVIRON International – Chris Emery
AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Clint Harper

Funding Amount: $106,970
($85,282 UT Austin, $21,688 Environ)

Executive Summary

Wildland fires and open burning can be substantial sources of nitrogen oxides (NO_x), carbon monoxide (CO), and non-methane hydrocarbons (NMHCs), which are precursors to ozone formation, as well as particulate matter (PM), sulfur dioxide (SO_2), and ammonia (NH_3). Fire emissions are often transported over long distances and can contribute to exceedances of air quality standards at local and regional levels. Achieving attainment with the National Ambient Air Quality Standards (NAAQS) for ozone has been the primary focus of State Implementation Plans (SIPs) for Texas. Accurate characterization of fire events is necessary for understanding their influence on measured ambient concentrations, for providing a weight of evidence for exceptional event exclusions if necessary, and for conducting air quality modeling for planning and attainment demonstrations. In addition, if more stringent federal standards for ozone are considered in the future, emissions of its precursors from regional sources, such as fires in the Western U.S., Mexico, and Central America, that can contribute to background concentrations will become increasingly important for understanding the relative effectiveness of local and regional emissions control programs. This project examines the effects of uncertainties in fire emissions estimates on modeled ozone and particulate matter concentrations in Texas using the Fire INventory from NCAR (FINN) and the Comprehensive Air Quality Model with extensions (CAMx).

Project Update

A climatology of fires in Texas, Louisiana, five central states (Arkansas, Kansas, Missouri, Mississippi, Oklahoma), eleven western states (New Mexico, Colorado, Wyoming, Montana, Idaho Washington, Oregon, California, Arizona, and Utah), Mexico, Central America (Guatemala, Belize Nicaragua, Costa Rica), and Western Canada was developed utilizing default FINN estimates from 2002-2012. A literature review of the effects of fires on air quality, climate change and fires, fire emissions estimation methods, and the FINN default model configuration and input parameters was completed.

ENVIRON/Alpine Geophysics transferred a 2008 CAMx modeling database, which spanned the time period of April 1 – October 15, 2008, to the University of Texas at Austin (UT). UT installed the episode on the Lonestar 4 system at the Texas Advanced Computing Center

(TACC). Fire emissions estimates for CO, NO_x, VOCs, and $PM_{2.5}$ from BlueSky/SMARTFire 2, which was utilized in the original CAMx episode, have been compared to estimates from FINN for the episode period. Because both emissions models are used for regional air quality model simulations in the U.S., it is valuable to compare their emissions estimates and effects on simulated air quality.

ENVIRON developed an EPS3 processing algorithm for FINN emissions that was used to spatially allocate estimates to the specific modeling grid (horizontally and vertically), temporally allocate daily estimates to each hour, and speciate VOC and other chemical species as appropriate for the CB05 chemical mechanism employed in CAMx. The CAMx-ready fire emissions inventory for the FINN default configuration replaced the BlueSky/SMARTFIRE 2 estimates for the April 1- October 18, 2008 episode as developed by Alpine Geophysics. UT completed a CAMx simulation with fire emissions based on the FINN default configuration that forms the base case to which the sensitivity analyses are being compared. Dr. Wiedinmyer visited Dr. McDonald-Buller's team at the University of Texas at Austin for three days during June 24-26, 2013. A primary goal of this trip was to develop the sensitivity analyses with FINN.

In order to assess the variability in estimated emissions to various uncertainties in the FINN model, the sensitivity simulations shown in Table 1 were performed. These included sensitivities to emission factors, land cover and land use inputs, fuel loading estimates, and fire location and area burned. Emission factors were updated with those published by Akagi et al. (2013) and Yokelson et al. (2013), downloaded from http://bai.acd.ucar.edu/Data/fire/). Uncertainties in the emissions factors were also tested using the uncertainties assigned by Akagi et al., (2013) and Yokelson et al. (2013) as upper and lower limits. The sensitivity of the emission estimates to global land cover classification was tested using the 2009 GlobCover global land cover map (http://due.esrin.esa.int/globcover/). A simulation was performed to test the fuel loadings assigned to each fire. For this case, the Fuels Characteristic Classification System (FCCS; http://www.fs.fed.us/pnw/fera/fccs/) was used in place of the default fuel loadings for vegetation identified. A simulation was also conducted in which SMARTFire was used to identify fire locations and estimated area burned, rather than the MODIS Rapid Response and the assumed area burned used by FINN. Data from the SMARTFire product were provided by Sim Larkin (US Department of Agriculture/US Forest Service) and Sean Raffuse (Sonoma Technology, Inc.) for the continental U.S.

In addition to analyzing the FINN emissions estimates from the sensitivity studies in Table 1 on state and regional scales, these inventories are being utilized in CAMx simulations by replacing estimates from the FINN default configuration in order to evaluate the effects on predicted air quality.

T**able 1.** Sensitivity simulations performed.

RUN NAME	**Land Cover/Fuel**	**Fuel Loading**	**Emission Factor**	**Fire Detection/Area Burned**
FINN default	default	default	default	default
Globcover	**GLOBCOVER**	default	default	default
newEmis	default	default	**New**	default
LOWemis	default	default	**Low**	default
HIGHemis	default	default	**High**	default
Fccsfuel	default	**FCCS**	default	default
SMARTFire2	default	default	default	SMARTFire2

*Default refers to inputs/parameters described by Wiedinmyer et al. (2011) for FINN version 1.

At this time, we intend to use all funds allocated to the project by 11/30/2013.

Project 13-022 **STATUS: Active – January 29, 2013**

Surface Measurements of PM, VOCs, and Photochemically Relevant Gases in Support of DISCOVER-AQ

Rice University – Robert Griffin
University of Houston – Barry Lefer

AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Jocelyn Mellberg

Funding Amount: $206,815
($89,912 Rice, $116,903 UH)

Executive Summary

In recent years, the National Aeronautics and Space Administration (NASA) has placed considerable emphasis on the use of satellite remote sensing in the measurement of species such as O_3 and PM that constitute air pollution. However, additional data are needed to aid in the development of methods to distinguish between low- and high-level pollution in these measurements. To that end, NASA has established a program titled Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ). DISCOVER-AQ began in summer 2011 with work in the Mid-Atlantic Coast that featured satellite, airborne, and ground-based sampling. The DISCOVER-AQ program will conduct operations in and near Houston in September 2013.

During the Houston operations of DISCOVER-AQ, there will be a need for ground-based measurement support. This project will fill that need by providing quantitative measurements of sub-micron particle size and composition and mixing ratios of volatile organic compounds (VOCs) and other photochemically relevant gases such as O_3 and oxides of nitrogen (NO_x = nitric oxide (NO) plus nitrogen dioxide (NO_2)). The instrumentation for these measurements will be deployed using the University of Houston (UH) mobile laboratory.

The measurements made on the mobile laboratory generally will operate in two modes. First, during periods when DISCOVER-AQ flight patterns spiral over a given location, the mobile laboratory will operate at the ground surface beneath these spirals in a stationary mode in which surface air quality parameters are monitored continuously. Additional stationary mode measurements will be made at other locations of interest. When not in stationary mode, the mobile laboratory will be deployed to perform Lagrangian studies of air quality within plumes from major sources of primary pollutants, as well as downwind of the major metropolitan area, to characterize secondary processes at surface level.

Project Update

The bulk of the activity focused on preparation for the September deployment. Based on expected load, the power system, air conditioning, shocks, and wheels for the mobile laboratory were upgraded to accommodate all of the planned instrumentation. This will ensure smooth operation during the campaign. In addition, the instrument configuration plan within the bed was

finalized, as was the layout and design for the inlets. Mock frames of all instruments were constructed and placed into the mobile laboratory to ensure that the layout will work geometrically. Team members also participated in conference calls with NASA and TCEQ to discuss flight plans, which in turn determined locations for surface deployments. This also entailed coordination with other mobile laboratory facilities (most specifically NASA, Princeton University, and Aerodyne Research, Inc.). In mid-August, NASA and TCEQ made a request that the Rice-UH group sample in the northwest section of the greater Houston area on flight days in order to characterize Houston outflow and to be co-located at least part of the time with instrumentation being operated by University of Texas researchers at the Conroe site. A preliminary plan for overnight locations also was created at the request of TCEQ staff. Part of the preparation for the campaign included training of students and staff from both universities on the relevant equipment; this is especially true of the Rice group, who deployed the PILS and a high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS) to a stationary ground site in early summer, in part so that the staff could be better prepared for the September deployment. Students and staff from both universities also continued to purchase supplies necessary to perform the campaign.

In mid-August, the uploading process began. Each piece of equipment was uploaded onto the mobile laboratory during the week of August 19, 2013. This was followed by checks for power, air conditioning, shocks, etc. Based on HR-ToF-AMS overheating errors, installation of an additional air conditioner within the mobile laboratory shell was deemed necessary, which has been completed. During a test drive in late August, despite significant shock prevention efforts, the filaments on the HR-ToF-AMS were found to trip whenever the mobile laboratory went over even the smallest of bumps. It was decided that the laboratory would perform semi-mobile sampling (sample for a period of time, move a short distance, sample for another period of time, move a short distance, etc.) until replacement parts arrived. These are expected in early September. This limitation is expected to have limited overall impact on the data generated besides the existence of small gaps in data continuity during the early part of DISCOVER-AQ. The PILS and all associated required materials were deployed to the Manvel Croix site on August 26, 2013. As of the end of August, the team was ready to sample.

In addition, plans were made for non-flight days. On non-flight days, sampling locations and patterns will be based on meteorological patterns, needs (calibrations, rest for the staff, etc.), and specific questions. Several scientific objectives were discussed, including measurements in the Houston Ship Channel and Texas City areas and along roadways to investigate primary emissions, co-location at Manvel Croix to compare HR-ToF-AMS and PILS data to determine HR-ToF-AMS collection efficiency, co-location with the Princeton mobile laboratory that is measuring ammonia to investigate ammonia-ammonium equilibrium, deployment to Galveston to measure inflow, and deployment near special types of emission sources such as landfills and wastewater treatment facilities.

Project 13-024 **STATUS: Active – February 20, 2013**

Surface Measurement of Trace Gases in Support of DISCOVER-AQ in Houston in Summer 2013

University of Maryland – Xinrong Ren

AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Erik Gribbon

Funding Amount: $90,444

Executive Summary:
The link between ozone (O_3) and NO_X (= NO + NO_2) photochemistry has been extensively studied for decades, yet new discoveries have revealed the need to improve scientific understanding of ozone formation chemistry. In order to improve the interpretation of aircraft and satellite observations to diagnose near-surface conditions relating to air quality, high-quality surface observations of ozone and particulate matter (PM) precursors are needed, especially in urban environments like Houston. To support the NASA DISCOVER-AQ study in Houston in summer 2013, we will make surface measurements of trace gases, including O_3, NO/NO_2/NO_Y, and SO_2. Research-grade instrumentation to measure these traces gases will be deployed at two of the science sites identified by TCEQ/AQRP. These measurements will be compared to concurrent aircraft measurements for the periods when the NASA P-3B aircraft conducts spiral profiles over the sites. Vertical distributions of these gases will be observed and compared with surface observations with the aim of improving the capability of transport models for air quality simulations. Data collected in the field study will be analyzed with regard to the source regions and emission profiles, reactive nitrogen budget, and relationship between NO_Z and O_3.

Project Update:
During the period from June 1, 2013 to August 31, 2013, the teams at University of Maryland College Park and NOAA's Air Resources Laboratory have accomplished the following tasks:

(1) Preparation for the DISCOVER-AQ field study in Houston, including
   a. the rebuild of the vacuum pump to be used for the NO-NO_2-NO_Y system with high ozone level during its operation;
   b. tests and calibration of the NO-NO_2-NO_Y system,
   c. calibrations of the ozone and SO_2 analyzers;
   d. preparation of data acquisition software based on Lab View;
   e. calibration of the Cavity Ring Down NO_2 analyzer,
   f. preparation of sample lines for the both the Galveston and Manvel Croix sites;
   g. further communication with Vincent Torres and Jim Thomas at University of Texas regarding the space and modification requirements for the Mobile Mini trailers at the sites.

(2) Completion of the final testing and calibrations for all instruments in the laboratory that were deployed in the DISCOVER-AQ field study in late August.

(3) Transport of the instruments to the Galveston and Manvel Croix sites and installation at both sites at the end of August.

(4) Completion of further testing and calibrations of the instruments in the field.

(5) Starting in August 31, all instruments were fully operational at the both sites.

(6) Preliminary data files have been submitted to the DISCOVER-AQ data archive on a daily basis.

During the next quarter, the following tasks are anticipated to be accomplished:

(1) To complete the data collection during DISCOVER-AQ in September 2013.

(2) Post-campaign calibrations of the instruments in the laboratory in October 2013.

(3) To finalize the data and submit them to the DISCOVER-AQ data archive

(4) To present the preliminary results from this project at the AQRP/TCEQ meeting in November 2013.

Project 10-028 **STATUS: Active – January 29, 2013**

Implementation and evaluation of new HONO mechanisms in a 3-D Chemical Transport Model for Spring 2009 in Houston

University of Houston – Barry Lefer
UCLA – Jochen Stutz
Environ – Greg Yarwood
UNC at Chapel Hill – Will Vizuette

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Doug Boyer

Funding Amount: $117,269
($19,599 UH, $17,944 UCLA, $44,496 Environ, $35,230 UNC)

Executive Summary

Although portions of the chemistry that lead to the formation of ozone have been understood for decades, new discoveries have revealed the need to improve scientific understanding of ozone formation chemistry. Radical production in Houston and other urban areas appear to be underestimated by chemical mechanisms. The roles of some radical precursors such as HONO, HCHO, and reactive VOCs in ozone formation in Houston and other Texas cities have not been well understood. Research based on both modeling and field measurements by the University of Houston, ENVIRON, University of California – Los Angeles, and the University of North Carolina – Chapel Hill has shown that nitrous acid (HONO) significantly affects the HOx budget in urban environments like Houston. These chemical processes connect surface emissions, both anthropogenic and natural, to local and regional air quality.

From April 15th to May 30th, 2009, a team of more than 40 scientists representing more than 15 different institutions collected a relatively complete suite of atmospheric measurements, including NO, NO_2, NO_Y, HONO, HNO_3, O_3, CO, SO_2, HCHO, HOOH, OH, HO_2, OVOCs, VOCs, actinic flux, PBL height, O_3 production rates, and vertical profiles (nominally 40m, 150m, 300m) of NO_2, HONO, O_3, SO_2, and HCHO, during the Study of Houston Atmospheric Radical Precursor (SHARP). The SHARP dataset provides us a unique opportunity to examine and improve our understanding of atmospheric HONO formation processes and how they may be implemented into the Comprehensive Air quality Model with extensions (CAMx) 3-D chemical transport model commonly used for SIP evaluations. The objective of this study is to develop, implement, and evaluate missing pathways for HONO formation in a photochemical model, CAMx, that is used routinely for regulatory applications in Texas and other areas. This model update is expected to improve the model's ability to simulate ozone concentrations, because HONO is a potential daytime source of the hydroxyl radical, OH, which plays an important role in the ozone formation cycle. Measurements during the SHARP study in Houston showed that radical production in the early morning was dominated by HONO photolysis.

The modeling strategy is to take advantage of the SHARP data analysis in a previous AQRP project (Project 10-032) to develop parameterizations, based on current understanding of the important processes governing HONO formation, and implement and refine these parameterizations in CAMx using existing modeling databases for the Houston area during the SHARP period. Model performance evaluation will make use of process analysis tools to evaluate how HONO formation pathways influence radical budgets and ozone formation within CAMx simulations.

Project Update

The project team (UH, UCLA, UNC, and ENVIRON) has developed new CAMx HONO production mechanisms. As part of this effort, the ENVIRON team has rewritten the CAMx surface model to enable us to implement the following HONO processes into CAMx:

A) Unimolecular conversion of NO_2 to HONO in the dark as a function of relative humidity.

B) Photo-induced conversion of NO_2 to HONO during the daytime.

C) Photolysis of surface HNO_3 to HONO.

The UNC group has successfully run the new CAMx HONO parameterizations for the Spring 2009 SHARP period using CAMx 6.0. The preliminary process analysis results showed that very little HONO was being generated by HNO_3 deposition to the land surface. Further investigation revealed that HNO_3 surface loadings were too low by several orders of magnitude. The project identified an error in the new CAMx land surface model where the e-folding lifetime of the deposited species was too low. This error was corrected and new model runs look significantly better.

In contrast the homogenous HONO production mechanism was generating significant levels of HONO, often times much greater than the daytime observations at the UH Moody Tower during SHARP. The cause of the high homogenous HONO production resulted from unrealistically high ambient NOx levels in the CAMx model in the UH Moody Tower grid cell only during periods of easterly winds. This was traced to several off-road NOx sources (cranes and construction equipment) several kilometers east of Moody Tower in the particular 2009 inventory used by this project. Simply looking at the results of an adjacent grid cell to the southwest of the Moody Tower showed much better agreement with both NOx and HONO.

The project team has completed the implementation of HONO production mechanisms via the new CAMx land surface model and run this new code for the Spring of 2009. We are currently finishing up the CAMx Process analysis and writing the draft final project report.

Project 10-032 **STATUS: Active – January 25, 2013**

Collect, Analyze, and Archive Filters at two DISCOVER-AQ Houston Focus Areas: Initial Characterization of PM Formation and Emission Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms

Baylor University – Rebecca Sheesley

AQRP Project Manager – Dave Sullivan
TCEQ Project Liaison – Fernando Mercado

Funding Amount: $45,972

Executive Summary

DISCOVER-AQ (Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality) is a multi-year air quality research study set to focus on Houston, TX in September 2013. NASA's P-3B and B200 aircraft will be deployed to sample vertical profiles over specific focus areas using a spiraling vertical profile flight plans for selected days during the one month sampling campaign. In this study, we will measure elemental carbon (EC), organic carbon (OC), and optical black carbon (BC) at two of these vertical spiral sites during the DISCOVER-AQ mission. Baylor University's research group will collect, analyze, and archive particulate filters collected concurrently with DISCOVER-AQ 2013 Houston-based sampling campaign. Specifically, we will continuously measure OC, EC and BC at two surface sites on each day of the month that the NASA aircraft will be deployed. Collection will occur at two field stations located directly below aircraft focus areas (i.e. vertical profile sites). Results from the carbon measurements taken during the campaign will be disseminated to DISCOVER-AQ investigators and other external research groups. We will also archive particulate filters for future research opportunity. Access to these archived filters will be provided to DISCOVER-AQ investigators and external research groups.

Specific goals of this project are to:

1) Characterize OC and EC concentrations using fine particulate matter ($PM_{2.5}$) and total suspended particulate (TSP) air filter samples collected at two of DISCOVER-AQ Houston's focus areas.
    a. Focus areas include ground stations near Katy and H-NET Jones Forest.
    b. Archive filters for two years at -10°C for future research opportunities.
    c. Provide access of filters to DISCOVER-AQ project leadership and external research groups and collaborators.
2) Measure optical BC using a seven channel aethalometer at the H-NET Jones Forest ground station.
3) Compare ground-based OC, EC, and optical BC with other aerosol measurements made directly over focus areas on NASA's P-3B and B200 aircraft (i.e**.** water soluble organic carbon and BC).

Project Update

Significant progress has been made in the planning and preparation for the September DISCOVER-AQ sampling campaign. The two sites have been completely outfitted and students are on-site to begin sampling the first week of September. PIs Sheesley and Usenko have participated in the field campaign conference calls led both by AQRP and by NASA. PIs Sheesley and Usenko have also been working directly with Vince Torres and Raj Nadkarni to finalize site details and coordination for Manvel Croix. A site visit was made to Moody Tower to define sampler locations and discuss site logistics with Dr. Barry Lefer at University of Houston. Preliminary collaboration discussions of plans to share filter media collected by Baylor during the September campaign were conducted with Dr. Sarah Brooks at TAMU during a visit to TAMU; this is responsive to the goal of the Baylor AQRP project to distribute filter media to research collaborators. The study team discussed collaboration and filter media sharing with Dr. Rachelle Duvall, Dr. Tad Kleindienst, Dr. John Offenberg and Dr. Michael Lewandowski of the US EPA, NERL; this is also responsive to the goals of the Baylor PIs. Additional collaboration with Lea Hildebrandt Ruiz of UT was planned and a filter sampler plus training was provided to her to enable filter collection by her group at the Conroe site during the September campaign; this was coordinated with Rachelle Duvall of the US EPA and will enable additional filter media sharing among the institutions.

Field instrumentation preparation including filter substrate prep and aethalometer maintenance, testing and site setup has been completed. A preliminary week-long sample was collected to provide mass for preliminary analysis and to test additional analytical techniques. This sample will also provide information on the site conditions at Moody Tower leading into the September campaign. Three graduate students have been trained to use all sampling equipment and in proper QAQC during field work. An undergraduate student has been trained in filter substrate preparation and OCEC analysis.

In addition, we are finalizing collaborations with other AQRP funded and NASA DISCOVER-AQ collaborators: specifically focusing on sampling logistics and aerosol research. By reaching out to various AQRP and NASA collaborators we have succeeded in expanding the number of samplers at Manvel Croix and Moody Towers. This will:

a. Improve sampling logistics.

b. Increase sampling resolution: Improve coverage of events (i.e. pollution or fights).

c. Increase mass of particulates sampled.

d. Expand opportunities for collaboration.

There were no delays in site preparation which affected the sample setup. Potential issues with electrical power and air conditioning at Manvel Croix was immediately fixed by Jim Thomas.

The rewiring of one circuit at Manvel Croix allowed for higher time resolution sampling to better match DISCOVER-AQ flight days; this was accommodated within 24 hours.

We are anticipating that all funds allocated to this project will be utilized by November 30th, 2013.

Project 12-TN1 **STATUS: Active – February 21, 2013**

Investigation of surface layer parameterization of the WRF model and its impact on the observed nocturnal wind speed bias

University of Maryland – Daniel Tong
Pius Lee
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Bright Dornblaser

Funding Amount: $64,994

Executive Summary

This study investigates surface layer parameterizations in the Weather Research and Forecasting (WRF) model. The parameterization of energy fluxes from the surface layer significantly impacts the modeled near-surface winds. The WRF model tends to over-predict the surface wind speeds in eastern Texas in the evening hours, especially in coastal regions. This project examines the various similarity theories that parameterize the momentum fluxes of the surface layer used in the WRF meteorological model.

The investigation and possible remedy recommendation for rectifying the high wind-speed-bias is carried out in multiple steps: (A) Understand the sensitivities of the different surface layer schemes, (B) Examine the sensitivity of the flux-profile relationships with regards to synoptic and atmospheric stability conditions, and (C) Investigate the universal flux profile functions and the range of parameter values used by the functions to suggest potential modifications for improvement – especially for the stable regimes. These details of the surface layer schemes are important as they govern the correct timing of the decoupling of near-surface and surface phenomena which are critical in the redistribution of kinetic energy from the residual layer to the surface. The rate of transfer of energy affects the evolution of wind speeds in the lowest layers.

A series of sensitivity runs of the WRF model is devised and conducted with possible recommendation on adjusted values for several of the tunable constants in the surface layer similarity theory parameterizations. Although the runs will focus on an early summer period for the Houston-Galveston-Brazoria area, they should provide insight on the rate and strength of the coupling and decoupling between the surface layer and the lowest model level in a large range of land-use and meteorological conditions.

Project Update

We continued the effort to rerun the simulation with WRF Model version 3.4.1 for the innermost nest for Eastern Texas. This effort stemmed from a relevant decision that this upgraded version included two bug fixes with respect to WRF version 3.2.1 that we used in the previous TCEQ-funded project addressing the wind-bias problem described in the title of this project. Both fixes dealt with the Yonsei University (YSU) planetary boundary layer (PBL) parameterization

scheme under stable atmospheric conditions and are directly binding on our model results for nocturnal wind speeds.

Figure 1 shows a comparison of measured and predicted wind speeds in the lowest levels over UHCC. The measurements were made at 43 meters. The predicted winds shown are at 16.9 m (first model level) and 59.4 m (second model level), respectively. The primary challenge of reducing the positive biases in low level wind at early evening hours at coastal sites was not addressed by the results of the newer WRF.

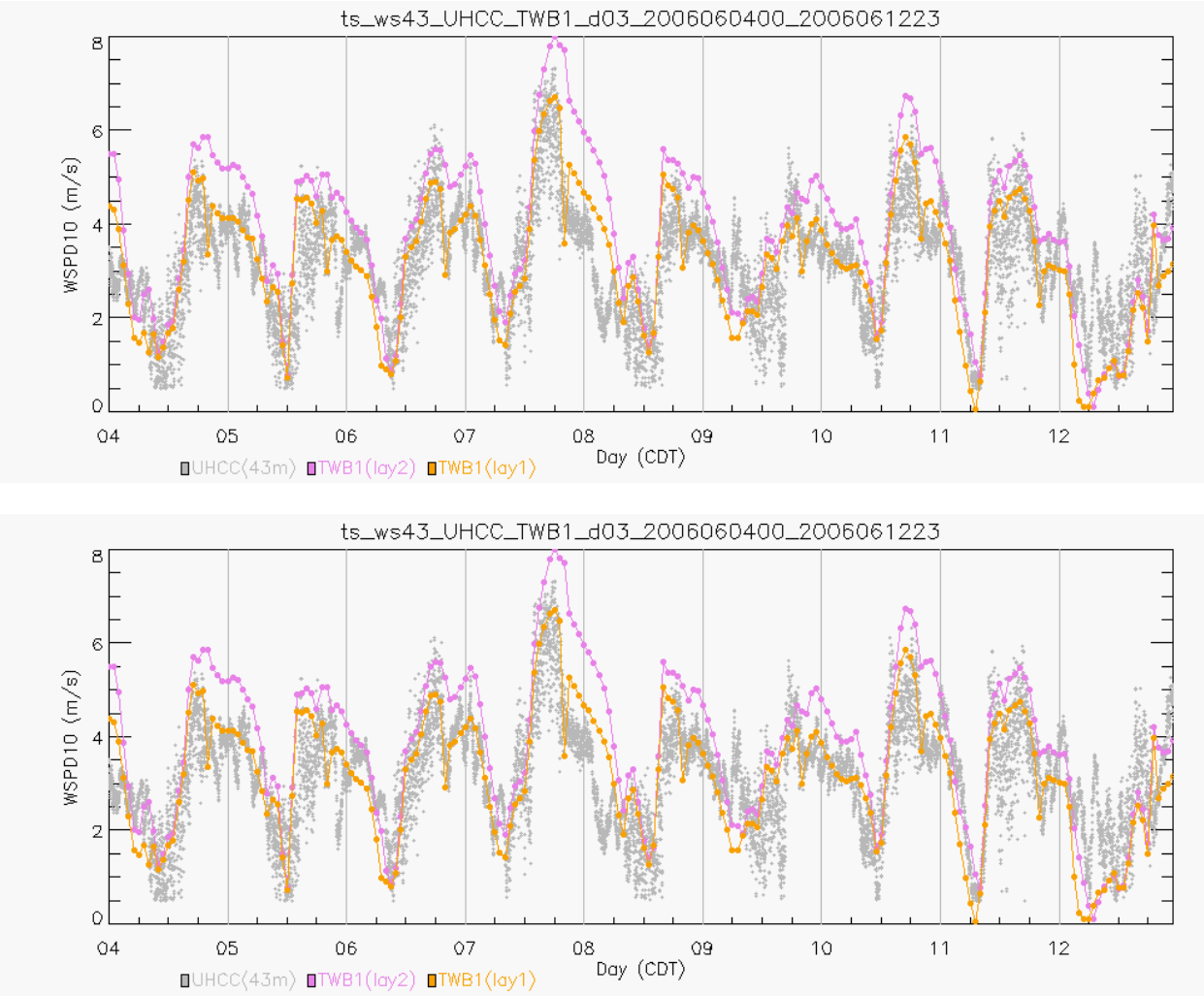

Fig. 1 Time series comparison of 43-m height observed wind (gray color) with 1st layer model wind (~16.9 m, pink line) and 2nd layer model wind (~59.4 m, red line) for large wind bias period at UHCC station for model results by (a) WRF3.2.1, and (b) WRF3.4.1.

We also explored the impact of changing the model physics option for land surface model (LSM) from the MM5's 5-layer slab model to a more sophisticated model – the National Centers for Environmental Prediction; Oregon State University; Air Force; Hydrological Research Laboratory (Noah) LSM. The model results showed some promise as bias was reduced for results by the newer WRF version 3.4.1 for some of these prognostic variables such as the reduced surface sensible heat flux biases over the large period between June 4 and June 13 2006 (See Fig. 2c). However the other variables such as 10 meter wind speed and wind direction did not necessarily see the same degree of improvement (See Fig 2 b and d).

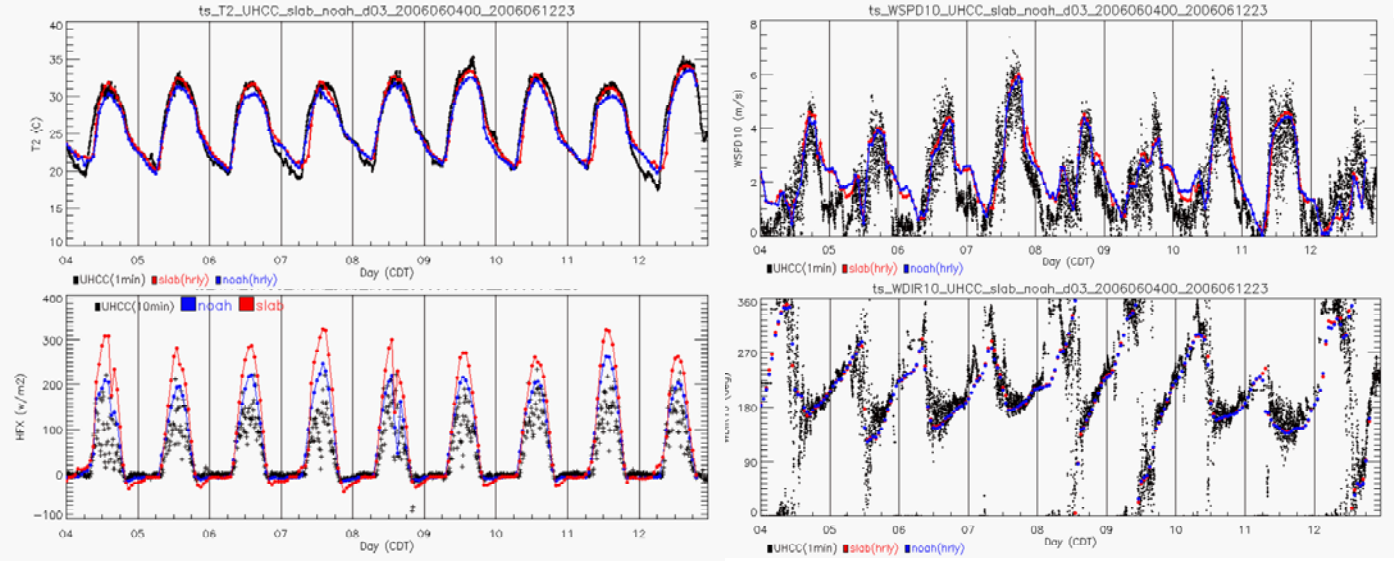

Fig. 2 Comparison of model results between Slab LSM (red) and NOAH LSM (blue) simulations between June 4 and June 13 2006 over UH Coastal Site for (a) 2 m temperature, (b) 10 m wind speed, (c) sensible heat flux and (d) 10 m wind direction.

Modification of WRF to generate extra intermediate output from the surface layer model

As the effort of model rerun did not completely rectify the nocturnal wind bias problem, we embarked to modify the surface layer module of the WRF model to generate extra intermediate output per time step to examine variables that may be an obvious cause of the biases. We started to analyze the stability regimes pertinent to the UHCC site. We had tried two approaches to generate extra intermediate output, such as the stability parameter z/L, where z is height and L is the Monin-Obukhov length scale. The first attempt was to modify the segment of the code where it was derived. We simply added a "print statement" to screen-dump the value at every time step in module "sfclay.F" that performs the surface similarity parameterization calculations. The calculation of z/L was based on Holtslag and De Bruin (1988) and Launiainen (1995). We

noticed that there was a strong tendency of z/L to give the "zero" value as noted by Jimenez et al. (2012).

We will continue this time series analysis of the governing parameters of the surface layer model to identify possibilities to adjust one or several parameters to test for reductions in the modeled wind biases.

Project 12-TN2 **STATUS: Active – February 21, 2013**

Development of IDL-based geospatial data processing framework for meteorology and air quality modeling

University of Maryland – Daniel Tong
HyunCheol Kim
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Bright Dornblaser

Funding Amount: $69,985

Executive Summary

This project investigates basic computational algorithms to handle Geographic Information System (GIS) data and satellite data, which are essential in regional meteorological and chemical modeling. It develops a set of generalized libraries within a geospatial data processing framework aiming to process geospatial data more efficiently and accurately. The tool can process GIS data both in vector format (e.g., ESRI shapefiles) and raster format (e.g., GEOTIFF and IMG) for any given domain. Processing speeds will be improved through selective usages of polygon-clipping routines and other algorithms optimized for specific applications. The raster tool will be developed utilizing a histogram reverse-indexing method that enables easy access of grouped pixels. It generates statistics of pixel values within each grid cell with improved speed and enhanced control of memory usage. Spatial allocating tools that use polygon clipping algorithms require huge computational power to calculate fractional weighting between GIS polygons (and/or polylines) and gridded cells. To overcome the speed and computational accuracy deterioration issues, an efficient polygon/polyline clipping algorithm is crucial. A key for faster spatial allocation is to optimize computational iterations in both polygon clipping and map projection calculations.

The project has the following specific objectives: (A) To develop an optimized geospatial data processing tool that can handle raster data format and vector data format with enhanced processing time and accuracy, for any given target domain. (B) To collect and to process sample GIS and satellite data. Applications will include a spatial regridding method for emissions and satellite data, such as the Moderate Resolution Imaging Spectroradiometer (MODIS) Aerosol Optical Depth (AOD), the Ozone Monitoring Instrument (OMI), and the Global Ozone Monitoring Experiment (GOME)-2 NO_2 column data. (C) To perform an engineering test with processed fine resolution LULC data.

Project Update

We have focused on the development of a vector and raster data processing tool, by implementing polygon clipping and pixel statistics algorithms in IDL.

1. Development of GIS vector data processing tools

Handling vector data is essential to convert irregular-shaped GIS vector data into a designated model grid. We have developed two algorithms for spatial data regridding. Spatial regridding is a commonly performed procedure in satellite data processing. It converts a data set between different map projections and resolutions. Among numerous spatial regridding methods, interpolation and pixel aggregation are two of the most common methods. Interpolation is preferred when the target domain resolution is higher than the raw data pixels, while pixel aggregation is the preferred way to average all the pixels inside each domain cell when the grid cell size is bigger than the raw data pixel size. Despite their popularity, the need for more mathematically complete methods for spatial regridding has been raised, especially in dealing with fine resolution data and/or where conservation of a measured quantity is required. A case in point is processing emission data. It requires great caution on spatial data handling because mass conservation is strictly applied. EPA's spatial allocator used in their emission model Sparse Matrix Operator Kernel Emissions (SMOKE) is one of the examples to reproject emission data without a loss of emission quantity. It calculates fractional areas of overlapping polygons between raw data pixels and modeling grid cells. In order to build a lossless spatial regridding tool, we have utilized polygon clipping algorithms, and have developed a tool to perform accurate spatial regridding of satellite data. Two key algorithms for the regridding tool are developed and implemented: the "Conservative remapping" algorithm performs lossless spatial remapping, and the "Downscaling" algorithm is designed to generate fine structure out of coarse resolution input data (e.g. satellite pixels), with additional information from fine resolution data set (e.g. fine resolution model simulation)

2. Raster data processing tool

Algorithms for raster data processing are rather straightforward compared to vector processing algorithms that use complicated polygon clipping algorithms. However, optimizations of raw data accessing methods and pixel indexing are required to efficiently handle huge raster data. We have built partial data accessing routines for several GIS raster data formats such as Geo Tagged Image File (GeoTIFF) and ERDAS IMAGINE (.IMG) files, to avoid unnecessary access of whole data set that often causes memory problems. We also utilized histogram reverse-indexing methods from the IDL histogram routine, which enables easy access of grouped pixels for given indices (e.g. target domain cell index). In addition, it generates statistics of pixel values within each grid cell with improved efficiency and enhanced control of memory usage. Pixel statistics algorithm was further extended to be applied to any given polygons with arbitrary shapes, which enables the conversion of raster data information not only into domain cells but also to any GIS boundary (e.g. raster data statistics in any Federal Information Processing Standards (FIPS) boundary).

FINANCIAL STATUS REPORT

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May 2010 an amendment was issued increasing the budget by $40,000. Funding for fiscal year 2011 was established at $2,106,071, for a total award of $4,878,142 for the FY 2010/2011 biennium. FY 2010 funds were fully expended in early 2012 and the FY 2011 funds expired on June 30, 2013 with a remaining balance of $0.11.

In February 2012, funding of $1,000,000 was awarded for FY 2012. In June 2012, an additional $160,000 was awarded in FY 2012 funds and $1,000,000 was awarded in FY 2013 funds, for a total of $2,160,000 in funding for the FY 2012/2013 biennium.

In April 2013, the grant was amended to reduce the FY 2012 funds by $133,693.60 and increase the FY 2011 funds by the same amount.

In June 2013, the grant was amended to increase the FY 2013 funds by $2,500,000.

All of these funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

Program Administration – limited to 10% of the overall funding (per Fiscal Year)
This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC
These funds are to cover the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project will be assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual
These are the funds available to support the research projects that are selected for funding.

Program Administration

Program Administration includes salaries and fringe benefits for those overseeing the program as a whole, as well as, materials and supplies, travel, equipment, and other expenses. This category allows indirect costs in the amount of 10% of salaries and wages.

During the reporting period several staff members were involved, part time, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. James Thomas, AQRP Manager, is responsible for assisting Dr. Allen in the program administration. Maria Stanzione, AQRP Grant Manager, with assistance from Rachael Bushn, Melanie Allbritton, and Susan McCoy each provided assistance with program organization and financial management. This included assisting with the

contracting process. Denzil Smith is responsible for the AQRP Web Page development and for data management.

Fringe benefits for the administration of the AQRP were initially budgeted to be 22% of salaries and wages across the term of the project. It should be noted that this was an estimate, and actual fringe benefit expenses have been reported for each month. The fringe benefit amount and percentage fluctuate each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. For example, the amount of fringe benefits is greater for a person with family medical insurance versus a person with individual medical insurance. At the end of the project, the overall total of fringe benefit expensed is expected to be at or below 22% of the total salaries and wages. Actual fringe benefit expenses to date are included in the spreadsheets above.

As discussed in previous Quarterly Reports, the AQRP Administration requested and received permission to utilize funds in future fiscal years. This is for all classes of funds including Administration, ITAC, Project Management, and Contractual. As of the writing of this report, the FY 10 and 11 funds have been fully expended. This same procedure will be followed for the FY 12 and 13 funds.

In June 2013, UT-Austin received a Contract Extension for the AQRP. This extension will continue the program through December 29, 2015.

Table 1: AQRP Administration Budget

Administration Budget (includes Council Expenses)
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$202,816.67	$172,702.06	$375,518.73	$375,518.73	$0	$0
Fringe Benefits		$38,665.65	$33,902.95	$72,568.60	$72,568.60	$0	$0
Travel		$346.85	$0	$346.85	$346.85		$0
Supplies		$15,096.14	$101.25	$15,197.39	$15,197.39	$96.73	$0
Equipment		$0	$0	$0			$0
Total Direct Costs		$256,925.31	$206,706.26	$463,631.57	$463,631.57	$0	$0
Authorized Indirect Costs		$20,281.69	$17,270.20	$37,551.89	$37,551.89		$0
10% of Salaries and Wages							
Total Costs		**$277,207**	**$223,976.46**	**$501,183.46**	**$501,183.46**	**$0**	**$0**
Fringe Rate		22%	22%		19%		

Administration Budget (includes Council Expenses)
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$68,340.00	$265,040.00	$333,380.00	$83,579.16	$0.00	$249,800.84
Fringe Benefits		$14,606.64	$47,706.00	$62,312.64	$19,299.29	$0.00	$43,013.35
Travel		$2,850.00	$750	$3,600.00	$339.13		$3,260.87
Supplies		$10,000.00	$10,000	$20,000.00	$1,815.13	$0.00	$18,184.87
Equipment		$0.00	$0	$0			$0
Total Direct Costs		$95,796.64	$323,496.00	$419,292.64	$105,032.71	$0.00	$314,259.93
Authorized Indirect Costs		$6,834.00	$26,504.00	$33,338.00	$8,357.91	$0.00	$24,980.09
10% of Salaries and Wages							
Total Costs		**$102,630.64**	**$350,000.00**	**$452,630.64**	**$113,390.62**	**$0.00**	**$339,240.02**
Fringe Rate		22%	22%		23%		

ITAC

All ITAC activities in this period were conducted via email and webinar, therefore no expenses related to ITAC meetings were incurred. The remaining FY 2011 ITAC funds were rebudgeted to the Project Management and Research Project categories, so that the funds could be fully expended for research activities by the AQRP.

Table 2: ITAC Budget

ITAC Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$16,378.86	$6,292.97	$22,671.83	$22,671.83	$0.00	$0
Supplies		$1,039.95	$284.67	$1,324.62	$1,324.62	$0.00	0
Total Direct Costs		$17,418.81	$6,577.64	$23,996.45	$23,996.45	$0.00	$0
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$17,418.81**	**$6,577.64**	**$23,996.45**	**$23,996.45**	**$0.00**	**$0**

ITAC Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$10,000	$8,000.00	$18,000	$0	$0	$18,000.00
Supplies		$500	$2,000.00	$2,500	$0		$2,500.00
Total Direct Costs		$10,500	$10,000.00	$20,500	$0	$0	$20,500.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$10,500**	**$10,000.00**	**$20,500**	**$0**	**$0**	**$20,500.00**

Project Management

In August 2012, Project Managers were assigned to the FY 2012-2013 Research Projects. Project Managers continued to work with Investigators to make sure they met reporting deadlines.

Table 3: Project Management Budget

Project Management Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$145,337.70	$121,326.64	$266,664.34	$266,664.34	$0	$0
Fringe Benefits		$28,967.49	$23,102.60	$52,070.09	$52,070.26	$0	($0.17)
Travel		$0	$0	$0	$0		$0
Supplies		$778.30	$207.98	$986.28	$986.22	$0	$0.06
Total Direct Costs		$175,083.49	$144,637.22	$319,720.71	$319,720.82	$0	($0.11)
Authorized Indirect Costs		$14,533.77	$12,132.66	$26,666.43	$26,666.32	$0	$0.11
10% of Salaries and Wages							
Total Costs		**$189,617.26**	**$156,769.88**	**$346,387.14**	**$346,387.14**	**$0**	**$0.00**

Project Management Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$48,900.00	$152,000	$200,900.00	$40,921.65	$0.00	$159,978.35
Fringe Benefits		$9,106.00	$31,800	$40,906.00	$8,409.23	$0.00	$32,496.77
Travel		$500	$0	$500.00	$0.00		$500.00
Supplies		$7,279.76	$6,000	$13,279.76	$392.98		$12,886.78
Total Direct Costs		$65,785.76	$189,800	$255,585.76	$49,723.86	$0.00	$205,861.90
Authorized Indirect Costs		$4,890.00	$15,200	$20,090.00	$4,092.16	$0.00	$15,997.84
10% of Salaries and Wages							
Total Costs		**$70,675.76**	**$205,000**	**$275,675.76**	**$53,816.02**	**$0.00**	**$221,859.74**

Research Projects

FY 2010-2011

The FY 2010 Research/Contractual budget was originally funded at $2,286,000. After all transfers, it was increased by $1,827.93. The FY 2011 Research/Contractual budget was originally funded at $1,736,063. After all transfers, it was increased by $377.62, plus an additional $116,000 from FY 2012 funds that were changed to FY 2011 funds. This is an overall net increase of $13,205.55 to the Research/Contractual funds (and net reduction in Project Management/ITAC funds). ($105,000 in FY 2012 research funds were transferred to FY 2011, the remaining $11,000 were transfers from Project Management funds.)

All FY 2010 Research Project funding was fully expensed before the expiration of FY 2010 funds in June 2012. The FY 2011 Research Project funding that remained after all FY 2011 research projects were completed was allocated to FY 2012-2013 projects. This included the funds that were reallocated from FY 2012 to FY 2011. The funds were allocated to project 13-016 Valparaiso and project 13-004 Discover AQ Infrastructure. Both projects utilized their FY 2011 funds (project 13-004 $116,000 and project 13-016 $20,168.90) by June 30, 2013. A remaining balance of $0.11 was returned to TCEQ.

Table 4 on the following 2 pages illustrates the 2010-2011 Research Projects, including the funding awarded to each project and the total expenses reported on each project through the expiration of the FY 2011 funds on June 30, 2013.

FY 2012-2013

The FY 2012 Research/Contractual budget was originally funded at $815,000. Transfers to date have increased the budget by $27,500. The FY 2013 Research Contractual budget was originally funded at $835,000. In June 2013, Amendment 9 increased this budget by $2,100,000. (The remaining $400,000 was allocated to Admin and Project Management.) $1,402,744 of these funds were allocated to Project 13-004 to allow for the purchase of additional infrastructure equipment and expand the number of Discover-AQ sites. The funds that have not yet been allocated to research projects will be allocated from the next RFP.

Table 5 illustrates the 2012-2013 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of August 31, 2013.

Table 4: 2010/2011 Contractual Expenses

Contractual Expenses

FY 10 Contractual Funding	$2,286,000
FY 10 Contractual Funding Transfers	$1,827.93
FY 10 Total Contractual Funding	**$2,287,827.93**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-008	Rice University	$128,851	$126,622.32	$2,228.68
10-008	Environ International	$49,945	$49,944.78	$0.22
10-009	UT-Austin	$591,332	$591,306.66	$25.34
10-021	UT-Austin	$248,786	$248,786.41	-$0.41
10-022	Lamar University	$150,000	$132,790.80	$17,209.20
10-032	University of Houston	$176,314	$176,314	$0
10-032	University of New Hampshire	$23,054	$18,850.65	$4,203.35
10-032	UCLA	$49,284	$47,171.32	$2,112.68
10-034	University of Houston	$195,054	$186,657.54	$8,396.46
10-042	Environ International	$237,481	$237,479.31	$1.69
10-045	UCLA	$149,773	$142,930.28	$6,842.72
10-045	UNC - Chapel Hill	$33,281	$33,281	$0
10-045	Aerodyne Research Inc.	$164,988	$164,988.10	-$0.10
10-045	Washington State University	$50,000	$50,000	$0
10-DFW	UT-Austin	$37,857	$37,689.42	$167.58
FY 10 Total Contractual Funding Awarded		$2,286,000		
FY 10 Contractual Funding Expended (Init. Projects)			$2,244,812.59	
FY 10 Contractual Funds Remaining Unspent after Project Completion				$41,187.41
FY 10 Additional Projects				
	Data Storage	$7,015.34	$7,015.34	$0
10-SOS	State of the Science	$36,000.00	$36,000.00	$0
FY 10 Contractual Funds Expended to Date*			$2,287,827.93	
FY 10 Contractual Funds Remaining to be Spent				$0

FY 11 Contractual Funding		$1,736,063.00		
FY 11 Contractual Funding Transfers		$116,377.62		
FY 11 Total Contractual Funding		**$1,852,440.62**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179	$262,179	$0
10-006	University of Houston	$222,483	$217,949.11	$4,533.89
10-015	Environ International	$201,280	$201,278.63	$1.37
10-020	Environ International	$202,498	$202,493.48	$4.52
10-024	Rice University	$225,662	$223,769.99	$1,892.01
10-024	University of New Hampshire	$70,747	$70,719.78	$27.22
10-024	University of Michigan	$64,414	$60,597.51	$3,816.49
10-024	University of Houston	$98,134	$88,914.46	$9,219.54
10-029	Texas A&M University	$80,108	$78,276.97	$1,831.03
10-044	University of Houston	$279,642	$277,846.38	$1,795.62
11-DFW	UT-Austin	$50,952	$29,261.75	$21,690.25
FY 11 Total Contractual Funding Awarded		$1,758,099		
FY 11 Contractual Funds Expended (Init. Projects)			$1,713,287.06	
FY 11 Contractual Funds Remaining Unspent after Project Completion				$44,811.94
FY 11 Additional Projects				
	Data Storage	$2,984.66	$2,984.66	$0.00
	12-016 Valparaiso	$20,168.90	$0.00	$21,168.90
	12-004 Discover AQ Infrastructure	$116,000.00	$115,999.89	$0.11
FY 11 Contractual Funds Expended to Date*			$1,852,440.51	
FY 11 Contractual Funds Remaining to be Spent				$0.11
Total Contractual Funding		$4,022,063.00		
Total Contractual Funding Transfers		$118,205.55		
Total Contractual Funding Available		$4,140,268.55		
Total Contractual Funds Expended to Date			$4,140,268.44	
Total Contractual Funds Remaining				$0.11

Table 5. 2012/2013 Contractual Expenses

Contractual Expenses

FY 12 Contractual Funding	$815,000
FY 12 Contractual Funding Transfers	$27,500
FY 12 Total Contractual Funding	**$842,500**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
12-004	UT-Austin (Torres)	$4,820		$4,820.00
12-006	UC-Riverside	$101,765	$51,991.58	$49,773.42
12-006	TAMU/TEES	$44,494	$6,553.52	$37,940.48
12-011	Environ International	$77,420	$51,302.43	$26,117.57
12-012	UT-Austin (Hildebrandt)	$79,463	$40,805.64	$38,657.36
12-012	Environ International	$69,374	$20,951.90	$48,422.10
12-013	Environ International	$59,974	$43,353.42	$16,620.58
12-018	UT-Austin (McDonald-Buller)	$85,282	$33,615.73	$51,666.27
12-018	Environ International	$21,688	$4,053.96	$17,634.04
12-028	University of Houston	$19,599	$15,724.01	$3,874.99
12-028	UCLA	$17,944	$15,232.40	$2,711.60
12-028	Environ International	$44,496	$26,903.01	$17,592.99
12-028	UNC - Chapel Hill	$35,230	$30,465.25	$4,764.75
12-032	Baylor	$45,972	$23,478.80	$22,493.20
12-TN1	Maryland	$64,994		$64,994.00
12-TN2	Maryland	$69,985		$69,985.00
FY 12 Total Contractual Funding Awarded		$842,500		
FY 12 Contractual Funds Remaining to be Awarded		$0		
FY 12 Contractual Funds Expended to Date			$364,431.65	
FY 12 Contractual Funds Remaining to be Spent				$450,568

FY 13 Contractual Funding		$835,000		
FY 13 Contractual Funding Transfers		$2,100,000		
FY 13 Total Contractual Funding		**$2,935,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
13-004	UT-Austin (Torres)	$1,571,124	$412,081.85	$1,159,042.15
13-005	Chalmers University of Tech	$129,047	$19,150.31	$109,896.69
13-005	University of Houston	$48,506	$23,027.69	$25,478.31
13-016	Valparaiso	$46,652	$18,289.37	$28,362.73
13-016	University of Houston	$19,846	$6,572.16	$13,273.84
13-022	Rice University	$89,912	$28,181.62	$51,730.38
13-022	University of Houston	$116,903	$68,302.16	$48,600.84
13-024	Maryland	$90,444	$33,911.99	$56,532.01
FY 13 Total Contractual Funding Awarded		$2,112,434		
FY 13 Contractual Funding Remaining to be Awarded		$822,566		
FY 13 Contractual Funds Expended to Date			$619,517.15	
FY 13 Contractual Funds Remaining to be Spent				$215,483
Total Contractual Funding		$3,777,500		
Total Contractual Funding Awarded		$2,954,934		
Total Contractual Funding Remaining to be Awarded		$822,566		
Total Contractual Funds Expended to Date			$983,948.80	
Total Contractual Funds Remaining to be Spent				$2,793,551

Appendix A

Financial Reports by Fiscal Year

FY 10 and 11

(Expenditures reported as of May 31, 2013.)

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67		$0
Fringe Benefits		$38,665.65	$38,665.65		$0
Travel		$346.85	$346.85		$0
Supplies		$15,096.14	$15,096.14		$0
Equipment		$0.00			$0
Other					
Contractual					
Total Direct Costs		$256,925.31	$256,925.31		$0
Authorized Indirect Costs		$20,281.69	$20,281.69		$0
10% of Salaries and Wages					
Total Costs		**$277,207.00**	**$277,207.00**	**$0**	**$0**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00		$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment					
Other		$0.00			$0.00
Contractual					
Total Direct Costs		$206,706.26	$206,706.26	$0.00	$0.00
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$223,976.46**	**$223,976.46**	**0.00**	**$0.00**

ITAC Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,378.86	$16,378.86	$0	$0
Supplies		$1039.95	$1,039.95		$0
Equipment					
Other					
Total Direct Costs		$17,418.81	$17,418.81	$0	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$17,418.81**	**$17,418.81**	**$0**	**$0**

ITAC Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$6,292.97	$6,292.97	$0.00	$0
Supplies		$284.67	$284.67	$0.00	$0
Equipment					
Other					
Total Direct Costs		$6,577.64	$6,577.64	$0.00	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$6,577.64**	**$6,577.64**	**$0.00**	**$0**

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$145,337.70	$145,337.70		$0
Fringe Benefits		$28,967.49	$28,967.49		$0
Travel		$0	$0		$0
Supplies		$778.30	$778.30		$0
Equipment					
Other					
Total Direct Costs		$175,083.49	$175,083.49	$0	$0
Authorized Indirect Costs		$14,533.77	$14,533.77		$0
10% of Salaries and Wages					
Total Costs		**$189,617.26**	**$189,617.26**	**$0**	**$0**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$121,326.64	$121,326.64	$0	$0
Fringe Benefits		$23,102.60	$23,102.77	$0	($0.17)
Travel		$0			$0
Supplies		$207.98	$207.92	$0	$0.06
Equipment					
Other					
Total Direct Costs		$144,637.22	$144,637.33	$0	($0.11)
Authorized Indirect Costs		$12,132.66	$12,132.55	$0	$0.11
10% of Salaries and Wages					
Total Costs		**$156,769.88**	**$156,769.88**	**$0**	**$0.00**

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67	$0.00	$0.00
Fringe Benefits		$38,665.65	$38,665.65	$0.00	$0.00
Travel		$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$15,096.14	$0.00	$0.00
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,287,827.93	$2,287,827.93	$0.00	$0.00
ITAC		$17,418.81	$17,418.81	$0.00	$0.00
Project Management		$189,617.26	$189,617.26	$0.00	$0.00
Total Direct Costs		$2,751,789.31	$2,751,789.31	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$20,281.69	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,772,071.00**	**$2,772,071.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$1,852,440.62	$1,852,440.51	$0.00	$0.11
ITAC		$6,577.64	$6,577.64	$0.00	($0.00)
Project Management		$156,769.88	$156,769.88	$0.00	$0.00
Total Direct Costs		$2,222,494.40	$2,222,494.29	$0.00	$0.11
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,239,764.60**	**$2,239,764.49**	**$0.00**	**$0.11**

Appendix B

Financial Reports by Fiscal Year

FY 12 and 13

(Expenditures reported as of May 31, 2013.)

Administration Budget (includes Council Expenses)

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$68,340.00	$67,920.86	$0.00	$419.14
Fringe Benefits		$14,606.64	$15,700.48	$0.00	($1,093.84)
Travel		$2,850.00	$339.13		$2,510.87
Supplies		$10,000.00	$1,738.80	$0.00	$8,261.20
Equipment		$0.00			$0.00
Other					
Contractual					
Total Direct Costs		$95,796.64	$85,699.27	$0.00	$10,097.37
Authorized Indirect Costs		$6,834.00	$6,792.08	$0.00	$41.92
10% of Salaries and Wages					
Total Costs		**$102,630.64**	**$92,491.35**	**$0.00**	**$10,139.29**

Administration Budget (includes Council Expenses)

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$265,040.00	$15,658.30		$249,381.70
Fringe Benefits		$47,706.00	$3,598.81		$44,107.19
Travel		$750.00	$0.00		$750.00
Supplies		$10,000.00	$76.33		$9,923.67
Equipment					
Other		$0.00	$0.00		$0.00
Contractual					
Total Direct Costs		$323,496.00	$19,333.44	$0.00	$304,162.56
Authorized Indirect Costs		$26,504.00	$1,565.83		$24,938.17
10% of Salaries and Wages					
Total Costs		**$350,000.00**	**$20,899.27**	**$0.00**	**$329,100.73**

ITAC Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$10,000.00	$0.00	0.00	$10,000.00
Supplies		$500.00			$500.00
Equipment					
Other					
Contractual					
Total Direct Costs		$10,500.00	$0.00	$0.00	$10,500.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$10,500.00**	**0.00**	**$0.00**	**$10,500.00**

ITAC Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$8,000.00	$0.00		$8,000.00
Supplies		$2,000.00	$0.00		$2,000.00
Equipment					
Other					
Contractual					
Total Direct Costs		$10,000.00	$0.00	$0.00	$10,000.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$10,000.00**	**$0.00**	**$0.00**	**$10,000.00**

Project Management Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$48,900.00	$40,921.65	$0.00	$7,978.35
Fringe Benefits		$9,106.00	$8,409.23	$0.00	$696.77
Travel		$500.00			$500.00
Supplies		$7,279.76	$392.98		$6,886.78
Equipment					
Other					
Contractual					
Total Direct Costs		$65,785.76	$49,723.86	$0.00	$16,061.90
Authorized Indirect Costs		$4,890.00	$4,092.16	$0.00	$797.84
10% of Salaries and Wages					
Total Costs		**$70,675.76**	**53,816.02**	**$0.00**	**$16,859.74**

Project Management Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$152,000.00			$152,000.00
Fringe Benefits		$31,800.00			$31,800.00
Travel		$0.00			$0.00
Supplies		$6,000.00			$6,000.00
Equipment					
Other					
Contractual					
Total Direct Costs		$189,800.00	$0.00	$0	$189,800.00
Authorized Indirect Costs		$15,200.00			$15,200.00
10% of Salaries and Wages					
Total Costs		**$205,000.00**	**0.00**	**$0.00**	**$205,000.00**

AQRP Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$68,340.00	$67,920.86	$0.00	$419.14
Fringe Benefits		$14,606.64	$15,700.48	$0.00	($1,093.84)
Travel		$2,850.00	$339.13	$0.00	$2,510.87
Supplies		$10,000.00	$1,738.80	$0.00	$8,261.20
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$842,500.00	$364,431.65	$0.00	$478,068.35
ITAC		$10,500.00	$0.00	$0.00	$10,500.00
Project Management		$70,675.76	$53,816.02	$0.00	$16,859.74
Total Direct Costs		$1,019,472.40	$503,946.94	$0.00	$515,525.46
Authorized Indirect Costs		$6,834.00	$6,792.08	$0.00	$41.92
10% of Salaries and Wages					
Total Costs		**$1,026,306.40**	**$510,739.02**	**$0.00**	**$515,567.38**

AQRP Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$265,040.00	$15,658.30	$0.00	$249,381.70
Fringe Benefits		$47,706.00	$3,598.81	$0.00	$44,107.19
Travel		$750.00	$0.00	$0.00	$750.00
Supplies		$10,000.00	$76.33	$0.00	$9,923.67
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$2,935,000.00	$619,517.15	$0.00	$2,315,482.85
ITAC		$10,000.00	$0.00	$0.00	$10,000.00
Project Management		$205,000.00	$0.00	$0.00	$205,000.00
Total Direct Costs		$3,473,496.00	$638,850.59	$0.00	$2,834,645.41
Authorized Indirect Costs		$26,504.00	$1,565.83	$0.00	$24,938.17
10% of Salaries and Wages					
Total Costs		**$3,500,000.00**	**$640,416.42**	**$0.00**	**$2,859,583.58**

AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-10-94300
Awarded to The University of Texas at Austin

Annual Report

September 1, 2013 through August 31, 2014

Submitted to

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Texas Air Quality Research Program

Annual Report

September 1, 2013 – August 31, 2014

Overview

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the 2010-2011 biennium, the AQRP had approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released its first request for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received. After review by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs, the results of the reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. A total of 15 proposals were selected for funding. As of November 30, 2011, all projects have been completed. Final reports have been posted to the AQRP website.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding of $1,000,000 for the FY 2012 period was awarded in February 2012. An additional $1,000,000 for the FY 2013 period was awarded in June 2012. At the same time an additional $160,000 was awarded for FY 2012, to support funding for two specific air quality projects recommended by the TCEQ. A call for proposals was released in May 2012. Thirty-two proposals, requesting $5 million in research funding were received. The proposals were reviewed by the ITAC and the TCEQ. The Advisory Council selected 14 projects for funding.

In June 2013, the TCEQ issued Amendment 9 to the AQRP grant. This amendment had two purposes, 1) it renewed the AQRP for the 2014-2015 biennium (but did not award any funding for that biennium), and 2) it awarded an additional $2,500,000 in FY 2013 funds. Ten percent (10%) of these funds were allocated for Project Administration, and the remaining funds were allocated to the Research program per the terms of the AQRP grant. A portion of the research funds were awarded to the 2012-2013 Discover-AQ Ground Sites Infrastructure Support project, in order to expand logistical support for the Discover-AQ study, at the request of TCEQ and with the Advisory Council's approval.

All 2012 – 2013 research projects were completed by November 30, 2013. The final reports for the projects have been posted to the AQRP website. All FY 2012 funds were fully expended and the remaining FY 2013 funds were held for use on future projects.

After the TCEQ issued Amendment 9 to renew the grant, the AQRP developed the FY 2014/2015 research priorities and submitted them to the ITAC for input and to the TCEQ for review. Funding of $1,000,000 for FY 2014 and $1,000,000 for FY 2015 was awarded via Amendment 10 in October 2013. A call for proposals was released and by the November 22, 2013 due date, 31 proposals requesting $5.8 million in research funding were received. In December and January the ITAC and the TCEQ reviewed the proposals. On February 21, the Advisory Council selected 15 projects for funding, with one project on hold while TCEQ completed their review. These projects were funded with a combination of FY 2013, 2014, and 2015 funds.

In early March, project Principal Investigators (PIs) were notified of the decision of the Advisory Council. AQRP Project Managers and TCEQ Project Liaisons were assigned to each project. A kick-off call was held with the project teams to discuss the development of the Work Plans which consist of the project scope of work, budget and justification, and quality assurance project plan (QAPP). The TCEQ completed their review of the final projects to be recommended for funding and the Council approved the final project on April 2, 2014.

During the spring and summer, project administration staff focused on putting contracts in place with each entity involved in the research projects. Project Managers worked with the project teams to complete and approve the Work Plans. As of August 31, 2014, all project Work Plans were approved, one project entity was still negotiating the Master Agreement with UT, and all other projects had begun work. An update of the status of each project is listed in the Research Projects section of this report.

BACKGROUND

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.

(b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.

(c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.

(d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.

(e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.

(f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010 for the 2010-2011 biennium, and was renewed in June 2011 for the 2012-2013 biennium and in June 2013 for the 2014-2015 biennium. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

RESEARCH PROJECT CYCLE

The Research Program is being implemented through a 9 step cycle. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle.

1.) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and the TCEQ, develop research priorities; the research priorities are released along with a Request for Proposals.

2.) Project proposals relevant to the research priorities are solicited. The Request for Proposals can be found at http://aqrp.ceer.utexas.edu/ .

3.) The Independent Technical Advisory Committee (ITAC) performs a scientific and technical evaluation of the proposals.

4.) The project proposals and ITAC recommendations are forwarded to the TCEQ. The TCEQ evaluates the project recommendations from the ITAC and comments on the relevancy of the projects to the State's air quality research needs.

5.) The recommendations from the ITAC and the TCEQ are presented to the Council and the Council selects the proposals to be funded. The Council also provides comments on the strategic research priorities.

6.) All Investigators are notified of the status of their proposals, either funded, not funded, or not funded at this time, but being held for possible reconsideration if funding becomes available.

7.) Funded projects are assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin is responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The Project Manager has responsibility for documenting progress toward project measures of success for each project. The Project Manager works with the researchers, and the TCEQ, to create an approved work plan for the project.

    The Project Manager also works with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved Quality Assurance Project Plan (QAPP) for each project. The Project Manager reviews monthly, annual and final reports from the researchers and works with the researchers to address deficiencies.

8.) The AQRP Director and the Project Manager for each project describe progress on the project in the ITAC and Council meetings dedicated to on-going project review.

9.) The project findings are communicated through multiple mechanisms. Final reports are posted to the Program web site; research briefings are developed for the public and air quality decision makers; and a bi-annual research conference/data workshop is held.

Steps 1 – 9 have all been completed for both the 2010-2011 and 2012 - 2013 biennia. For the 2014-2015 biennium Steps 1 through 6 have been completed. Steps 7 and 8 are in progress.

Independent Technical Advisory Committee (ITAC)

The AQRP funding is used primarily for research projects, and one of three groups responsible for selecting the projects is the Independent Technical Advisory Committee (ITAC). The ITAC, composed of up to 15 individuals with scientific expertise relevant to the Program, is charged with recommending technical approaches, and establishing research priorities. Initially, the ITAC was to meet at least twice per year at locations rotating between Austin, Dallas and Houston. As the Program proceeded, it was more efficient for the ITAC to meet once in Austin and as needed via conference call/webinar. Generally, the meetings in Austin are dedicated to new project review, reviewing progress on funded projects, and reviewing the Program's strategic plan.

Members of the ITAC consist of the TCEQ Project Director (or designee), representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC are drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas. The members of the ITAC are listed in Table 1.

As the ITAC membership is intentionally drawn from air quality researchers who have experience in Texas; these researchers and their colleagues will likely have interest in responding to the requests for research proposals issued by the AQRP. This raises potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas requires that the AQRP shall maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members are required to certify:

> *Confidentiality:* As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)
>
> *Conflict of Interest:* As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or the TCEQ Project Director. If there is a question of interpretation regarding whether a conflict of interest exists, I agree that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Table 1: Members of the Independent Technical Advisory Committee

Name	Title	Organization
David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	University of Colorado - Boulder
Sarwar Golam	Research Physical Scientist, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Tho (Thomas) Ching Ho	Chairman, Dan F. Smith Dept. of Chemical Engineering	Lamar University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Associate Professor, Department of Earth and Atmospheric Sciences	The University of Houston
John Nielsen-Gammon	Professor and Texas State Climatologist Center for Atmospheric Chemistry and the Environment	Texas A&M University
David Parrish	Program Lead, Tropospheric Chemistry, NOAA/ESRL/Chemical Sciences Division	National Oceanic and Atmospheric Administration
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Associate Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ

TCEQ Relevancy Review

Once the ITAC has reviewed and ranked research project proposals according to technical merit, they are submitted to the TCEQ for a relevancy review. The TCEQ reviews proposals for relevancy to the State's air quality research needs. TCEQ approval is required for a project to receive funding from the Program.

Advisory Council

The final group responsible for selecting AQRP research projects is the Advisory Council. The Council consists of up to 11 members, all residents of the State of Texas. Two Council members with relevant scientific expertise are nominated by the TCEQ. As defined in the AQRP contract, up to four members of the Council can be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. Additional members include government officials from Texas Near-Non-Attainment Areas active in air quality management. The purpose of the Council is to give final approval to projects recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. At least one meeting in Austin is dedicated to new project selection. Additional meetings, either in person or via webinar, and email updates are dedicated to providing summaries of on-going projects and review of the strategic plan.

Table 2: Members of the Advisory Council

Name	**Title**	**Organization**
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

PROJECT TIMELINE

During the project period covered by this report (September 1, 2013-August 31, 2014), five primary activities took place:

- FY 2012-2013 projects completed
- Data Workshop
- New funding for FY 2014-2015
- A Request for proposals (RFP) issued for FY 2014-2015
- FY 2014-2015 projects selected/funded

September 2013 – November 2013

At the beginning of fiscal year 2013-2014, the FY 2012-2013 projects were still active. The Discover-AQ activities (see description under Research Projects) took place in September. On November 14, 2013, the AQRP hosted a Data Workshop at The University of Texas at Austin's Pickle Research Campus. A representative from each project presented a report on research project findings and recommendations to the TCEQ, AQRP, and to the other AQRP researchers. All FY 2012-2013 projects ended on November 30, 2013, and final reports were submitted to the Project Managers for review.

Funding of $1,000,000 for FY 2014 and $1,000,000 for FY 2015 was awarded via Amendment 10 in October 2013. A call for proposals was released and by the November 22, 2013 due date, 31 proposals requesting $5.8 million in research funding were received.

Program Administration during this period focused on the payment of monthly invoices for projects, reporting activities, the planning and execution of the Data Workshop, and the issuance of the RFP.

Table 3 under Research Projects, page 13, lists all FY 2012-2013 Research Projects, the amount they were funded, the amount they expended, and the amount they returned to the AQRP.

December 2013 – Feb 2014

During the second quarter of FY 2013-2014, Program Administration focused on the close-out and final payment of invoices for projects, as well as the completion of reporting activities. Project Managers and TCEQ Liaisons completed the review of the Final Reports.

Once all reviews were completed, the Final Report for each project was posted on the AQRP website at http://aqrp.ceer.utexas.edu/projects.cfm. All Final Reports have been posted to the website. Principal Investigators notified Project Managers and TCEQ Liaisons of impending publications developed from the AQRP Projects. A reference list of the publications from all AQRP projects can be found in Appendix D.

The ITAC conducted the scientific and technical review of the proposals received under the FY 2014-2015 RFP via a conference call on December 17, 2013 and in a meeting held in Austin, Texas, on January 10, 2014. Seven proposals were highly recommended for funding; seven

proposals were recommended for funding; five proposals were recommended for funding, if additional funds were available; and twelve proposals were not recommended for funding.

On January 13, 2014, the project proposals and ITAC recommendations were forwarded to TCEQ. The TCEQ evaluated the project recommendations from the ITAC and provided comment on the relevancy of the projects to the State's air quality research needs. The TCEQ recommended for funding thirteen (13) of the fourteen (14) proposals that the ITAC either highly recommended or recommended, and two (2) of the five (5) proposals that the ITAC recommended if funding was available. While it was ultimately recommended, the TCEQ took additional time to review one of the proposals that was recommended by the ITAC until after the initial Advisory Council meeting, held on February 21, 2014. On this date, the Advisory Council selected 15 projects for funding.

March 2014 – May 2014

In early March, project Principal Investigators (PIs) were notified of the decision of the Advisory Council. AQRP Project Managers and TCEQ Project Liaisons were assigned to each project. A kick-off call was held with the project teams to discuss the development of the Work Plans which consist of the project scope of work, budget and justification, and quality assurance project plan (QAPP). The TCEQ completed their review of the final project to be recommended for funding and the Council approved the sixteenth project on April 2, 2014.

Throughout March, April, and May, project administration staff focused on putting contracts in place with each entity involved in the research projects. Project Managers worked with the project teams to complete and approve the Work Plans. Several of the proposals that were selected for funding came from institutions that had received AQRP funding in the prior biennia. Because Master Agreements were already in place with these organizations, the AQRP was able to issue amendments, decreasing the amount of time spent on contract negotiations. For those organizations that were new to the AQRP, new Master Agreements were negotiated. At the end of this quarter, all of the amendments to the Master Agreements were in place. All sixteen (16) of the projects had submitted Work Plans for review and seven (7) of the sixteen (16) Work Plans were approved. (The Work Plan consists of the Project Plan, Budget and Justification, and Quality Assurance Project Plan (QAPP).)

June 2014 – August 2014

During this period, all project work plans were approved, and contracts were finalized for all but two projects. Work either began or continued for the remaining projects. Projects were assigned funding from fiscal year 2013, 2014, or 2015 with multiple projects assigned partial funding from multiple fiscal years. This allowed the AQRP to fully expend all FY 2013 Research funds before they expired, and allow projects to continue through June 2015.

Project managers continued to work with principal investigators to ensure that all project goals were met, as well as all reporting and invoicing requirements. In August, the AQRP was notified that two projects were undergoing significant changes:

Project 14-026, led by Environ International, was authorized to begin work even though contract negotiations were still on-going with the project partner, the California Institute of Technology (Cal Tech). In August, Environ notified AQRP that Cal Tech wanted to terminate contract negotiations with the AQRP and would no longer be involved with the project. Cal Tech's contract negotiations office confirmed this with AQRP's contract negotiations office. Environ submitted a revised Work Plan to the AQRP to modify the scope and budget of the project in light of the change in participants. The change included bringing on David Parrish as a consultant. The revised Work Plan will be reviewed by the AQRP Review Panel in September.

Project 14-023, led by The University of Texas at Austin, began work in May. In July, the host of the site where the work was to be performed notified the PI that the company was being sold, and the new owners would not allow the project to take place on that site. The PI tried to locate an alternate site for the project, but was unable to find a host. In August, the PI officially notified the AQRP that the project could not be completed. At this point the project was ended and all unspent funds were returned to the AQRP Research Projects fund.

At this time, the AQRP is working with the TCEQ to identify alternate projects for funding. This will be further discussed by the Review Panel during their call in September.

An update of the status of each project is listed in the Research Projects section of this report.

RESEARCH PROJECTS

Research projects for FY 2010-2011 are complete. The FY 2012-2013 research projects were completed in November 2013. All projects have submitted final invoices and those invoices have been paid. The Final Report for each project is posted on the AQRP website at http://aqrp.ceer.utexas.edu/projects.cfm.

A final summary of the FY 2012-2013 projects is shown in Table 3 below. It is followed by a description of the new projects approved for funding for FY 2014-2015. A list of publications resulting from all research projects to date is provided in Appendix D and can also be found on the AQRP website.

FY 2012 – 2013 Projects

Discover AQ

In September of 2013, the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program deployed NASA aircraft to make a series of flights with scientific instruments on board to measure gaseous and particulate pollution in the Houston, Texas area. The purpose, for NASA, of this campaign was to better understand how satellites could be used to monitor air quality for public health and environmental benefit.

To complement the NASA flight-based measurements, and to leverage the extensive measurements being funded by NASA to better understand factors that control air quality in Texas, ground-based air quality measurements were made simultaneously by researchers from collaborating organizations, including research scientists and engineers funded wholly or in part by the AQRP and the TCEQ. Because of the opportunity to leverage NASA measurements, projects related to DISCOVER-AQ were a high priority for the 2012-2013 biennium.

Table 3: FY 2012-2013 Funded Research Projects

AQRP Project Number	Title	Start Date	End Date	Total Project Funding Awarded	Total Project Expenditures	Funding Returned to AQRP
	Institution (*Institution = Lead Institution and PI)	Principal Investigator		Project Funding Awarded to Institution	Institution Project Expenditures	Institution Funding Returned to AQRP
12-004	**DISCOVER-AQ Ground Sites Infrastructure Support**	**3/1/2013**	**11/30/2013**	**$1,691,944**	**$941,402.05**	**$750,541.95**
	*The University of Texas at Austin	Vincent Torres				
13-005	**Quantification of industrial emissions of VOCs, NO2 and SO2 by SOF and mobile DOAS during DISCOVER AQ**	**1/15/2013**	**11/30/2013**	**$177,553.00**	**$173,975.24**	**$3,577.76**
	*Chalmers University of Technology	Johan Mellqvist		$129,047.00	$129,047.00	$0.00
	University of Houston	Barry Lefer		$48,506.00	$44,928.24	$3,577.76
12-006	**Environmental chamber experiments and CMAQ modeling to improve mechanisms to model ozone formation from HRVOCs**	**2/8/2013**	**11/30/2013**	**$146,259.00**	**$143,899.22**	**$2,359.78**
	*University of California - Riverside	Gookyoung Heo		$101,765.00	$101,765.00	$0.00
	Texas A&M University	Qi Ying		$44,494.00	$42,134.22	$2,359.78
12-011	**Investigation of Global Modeling and Lightning NOx Emissions as Sources of Regional Background Ozone in Texas**	**1/17/2013**	**11/30/2013**	**$77,420.00**	**$77,410.16**	**$9.84**
	*ENVIRON International	Chris Emery				
12-012	**Interactions Between Organic Aerosol and NOy: Influence on Oxidant Production**	**12/19/2012**	**11/30/2013**	**$148,837.00**	**$148,546.58**	**$290.42**
	*The University of Texas at Austin	Lea Hildebrandt Ruiz		$79,463.00	$79,173.94	$289.06
	ENVIRON International	Greg Yarwood		$69,374.00	$69,372.64	$1.36
12-013	**Development of Transformation Rate of SO2 to Sulfate for the Houston Ship**	**12/14/2012**	**11/30/2013**	**$59,974**	**$59,960.93**	**$13.07**

	Channel using the TexAQS 2006 Field Study Data					
	* ENVIRON International	Ralph Morris				
13-016	**Ozonesonde launches from the University of Houston and Smith Point, Texas in Support of DISCOVER AQ**	**11/20/2012**	**11/30/2013**	**$86,667.00**	**$80,922.40**	**$5,744.60**
	*Valparaiso University	Gary Morris		$66,821.00	$66,821.00	$0.00
	University of Houston	Barry Lefer		$19,846.00	$14,101.40	$5,744.60
12-018	**The Effects of Uncertainties in Fire Emissions Estimates on Predictions of Texas Air Quality**	**1/8/2013**	**11/30/2013**	**$106,970.00**	**$106,884.06**	**$85.94**
	*The University of Texas at Austin	Elena McDonald-Buller		$85,282.00	$85,197.80	$84.20
	ENVIRON International	Chris Emery		$21,688.00	$21,686.26	$1.74
13-022	**Surface Measurements of PM, VOCs, and Photochemically Relevant Gases in Support of DISCOVER-AQ**	**1/29/2013**	**11/30/2013**	**$206,815.00**	**$192,004.33**	**$14,810.67**
	*Rice University	Robert Griffin		$89,912.00	$75,881.86	$14,030.14
	University of Houston	Barry Lefer		$116,903.00	$116,122.47	$780.53
13-024	**Surface Measurement of Trace Gases in Support of DISCOVER-AQ in Houston in Summer 2013**	**2/20/2013**	**11/30/2013**	**$90,444.00**	**$89,658.88**	**$785.12**
	*University of Maryland	Xinrong Ren				
12-028	**Implementation and evaluation of new HONO mechanisms in a 3-D Chemical Transport Model for Spring 2009 in Houston**	**1/29/2013**	**11/30/2013**	**$117,269.00**	**$114,022.02**	**$3,246.98**
	*University of Houston	Barry Lefer		$19,599.00	$16,586.51	$3,012.49
	University of California - Los Angeles	Jochen Stutz		$17,944.00	$17,709.51	$234.49
	ENVIRON International	Greg Yarwood		$44,496.00	$44,496.00	$0.00
	University of North Carolina – Chapel Hill	Will Vizuette		$35,230.00	$35,230.00	$0.00

12-032	**Collect, Analyze, and Archive Filters at two DISCOVER-AQ Houston Focus Areas: Initial Characterization of PM Formation and Emission Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms**	**1/25/2013**	**11/30/2013**	**$45,972.00**	**$43,642.21**	**$2,329.79**
	*Baylor University	Rebecca Sheesley				
12-TN1	**Investigation of surface layer parameterization of the WRF model and its impact on the observed nocturnal wind speed bias**	**2/21/2013**	**11/30/2013**	**$64,994.00**	**$64,537.12**	**$456.88**
	*University of Maryland	Daniel Tong / Pius Lee				
12-TN2	**Development of IDL-based geospatial data processing framework for meteorology and air quality modeling**	**2/21/2013**	**11/30/3013**	**$69,985.00**	**$68,362.27**	**$1,622.73**
	*University of Maryland	Daniel Tong / HyunCheol Kim				
Notes:						

Project 14-002 **STATUS: Work Plan Approved**
Master Agreement Negotiations Pending

Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC4RS Campaigns

University of Colorado - Boulder – Alan Fried
University of Maryland – Christopher Loughner
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Jim Smith

Funding Amount: $199,895

($150,508 UC-Boulder, $49,387 U of Maryland)

Executive Summary

During summer months the greater Houston-Galveston-Brazoria Metropolitan Area (HGBMA) often experiences elevated levels of ozone exceeding federal standards, particularly during hot and stagnant wind conditions. Although significant progress has been achieved understanding the major causes of these events over the past 10 years, there are still major unanswered questions related to sources of ozone from highly reactive volatile organic compounds (HRVOC's) emitted by large petrochemical facilities throughout the HGBMA. The toxic trace gas formaldehyde (CH_2O) is produced as an intermediate when these HRVOC's breakdown in the atmosphere, and ozone and radicals are formed when CH_2O further breaks down. Therefore a comprehensive understanding of CH_2O emissions, photochemical production rates, and transport processes is needed. Unfortunately, despite extensive efforts and advances from past studies, there are still major gaps in understanding related to the importance of directly emitted CH_2O from sources such as petrochemical flaring operations and automotive emissions relative to secondarily produced CH_2O from HRVOC's produced downwind, affecting large geographic areas far removed from the petrochemical facilities. Updating the emission inventories and temporal trends for CH_2O and its HRVOC precursors are two additional areas requiring attention.

To address these issues, a collaborative team, comprised of scientists from the University of Colorado, the University of Maryland, and the NASA Goddard Space Flight Facility, will analyze ambient measurements of CH_2O they acquired on the NASA P3 and DC-8 aircraft during the 2013 DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) and 2013 SEAC^{4}RS (Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys) studies, respectively.

The analysis will rely on the Community Multiscale Air Quality (CMAQ) model with Process Analysis, in very high-resolution mode (1 km resolution), driven by the WRF (Weather Research and Forecasting) meteorological model. The analysis will begin by identifying favorable time periods, such as Sept. 25, 2013, when sampling large petrochemical and refinery plumes under favorable meteorological conditions as well as other clearly identifiable sources (e.g., ship plumes, etc.) close to their source and downwind. The high resolution WRF-CMAQ model results will be compared with observations downwind at various times to arrive at updated

emission rates for CH_2O and to help in validating the model meteorology and chemistry. The CMAQ model will be run in the Process Analysis Mode to quantify the relative importance of the major CH_2O sources. The analysis will conclude with an effort to compare select airborne CH_2O measurements with 24-hour averaged cartridge measurements acquired by The Texas Commission on Environmental Quality (TCEQ) every 6th day at the Clinton, Deer Park and Channelview sites as a means to further validate and/or provide error bounds, for such long-term CH_2O data in the greater HGBMA.

Project Update

The Work Plan for Project 14-002 was approved on June 5, 2014. Contract negotiations are still on-going between the University of Colorado-Boulder and UT Austin. Final terms are very close to completion and the project is expected to begin in September. The project start date will be the date the project Work Plan was approved.

Project 14-003 **STATUS: Active – May 28, 2014**

Update and evaluation of model algorithms needed to predict Particulate Matter from Isoprene

University of North Carolina – Chapel Hill – William Vizuete

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Jim Price

Funding Amount: $200,000

Executive Summary

Terrestrial vegetation emits into the atmosphere large quantities (~500 teragrams C) of the reactive di-olefin isoprene (C_5H_8). Isoprene emissions in eastern Texas and northern Louisiana are some of the largest in the United States. Photochemical oxidation of isoprene leads to significant yields of gas-phase intermediates that contribute to fine particulate matter (PM2.5). The production of isoprene-derived PM2.5 is enhanced when mixed with anthropogenic emissions from urban areas like those found in Houston. To predict PM production from isoprene requires fundamental parameters needed to describe the efficiency with which gas phase intermediates react on the surface of atmospheric particles. Recently, EPA updated a regulatory chemical mechanism to include the formation of these new gas-phase isoprene-derived intermediates. Furthermore, the project investigators recently collaborated with the EPA to update the CMAQ model to predict isoprene-derived PM explicitly across the eastern US. This updated gas- and aerosol-phase framework found in CMAQ remains to be validated against systematically conducted chamber experiments. Thus, we first propose to conduct a series of new experiments at UNC to quantitatively measure the reactive uptake of the two predominant isoprene-derived gas phase intermediates to PM of different inorganic compositions. By providing these new fundamental measurements, we will be able to more directly evaluate the aerosol-phase processes added to the model. This work will produce a model evaluation of isoprene SOA formation against existing UNC outdoor smog chamber experiments. This project will also deliver performance data needed to bound uncertainties in key parameters used by CAMx to predict isoprene derived PM. This work directly addresses the stated priority area of investigating the transformation of gas-phase pollutants to particulate matter that impact Texas air quality.

Project Update

Progress on Project 14-003 is summarized below by Task:

Task 1. Integration of Gas-Phase Epoxide Formation and Subsequent SOA Formation into UNC MORPHO Box Model

Thus far the integration and simulations using the updated SAPRAC07TC chemical mechanism are complete. These simulations include characterization experiments using wall reaction rate constants. Implementation of the multiphase chemistry of isoprene derived epoxides continues. In the past month the team has been debugging and refining the box model which simulates the uptake of gaseous IEPOX onto an aerosol of variable acidity,

temperature, and relative humidity. In particular, a time stepping algorithm has been implemented that finds a time step that is small enough to keep the solution error within a particular tolerance while keeping it large enough so that the solution is found within a reasonable amount of computing time. Additionally, errors in the code related to wall loss calculations have been corrected. The team intends to complete implementation and begin simulations of existing experiments in the next quarter.

Task 2. Synthesis of Isoprene-derived Epoxides and Known SOA Tracers

Discussions with Dr. Avram Gold concerning synthesis protocols are complete. As a result of these meetings, the synthesis protocols for SOA constituents are now finalized and scheduled for his lab. Starting materials for synthesis of the SOA constituents have been ordered.

Task 3. Indoor Chamber Experiments Generating SOA Formation Directly from Isoprene Derived Epoxides

Preparation of the UNC indoor 10---m3 flexible Teflon chamber for use in this project. The team also trained students, prepared teflon filters, and calibrated GC/MS, IC, CIMS, and LC/DAD---ESI---QTOFMS instruments. Finally, an experimental plan has been proposed and experiments placed on the calendar. The next 2---3 months will yield enough experimental data to evaluate by the model. These will include wall---loss experiments (including for IEPOX and MAE), as well as actual experiments outlined in the work plan.

Task 4. Modeling of Isoprene-derived SOA Formation From Environmental Simulation Chambers

Work on this task has not yet begun.

All funds allocated to the project are intended to be utilized by June 30, 2015.

Project 14-004 **STATUS: Active – June 20, 2014**

Emission Source region contributions to a high surface ozone episode during DISCOVER-AQ

University of Maryland – Christopher Loughner
Morgan State University – Melanie Follette-Cook
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Doug Boyer

Funding Amount: $109,111
($55,056 Univ. of Maryland, $54,055 Morgan State Univ.)

Executive Summary

The highest ozone air pollution episode in the Houston, TX region in 2013 occurred September 24-26, which coincided with the DISCOVER-AQ (Deriving Information on Surface Conditions and Vertically Resolved Observations Relevant to Air Quality) field campaign. The maximum 8-hour average ozone peaked on September 25 at LaPorte Sylvan Beach reaching 124 ppbv. We propose to analyze this air pollution episode to quantify how emissions from various source regions (i.e., Houston, Dallas, Beaumont/Port Arthur, Lake Charles, LA, Oklahoma, etc.) contributed to Houston's poor air quality. This work will examine the importance of regional emissions and transport on local air quality.

The investigators will use a combination of model simulations and space-, aircraft-, and ground-based observations to investigate the roles of both regional transport and local emissions on air quality in Houston, TX for this event. This work will improve understanding of ozone formation and accumulation by examining the spatial patterns of emissions within and outside of Texas and the transport processes that contributed to high ozone in Houston.

The investigators will use Weather Research and Forecasting (WRF) and Community Multi-scale Air quality (CMAQ) model output along with ground- and aircraft-based observations obtained during the DISCOVER-AQ field campaign to identify plumes that entered the Houston metropolitan area and contributed to high surface ozone concentrations. The investigators will identify the origins of plumes by calculating back trajectories from the WRF simulation. CMAQ simulations performed with source apportionment will be analyzed to determine the contributions of various source regions on surface ozone concentrations in the Houston metropolitan area. In addition, satellite observations (Ozone Monitoring Instrument (OMI) tropospheric nitrogen dioxide, OMI ozone profiles, Measurement Of Pollution In The Troposphere (MOPITT) carbon monoxide, and Moderate Resolution Imaging Spectrometer (MODIS) and Visible Infrared Imaging Radiometer Suite (VIIRS) aerosol optical depth) will be analyzed to determine if they were able to detect the regional transport of air pollution and subsequent buildup in the Houston metropolitan area.

Project Update

The contracts with the University of Maryland and Morgan State University are in place and the Work Plan and QAPP are approved. During this quarter, the team reviewed the Work Plan and QAPP. The team developed a plan to accomplish the project tasks. The team will begin by processing WRF model output to prepare input files for the RIP (Read/Interpolate/Plot) program for calculating back trajectories, run RIP, create CMAQ input files, and perform CMAQ model simulations.

Project 14-006 **STATUS: Active – June 12, 2014**

Characterization of Boundary-Layer Meteorology during DISCOVER-AQ Using Radar Wind Profiler and Balloon Sounding Measurements

Sonoma Technology, Inc. – Clinton MacDonald
Valparaiso University – Gary Morris
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Dave Westenbarger

Funding Amount: $65,588
($49,979 Sonoma Technology, $15,609 Valparaiso)

Executive Summary
As part of the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program in August and September 2013, Sonoma Technology, Inc. and the National Oceanic and Atmospheric Administration, with support from the AQRP, operated radar wind profilers (RWPs) at four sites in the greater Houston area to collect boundary layer wind data. In addition, a permanent network of three RWPs also provided data during this study. Also, Pennsylvania State University and the Valparaiso University/University of Houston team conducted daily meteorological and ozone soundings on most days during DISCOVER-AQ. The combination of these data offers a rich source of boundary layer meteorological data and can be used to provide insight into the processes that influence the air quality in Houston.

To address questions about meteorological conditions during the DISCOVER-AQ study and to provide useful information to other researchers, this project will (1) characterize boundary layer meteorological processes on all aircraft flight days and high ozone days during the DISCOVER-AQ study period; (2) provide context to the DISCOVER-AQ boundary layer characteristics by comparing them to characteristics observed on high ozone days during the TexAQS-II project in 2005 and 2006 and over the past 10 years for the month of September; and (3) provide continuous daytime boundary layer height data at the seven RWP sites for the entire study period. The results from this project will be documented in a final report, distributed to other researchers, and presented at an end-of-project meeting in Austin in June 2015.

Project Update
During June, July, and August, 2014, the project team held internal project progress meetings to discuss project roles, assignments, and deadlines; began gathering relevant meteorological and air quality data from the DISCOVER-AQ program necessary to complete the project; calculated mixing heights from radar wind profilers and ozonesondes operated in the Houston area during DISCOVER-AQ, and performed an initial assessment of meteorological and air quality conditions on DISCOVER-AQ flight days and other days with high ozone levels in the Houston area.

Data gathered for this project during the June-August 2014 period included surface and upper-level meteorological plots, ozonesonde data from the three Houston-area launch sites, radar wind profiler data from the seven Houston-area profilers, surface ozone data, and radar and satellite imagery. The bulk of the work performed during this time period involved calculating mixing

heights (Task 3 of this project), as these data will be necessary for the comprehensive characterization of weather and air quality conditions in the Houston-area during the DISCOVER-AQ program (Task 1) and the comparison of the results from Task 1 to weather and air quality conditions observed during the 2006 TexAQS program (Task 2).

Over the next quarter, work will focus on concluding the calculation of mixing heights (Task 3), completing the characterization of weather and air quality conditions in the Houston-area during the DISCOVER-AQ program (Task 1), and comparing the results found in Task 1 to weather and air quality conditions observed during the 2006 TexAQS program (Task 2), with the anticipation of completing a draft final report by November 30, 2014.

Project 14-007 **STATUS: Active – June 23, 2014**

Improved Analysis of VOC, NO2, SO2 and HCHO data from SOF, mobile DOAS and MW-DOAS during DISCOVER-AQ

Chalmers University – Johan Mellqvist
University of Houston – Barry Lefer
AQRP Project Manager – David Sullivan
TCEQ Project Liaison – John Jolly

Funding Amount: $97,260
($74,179 Chalmers, $23,081 UH)

Executive Summary

Mobile optical remote sensing measurements by the SOF and mobile DOAS techniques were carried out in the Houston area during September 2013 as part of the NASA Discover Air Quality experiment. Atmospheric gas column measurements of SO_2, NO_2, HCHO and VOCs were carried out in a box around the Houston Ship channel, in parallel with flights by two aircraft from NASA. In this project the collected optical remote sensing data will be reanalyzed, improved and compared to other data. In particular, the investigators will work with radiative transfer modeling to minimize cloud effects.

In addition, during the 2013 field campaign a new VOC sensor was used to map ratios of the ground concentrations of alkanes and aromatic VOCs downwind of various industries. In this project the investigators will refine the spectral analysis for measurements of the aromatic VOCs from this sensor and compare the data to parallel measurements with other techniques and write a scientific paper.

This project will support the AQRP priority research area: "Improving the understanding of ozone and particulate matter (PM) formation, and quantifying the characteristics of emissions in Texas through analysis of data collected during the DISCOVER-AQ and SEAC4RS campaigns."

Project Update

During the period June 21 to August 31 the following tasks have been carried out in collaboration between Chalmers University of technology and University of Houston:

a) A retrieval scheme and automatic retrieval algorithm has been developed for multiple angle measurements by DOAS.

b) A radiative transfer model named Sciatran has been installed and compiled on a computer with the objective to improve the column measurements from DOAS. Various test cases have been run and appropriate input data from the NASA discover database has been compiled (partly).

c) Comparative data from ground sites and the two airplanes within NASA DISCOVER-AQ has been compiled (partly).

Project 14-008 **STATUS: Active – April 17, 2014**

Investigation of Input Parameters for Biogenic Emissions Modeling in Texas during Drought Years

The University of Texas at Austin – Elena McDonald-Buller

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Barry Exum

Funding Amount: $175,000

Executive Summary

The role of isoprene and other biogenic volatile organic compounds (BVOCs) in the formation of tropospheric ozone has been recognized as critical for air quality planning in Texas. In the southwestern United States, drought is a recurring phenomenon and, in addition to other extreme weather events, can impose profound and complex effects on human populations and the environment. Understanding these effects on vegetation and biogenic emissions is important as Texas concurrently faces requirements to achieve and maintain attainment with the National Ambient Air Quality Standard (NAAQS) for ozone in several large metropolitan areas. Previous research has indicated that biogenic emissions estimates are influenced by potentially competing effects in model input parameters during drought and that uncertainties surrounding several key input parameters remain high. The primary objective of the project is to evaluate and inform improvements in the representation of one of these key input parameters, soil moisture, through the use of simulated and observational datasets. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) will be used to explore the sensitivity of biogenic emission estimates to alternative soil moisture representations.

Project Update

Progress on Project 14-008 is summarized below by Task:

Task 1. Investigation and Evaluation of Soil Moisture Datasets

Work during this quarter has focused on identifying and describing the networks [West Texas Mesonet, Climate Research Network (CRN), Soil Climate Analysis Network (SCAN), Cosmic Ray Soil Moisture Observing System (COSMOS)] that operate soil moisture observation stations in Texas as well as an analysis of data collected during 2006-2013 at selected stations (including two in the Oklahoma Mesonet representative of soil moisture conditions for northeast Texas).

Seven soil types are found in Texas, including Alfisols, Aridsols, Entisols, Inceptisols, Mollisols, Ultisols, and Vertisols; their spatial distribution is shown in Figure 1. The Soil Survey Geographic Data Base (SSURGO), which was created using field methods and aerial photos, provides the most detailed level of soil information. The detailed SSURGO soil survey maps, or if unavailable data on geology, topography, vegetation, and climate together with satellite images, have been generalized to create the State Soil Geographic Data Base

(STATSGO). STATSGO is mapped on USGS 1:250,000-scale topographic quadrangle series and is the source of the USDA soil taxonomy classification (order) mapping shown in Figure 1.

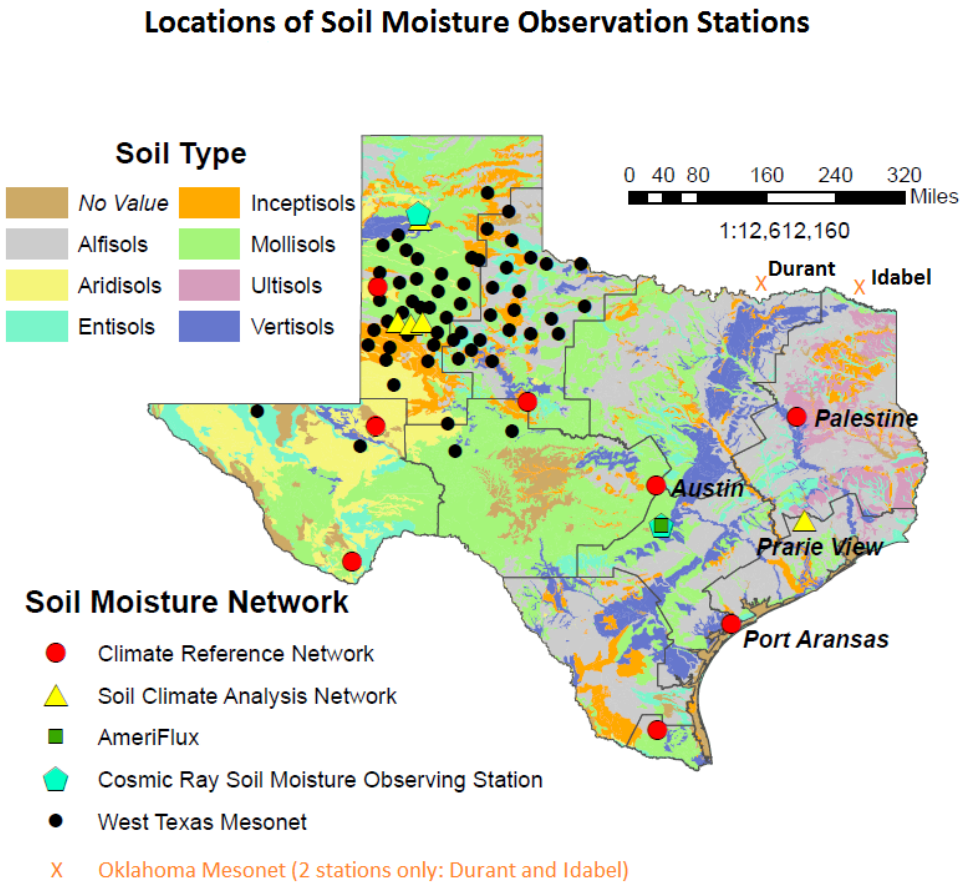

Figure 1. Locations of soil moisture observation stations in Texas overlain on a soils type map. The boundaries show the ten Texas climate divisions. Measurement data collected at the labeled sites in eastern Texas and southeastern Oklahoma during 2006-2013 are currently being investigated.

Initial analyses of observational soil moisture data are focusing on the four labeled sites in Texas in Figure 1 (i.e., “Palestine”, “Austin”, “Prairie View”, “Port Aransas”) in addition to two Oklahoma Mesonet stations (representative of conditions in northeastern Texas) adjacent to the Red River in southeastern Oklahoma (“Durant” and “Idabel”). The hourly data for Texas stations were retrieved directly from the SCAN and CRN websites; summary daily data for the Oklahoma Mesonet stations were accessed via the North American Soil Moisture Database (NASMD) and were only available (at this time) through September 2012.

A completeness criteria of 70% for individual annual seasons was applied. (For our purposes: winter=Dec/Jan/Feb, spring=Mar/Apr/May, summer=Jun/Jul/Aug, fall=Sep/Oct/Nov). On average across all years, seasonal soil moisture increases with increasing depth All depths show a similar seasonality with lowest soil moisture values during summer and fall and relatively higher values during spring and, especially, winter; this seasonal trend was observed across all locations. Results at each available location at 100 cm show strong seasonality (though with less consistency) and increased soil moisture compared to 5 cm; values at Port Aransas are substantially lower compared to the other locations. The investigation of observed soil moisture at these stations (hourly, daily, and seasonal), including an analysis of inter-annual variability with particular attention to drought year 2011, is on-going.

Task 2. Comparison of Simulated and Observed Soil Moisture

The North American Land Data Assimilation System Phase 2 (NLDAS-2) provides high-resolution simulations of land surface variables, including soil moisture. This dataset cover the period from Jan 1979 up to present. NLDAS-2 (Mitchell et al., 2004; Xia et al., 2012) integrates a large quantity of observation-based and model reanalysis data to drive land-surface models, and executes at 1/8th-degree grid spacing over central North America. Three land-surface models are included in NLDAS-2: NASA's Mosaic, NOAA's Noah, and Princeton's VIC. Mosaic was developed by Koster and Suarez (1994, 1996) to account for subgrid vegetation variability. Analysis of the Mosaic and Noah dataset and comparisons with in-situ measurements at the four sites of Prairie View, Port Aransas, Austin and Palestine are being conducted for the time period of 2006-2013.

Task 3. Preparation of MEGAN Simulations

This task has not yet been initiated.

Task 4. Sensitivity of Biogenic Emission Estimates to Soil Moisture

This task has not yet been initiated.

All funds allocated to the project are intended to be utilized by June 30, 2015.

Project 14-009 **STATUS: Active – July 1, 2014**

Analysis of Surface Particulate Matter and Trace Gas Data Generated during the Houston Operations of DISCOVER-AQ

Rice University – Robert Griffin
University of Houston – Barry Lefer
AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $219,232
($109,867 Rice, $109,365 UH)

Executive Summary

In recent years, the National Aeronautics and Space Administration (NASA) has placed considerable emphasis on the use of satellite remote sensing in the measurement of species such as O_3 and PM that constitute air pollution. However, additional data are needed to aid in the development of methods to distinguish between low- and high-level pollution in these measurements. To that end, NASA established a program titled Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ). DISCOVER-AQ began in summer 2011 with work in the Mid-Atlantic Coast that featured satellite, airborne, and ground-based sampling. The DISCOVER-AQ program conducted operations in and near Houston in September 2013.

During the Houston operations of DISCOVER-AQ, there was a need for ground-based measurement support. The predecessor to this project filled that need by providing quantitative measurements of sub-micron particle size and composition and mixing ratios of volatile organic compounds (VOCs) and other photochemically relevant gases such as O_3 and oxides of nitrogen (NO_x = nitric oxide (NO) plus nitrogen dioxide (NO_2)). The instrumentation for these measurements was deployed using the University of Houston (UH) mobile laboratory. The current project focuses on the analysis of data generated during the mobile laboratory operations during DISCOVER-AQ. To date, work has focused simply on contracting issues and development of a work plan and a quality assurance plan.

Project Update

During June 2014, most effort related to Project 14 was focused on development of a Work Plan and Quality Assurance Project Plan. These documents were approved late in the month, and the Project commenced officially at the beginning of July.

During July and August 2014, significant effort was placed on determination of particle emission factors as a function of size (if possible) when mobile laboratory sampling was obviously occurring within a specific plume from gasoline-fueled motor vehicles. Generally this occurred while the mobile laboratory was on-road. As such, determination of emissions factors predominantly is focused on organic aerosol of particle diameter smaller than one micron. A protocol for determination of these emission factors has been developed. A ratio of enhancements in organic aerosol to enhancements in either carbon monoxide (CO) or nitric oxide (NO) is being compared to known emission factors for CO or NO (taken from Environmental Protection Agency (EPA) modeling). Enhancements are defined relative to the

background immediately before and after the plume sampling. Plumes of organic aerosol while the mobile laboratory was on-road have been identified for the DISCOVER-AQ period, and the corresponding enhancements in organic aerosol have been calculated. Eight specific episodes have been identified; enhancements in sub-micron organic aerosol ranged from 14 to 215 micrograms per cubic meter. Current efforts are focused on calculating the ratio of these values to appropriate values of CO or NO. With the high-definition cameras available on the mobile laboratory, the type of vehicle is being identified for each on-road event. Therefore, multiple points will be combined to provide data across vehicle type. An additional approach is to combine points across location type. The appropriate emission factor for vehicle type or location is being determined by regression between the enhancement ratios and the EPA estimates.

Other large aerosol enhancements (beyond those from gasoline-powered motor vehicles) also are being characterized as part of these analysis activities. The time series generated during the periods of operation of the mobile laboratory were examined, and the emission sources associated with these peak events were identified based on field observations and thorough analysis of video footage obtained from the four different cameras installed in the mobile laboratory. The continuous operation of these video cameras allowed capture of a peripheral view of the different events occurring while the mobile laboratory was in transit. For consistency purposes, short-term increases in concentrations of sub-micron PM were classified as peak events when the average PM background concentration for the specific time interval and location was exceeded by at least three standard deviations. Twenty-six peak events (in addition to those described above) associated with both mobile and point sources were identified during the period of monitoring. Mobile sources including heavy and light duty diesel vehicles and a tanker ship transporting bulk-liquid chemicals were identified as the responsible sources for the PM concentration peaks in twelve events. Point sources corresponding to petrochemical facilities (e.g., storage tanks, stack emissions, and gas flares) and biomass burning activities were associated with nine and five of the observed peak events, respectively. Significant increases in the organic fraction of PM were primarily detected in the peak events attributed to mobile sources and biomass burning, while sulfate was generally the largest component observed in the peak events attributed to emissions from petrochemical facilities. Concentrations of PM with maximum levels between 15 and 100 micrograms per cubic meter were observed in events related to mobile sources and biomass burning activities, while more moderate increases were detected for PM concentration peaks associated with operations in petrochemical facilities (maximum concentration between 4 and 30 micrograms per cubic meter). Analysis of the mass spectra of the observed peak events is being conducted in order to gain further insight into the chemical characteristics of the associated source profiles. Analysis of mass spectra in conjunction with aerosol size distributions corresponding to each observed PM peak event is being conducted currently as well to investigate how chemical characteristics of PM vary with particle size.

Work has begun to characterize the oxidized nature of the PM as well, which provides insight into whether the particle was emitted from a primary source or formed directly in the atmosphere. This is first being approached via the application of factor analysis by positive matrix factorization (PMF) for identification of aerosol components (e.g., hydrocarbon-like organic aerosol and various forms of oxidized organic aerosol). In addition, the feasibility of conducting a three-dimensional (3D) factorization technique, specifically called parallel factor

analysis (PARAFAC), is being evaluated. The extension of the two-dimensional analysis (PMF) to a 3-D analysis of size resolved organic composition data set has been reported recently, but only a few studies have employed this technique for analysis of HR-AMS data sets. Application of PARAFAC (sometimes referred as PMF3) on the HR data set generated during DISCOVER-AQ likely will allow the identification of additional aerosol components and provide more robust information on their size distribution. The necessary formatting of the data set is being conducted currently, and preliminary PARAFAC application will be performed once the formatting is complete.

Lastly, significant effort was made to have all promised data in a form that will be readily shared with other AQRP investigators. It is expected that all data for sharing will be provided to collaborators during September 2014.

Project 14-011 **STATUS: Active – June 23, 2014**

Targeted Improvements in the Fire Inventory from NCAR (FINN) Model for Texas Air Quality Planning

The University of Texas at Austin – Elena McDonald-Buller
Environ – Christopher Emery

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Jim MacKay

Funding Amount: $179,586
($151,167 UT-Austin, $28,419 Environ)

Executive Summary

Wildland fires and open burning can be substantial sources of ozone precursors and particulate matter. The influence of fire events on air quality in Texas has been well documented by observational studies. During the 2012-2013 fiscal year of the Air Quality Research Program (AQRP), Dr. Elena McDonald-Buller, Dr. Christine Wiedinmyer, and Mr. Chris Emery led a project (#12-018) that evaluated the sensitivity of emissions estimates from the Fire INventory from NCAR (FINNv1; Wiedinmyer et al. 2011) to the variability in input parameters and the effects on modeled air quality using the Comprehensive Air Quality Model with Extensions (CAMx; ENVIRON, 2011). The project included an analysis of the climatology of fires in Texas and neighboring regions, comparisons of fire emission estimates between the FINN and BlueSky/SmartFire (Larkin 2009; Chinkin et al., 2009) modeling frameworks, evaluation of the sensitivity of FINN emissions estimates to key input parameters and data sources, and assessment of the effects of FINN sensitivities on Texas air quality. Among the many findings of the study were the needs for targeted improvements in land cover characterization, burned area estimation, fuel loadings, and emissions factors. These needs were particularly pronounced in areas with agricultural burning. This project addresses specific improvements in FINN that will support fire emissions estimates for Texas and the next public release of the FINN model. Fire emissions and air quality modeling will focus on 2012 to support TCEQ's air quality planning efforts.

Project Update

Progress on Project 14-011 is summarized below by Task:

Task 1. Regional Land Cover Characterization

Task 1 of this work is applying land cover data specific to Texas, as an alternative to global scale land cover mapping from the MODIS Land Cover Type (LCT) product, which is the FINN default. In addition, a mapping of crop types will be developed for incorporation in the FINN land cover database that focuses on Texas and surrounding states. The team is using a land use/land cover database for Texas and surrounding states developed by Popescu et al. (2011; *http://m.tceq.texas.gov/assets/public/implementation/air/am/contracts/reports/oth/5820564593FY0925-20110419-tamu-expension_tx_lulc_arboreal_vegetation.pdf*). For the

characterization of croplands, the team has selected the following: *U.S. Department of Agriculture (USDA), National Agricultural Statistical Service (NASS) Cropland Data Layer (CDL): http://nassgeodata.gmu.edu/CropScape/*.

Task 2. Mapping of Croplands

A mapping and cross-tabulation of land cover classifications associated with agricultural operations between the 2012 NASS and Popescu et al. (2011) databases is being developed for Texas using the spatial analyst package in ArcGIS for this task.

Task 3. Estimation of Burned Area

This task has not yet been initiated.

Task 4. Sub-grid scale Partitioning of NO_x Emissions to NO_z in Fire Plumes

This task has not yet been initiated.

Task 5. CAMx Sensitivity Studies

This task has not yet been initiated.

All funds allocated to the project are intended to be utilized by June 30, 2015.

Project 14-016 **STATUS: Active – June 4, 2014**

Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations

Environ – Greg Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Amount: $271,911

Executive Summary

The exchange of gases and aerosols between the Earth's surface and the atmosphere is an important factor in determining atmospheric composition and regional air quality. Accurate quantification of emission fluxes is a necessary step in developing air pollution control strategies. In some cases emissions can be directly measured (e.g., point sources with continuous emission monitors) or can be estimated with reasonable confidence (e.g., point sources that have well-defined operating parameters). In contrast, large uncertainties are associated with area sources including emissions from vegetation, and in particular, emissions of biogenic volatile organic compounds (BVOCs). Vegetation is the largest source of VOC emissions to the global atmosphere. The oxidation of BVOCs in the atmosphere affects ozone, aerosol and acid deposition. Current BVOC emission estimates are based on measurements for individual plants that must be scaled up to represent landscapes and adjusted for environmental conditions. There is a critical need for independent BVOC emission inputs for air quality models.

AQRP Project 14-016 will use aircraft observations from the 2013 Southeast Atmosphere Study (SAS) and the 2006 Texas Air Quality Study (TexAQS) to assess and reduce uncertainties associated with a widely-used BVOC emissions model, namely the Model of Emissions of Gases and Aerosol from Nature version (MEGAN). The eddy covariance technique will be used to directly quantify BVOC emission fluxes for all suitable aircraft observations from the SAS study. Using the relationship between BVOC fluxes and concentrations derived from this subset of SAS aircraft data, BVOC emission fluxes will be estimated for 2013 SAS and 2006 TexAQS flights in the southeastern U.S. and Texas, respectively. In addition, the investigators will improve the land cover and emission factor input data sets that are considered the major uncertainties associated with BVOC emission estimates. The overall benefit of this project will be more accurate BVOC emission estimates that can be used in Texas air quality simulations that are critical for scientific understanding and the development of effective regulatory control strategies that will enhance efforts to improve and maintain clean air.

Project Update

This AQRP project is being performed by ENVIRON International Corporation (ENVIRON) as prime contractor, and NOAA and Battelle/Pacific Northwest National Laboratory as sub-contractors. A summary of activities for the period June 1, 2014 through August 31, 2014 is presented below.

Task 4: Development of MEGAN Biogenic Emission Inventories and Inventory Evaluation using Regional Photochemical Modeling

ENVIRON carried out mesoscale meteorological modeling of the period June 1-July 15, 2013 with the Weather Research and Forecast (WRF) Model (Skamarock et al. 2008). ENVIRON developed model inputs and ran the model on the nested 36/12 km modeling grids that encompass the NOAA/NCAR aircraft flight tracks to be used to develop biogenic emissions. ENVIRON began evaluation of WRF output fields against CAMS station wind and temperature data within Texas and ds472 airport meteorological data within and outside of Texas.

ENVIRON prepared a biogenic emission inventory for June 1-July 15, 2013 using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) (Guenther et al., 2012). In the past, ENVIRON has used MEGAN input data available in ArcGIS format, but the developers of MEGAN plan to release future MEGAN inputs (including inputs for this project) in NetCDF format. ENVIRON developed software that takes MEGAN input data in NetCDF format and reformats the data into the ASCII format used by MEGAN. Using the WRF output from the initial model run to generate weather data for MEGAN, we ran MEGAN for the June 1-July 15, 2013 episode with default landcover and emission factor inputs. Episode average isoprene and monoterpene emissions on the 12 km modeling domain are shown in Figure 1. We verified that the NetCDF reformatting tool and MEGAN modeling system are functioning properly by comparing the magnitude and spatial patterns of episode average isoprene and terpenes across the 36 km and 12 km grids with July episode average maps from the biogenic emission inventory prepared for the Western Governors Association by ENVIRON and Dr. Guenther (Sakulyanontvittaya et al., 2012). If no further WRF runs are needed, this MEGAN emission inventory will serve as the base case default biogenic emission inventory against which we will compare MEGAN inventories developed with new inputs developed in Tasks 1-3.

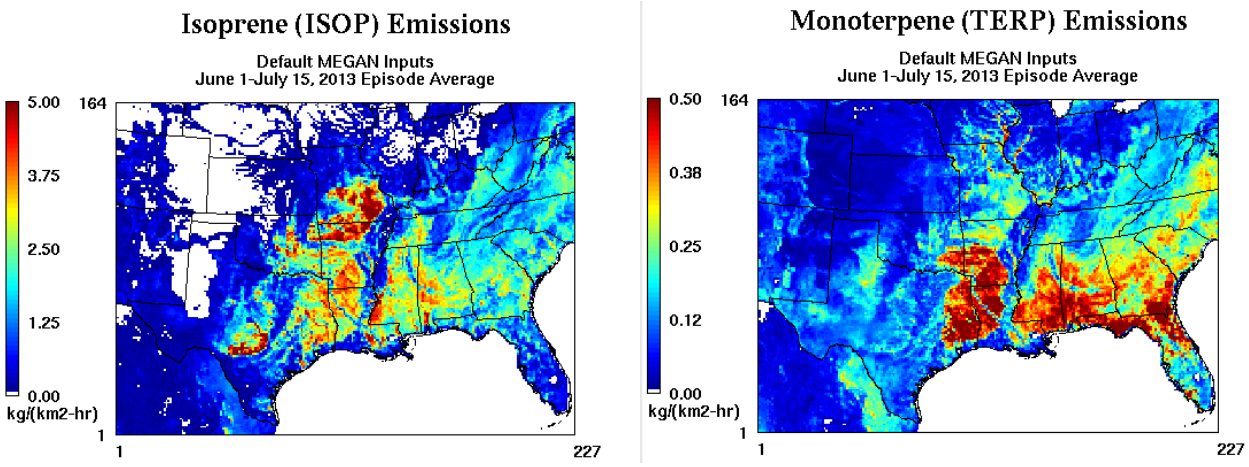

Figure 1. June 1-July 15, 2013 episode average MEGAN isoprene (left panel) and monoterpene (right panel) emissions developed using default land cover and emission factor assumptions.

Task 5: Project Management

ENVIRON, NOAA and PNNL/Battelle developed subcontracting agreements for NOAA and PNNL/Battelle for work to be done under Tasks 1-3.

The development of subcontracting agreements has progressed more slowly than expected. We expect that the schedule for Tasks 1-3 will be extended by 3-4 months. However, sufficient progress on Task 4 has been made that the project remains on schedule for completion with delivery of the final AQRP-reviewed report by June 30, 2015.

We intend to use all funds allocated to the project by 06/30/2015.

References

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Project 14-017 **STATUS: Active – July 8, 2014**

Incorporating Space-borne Observations to Improve Biogenic Emission Estimates in Texas

University of Alabama - Huntsville – Arastoo Pour Biazar
Rice University – Daniel Cohan

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Amount: $199,982
($137,003 UAH, $62,979 Rice)

Executive Summary

One of the challenges in understanding the Texas air quality has been the uncertainties in estimating the biogenic hydrocarbon emissions. Biogenic volatile organic compounds, BVOCs, play a critical role in atmospheric chemistry, particularly in ozone and particulate matter (PM) formation. In southeast Texas, BVOCs (mostly as isoprene) are the dominant summertime source of reactive hydrocarbon. Despite significant efforts by the State of Texas in improving BVOC estimates, the errors in emission inventories remain a concern. This is partly due to the diversity of the land use/land cover (LU/LC) over southeast Texas coupled with a complex weather pattern, and partly due to the fact that isoprene is highly reactive and relating atmospheric observations of isoprene to the emissions source (vegetation) relies on many meteorological factors that control the emission, chemistry, and atmospheric transport.

BVOC estimates depend on the amount of radiation reaching the canopy (Photosynthetically Active Radiation, PAR), and temperature. However, the treatment of temperature and PAR is not uniform across emissions models and still poses a problem when evaluating the inventories. Recent studies show that the largest uncertainty comes from the model solar radiation estimates and that using satellite-based PAR would be preferable. Emissions from soils also remain as one of the poorly quantified sources of NOx (nitrogen oxides) in most air quality models. Soils can be the largest source of NOx in rural regions where low-NOx conditions make ozone production efficiency especially high, contributing to background ozone levels.

The overall objective of the current activity is to advance our understanding of Texas Air Quality by utilizing satellite observations and the new advances in biogenic emissions modeling to improve biogenic emission estimates. This work specifically addresses a priority area in Texas AQ studies by improving biogenic emission estimates. In particular, the objectives are:

(1) To provide satellite-based PAR estimates for Texas during selected periods of 2006 and the Discover-AQ period (September, 2013).

(2) To produce an improved biogenic emission estimate for Texas and help in the evaluation of biogenic emission inventories over Texas by providing the best model representation of the atmospheric condition during the observations used for evaluation.

(3) To prepare and use a new soil NOx scheme that provides more mechanistic representation of how emissions respond to nitrogen deposition, fertilizer application, and changing meteorology.

The University of Alabama in Huntsville (UAH) currently generates a set of products from the Geostationary Operational Environmental Satellite (GOES) that includes surface incident short-wave radiation as well as cloud albedo and cloud top temperature. Under this activity, UAH will produce the Photosynthetically Active Radiation (PAR) needed in the estimation of biogenic hydrocarbon emissions. Satellite-derived PAR will be evaluated against previous satellite-based products as well as surface observations for the summer of 2006 and also during Texas Discover-AQ campaign. Furthermore, the new PAR retrievals will be used in MEGAN (the Model of Emissions of Gases and Aerosols from Nature) to generate BVOC emissions.

The new soil NOx scheme to be used is an implementation of the Berkeley-Dalhousie Soil NOx Parameterization (BDSNP) within MEGAN. A series of sensitivity simulations will be performed and evaluated against Discover-AQ observations to test the impact of satellite-derived PAR and the new soil NOx emission model on air quality simulations.

Project Update

Contract negotiations were completed on August 22, 2014, and the project start date was back dated to July 8, 2014, when the Work Plan was approved. Project activities to date have been limited, but are expected to proceed in the coming months.

Project 14-023 **STATUS: Active – May 23, 2014**

Assessment of Two Remote Sensing Technologies to Control Flare Performance

The University of Texas at Austin – Vincent Torres
Aerodyne Research, Inc. – Scott Herndon
Leak Surveys, Inc. – Joshua Furry
Providence Photonics, LLC – Yongshen Zeng

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Russell Nettles

Funding Amount: $480,741
($239,773 UT-Austin, $157,066 Aerodyne, $26,716 Leak Survey, $57,186 Providence Photonics)

Executive Summary
Industrial flares are devices used at industrial facilities to safely dispose of relief gases in an environmentally compliant manner through the use of combustion. Recent studies of industrial air- and steam-assisted flares have shown that merely complying with federal regulations like the Environmental Protection Agency's 40CFR § 60.18 and 40CFR § 63.11, do not ensure the flare will operate with at high combustion efficiency when combusting hydrocarbons over the entire range of operating scenarios for dual service flares. For vent gas streams containing hydrocarbons, the combustion efficiency (CE) is the percentage of the total hydrocarbon stream entering the flare that burns completely to form only carbon dioxide and water. It is desirable to have high combustion efficiency at all times to maximize flare performance.

The purpose of the proposed project is to conduct a series of field tests using an operational, full-scale industrial flare at a Petrologistics, LLC plant in Houston, Texas, to determine the technical, economic and operational feasibility of two approaches designed to maximize flare performance. These approaches continuously measure or determine the flare's combustion efficiency and would use this information to adjust the steam assist to the flare to adjust the flare's performance. To assess the technical performance of the approaches, the combustion efficiency measurements of each approach will be compared to an independent direct sampling measurement (the reference measurement) of the flare's combustion efficiency to determine the accuracy and completeness of the measurements obtained from the two approaches. For the field tests, the performance of the flare will not be controlled by either of the two approaches so that the prescribed test plan can be conducted with the flare. After the test series, the economic and operational feasibility will be evaluated based on the operational and safety characteristics observed during the tests and the estimated cost to implement each approach.

Project Update
An initial site visit to the Petrolgistics, LLC plant was conducted on June 12. The project team spent most of the morning reviewing, understanding and discussing the process flows, typical compositions of the vent gas and plant fuel gas (C2s and lighter), ability of the plant to vary these flows and compositions, and other information required to update the QAPP and develop the field test plan. Agreements were made on how the sampling would be conducted and a date (December 1-5, 2014) for the field tests was selected.

On June 26, 2014, the flare site contact for Petrologistics, Vance Darr, notified the Principal Investigator that the representative from Flint Hills Resources (FHR), who was present during the planning meeting on June 12, informed Petrologistics that FHR will not continue participation in the study after the acquisition of Petrologistics is complete. FHR is in the process of purchasing Petrologisitics and this acquisition will be concluded before the study can be completed. Mr. Darr reviewed the purpose and scope of the study with FHR, and Petrologisitcs involvement with the TCEQ and EPA. Nonetheless, FHR has elected not to participate in this study.

From June 26 until August 12, the project team, along with the project's Industry Advisory Committee, attempted to find another host site for the project. We were unable to find one and made the decision to terminate the project as time to locate another host site had expired. Therefore, on August 15, 2014, notice was sent to the AQRP Project Manager that the project would need to be terminated and all unspent funds returned to the AQRP.

No further work will be performed or costs incurred on this project.

Project 14-024 **STATUS: Active – June 18, 2014**

Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ Data, Modeling and Experiments

The University of Texas at Austin – Lea Hildebrandt Ruiz
Environ – Greg Yarwood
University of California – Riverside – Gookyoung Heo

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $300,000
($163,282 UT-Austin, $101,404 Environ, $35,314 UC – Riverside)

Executive Summary

The United States Environmental Protection Agency recently lowered the annual National Ambient Air Quality Standard (NAAQS) for particulate matter smaller than 2.5 μm in diameter ($PM_{2.5}$) from 15 to 12 μg m^{-3}. This new annual standard brings the Houston region near to non-attainment for $PM_{2.5}$, underlining the importance of understanding the composition and sources of $PM_{2.5}$ in Houston. Recent measurements made during the month of September indicate that a majority of $PM_{2.5}$ in the Houston region is composed of organic material. An improved understanding of Houston organic aerosol is therefore essential and will directly benefit the Texas Commission on Environmental Quality (TCEQ) in understanding how to manage Houston's air quality.

Project 14-024 will focus on improving our understanding of the contributions of intermediate volatility organic compounds (IVOC) to formation of secondary organic aerosol (SOA). IVOCs, specifically large alkanes and polycyclic aromatic hydrocarbons, are largely excluded from current emission inventories because these compounds fall between the definitions of volatile organic compounds (VOC) and primary organic $PM_{2.5}$. Emissions of IVOC are expected to be high in Houston, due to the combination of petrochemical industry and mobile source emissions, and the contributions of IVOC to SOA appear to be important but underestimated. Work will include analysis of recently collected ambient data during DISCOVER-AQ on PM concentration and composition, new environmental chamber experiments on the SOA formation potential of IVOC, and photochemical modeling of the Houston region. Modeling of the formation of SOA from VOC and IVOC precursors will use a new state of the art approach based on the Volatility Basis Set (VBS) that has recently been implemented in the Comprehensive Air-quality Model with extensions (CAMx).

Project Update

In this quarter the team conducted a literature review to identify the most recent emission estimates for intermediate volatility organic compounds (IVOCs). Early modeling studies estimated IVOC by scaling from primary organic aerosol (POA) emissions. A limitation of this approach is that the ratio of IVOC to POA emissions would depend on gas-particle partitioning of POA at the measurement condition. A more recent approach estimates IVOC from the un-speciated fraction of total non-methane organic gas (NMOG) emissions. Recently published

chamber data provide source-specific un-speciated fractions of NMOG (i.e., approximate IVOC-to-NMOG ratios) for on-road gasoline and diesel vehicle emissions and biomass burning emissions.

The team also conducted a literature review to identify previous studies on mass yields of SOA formed from oxidation of IVOCs. This effort resulted in the creation of a preliminary list of IVOCs to study in chamber experiments. The team also designed and ordered the heated injector, which will be used to inject low-volatility IVOCs into the laboratory chamber and the thermodenuder, which will be used to measure the volatility of the organic aerosol formed. DISCOVER-AQ data has been shared with investigators of AQRP projects 14-009 and 14-029.

All funds allocated to the project are expected to be used by June 30, 2015.

Project 14-025 **STATUS: Active – May 21, 2014**

Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model

Environ – Christopher Emery
Texas A&M University – John Nielson-Gammon
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Khalid Al-Wali

Funding Amount: $256,261
($135,735 Environ, $120,526 TAMU)

Executive Summary

The US Environmental Protection Agency (EPA) requires the use of photochemical models to demonstrate that emission control plans will achieve the federal standard for ground-level ozone (EPA, 2007). The TCEQ uses the Comprehensive Air quality Model with extensions (CAMx) for research and regulatory photochemical modeling. Previous research conducted for the TCEQ has concluded that improvements to the CAMx modeling system, including a sub-grid cloud convection treatment, are necessary to reduce model under prediction biases in oxidized nitrogen compounds in the upper troposphere. Cloud convection at sub-grid scales is an important mechanism for exchanging boundary layer air with the free troposphere and for chemical processing. The current sub-grid cloud approach within CAMx influences photolysis rates, scavenging by rainfall, and aqueous chemistry at grid scale, but does not explicitly treat these processes at cloud scale and does not include sub-grid convective transport.

Small-scale clouds are often widespread but they are not explicitly resolved by the grid scales employed in regional meteorological and photochemical modeling applications. The physical effects from these sub-grid clouds are difficult to characterize accurately, but they can substantially influence many different atmospheric processes, including: boundary layer mixing, ventilation, and deep vertical transport of heat, moisture, and chemical tracers; radiative transfer and surface heat budgets; spatio-temporal precipitation patterns, intensity and wet scavenging rates; chemistry via photolysis and aqueous reactions; and certain environmentally-sensitive emission sectors (e.g., biogenic). Cloud convection is also an important component for long-range transport of ozone, PM, and precursors. The effects of sub-grid clouds on vertical transport, chemistry, and wet scavenging are addressed to varying degrees in off-line photochemical models (i.e., models like CAMx that operate separately from meteorological models that supply environmental inputs). However, the spatio-temporal distributions of such clouds, and all the processes that occur within them, must be re-diagnosed because meteorological models do not export necessary information from their sub-grid cloud parameterizations. This leads to potentially large inconsistencies between the models.

Under this AQRP Project, ENVIRON and collaborators at the Texas A&M University (TAMU) will incorporate and extensively evaluate an explicit sub-grid cloud model within CAMx. The primary goal of this work is to introduce shallow and deep convective cloud mixing at sub-grid scales. Further, the investigators will develop an approach to improve interactions with chemistry and wet deposition to operate explicitly at sub-grid scales in tandem with the cloud mixing scheme. The approach will tie into recent updates implemented in the Weather Research and

Forecasting (WRF) model by researchers at EPA, whereby specific sub-grid cloud fields will be passed to CAMx to define their spatio-temporal distributions and mixing rates for the new sub-grid cloud algorithm. This will yield a more consistent cloud-mixing-chemistry system across the WRF and CAMx models. The new CAMx treatment will be tested for three convective episodes that occurred during the September 2013 Houston DISCOVER-AQ field study and the Spring 2008 START08 field study, particularly addressing tropospheric profiles of NOx, ozone, and other chemical tracers by comparing to in situ profiles from aircraft measurements. The new model will be provided to TCEQ to support future regulatory and research-oriented ozone and PM modeling.

Project Update

This AQRP project is being performed by ENVIRON International Corporation (ENVIRON) and the Texas A&M University. A summary of activities for the period June 1, 2014 through August 31, 2014 is presented below.

The team has commenced modeling database setup and measurement data acquisition. We have obtained the latest WRF model source code (v3.6) from NCAR, which includes EPA's updates to the Kain-Fritsch (K-F) sub-grid convection algorithm. We have discussed these updates via e-mail correspondence with EPA to define the specific variables available to support the CAMx cloud model framework. Additional updates to make the K-F parameterization applicable at small spatial scales (<10 km) are currently under development at EPA. This "scale-aware" version of WRF K-F is expected to be available from EPA this fall. From this information we have begun to refine details of the methodology to incorporate a sub-grid cloud model in CAMx.

The interactive sub-grid cloud framework in CAMx will address shallow mixing, deep convective transport, gas and aqueous chemistry, and wet scavenging. All processes will be driven by specific data obtained from output fields generated by the WRF K-F scheme. The CAMx sub-grid cloud model framework will operate separately from the normal grid processes in a manner similar to the Plume-in-Grid (PiG) model. This "cloud-in-grid" (CiG) approach will define at each hour the physical attributes of a multi-layer cloud "reactor" according to the hourly cloud data provided by WRF. Each CiG reactor configuration will be unique to each grid column (or entirely absent from it) and characterize a steady-state sub-grid cloud environment between each hourly meteorological update time. Fractions of pollutant vertical mass profiles from each host grid column will be allocated to each CiG reactor layer, which will then operate on that mass to include vertical transport, entrainment/ detrainment with the ambient grid column, chemistry, and wet removal.

The project team has conferred on the model design and implementation approach. The general approach and certain technical implementation issues to consider in the final design of the CAMx cloud treatment were discussed at length. Some of the most important issues included: need for additional variables to be output from the WRF K-F algorithm; addressing "layer collapsing" of WRF layers to the CAMx layer structure; use of hourly-instantaneous or averaged fields; approach to partition CAMx grid mass to the ambient and in-cloud environments; approach to integrate chemistry and wet scavenging; numerical solvers to employ for convective transport; and compatibility with and inclusion of Probing Tool tracers. To gain insight and perspective on how sub-grid cloud processes are handled in other models, we have reviewed literature on the K-F approach, the sub-grid cloud technique in CMAQ, and the techniques

employed in two European air quality models (TOMCAT and CHIMERE). A detailed implementation design has been developed that addresses all of these issues; it is documented in the August monthly progress report.

Establishment of an AQRP sub-contract with co-principal investigators at Texas A&M has been delayed. Once a contract is established with Texas A&M, collection of field study measurements from DISOVER-AQ and START08 will commence. Other than addressing technical details in the design and implementation of the sub-grid cloud system into CAMx, no major technical issues have been encountered during the course of this project.

We intend to use all funds allocated to the project by 6/30/2015.

Project 14-026 **STATUS: Active – May 21, 2014**

Quantifying ozone production from light alkenes using novel measurements of hydroxynitrate reaction products in Houston during the NASA SEAC4RS project

Environ – Thomas Ryerson AQRP Project Manager – Gary McGaughey
California Institute of Technology – Paul Wennberg TCEQ Project Liaison – Chris Kite

Funding Amount: $231,182
($135,782 Environ, $95,400 CalTech)

Executive Summary

The objective of this project is to improve and quantify our understanding of ozone (O_3) and formaldehyde (HCHO) production from industrial emissions of Highly Reactive Volatile Organic Compounds (HRVOCs) in the Houston area. Aircraft flights during the National Aeronautics and Space Administration (NASA) Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys ($SEAC^4RS$) project encountered plumes with enhanced O_3 downwind of petrochemical facilities in Houston. For example, on 25 September 2013, ground monitoring downwind of the Ship Channel showed 5-minute average O_3 values peaking at 165 ppb and are associated with elevated concentrations of the oxidation products of HRVOCs. HRVOCs, specifically ethene, propene, butenes and 1,3-butadiene, have been implicated in these types of high ozone events but quantifying the relative contributions of individual HRVOCs to O_3 formation has been difficult.

The project objective will be accomplished by a combination of data analysis and reactive plume modeling. Data taken aboard the NASA DC-8 research aircraft during the 2013 $SEAC^4RS$ project in Houston will be analyzed. Chemical compounds called β-hydroxynitrates are formed when HRVOCs react in the atmosphere in the presence of nitrogen oxides (NOx). Measurements of the C_2-C_4 hydroxynitrates aboard the DC-8 provide a novel means to link observed enhancements of O_3 and HCHO to reactions of specific HRVOCs. Analyzing the data will provide a robust first-order attribution of observed O_3 and HCHO enhancements to the oxidation of individual HRVOCs emitted from the Houston Ship Channel. The plumes of HRVOCs and O_3 that the DC-8 intercepted will be analyzed further to estimate what emissions of HRVOCs and NOx gave rise to each plume. A reactive plume model (SCICHEM) will be used to model these plumes and test chemical reaction mechanisms for individual HRVOCs. The model sensitivity to plume expansion rates will be evaluated to test how plume dilution influences chemical processing and therefore how grid model resolution can influence assessments for HRVOC sources. The benefits of this project to the TCEQ will be a data-driven assessment of the contributions of individual HRVOCs to O_3 and HCHO enhancements downwind of the Houston ship channel and improved modeling tools for assessing the air quality impacts of HRVOC emissions in the Texas State Implementation Plan (SIP).

Project Update

This AQRP project is being performed by ENVIRON International Corporation (ENVIRON), NOAA (under sub-contract to ENVIRON), and Caltech. A summary of activities for the period June 1, 2014 through August 31, 2014 is presented below.

Task 1: QA/QC Alkene Hydroxynitrate Measurements by the Caltech TOF-CIMS aboard the DC-8 during SEAC^{4}RS and Generate Final Data

This task is being conducted by Caltech. However, the contract between Caltech and AQRP has been delayed, and Caltech has not yet initiated work on this task.

Task 2: Analysis of DC-8 airborne data to quantify plume initial conditions, production rates, and yields of O_3 and HCHO from parent alkenes

This task is being conducted by NOAA with assistance from Caltech. Since it requires the products of Task 1 before it can be initiated, there has been no progress on this task in the reporting quarter.

Task 3: Photochemical plume modeling to assess effects of hydroxynitrate sinks and 2nd-generation reaction products on inferred plume ozone production

This task is being conducted by ENVIRON. As part of this task, ENVIRON began updating the chemical mechanisms in SCICHEM from CB05 to CB6r2. The remaining components of this task (updates to CB6r2 mechanism to include additional explicit reactions to represent hydroxynitrate production from individual HRVOCs; plume modeling) will require the products of Tasks 1 and 2 before the task can be completed.

Project Management

ENVIRON developed a subcontracting agreement for NOAA for work to be done under Task 2. Since the Caltech contract with AQRP has been delayed, ENVIRON submitted a revised Workplan and QAPP to AQRP on August 21, 2014 that takes this delay into account and provides a revised approach to accomplishing the objectives of this study on time. This approach includes removing Caltech from the project and bringing on David Parrish as a consultant.

The study has progressed more slowly than expected due to delays in the Caltech contract. We expect that the schedule for Tasks 1-2 will be extended by about 3 months. However, we expect the overall project to remain on schedule for completion with delivery of the final AQRP-reviewed report by June 30, 2015, as described in our revised workplan.

Project 14-029 **STATUS: Active – July 10, 2014**

Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ

Baylor University – Rebecca Sheesley

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $178,679

Executive Summary

This projects builds on a previously-funded AQRP project tasked at the initial elemental carbon (EC), organic carbon (OC), and optical black carbon (BC) characterization of particulate matter (PM) at Moody Tower and Manvel Croix during DISCOVER-AQ Houston Texas 2013 (AQRP 12-032). Under the original framework of PIs Sheesley and Usenko's AQRP ECOC Project, samples were to be collected over the entire DISCOVER-AQ sampling period at two primary sites in Houston: Moody Tower (urban) and Manvel Croix (southern suburb). Collaborations developed during the early stages of this project increased the sampling intensity at the two primary sites and expanded PM sampling efforts to Conroe (far north suburb) and La Porte (urban industrial).

The overall goals of this project are to analyze the filter samples collected in the previous project and to quantify the strength of PM formation and PM emission sources, including shipping emissions, motor vehicle exhaust, biomass burning and biogenic emissions, across the Houston metropolitan area. This work builds on the strengths of DISCOVER-AQ, specifically the spatial and temporal sampling strategies (i.e. multiple ground-based sites sampled for approximately 28 days). These strategies allow for the examination of both regional and long-range transport as well as anthropogenic and biogenic influences on air quality. The project will characterize PM through the quantification of water-soluble OC, organic tracers, EC, OC, ^{14}C, select inorganic ions, and elemental tracers from PM filters collected from four DISCOVER-AQ anchor sites including Moody Tower, Manvel Croix, Conroe, and La Porte. The PIs will apply a combination of radiocarbon source apportionment of organic and elemental carbon with source-specific organic and inorganic molecular tracers to tightly constrain urban and regional, fossil and biomass burning/biogenic sources.

Progress Report

In July and August, 2014 research efforts focused on training students and method optimization. Specifically, students were trained in quality assurance and quality control protocols. In addition, students performed a reproducibility study to ensure the ability of each analyst participating in the study. Research efforts focused on tasks outlined in the project timeline specifically water-soluble organic carbon (WSOC) and organic tracer analysis. The initial WSOC analysis focused on airborne particulate matter samples collected from Manvel Croix, TX. PI Sheesley and PI Usenko participated in a conference call with the AQRP program officer and DISCOVER-AQ aerosol focus group collaborators (grants 14-024 and 14-009). The WSOC is on target to be completed and shared with Dr. Hildebrandt-Ruiz by the end of September. An analytical method capable of measuring all of the necessary organic tracers was optimized for airborne particulate

matter samples collected in Houston, TX. A manuscript describing this method and its optimization is currently underway with an anticipated submission date of Dec 2014. Laboratory consumables were purchased for both analyses.

Two abstracts were submitted to the national conference of the American Geophysical Union covering the DISCOVER-AQ analysis under 14-029:

"Spatial trends in surface-based carbonaceous aerosol, including organic, water-soluble and elemental carbon, during DISCOVER-AQ in Houston, TX"

"The application of a novel pressurized liquid extraction method to quantify organic tracers combined with historic and novel organic contaminants for the DISCOVER-AQ Houston field experiment"

No data is ready to be shared at this point.

Water blank issues arose during August for the WSOC analysis, but have since been resolved. This caused a small delay, but time had been included within the timeline for analysis issues and there will be no delay in the WSOC data sharing.

Supplies and salary expenses for August 2014 were reported by Phyllis Doughty of Baylor University. Supply expenses were associated with WSOC and organic tracer analysis. Salary expenses for August were associated with PI Sheesley.

Project 14-030 **STATUS: Active – June 25, 2014**

Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation

Texas A&M University – Qi Ying

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Amount: $176,109

Executive Summary

Isoprene emitted from biogenic sources plays an important role in atmospheric chemistry that leads to the formation of ozone and secondary particulate matter (PM). Although drought has been thought to affect biogenic emissions, the capability of the current drought parameterization to adjust the impact of soil moisture on isoprene emissions has not been critically evaluated, especially under severe drought conditions in Texas. The impact of this change in isoprene emissions on regional ozone concentrations is also unclear. In this study, biogenic isoprene emissions during two seven-month episodes, one representing a relatively wet year (2007) and one representing a severe drought year (2011) will be estimated using the most recent version of the MEGAN biogenic emission model (MEGAN v2.1). Emissions during the severe drought year 2011 will be estimated using several different soil moisture parameterization schemes, including one that will be developed in this study based on additional field and climate-controlled laboratory measurements of isoprene emissions at leaf-level for selected Texas tree species. The Community Multiscale Air Quality Model (CMAQ) will be used to simulate isoprene, isoprene oxidation products and ozone concentrations during the dry and wet episodes. The predicted concentrations will be evaluated against all available measurements to evaluate the ability of different drought parameterization schemes and quantify the impact of drought on biogenic isoprene emission and ozone concentrations in Texas. Optimal configuration of the WRF model that is most appropriate for meteorology and soil moisture simulations during the drought seasons will also be investigated.

Project Update

Due to delays in project setting up, the project started on June 25. The current report generally covers the activities during the month of July and August, 2014. The following summarized the progress on each Task in the Work Plan.

Task 1: Meteorology simulation with WRF.

A base case WRF simulation for May – November 2007 and 2011 have been completed using the TACC supercomputer at UT Austin. The WRF domains followed the same domains used by the TCEQ (na_36km, sus_12km, tx_4km), as proposed in the Work Plan. The base case simulation uses the default MODIS land use/land cover. Initial and boundary conditions, including initial soil moisture, were taken from the 3-h resolution North American Regional Reanalysis (NARR) data. The MM5 land surface model was used in this simulation. Observation data from ~100 surface weather stations in the 4-km domain were downloaded from the National Climatic Data Center (NCDC), dataset ds463.3, and soil moisture data for

both 2007 and 2011 were downloaded from TAMU North American Soil Moisture Database. Model performance analysis is currently underway. Based on the results from the initial model performance analysis, we will repeat the WRF simulations using Noah Land Surface Model and initial soil moisture data from the North American Land Data Assimilation System (NLDAS) archive, according to the Work Plan. The National Land Cover Database (NLCD) 2011 land cover data has been downloaded and processed and a sensitivity run will also be conducted. Currently, we can run the WRF simulations using TACC at 2 wall-clock hours for one day and multiple runs can be issued at the same time. We expect to finish WRF simulation in September.

Task 2: Perform field and laboratory measurements on common Texas tree species.

In this quarter, the Schade group assessed the seeding mortality rates and began leaf-level physiology and isoprene emission baseline measurements. The tree seedlings grown for this study were being nurtured in the greenhouse but unfortunately, they were forced to switch greenhouses, which caused additional delays and further increased seedling mortality. Nevertheless, a watering schedule was established in July, the soil used for potting was physically and chemically analyzed, the soil moisture sensors to be used were calibrated in the soil mix, and first photosynthesis baseline measurements on tree seedling leaves were initiated in August. Consumables were acquired throughout July and August and testing of the Tenax VOC sampling cartridges intended for isoprene emissions quantification commences.

Task 5: Perform regional air quality simulations.

Emission inventory for 2007 based on the 2007v5 modeling platform was downloaded from ftp://ftp.epa.gov/EmisInventory/2007v5/; and emission inventory for 2011 based on 2011 NEIv1 modeling platform was download from ftp://ftp.epa.gov/EmisInventory/2011v6/v1platform/. Spatial allocation surrogates were prepared for the RPO 36-km, Texas 12-km, and 4-km domains. Anthropogenic emissions (except point sources) for 2007 and 2011 have been prepared.

FINANCIAL STATUS REPORT

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May 2010 an amendment was issued increasing the budget by $40,000. Funding for fiscal year 2011 was established at $2,106,071, for a total award of $4,878,142 for the FY 2010/2011 biennium. FY 2010 funds were fully expended in early 2012 and the FY 2011 funds expired on June 30, 2013 with a remaining balance of $0.11.

In February 2012, funding of $1,000,000 was awarded for FY 2012. In June 2012, an additional $160,000 was awarded in FY 2012 funds and $1,000,000 was awarded in FY 2013 funds, for a total of $2,160,000 in funding for the FY 2012/2013 biennium.

In April 2013, the grant was amended to reduce the FY 2012 funds by $133,693.60 and increase the FY 2011 funds by the same amount.

In June 2013, the grant was amended to increase the FY 2013 funds by $2,500,000.

In October 2013, the grant was amended to award FY 2014 funds of $1,000,000 and FY 2015 funds of $1,000,000. The budget for each fiscal year can be found in Appendix C.

FY 2012 funds were fully expended at the end of April 2014.

For each biennium (and fiscal year) the funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

Program Administration – limited to 10% of the overall funding (per Fiscal Year)
This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC
These funds are to cover the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project will be assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual
These are the funds available to support the research projects that are selected for funding.

Program Administration

Program Administration includes salaries and fringe benefits for those overseeing the program as a whole, as well as, materials and supplies, travel, equipment, and other expenses. This category allows indirect costs in the amount of 10% of salaries and wages.

During the reporting period several staff members were involved, part time, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. James Thomas, AQRP Manager, is responsible for assisting

Dr. Allen in the program administration. Maria Stanzione, AQRP Grant Manager, with Rachael Bushn, Melanie Allbritton, and Susan McCoy each provided assistance with program organization and financial management. This included assisting with the contracting process. Denzil Smith is responsible for the AQRP Web Page development and for data management.

Fringe benefits for the administration of the AQRP were initially budgeted to be 22% of salaries and wages across the term of the project. It should be noted that this was an estimate, and actual fringe benefit expenses have been reported for each month. The fringe benefit amount and percentage fluctuate each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. For example, the amount of fringe benefits is greater for a person with family medical insurance versus a person with individual medical insurance. At the end of the project, the overall total of fringe benefit expensed is expected to be at or below 22% of the total salaries and wages. Actual fringe benefit expenses to date are included in the spreadsheets above.

As discussed in previous Quarterly Reports, the AQRP Administration requested and received permission to utilize funds in future fiscal years. This is for all classes of funds including Administration, ITAC, Project Management, and Contractual. As of the writing of this report, the FY 2010, FY 2011, and FY 2012 funds have been fully expended. This same procedure will be followed for the FY 2013, FY 2014, and FY 2015 funds.

In May 2014, UT-Austin received a Contract Extension for the AQRP. This extension will continue the program through April 27, 2016.

Table 1: AQRP Administration Budget

Administration Budget (includes Council Expenses)
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$202,816.67	$172,702.06	$375,518.73	$375,518.73	$0.00	$0.00
Fringe Benefits		$38,665.65	$33,902.95	$72,568.60	$72,568.60	$0.00	$0.00
Travel		$346.85	$0	$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$101.25	$15,197.39	$15,197.39	$0.00	$0.00
Equipment		$0	$0	$0			$0.00
Total Direct Costs		$256,925.31	$206,706.26	$463,631.57	$463,631.57	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$17,270.20	$37,551.89	$37,551.89	$0.00	$0.00
10% of Salaries and Wages							
Total Costs		**$277,207.00**	**$223,976.46**	**$501,183.46**	**$501,183.46**	**$0.00**	**$0.00**
Fringe Rate		22%	22%		19%		

Administration Budget (includes Council Expenses)
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$74,238.65	$265,040.00	$339,278.65	$226,107.70	$0.00	$113,170.95
Fringe Benefits		$17,068.38	$47,706.00	$64,774.38	$51,188.43	$0.00	$13,585.95
Travel		$339.13	$750	$1,089.13	$339.13		$750.00
Supplies		$3,560.62	$10,000	$13,560.62	$9,731.07	$0.00	$3,829.55
Equipment		$0.00	$0	$0			$0
Total Direct Costs		$95,206.78	$323,496.00	$418,702.78	$287,366.33	$0.00	$131,336.45
Authorized Indirect Costs		$7,423.86	$26,504.00	$33,927.86	$22,610.76	$0.00	$11,317.10
10% of Salaries and Wages							
Total Costs		**$102,630.64**	**$350,000.00**	**$452,630.64**	**$309,977.09**	**$0.00**	**$142,653.55**
Fringe Rate		22%	22%		23%		

Administration Budget (includes Council Expenses)
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$70,000.00	$70,000.00	$140,000.00	$0.00	$0.00	$140,000.00
Fringe Benefits		$15,150.00	$15,150.00	$30,300.00	$0.00	$0.00	$30,300.00
Travel		$350.00	$350.00	$700.00	$0.00	$0.00	$700.00
Supplies		$7,500.00	$7,500.00	$15,000.00	$0.00	$0.00	$15,000.00
Equipment							
Total Direct Costs		$93,000.00	$93,000.00	$186,000.00	$0.00	$0.00	$186,000.00
Authorized Indirect Costs		$7,000.00	$7,000.00	$14,000.00	$0.00	$0.00	$14,000.00
10% of Salaries and Wages							
Total Costs		**$100,000.00**	**$100,000.00**	**$200,000.00**	**$0.00**	**$0.00**	**$200,000.00**
Fringe Rate		22%	22%		0%		

ITAC

During December 2013and January 2014 the ITAC conducted their review of the proposals submitted in response to the 2014 – 2015 Request for Proposals. In November 2013 each proposal was assigned to 3 different ITAC members for review. On December 17, 2013, the individual reviews were submitted to AQRP and a conference call was held to perform an initial discussion and ranking of the proposals. On January 10, 2014, the ITAC met for a full day to review the proposals for technical merit and provide a ranking to the TCEQ and the Advisory Council. Expenses during this period were for travel for the ITAC members to attend the meeting and lunch provided during the meeting.

All remaining FY 2012 and FY 2013 ITAC funds were transferred to Research Projects/Contractual, as they were no longer needed for ITAC expenses and could be better utilized as additional research funding.

Table 2: ITAC Budget

ITAC Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$16,378.86	$6,292.97	$22,671.83	$22,671.83	$0.00	$0
Supplies		$1,039.95	$284.67	$1,324.62	$1,324.62	$0.00	0
Total Direct Costs		$17,418.81	$6,577.64	$23,996.45	$23,996.45	$0.00	$0
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$17,418.81**	**$6,577.64**	**$23,996.45**	**$23,996.45**	**$0.00**	**$0**

ITAC Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$5,323.31	$0.00	$5,323.31	$5,323.31	$0	$0.00
Supplies		$231.86	$0.00	$231.86	$231.86		$0.00
Total Direct Costs		$5,555.17	$0.00	$5,555.17	$5,555.17	$0	$0.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$5,555.17**	**$0.00**	**$5,555.17**	**$5,555.17**	**$0**	**$0.00**

ITAC Budget
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$7,000.00	$7,000.00	$14,000.00	$0.00	$0.00	$14,000.00
Supplies		$500.00	$500.00	$1,000.00	$0.00	$0.00	$1,000.00
Total Direct Costs		$7,500.00	$7,500.00	$15,000.00	$0.00	$0.00	$15,000.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$7,500.00**	**$7,500.00**	**$15,000.00**	**$0.00**	**$0.00**	**$15,000.00**

Project Management

During the first quarter of FY 2013-2014, Project Managers assisted with project questions, reporting requirements, and budget amendment requests as projects drew to a close. They also reviewed draft final reports and provided feedback. This transitioned to reviewing final project reports for the FY 2012-2013 research cycle as projects closed at the end of November 2013. This included a thorough review of each project against its Quality Assurance Project Plan (QAPP). Final reports were approved for all projects and are now available on the AQRP web page.

During third quarter, Project Managers worked with the project teams to complete the project Work Plans and begin work on the projects. As these were approved and projects became active, Project Managers focused on making sure all reporting requirements were met and projects were moving forward as described in the Work Plans.

Table 3: Project Management Budget

Project Management Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$145,337.70	$121,326.64	$266,664.34	$266,664.34	$0	$0
Fringe Benefits		$28,967.49	$23,102.60	$52,070.09	$52,070.26	$0	($0.17)
Travel		$0	$0	$0	$0		$0
Supplies		$778.30	$207.98	$986.28	$986.22	$0	$0.06
Total Direct Costs		$175,083.49	$144,637.22	$319,720.71	$319,720.82	$0	($0.11)
Authorized Indirect Costs		$14,533.77	$12,132.66	$26,666.43	$26,666.32	$0	$0.11
10% of Salaries and Wages							
Total Costs		**$189,617.26**	**$156,769.88**	**$346,387.14**	**$346,387.14**	**$0**	**$0.00**

Project Management Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$53,384.46	$77,000.00	$130,333.63	$130,333.63	$0.00	$50.83
Fringe Benefits		$10,991.04	$13,500.00	$26,291.04	$25,496.30	$0.00	$794.74
Travel		$0.00	$0	$0.00	$0.00		$0.00
Supplies		$967.98	$6,000.00	$6,967.98	$1,452.52		$5,515.46
Total Direct Costs		$65,343.48	$98,300.00	$163,643.48	$157,282.45	$0.00	$6,361.03
Authorized Indirect Costs		$5,338.44	$7,700.00	$13,038.44	$13,033.36	$0.00	$5.08
10% of Salaries and Wages							
Total Costs		**$70,681.92**	**$106,000.00**	**$176,681.92**	**$170,315.81**	**$0.00**	**$6,366.11**

Project Management Budget
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$52,000.00	$52,000.00	$104,000.00	$3,869.46	$0.00	$100,130.54
Fringe Benefits		$9,300.00	$9,300.00	$18,600.00	$785.46	$0.00	$17,814.54
Travel							
Supplies		$1,000.00	$1,000.00	$2,000.00	$0.00	$0.00	$2,000.00
Total Direct Costs		$62,300.00	$62,300.00	$124,600.00	$4,654.92	$0.00	$119,945.08
Authorized Indirect Costs		$5,200.00	$5,200.00	$10,400.00	$386.94	$0.00	$10,013.06
10% of Salaries and Wages							
Total Costs		**$67,500.00**	**$67,500.00**	**$135,000.00**	**$5,041.86**	**$0.00**	**$129,958.14**

Research Projects

FY 2010-2011

The FY 2010 Research/Contractual budget was originally funded at $2,286,000. After all transfers, it was increased by $1,827.93. The FY 2011 Research/Contractual budget was originally funded at $1,736,063. After all transfers, it was increased by $377.62, plus an additional $116,000 from FY 2012 funds that were changed to FY 2011 funds. This is an overall net increase of $13,205.55 to the Research/Contractual funds (and net reduction in Project Management/ITAC funds). ($105,000 in FY 2012 research funds were transferred to FY 2011, the remaining $11,000 were transfers from Project Management funds.)

All FY 2010 Research Project funding was fully expensed before the expiration of FY 2010 funds in June 2012. The FY 2011 Research Project funding that remained after all FY 2011 research projects were completed was allocated to FY 2012-2013 projects. This included the funds that were reallocated from FY 2012 to FY 2011. The funds were allocated to project 13-016 Valparaiso and project 13-004 Discover AQ Infrastructure. Both projects utilized their FY 2011 funds (project 13-004 $116,000 and project 13-016 $20,168.90) by June 30, 2013. A remaining balance of $0.11 was returned to TCEQ.

Table 4 on the following 2 pages illustrates the 2010-2011 Research Projects, including the funding awarded to each project and the total expenses reported on each project through the expiration of the FY 2011 funds on June 30, 2013.

FY 2012-2013

The FY 2012 Research/Contractual budget was originally funded at $815,000. Transfers to date have increased the budget by $32,438.67. These funds were fully expended as of April 2014. The FY 2013 Research Contractual budget was originally funded at $835,000. In June 2013, Amendment 9 increased this budget by $2,100,000. (The remaining $400,000 was allocated to Admin and Project Management.) Transfers to date have increased that by an additional $109,000 for a total FY 2013 Research Contractual budget of $3,044,000. This includes funds transferred from the FY 13 Project Management budget to the Research Projects budget, in order to fund as many research projects as possible.

Total FY 2013 research project expenditures are $1,321,620.01. Funds that were not expended by the FY 2012 – 2013 research projects totaling $1,716,844.99 have been allocated to projects from the FY 2014-2015 RFP.

Table 5 illustrates the 2012-2013 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of August 31, 2014. FY 2013 funding will be fully expended by June 30, 2015.

FY 2014-2015

The FY 2014 and 2015 Research/Contractual budgets were originally funded at $825,000 each. Research projects have been awarded to FY 2013, 2014, and 2015 funds.

Table 4: 2010/2011 Contractual Expenses

Contractual Expenses

FY 10 Contractual Funding	$2,286,000
FY 10 Contractual Funding Transfers	$1,827.93
FY 10 Total Contractual Funding	**$2,287,827.93**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-008	Rice University	$128,851	$126,622.32	$2,228.68
10-008	Environ International	$49,945	$49,944.78	$0.22
10-009	UT-Austin	$591,332	$591,306.66	$25.34
10-021	UT-Austin	$248,786	$248,786.41	-$0.41
10-022	Lamar University	$150,000	$132,790.80	$17,209.20
10-032	University of Houston	$176,314	$176,314	$0
10-032	University of New Hampshire	$23,054	$18,850.65	$4,203.35
10-032	UCLA	$49,284	$47,171.32	$2,112.68
10-034	University of Houston	$195,054	$186,657.54	$8,396.46
10-042	Environ International	$237,481	$237,479.31	$1.69
10-045	UCLA	$149,773	$142,930.28	$6,842.72
10-045	UNC - Chapel Hill	$33,281	$33,281	$0
10-045	Aerodyne Research Inc.	$164,988	$164,988.10	-$0.10
10-045	Washington State University	$50,000	$50,000	$0
10-DFW	UT-Austin	$37,857	$37,689.42	$167.58
FY 10 Total Contractual Funding Awarded		$2,286,000		
FY 10 Contractual Funding Expended (Init. Projects)			$2,244,812.59	
FY 10 Contractual Funds Remaining Unspent after Project Completion				$41,187.41
FY 10 Additional Projects				
	Data Storage	$7,015.34	$7,015.34	$0
10-SOS	State of the Science	$36,000.00	$36,000.00	$0
FY 10 Contractual Funds Expended to Date*			$2,287,827.93	
FY 10 Contractual Funds Remaining to be Spent				$0

FY 11 Contractual Funding		$1,736,063.00		
FY 11 Contractual Funding Transfers		$116,377.62		
FY 11 Total Contractual Funding		**$1,852,440.62**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179	$262,179	$0
10-006	University of Houston	$222,483	$217,949.11	$4,533.89
10-015	Environ International	$201,280	$201,278.63	$1.37
10-020	Environ International	$202,498	$202,493.48	$4.52
10-024	Rice University	$225,662	$223,769.99	$1,892.01
10-024	University of New Hampshire	$70,747	$70,719.78	$27.22
10-024	University of Michigan	$64,414	$60,597.51	$3,816.49
10-024	University of Houston	$98,134	$88,914.46	$9,219.54
10-029	Texas A&M University	$80,108	$78,276.97	$1,831.03
10-044	University of Houston	$279,642	$277,846.38	$1,795.62
11-DFW	UT-Austin	$50,952	$29,261.75	$21,690.25
FY 11 Total Contractual Funding Awarded		$1,758,099		
FY 11 Contractual Funds Expended (Init. Projects)			$1,713,287.06	
FY 11 Contractual Funds Remaining Unspent after Project Completion				$44,811.94
FY 11 Additional Projects				
	Data Storage	$2,984.66	$2,984.66	$0.00
	12-016 Valparaiso	$20,168.90	$0.00	$21,168.90
	12-004 Discover AQ Infrastructure	$116,000.00	$115,999.89	$0.11
FY 11 Contractual Funds Expended to Date*			$1,852,440.51	
FY 11 Contractual Funds Remaining to be Spent				$0.11
Total Contractual Funding		$4,022,063.00		
Total Contractual Funding Transfers		$118,205.55		
Total Contractual Funding Available		$4,140,268.55		
Total Contractual Funds Expended to Date			$4,140,268.44	
Total Contractual Funds Remaining				$0.11

Table 5. 2012/2013 Contractual Expenses

Contractual Expenses

FY 12 Contractual Funding	$815,000.00
FY 12 Contractual Funding Transfers	$32,438.67
FY 12 Total Contractual Funding	**$847,438.67**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
12-004	UT-Austin (Torres)	$20,174.10	$20,174.10	$0.00
12-006	UC-Riverside	$101,765.00	$101,765.00	$0.00
12-006	TAMU/TEES	$44,494.00	$42,134.22	$2,359.78
12-011	Environ International	$77,420.00	$77,410.16	$9.84
12-012	UT-Austin (Hildebrandt)	$79,463.00	$79,173.94	$289.06
12-012	Environ International	$69,374.00	$69,372.64	$1.36
12-013	Environ International	$59,974.00	$59,960.93	$13.07
12-018	UT-Austin (McDonald-Buller)	$85,282.00	$85,197.80	$84.20
12-018	Environ International	$21,688.00	$21,686.26	$1.74
12-028	University of Houston	$19,599.00	$16,586.51	$3,012.49
12-028	UCLA	$17,944.00	$17,709.51	$234.49
12-028	Environ International	$44,496.00	$44,496.00	$0.00
12-028	UNC - Chapel Hill	$35,230.00	$35,230.00	$0.00
12-032	Baylor	$45,972.00	$43,642.21	$2,329.79
12-TN1	Maryland	$64,994.00	$64,537.12	$456.88
12-TN2	Maryland	$69,985.00	$68,362.27	$1,622.73
FY 12 Total Contractual Funding Awarded		$847,438.67		
FY 12 Contractual Funds Expended to Date			$847,438.67	
FY 12 Contractual Funds Remaining to be Spent				$0.00

Note:
Project 12-004 on this page and Project 13-004 on the following page were the same project, with funding split across fiscal years. After all FY12 projects were completed and fully invoiced, the remaining FY12 funds were transferred to 12-004 and 13-004 was reduced by the same amount, so that the total project budget remained the same, but all FY12 funds could be expended.

FY 13 Contractual Funding	$835,000

FY 13 Contractual Funding Transfers		$2,209,000		
FY 13 Total Contractual Funding		**$3,044,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
13-004	UT-Austin (Torres)	$1,555,770	$805,228.06	$750,541.84
13-005	Chalmers University of Tech	$129,047	$129,047.00	$0.00
13-005	University of Houston	$48,506	$44,928.24	$3,577.76
13-016	Valparaiso	$46,652	$46,652.10	$0.00
13-016	University of Houston	$19,846	$14,101.40	$5,744.60
13-022	Rice University	$89,912	$75,881.86	$14,030.14
13-022	University of Houston	$116,903	$116,122.47	$780.53
13-024	Maryland	$90,444	$89,658.88	$785.12
FY 13 Total Contractual Funding Awarded		$2,097,080		
FY 13 Contractual Funds Expended (Init. Projects)			$1,321,620.01	
FY 13 Contractual Funds Remaining Unspent				$1,722,379.99
FY 13 Additional Expenditures				
	DATA Storage	$5,535	$5,535	$0.00
FY 13 Contractual Funds Expended			$1,327,155.01	
FY 13 Contractual Funds Remaining Unspent				$1,716,844.99

Note:
After all FY13 projects were completed contractual funds in the amount of $1,716,844.99 remained. The funds will be utilized for FY14 projects and will be accounted for on the following page.

FY 13 Remaining Contractual Funding	**$1,716,844.99**

Awarded to FY 2014-2015 Projects				
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-003	UNC Chapel Hill	$180,000.00	$0.00	$180,000.00
14-006	Sonoma Technology	$47,979.00	$1,886.50	$46,092.50
14-006	Valparaiso	$15,609.00	$0.00	$15,609.00
14-007	Chalmers Univ.	$15,233.00		$12,000.00
14-007	Univ. of Houston	$10,000.00		$10,000.00
14-008	UT-Austin (McDonald-Buller)	$175,000.00	$10,318.18	$164,681.82
14-011	UT-Austin (McDonald-Buller)	$131,166.00	$8,798.70	$122,367.30
14-011	Environ	$6,000.00	$492.51	$5,507.49
14-016	Environ	$240,000.00	$52,820.56	$187,179.44
14-017	University of Alabama - Huntsville	$25,000.00		$25,000.00
14-017	Rice University	$25,000.00		$25,000.00
14-023	UT-Austin (Torres)	$76,773.00	$17,233.89	$59,539.11
14-023	Aerodyne	$147,066.00		$147,066.00
14-024	UT-Austin (Hildebrandt Ruiz)	$143,282.00	$25,074.73	$118,207.27
14-024	Environ	$25,000.00	$5,855.68	$19,144.32
14-024	UC Riverside	$35,314.00	$0.00	$35,314.00
14-025	Environ	$40,000.00	$19,447.89	$20,552.11
14-025	TAMU	$20,000.00		$20,000.00
14-029	Baylor University	$150,000.00		$150,000.00
14-030	TEES	$132,227.43	$4,231.74	$127,995.69
FY 13 Total Remaining Contractual Funding Awarded		$1,640,649.43		
FY 13 Remaining Contractual Funds Expended			$146,160.38	
FY 13 Remaining Contractual Funds Unspent				$1,570,684.61
Total Contractual Funding		$3,891,439		

Total Contractual Funding Awarded	$3,815,243		
Total Contractual Funding Remaining to be Awarded	$76,196		
Total Contractual Funds Expended to Date		$2,320,754.06	
Total Contractual Funds Remaining to be Spent			$1,570,684.61

Table 6. 2014/2015 Contractual Expenses

Contractual Expenses

FY 14 Contractual Funding	**$825,000**
FY 14 Contractual Funding Transfers	**$0**
FY 14 Total Contractual Funding	**$825,000**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-002	CU - Boulder	$150,508.00		$150,508.00
14-002	Univ. of Maryland	$49,387.00		$49,387.00
14-003	UNC Chapel Hill	$20,000.00	$0.00	$20,000.00
14-004	Univ. of Maryland	$55,056.00		$55,056.00
14-004	Morgan State Univ.	$54,055.00		$54,055.00
14-009	Rice Univ.	$109,867.00		$109,867.00
14-009	Univ. of Houston	$109,635.00		$109,635.00
14-026	Environ	$135,782.00	$3,657.28	$132,124.72
14-030	TAMU/TEES	$43,881.57		$43,881.57
				$0.00
				$0.00
				$0.00
FY 14 Total Contractual Funding Awarded		$728,171.57		
FY 14 Contractual Funding Remaining to be Awarded		$96,828.43		
FY 14 Contractual Funds Expended to Date			$3,657.28	
FY 14 Contractual Funds Remaining to be Spent				$821,342.72

FY 15 Contractual Funding		**$825,000**		
FY 15 Contractual Funding Transfers		**$0**		
FY 15 Total Contractual Funding		**$825,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-006	Sonoma Technology	$2,000.00	$0.00	$2,000.00
14-007	Chalmers University	$58,946.00		$74,179.00
14-007	Univ. of Houston	$13,081.00		$23,081.00
14-011	Univ. of Texas - Austin	$20,001.00		$20,001.00
14-011	Environ	$22,419.00		$28,419.00
14-016	Environ	$31,911.00	$0.00	$31,911.00
14-017	Univ. of Alabama - Huntsville	$112,003.00		$112,003.00
14-017	Rice University	$37,979.00		$37,979.00
14-023	Aerodyne Research	$10,000.00	$0.00	$10,000.00
14-024	Univ. of Texas - Austin	$20,000.00	$0.00	$20,000.00
14-024	Environ	$76,404.00	$0.00	$101,404.00
14-025	Environ	$95,735.00	$0.00	$135,735.00
14-025	TAMU	$100,526.00		$100,526.00
14-029	Baylor University	$28,679.00		$28,679.00
FY 15 Total Contractual Funding Awarded		$629,684.00		
FY 15 Contractual Funding Remaining to be Awarded		$195,316.00		
FY 15 Contractual Funds Expended to Date			$0.00	
FY 15 Contractual Funds Remaining to be Spent				$825,000.00

Total Contractual Funding	$1,650,000		
Total Contractual Funding Awarded	$1,357,856		
Total Contractual Funding Remaining to be Awarded	$292,144		
Total Contractual Funds Expended to Date		$3,657.28	
Total Contractual Funds Remaining to be Spent			$1,646,343

Appendix A

Financial Reports by Fiscal Year

FY 10 and 11

(Expenditures reported as of August 31, 2014.)

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67		$0
Fringe Benefits		$38,665.65	$38,665.65		$0
Travel		$346.85	$346.85		$0
Supplies		$15,096.14	$15,096.14		$0
Equipment		$0.00			$0
Other					
Contractual					
Total Direct Costs		$256,925.31	$256,925.31		$0
Authorized Indirect Costs		$20,281.69	$20,281.69		$0
10% of Salaries and Wages					
Total Costs		**$277,207.00**	**$277,207.00**	**$0**	**$0**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00		$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment					
Other		$0.00			$0.00
Contractual					
Total Direct Costs		$206,706.26	$206,706.26	$0.00	$0.00
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$223,976.46**	**$223,976.46**	**0.00**	**$0.00**

ITAC Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,378.86	$16,378.86	$0	$0
Supplies		$1039.95	$1,039.95		$0
Equipment					
Other					
Total Direct Costs		$17,418.81	$17,418.81	$0	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$17,418.81**	**$17,418.81**	**$0**	**$0**

ITAC Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$6,292.97	$6,292.97	$0.00	$0
Supplies		$284.67	$284.67	$0.00	$0
Equipment					
Other					
Total Direct Costs		$6,577.64	$6,577.64	$0.00	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$6,577.64**	**$6,577.64**	**$0.00**	**$0**

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$145,337.70	$145,337.70		$0
Fringe Benefits		$28,967.49	$28,967.49		$0
Travel		$0	$0		$0
Supplies		$778.30	$778.30		$0
Equipment					
Other					
Total Direct Costs		$175,083.49	$175,083.49	$0	$0
Authorized Indirect Costs		$14,533.77	$14,533.77		$0
10% of Salaries and Wages					
Total Costs		**$189,617.26**	**$189,617.26**	**$0**	**$0**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$121,326.64	$121,326.64	$0	$0
Fringe Benefits		$23,102.60	$23,102.77	$0	($0.17)
Travel		$0			$0
Supplies		$207.98	$207.92	$0	$0.06
Equipment					
Other					
Total Direct Costs		$144,637.22	$144,637.33	$0	($0.11)
Authorized Indirect Costs		$12,132.66	$12,132.55	$0	$0.11
10% of Salaries and Wages					
Total Costs		**$156,769.88**	**$156,769.88**	**$0**	**$0.00**

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67	$0.00	$0.00
Fringe Benefits		$38,665.65	$38,665.65	$0.00	$0.00
Travel		$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$15,096.14	$0.00	$0.00
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,287,827.93	$2,287,827.93	$0.00	$0.00
ITAC		$17,418.81	$17,418.81	$0.00	$0.00
Project Management		$189,617.26	$189,617.26	$0.00	$0.00
Total Direct Costs		$2,751,789.31	$2,751,789.31	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$20,281.69	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,772,071.00**	**$2,772,071.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$1,852,440.62	$1,852,440.51	$0.00	$0.11
ITAC		$6,577.64	$6,577.64	$0.00	($0.00)
Project Management		$156,769.88	$156,769.88	$0.00	$0.00
Total Direct Costs		$2,222,494.40	$2,222,494.29	$0.00	$0.11
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,239,764.60**	**$2,239,764.49**	**$0.00**	**$0.11**

Appendix B

Financial Reports by Fiscal Year

FY 12 and 13

(Expenditures reported as of August 31, 2014.)

Administration Budget (includes Council Expenses)

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$74,238.65	$74,238.65	$0.00	$0.00
Fringe Benefits		$17,068.38	$17,068.38	$0.00	$0.00
Travel		$339.13	$339.13		$0.00
Supplies		$3,560.62	$3,560.62	$0.00	$0.00
Equipment		$0.00			$0.00
Other					
Total Direct Costs		$95,206.78	$95,206.78	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$7,423.86	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$102,630.64**	**$102,630.64**	**$0.00**	**$0.00**

Administration Budget (includes Council Expenses)

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$265,040.00	$151,869.05		$113,170.95
Fringe Benefits		$47,706.00	$34,120.05		$13,585.95
Travel		$750.00	$0.00		$750.00
Supplies		$10,000.00	$6,170.45		$3,829.55
Equipment					
Other		$0.00			
Total Direct Costs		$323,496.00	$192,159.55	$0.00	$131,336.45
Authorized Indirect Costs		$26,504.00	$15,186.90		$11,317.10
10% of Salaries and Wages					
Total Costs		**$350,000.00**	**$207,346.45**	**$0.00**	**$142,653.55**

ITAC Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$5,323.31	$5,323.31		$0.00
Supplies		$231.86	$231.86		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$5,555.17	$5,555.17	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$5,555.17**	**$5,555.17**	**$0.00**	**$0.00**

ITAC Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00		$0.00
Supplies		$0.00	$0.00		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$53,384.46	$53,384.46	$0.00	$0.00
Fringe Benefits		$10,991.04	$10,991.04	$0.00	$0.00
Travel		$0.00	$0.00		$0.00
Supplies		$967.98	$967.98		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$65,343.48	$65,343.48	$0.00	$0.00
Authorized Indirect Costs		$5,338.44	$5,338.44	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$70,681.92**	**$70,681.92**	**$0.00**	**$0.00**

Project Management Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$77,000.00	$76,949.17		$50.83
Fringe Benefits		$15,300.00	$14,505.26		$794.74
Travel					
Supplies		$6,000.00	$484.54		$5,515.46
Equipment					
Other					
Contractual					
Total Direct Costs		$98,300.00	$91,938.97	$0	$6,361.03
Authorized Indirect Costs		$7,700.00	$7,694.92		$5.08
10% of Salaries and Wages					
Total Costs		**$106,000.00**	**$99,633.89**	**$0.00**	**$6,366.11**

AQRP Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$74,238.65	$74,238.65	$0.00	$0.00
Fringe Benefits		$17,068.38	$17,068.38	$0.00	$0.00
Travel		$339.13	$339.13	$0.00	$0.00
Supplies		$3,560.62	$3,560.62	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$847,438.67	$847,438.67	$0.00	$0.00
ITAC		$5,555.17	$5,555.17	$0.00	$0.00
Project Management		$70,681.92	$70,681.92	$0.00	$0.00
Total Direct Costs		$1,018,882.54	$1,018,882.54	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$7,423.86	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$1,026,306.40**	**$1,026,306.40**	**$0.00**	**$0.00**

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$265,040.00	$151,869.05	$0.00	$113,170.95
Fringe Benefits		$47,706.00	$34,120.05	$0.00	$13,585.95
Travel		$750.00	$0.00	$0.00	$750.00
Supplies		$10,000.00	$6,170.45	$0.00	$3,829.55
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$3,044,000.00	$1,473,315.39	$0.00	$1,570,684.61
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$106,000.00	$99,633.89	$0.00	$6,366.11
Total Direct Costs		$3,473,496.00	$1,765,108.83	$0.00	$1,708,387.17
Authorized Indirect Costs		$26,504.00	$15,186.90	$0.00	$11,317.10
10% of Salaries and Wages					
Total Costs		**$3,500,000.00**	**$1,780,295.73**	**$0.00**	**$1,719,704.27**

Appendix C

Financial Reports by Fiscal Year

FY 14 and 15

(Expenditures reported as of August 31, 2014.)

Administration Budget (includes Council Expenses)

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment					
Other					
Total Direct Costs		$93,000.00	$0.00	$0.00	$93,000.00
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$0.00**	**$0.00**	**$100,000.00**

Administration Budget (includes Council Expenses)

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment					
Other					
Total Direct Costs		$93,000.00	$0.00	$0.00	$93,000.00
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$0.00**	**$0.00**	**$100,000.00**

ITAC Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$7,000.00	$0.00	$0.00	$7,000.00
Supplies		$500.00	$0.00	$0.00	$500.00
Equipment					
Other					
Total Direct Costs		$7,500.00	$0.00	$0.00	$7,500.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$7,500.00**	**$0.00**	**$0.00**	**$7,500.00**

ITAC Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$7,000.00	$0.00	$0.00	$7,000.00
Supplies		$500.00	$0.00	$0.00	$500.00
Equipment					
Other					
Total Direct Costs		$7,500.00	$0.00	$0.00	$7,500.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$7,500.00**	**$0.00**	**$0.00**	**$7,500.00**

Project Management Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$52,000.00	$3,869.46	$0.00	$48,130.54
Fringe Benefits		$9,300.00	$785.46	$0.00	$8,514.54
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$1,000.00	$0.00	$0.00	$1,000.00
Equipment					
Other					
Total Direct Costs		$62,300.00	$4,654.92	$0.00	$57,645.08
Authorized Indirect Costs		$5,200.00	$386.94	$0.00	$4,813.06
10% of Salaries and Wages					
Total Costs		**$67,500.00**	**5,041.86**	**$0.00**	**$62,458.14**

Project Management Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$52,000.00	$0.00	$0.00	$52,000.00
Fringe Benefits		$9,300.00	$0.00	$0.00	$9,300.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$1,000.00	$0.00	$0.00	$1,000.00
Equipment					
Other					
Total Direct Costs		$62,300.00	$0.00	$0.00	$62,300.00
Authorized Indirect Costs		$5,200.00	$0.00	$0.00	$5,200.00
10% of Salaries and Wages					
Total Costs		**$67,500.00**	**$0.00**	**$0.00**	**$67,500.00**

AQRP Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$825,000.00	$3,657.28	$0.00	$821,342.72
ITAC		$7,500.00	$0.00	$0.00	$7,500.00
Project Management		$67,500.00	$5,041.86	$0.00	$62,458.14
Total Direct Costs		$993,000.00	$8,699.14	$0.00	$984,300.86
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$8,699.14**	**$0.00**	**$991,300.86**

AQRP Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$825,000.00	$0.00	$0.00	$825,000.00
ITAC		$7,500.00	$0.00	$0.00	$7,500.00
Project Management		$67,500.00	$0.00	$0.00	$67,500.00
Total Direct Costs		$993,000.00	$0.00	$0.00	$993,000.00
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$0.00**	**$0.00**	**$1,000,000.00**

Appendix D

AQRP Publications and Presentations

FY10-11

10-006

Johansson, J., Johan Mellqvist, Jerker Samuelsson, Brian Offerle, Jana Moldanova , Bernhard Rappenglück, Barry Lefer, and James Flynn (2014) , Formaldehyde Quantitative Measurements and Modeling of Industrial Formaldehyde Emissions in the Greater Houston Area during Campaigns in 2009 and 2011, Journal of Geophysical Research: Atmospheres, 119, DOI: 10.1002/2013JD020159

Johansson, J. K. E., J. Mellqvist, J. Samuelsson, B. Offerle, B. Lefer, B. Rappenglück, J. Flynn, and G. Yarwood(2014), Emission measurements of alkenes, alkanes, SO2, and NO2 from stationary sources in Southeast Texas over a 5 year period using SOF and mobile DOAS, J. Geophys. Res. Atmos., 119, doi:10.1002/2013JD020485.

10-008

Digar, A., D.S. Cohan, X. Xiao, K.M. Foley, B. Koo, and G. Yarwood (2013). Constraining ozone-precursor responsiveness using ambient measurements. *Journal of Geophysical Research*, 118(2), 1005-1019, doi:10.1029/2012JD018100.

10-009

The following papers were published in the journal Industrial & Engineering Chemistry Research in a Special Issue on Industrial Flaring:

Torres, V.M., Herndon, S., Wood, E., Al-Fadhli, F.M., Allen, D.T., Emissions of Nitrogen Oxides from Flares Operating at Low Flow Conditions, *Industrial & Engineering Chemistry Research,* 51, 12600-12605, DOI: 10.1021/ie300179x (2012)

Pavlovic, R.T., Al-Fadhli, Kimura, Y., Allen, D.T., and McDonald-Buller, E.C. Impacts of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area, *Industrial & Engineering Chemistry Research,* 51, 12593-12599, DOI: 10.1021/ie203052w (2012).

Knighton, W.B., Herndon, S.C., Franklin, J.F., Wood, E.C., Wormhoudt, J., Brooks, W., Fortner, E.C., and Allen, D.T. Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy, *Industrial & Engineering Chemistry Research,* 51, 12674-12684, DOI: 10.1021/ie202695v (2012)

Torres, V.M., Herndon, S., Kodesh, Z., Nettles, R., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research,* 51, 12559-12568, DOI: 10.1021/ie202674t (2012).
Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research,* 51, 12569-12576, DOI: 10.1021/ie202675f (2012)

Herndon, S.C., Nelson, D.D., Wood, E.C., Knighton, W.B., Kolb, C.E., Kodesh, Z., Torres, V.M., and Allen, D.T., Application of the carbon balance method to flare emissions characteristics, *Industrial & Engineering Chemistry Research,* 51, 12577-12585, DOI: 10.1021/ie202676b (2012)

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research,* 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

The following presentations were given at the Air& Waste Management Association June 2012 Conference, and papers were published in the Conference Proceedings:

Torres, V.M., Allen, D.T., Herndon, S. and Kodesh, Z., Overview of the Texas Commission on Environmental Quality 2010 Flare Study, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-437-AWMA, San Antonio, June, 2012.

Torres, V.M., Al-Fadhli, F.M., Allen, D.T., Herndon, S., and Wood, E., NOx Emissions from Industrial Flaring, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-315-AWMA, San Antonio, June, 2012.

10-015
The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models
J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride
J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

10-020
Brown, S. S., et al. (2012), Effects of NO_xcontrol and plume mixing on nighttime chemical processing of plumes from coal-fired power plants, J. Geophys. Res., 117, D07304, doi:10.1029/2011JD016954.

Brown, S. S., Dubé, W. P., Bahreini, R., Middlebrook, A. M., Brock, C. A., Warneke, C., de Gouw, J. A., Washenfelder, R. A., Atlas, E., Peischl, J., Ryerson, T. B., Holloway, J. S., Schwarz, J. P., Spackman, R., Trainer, M., Parrish, D. D., Fehshenfeld, F. C., and

Ravishankara, A. R.: Biogenic VOC oxidation and organic aerosol formation in an urban nocturnal boundary layer: aircraft vertical profiles in Houston, TX, Atmos. Chem. Phys., 13, 11317-11337, doi:10.5194/acp-13-11317-2013, 2013.

In preparation for Atmosphere:
Reactive Plume Modeling to Investigate NOx Reactions and Transport at Night
Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:
Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique
Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021

The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the submitted abstract was *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022

Kanwar Devesh Singh, Tanaji Dabade, Hitesh Vaid, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, Kuyen Li, and Christopher B. Martin "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Model," *Industrial & Engineering Chemistry Research* **2012** *51* (39), 12611-12620

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, " Parametric Study of Ethylene Flare Operations and Validation of a Reduced Combustion Mechanism," Engineering Applications of Computational Fluid Mechanics, Vol. 8, No. 2, pp. 211–228 (2014).

Hitesh S. Vaid, Kanwar Devesh Singh, Helen H. Lou, Daniel Chen, Peyton Richmond, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale CFD Simulations," International Journal of Numerical Methods for Heat and Fluid Flow, Vol. 24 No. 1, 2014, pp. 21-35.

K. Singh, T. Dabade, H. Vaid, P. Gangadharan, D. Chen, H. Lou, X. Li, K. Li, C. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Ind. & Eng. Chem. Research, 51 (39), 12611-12620, October, 2012.

H. Lou, D. Chen, C. Martin, X. Li, K. Li, H. Vaid, K. Singh, P. Gangadharan, "Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, " Industrial & Engineering Chemistry Research, Industrial flares special issue, 51 (39), 12697-12705, October, 2012.

H. Lou, C. Martin, D. Chen, X. Li, K. Li, H. Vaid, A. Tula, K. Singh,"Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, Volume 14, Issue 4, pp 737-748, August 2012, DOI 10.1007/s10098-011-0441-6.

Helen H. Lou, Christopher B. Martin, Daniel Chen, Xianchang Li, Kyuen Li, Hitesh Vaid, Anjan Tula Kumar, Kanwar Devesh Singh, & Doyle P. Bean, "A reduced reaction mechanism for the simulation in ethylene flare combustion," Clean Technologies and Environmental Policy, Volume 14, Issue 2, pp 229-239, April 2012, doi:10.1007/s10098-011-0394-9.

10-024
The Project Investigators have submitted articles to the following journals:
J. Geophysical Research (in revision)
Atmospheric Environment (in review)

10-032
Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhan, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappengluck, K. W. Wong. C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke and P. Kelley (2013), Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *Journal of Geophysical Research-Atmospheres,118*,5770-5780,doi:10.1002/jgrd.50342.

10-042
Heo, G., McDonald-Buller, E.C., Carter, W.P.L., Yarwood, G., Whitten, G.Z. and Allen, D.T. "Modeling Ozone Formation from Alkene Reactions using the Carbon Bond Chemical Mechanism, *Atmospheric Environment*, 59, 141-150, DOI: 10.1016/j.atmosenv.2012.05.042 (2012).

Heo, G. Y. Kimura, E. McDonald-Buller, D. T. Allen, G. Yarwood, G. Z. Whitten Evaluation of a New Toluene Mechanism For Carbon Bond 05 Using Environmental Chamber Data and Ambient Data, Air and Waste Management Association Annual Meeting, Paper #154, Detroit, June 2009

In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate NOx removal and recycling represented in atmospheric mechanisms for air quality modeling*
Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen

In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial NOx*
Gookyoung Heo, William Carter, Greg Yarwood

10-045
Olga Pikelnaya, James H. Flynn, Catalina Tsai, and Jochen Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, Journal of Geophysical Reserch, Volume 118, Issue 15, pages 8716–8728, 16 August 2013, DOI: 10.1002/jgrd.50643

The following papers were published in Industrial & Engineering Chemistry Research Special Issue on Industrial Flaring. The paper edition of this special edition came out in Fall 2012.

W. Berk Knighton, Scott C. Herndon, Ezra C. Wood, Edward C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Detecting Fugitive Emissions of 1,3-Butadiene and Styrene from a Petrochemical Facility: An Application of a Mobile Laboratory and a Modified Proton Transfer Reaction Mass Spectrometer," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12706-12711

Ezra C. Wood, Scott C. Herndon, Ed C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, W. Berk Knighton, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Combustion and Destruction/Removal Efficiencies of In-Use Chemical Flares in the Greater Houston Area," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12685-12696

Pikelnaya, O., J. H. Flynn, C. Tsai, and J. Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, J. Geophys. Res. Atmos., 118,8716–8728, doi:10.1002/jgrd.50643.

This project has also resulted in the following publications:
Olga Pikelnaya, Jochen Stutz, Scott Herndon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuete, Evan Couzo, "*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview",* in preparation for Journal of Geophysical Research

Olga Pikelnaya, Scott Herndon, Ezra Wood, and Jochen Stutz, "*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign,"* under development.

FY12-13

12-006
Journal Papers:
Gookyoung Heo, Peng Wang, Qi Ying, Ron Thomas, William P.L. Carter. Using chemically detailed emissions data to test assumptions used in developing chemical mechanisms: a case study for southeast Texas, USA. [To be submitted to Atmospheric Environment in Summer 2014]

Peng Wang, Gookyoung Heo, William P.L. Carter, Qi Ying. Comparison of a detailed and a lumped version of SAPRC-11 photochemical mechanism during a summer ozone episode. [To be submitted to Atmospheric Environment in Summer 2014]

Gookyoung Heo, Chia-Li Chen, Ping Tang, William P.L. Carter. Evaluation of mechanisms for major terminal and internal alkenes with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2014]

Gookyoung Heo, Shunsuke Nakao, William P.L. Carter. Evaluation of mechanisms for 1,3-butadiene with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2014]

Conference Paper:
Heo, G., Carter, W.P.L., Wang, P., Ying, Q., Thomas, R. (2013). Evaluating and improving atmospheric chemical mechanisms used for modeling ozone formation from alkenes. Presented at the 12th Annual CMAS Conference, Chapel Hill, NC, October 28-30, 2013.

12-012
Conference presentations:
C. Faxon, J. Bean, L. Hildebrandt Ruiz. Evidence of atmospheric chlorine chemistry in Conroe, TX: Regional implications. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

J. Bean, C. Faxon, L. Hildebrandt Ruiz. Atmospheric processing of pollutants in the Houston Region: First insights from DISCOVER-AQ. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

L. Hildebrandt Ruiz, J. Bean, G. Yarwood, B. Koo, U. Nopmongcol. Formation and Gas-Particle Partitioning of Organic Nitrates: Influence on Ozone Production. American Association for Aerosol Research Annual Meeting, October 2013, Portland, OR.

Planned publications:
C. Faxon, J. Bean and L. Hildebrandt Ruiz. Preliminary title “Significant Inland Concentrations of ClNO2 Detected in Conroe TX during DISCOVER-AQ 2013”. Submission planned for August 2014.
J. Bean, C. Faxon and L. Hildebrandt Ruiz. Manuscript summarizing particle-phase measurements from DISCOVER-AQ. Submission planned for late 2014.

13-016
Gary Morris presented a poster entitled "Tropospheric Ozone Pollution Project (TOPP) Overview: A Context for DISCOVER-AQ Houston 2013" at the DISCOVER-AQ Science Team Meeting on February 27, 2014.

13-024
NASA AQAST meeting at Rice University in Houston, TX (Jan. 14-16, 2014), where Xinrong Ren gave a talk titled: "Measurements of trace gases at the Manvel Croix and Galveston sites during DISCOVER-AQ."

NASA DISCOVER-AQ science meeting at NASA Langley in Hampton, VA, where Winston Luke gave a talk titled: "NOAA/Air Resources Laboratory Surface Observations at Galveston and Manvel-Croix: Summary and Comparison with Aircraft Data."

A paper is in preparation with the intent to submit to Atmospheric Chemistry and Physics within about 3 months.

12-028

Implementation and Refinement of a Surface Model for HONO formation in a 3-D Chemical Transport Model. Prakash Karamchandani[1], Chris Emery[1], Greg Yarwood[1], Barry Lefer[2], Jochen Stutz[3], Evan Couzo[4], and William Vizuete[5]. ([1]ENVIRON, [2]University of Houston, [3]University of California-Los Angeles, [4]Massachusetts Institute of Technology, and [5]University of North Carolina.)

Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas. Evan Couzo[1], Barry Lefer[2], Jochen Stutz[3], Greg Yarwood[4], Prakash Karamchandani[4], Barron Henderson[5], and William Vizuete[1]. ([1]University of North Carolina (now at MIT), [2]University of Houston, [3]University of California-Los Angeles, [4]ENVIRON, [5]University of Florida.)

12-032

Poster at the American Geophysical Union national meeting (Dec 2013) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Poster at the DISCOVER-AQ Science Working Group meeting (Feb 2014) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Manuscript in preparation. Submission planned to Atmospheric Environment in summer 2014. Draft title: "*Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX*."

12-TN1

Presentation:

"A regional chemical reanalysis prototype" Pius Lee , Greg Carmichael, Tianfeng Chai, Rick Saylor, Li Pan, Hyuncheol Kim, Daniel Tong, and Ariel Stein

Poster:

"Preliminary analyses of flight measurements and CMAQ simulation during Southeast Nexus (SENEX) field experiment" Li Pan, Pius Lee , Hyun Cheol Kim, Daniel Tong ,Rick Saylor and Tianfeng Chai

Publication:
Pius Lee, Fantine Ngan, Hang Lei, Barry Baker, Bright Dornblaser, Gary McGauhey,and Daniel Tong. An Application for Improving Air Quality: a Houston Case Study, Earthzine 2014 [available at: http://www.earthzine.org/2014/03/29/an-application-for-improving-air-quality-a-houston-case-study/?shareadraft=baba698217_53330c8eab882]

12-TN2
The project team presented at the Community Modeling and Analysis System (CMAS) Conference in October 2013.

Presentations:
"HCHO and NO2 column comparisons between OMI, GOME-2 and CMAQ during 2013 SENEX campaign (21 slides)" Hyun Cheol Kim, Li Pan, Pius Lee, Rick Saylor, and Daniel Tong

Posters:
Fine-scale comparison of GOME-2, OMI and CMAQ NO2 columns over Southern California in 2008" Hyun Cheol Kim, Sang-Mi Lee, Fong Ngan, and Pius Lee

AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-10-94300
Awarded to The University of Texas at Austin

Annual Report

September 1, 2014 through August 31, 2015

Submitted to

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September 30, 2015

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Texas Air Quality Research Program

Annual Report

September 1, 2014 – August 31, 2015

Overview

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the 2010-2011 biennium, the AQRP had approximately $4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released its first request for proposals in May, 2010. Forty-five proposals, requesting $12.9 million in research funding were received. After review by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs, the results of the reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. A total of 15 proposals were selected for funding. As of November 30, 2011, all projects have been completed. Final reports have been posted to the AQRP website.

In June 2011, the TCEQ renewed the AQRP for the 2012-2013 biennium. Funding of $1,000,000 for the FY 2012 period was awarded in February 2012. An additional $1,000,000 for the FY 2013 period was awarded in June 2012. At the same time an additional $160,000 was awarded for FY 2012, to support funding for two specific air quality projects recommended by the TCEQ. A call for proposals was released in May 2012. Thirty-two proposals, requesting $5 million in research funding were received. The proposals were reviewed by the ITAC and the TCEQ. The Advisory Council selected 14 projects for funding.

In June 2013, the TCEQ issued Amendment 9 to the AQRP grant. This amendment had two purposes, 1) it renewed the AQRP for the 2014-2015 biennium (but did not award any funding

for that biennium), and 2) it awarded an additional $2,500,000 in FY 2013 funds. Ten percent (10%) of these funds were allocated for Project Administration, and the remaining funds were allocated to the Research program per the terms of the AQRP grant. A portion of the research funds were awarded to the 2012-2013 Discover-AQ Ground Sites Infrastructure Support project, in order to expand logistical support for the Discover-AQ study, at the request of TCEQ and with the Advisory Council's approval.

All 2012 – 2013 research projects were completed by November 30, 2013. The final reports for the projects have been posted to the AQRP website. All FY 2012 funds were fully expended and the remaining FY 2013 funds were held for use on future projects.

After the TCEQ issued Amendment 9 to renew the grant, the AQRP developed the FY 2014/2015 research priorities and submitted them to the ITAC for input and to the TCEQ for review. Funding of $1,000,000 for FY 2014 and $1,000,000 for FY 2015 was awarded via Amendment 10 in October 2013. A call for proposals was released and by the November 22, 2013 due date, 31 proposals requesting $5.8 million in research funding were received. In December and January the ITAC and the TCEQ reviewed the proposals. On February 21, the Advisory Council selected 15 projects for funding, with one project on hold while TCEQ completed their review. These projects were funded with a combination of FY 2013, 2014, and 2015 funds.

In March 2014, project Principal Investigators (PIs) were notified of the decision of the Advisory Council. AQRP Project Managers and TCEQ Project Liaisons were assigned to each project. A kick-off call was held with the project teams to discuss the development of the Work Plans which consist of the project scope of work, budget and justification, and quality assurance project plan (QAPP). The TCEQ completed their review of the final projects to be recommended for funding and the Council approved a final project on April 2, 2014.

All projects began work as their Work Plans were approved and contracts were finalized. In August, the AQRP was notified by the PI of Project 14-023 that the site where the project work was to take place was no longer able to participate in the project and an alternate site could not be located. A decision was made to end Project 14-023 and return the unspent funds to the Research Program account. The TCEQ then performed a relevancy review of the projects that were not funded in the first round, and forwarded a ranking to the AQRP Review Panel, with a recommendation to fund 5 additional projects. The Review Panel concurred with that recommendation. The Advisory Council then reviewed the proposals and in November 2014, approved funding for the 5 additional projects recommended by the Review Panel. During December, January and February, the Project Investigators of the 5 additional projects submitted Work Plans for approval and Master Agreements and Task Orders were put in place. Once approved, work began on all 5 projects.

On June 17 and 18, 2015, the AQRP held a Workshop at The University of Texas in which a representative from each project presented data and results. Several projects requested extensions to the end date of June 30, 2015. At this time, 12 projects have ended and the remaining 9 projects will end on September 30, 2015. Project Managers and TCEQ Liaisons are in the process of reviewing final reports and the Project Administration is closing out contracts and processing final invoices.

BACKGROUND

Section 387.010 of HB 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ, Commission) to establish the Texas Air Quality Research Program (AQRP).

> Sec. 387.010. AIR QUALITY RESEARCH. (a) The commission shall contract with a nonprofit organization or institution of higher education to establish and administer a program to support research related to air quality.
>
> (b) The board of directors of a nonprofit organization establishing and administering the research program related to air quality under this section may not have more than 11 members, must include two persons with relevant scientific expertise to be nominated by the commission, and may not include more than four county judges selected from counties in the Houston-Galveston-Brazoria and Dallas-Fort Worth nonattainment areas. The two persons with relevant scientific expertise to be nominated by the commission may be employees or officers of the commission, provided that they do not participate in funding decisions affecting the granting of funds by the commission to a nonprofit organization on whose board they serve.
>
> (c) The commission shall provide oversight as appropriate for grants provided under the program established under this section.
>
> (d) A nonprofit organization or institution of higher education shall submit to the commission for approval a budget for the disposition of funds granted under the program established under this section.
>
> (e) A nonprofit organization or institution of higher education shall be reimbursed for costs incurred in establishing and administering the research program related to air quality under this section. Reimbursable administrative costs of a nonprofit organization or institution of higher education may not exceed 10 percent of the program budget.
>
> (f) A nonprofit organization that receives grants from the commission under this section is subject to Chapters 551 and 552, Government Code.

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on April 30, 2010 for the 2010-2011 biennium, and was renewed in June 2011 for the 2012-2013 biennium and in June 2013 for the 2014-2015 biennium. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

RESEARCH PROJECT CYCLE

The Research Program is being implemented through a 9 step cycle. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle.

1.) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the strategic research priorities. The AQRP Director, in consultation with the ITAC, and

the TCEQ, develop research priorities; the research priorities are released along with a Request for Proposals.

2.) Project proposals relevant to the research priorities are solicited. The Request for Proposals can be found at http://aqrp.ceer.utexas.edu/ .

3.) The Independent Technical Advisory Committee (ITAC) performs a scientific and technical evaluation of the proposals.

4.) The project proposals and ITAC recommendations are forwarded to the TCEQ. The TCEQ evaluates the project recommendations from the ITAC and comments on the relevancy of the projects to the State's air quality research needs.

5.) The recommendations from the ITAC and the TCEQ are presented to the Council and the Council selects the proposals to be funded. The Council also provides comments on the strategic research priorities.

6.) All Investigators are notified of the status of their proposals, either funded, not funded, or not funded at this time, but being held for possible reconsideration if funding becomes available.

7.) Funded projects are assigned a Project Manager at UT-Austin and a Project Liaison at TCEQ. The project manager at UT-Austin is responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The Project Manager has responsibility for documenting progress toward project measures of success for each project. The Project Manager works with the researchers, and the TCEQ, to create an approved work plan for the project.

   The Project Manager also works with the researchers, TCEQ and the Program's Quality Assurance officer to develop an approved Quality Assurance Project Plan (QAPP) for each project. The Project Manager reviews monthly, annual and final reports from the researchers and works with the researchers to address deficiencies.

8.) The AQRP Director and the Project Manager for each project describe progress on the project in the ITAC and Council meetings dedicated to on-going project review.

9.) The project findings are communicated through multiple mechanisms. Final reports are posted to the Program web site; research briefings are developed for the public and air quality decision makers; and a bi-annual research conference/data workshop is held.

Steps 1 – 9 have been completed for the 2010-2011 and 2012 - 2013 biennia. For the 2014-2015 biennium Steps 1 through 6 have been completed. Steps 7, 8, and 9 are in progress.

Independent Technical Advisory Committee (ITAC)

The AQRP funding is used primarily for research projects, and one of three groups responsible for selecting the projects is the Independent Technical Advisory Committee (ITAC). The ITAC, composed of up to 15 individuals with scientific expertise relevant to the Program, is charged with recommending technical approaches, and establishing research priorities. Initially, the ITAC was

to meet at least twice per year at locations rotating between Austin, Dallas and Houston. As the Program proceeded, it was more efficient for the ITAC to meet once in Austin and as needed via conference call/webinar. Generally, the meetings in Austin are dedicated to new project review, reviewing progress on funded projects, and reviewing the Program's strategic plan.

Members of the ITAC consist of the TCEQ Project Director (or designee), representatives with air quality expertise from research institutions with extensive expertise in air quality research in Texas. The members of the ITAC are drawn from Texas universities active in air quality research, national laboratories that have participated in air quality studies in Texas, and institutions that have expertise not available in Texas and that have participated in air quality studies in Texas. The members of the ITAC are listed in Table 1.

As the ITAC membership is intentionally drawn from air quality researchers who have experience in Texas; these researchers and their colleagues will likely have interest in responding to the requests for research proposals issued by the AQRP. This raises potential confidentiality and conflict of interest issues, and the contract between TCEQ and the University of Texas requires that the AQRP shall maintain and implement an appropriate written policy on conflict of interest. Specifically for the ITAC, all members are required to certify:

> *Confidentiality:* As a member of ITAC I understand that I will have access to proposals submitted to the Air Quality Research Program. Subject to any legal requirements, I agree to keep the information in these proposals confidential until the selection process is completed and it is appropriate to release information to the public. I understand that there may be certain information that comes to me in my role as a member of ITAC that retains its confidential nature even after the process is concluded. I also understand that I will review said proposals and may have access to the reviews made by other ITAC members. I agree to keep these reviews and the identity of the reviewers confidential until such time as this information is released to the public. (NOTE: For the reviews and reviewers, this information may never be released.)
>
> *Conflict of Interest:* As a member of ITAC, I agree that I will not evaluate, comment on, or vote on proposals in which I or my home institution is involved, including but not limited to, any financial interest, or in which I have another form of conflict of interest. I understand that ITAC members with conflicts of interest must leave the meeting room or the conference line when a proposal with which they have a conflict is discussed, voted on or otherwise being considered. I understand that I must recuse myself from participating in or attempting to influence at any time the ITAC's or the AQRP Council's consideration or decision concerning such proposals. I agree to bring any issues concerning a possible conflict of interest to the attention of the Director of the Air Quality Research Program or the TCEQ Project Director. If there is a question of interpretation regarding whether a conflict of interest exists, I agree that the decision regarding whether a conflict of interest exists will be made by the Director of the Air Quality Research Program or the TCEQ Project Director.

All members of the ITAC agreed to abide by these conflict of interest and confidentiality provisions prior to participating in the review of proposals.

Table 1: Members of the Independent Technical Advisory Committee

Name	Title	Organization

David Allen	Gertz Regents Professor in Chemical Engineering	The University of Texas at Austin
Peter Daum	Head, Atmospheric Science Division	Brookhaven National Lab
Mark Estes	Senior Air Quality Scientist Air Modeling and Data Analysis Section	Texas Commission on Environmental Quality
Fred Fehsenfeld	Senior Scientist, Cooperative Institute for Research in Environmental Sciences	University of Colorado - Boulder
Sarwar Golam	Research Physical Scientist, Atmospheric Modeling and Analysis Division, Office of Research and Development	U.S. Environmental Protection Agency
Robert Griffin	Associate Professor, Civil and Environmental Engineering	Rice University
Tho (Thomas) Ching Ho	Chairman, Dan F. Smith Dept. of Chemical Engineering	Lamar University
Kuruvilla John	Professor of Mechanical and Energy Engineering Associate Dean for Research and Graduate Studies	University of North Texas
Barry Lefer	Associate Professor, Department of Earth and Atmospheric Sciences	The University of Houston
John Nielsen-Gammon	Professor and Texas State Climatologist Center for Atmospheric Chemistry and the Environment	Texas A&M University
David Parrish	Program Lead, Tropospheric Chemistry, NOAA/ESRL/Chemical Sciences Division	National Oceanic and Atmospheric Administration
Jay Turner	Associate Professor of Energy, Environmental and Chemical Engineering	Washington University in St. Louis
William Vizuete	Associate Professor, Gillings School of Global Public Health	The University of North Carolina at Chapel Hill
Christine Wiedinmyer	Scientist II, Atmospheric Chemistry Division	Nation Center for Atmospheric Research
Greg Yarwood	Principal	Environ

TCEQ Relevancy Review

Once the ITAC has reviewed and ranked research project proposals according to technical merit, they are submitted to the TCEQ for a relevancy review. The TCEQ reviews proposals for relevancy to the State's air quality research needs. TCEQ approval is required for a project to receive funding from the Program.

Advisory Council

The final group responsible for selecting AQRP research projects is the Advisory Council. The Council consists of up to 11 members, all residents of the State of Texas. Two Council members with relevant scientific expertise are nominated by the TCEQ. As defined in the AQRP contract,

up to four members of the Council can be county judges from the Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) non-attainment counties. Additional members include government officials from Texas Near-Non-Attainment Areas active in air quality management. The purpose of the Council is to give final approval to projects recommended by the ITAC and TCEQ, and to provide guidance on the Strategic Plan. At least one meeting in Austin is dedicated to new project selection. Additional meetings, either in person or via webinar, and email updates are dedicated to providing summaries of on-going projects and review of the strategic plan.

Table 2: Members of the Advisory Council

Name	**Title**	**Organization**
Ramon Alvarez	Senior Scientist	Environmental Defense Fund
Daniel Baker	Senior Consultant in Air Quality	Shell Global Solutions
Sam Biscoe	County Judge	Travis County
Jeff Branick	County Judge	Jefferson County
Edward M. Emmett	County Judge	Harris County
Ralph B. Marquez	Former TCEQ Commissioner	Environmental Strategies and Policy
Keith Self	County Judge	Collin County
Kim Herndon	Assistant Director Air Quality Division	Texas Commission on Environmental Quality
TCEQ 2	Pending appointment by TCEQ	

PROJECT TIMELINE

During the project period covered by this report (September 1, 2014-August 31, 2015), the following activities took place:

September 2014 – November 2014

For projects that were active, Project Managers continued to work with principal investigators to ensure that project goals were met, as well as all reporting and invoicing requirements. Contracts were finalized with the University of Colorado at Boulder and Texas A&M University. Two projects underwent significant changes:

Project 14-026, led by Environ International, was authorized to begin work in May, even though contract negotiations were still on-going with the project partner, the California Institute of Technology (Cal Tech). In August, Environ notified AQRP that Cal Tech was terminating contract negotiations with the AQRP and would no longer be involved with the project. Cal Tech's contract negotiations office confirmed this with AQRP's contract negotiations office. Environ submitted a revised Work Plan to the AQRP to modify the scope and budget of the project in light of the change in participants. The change included bringing on David Parrish as a consultant. The revised Work Plan was reviewed by the AQRP Review Panel in September and these changes were approved. Because this resulted in a reduction of funds for this project, Advisory Council approval was not needed; however, the Council was notified of this change.

Project 14-023, led by The University of Texas at Austin, began work in May. In July, the host of the site where the work was to be performed notified the PI that the company was being sold, and the new owners would not allow the project to take place on that site. The PI tried to locate an alternate site for the project, but was unable to find a host. In August, the PI officially notified the AQRP that the project could not be completed. The project was ended and all unspent funds were returned to the AQRP Research Projects fund.

The changes in the two projects listed above resulted in approximately $511,000 being returned to the AQRP Research Projects fund. The AQRP immediately began working with the TCEQ to identify alternate projects for funding. The TCEQ performed a relevancy review of the proposals that were submitted in response to the FY 14-15 RFP, but were not selected for funding in the initial round of reviews. The Review Panel met in September and identified 5 alternate projects for funding based on that relevancy review. Due to the limited amount of time available to complete the projects, a recommendation was also made to reduce the scope and budget by approximately 30%, so that the work could be completed by October 2015. These proposals were then submitted to the Advisory Council along with the recommendations for the scope and budget changes. The Council approved the funding for all 5 projects, at the level recommended by the AQRP and the Review Panel.

The additional projects are:

14-005 PI: Sarah Brooks, Texas A&M
Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation

14-010 PI: Yuxuan Wang, Texas A&M Galveston
Impact of large-scale circulation patterns on surface ozone concentrations in HGB

14-014 PI: Yunsoo Choi, University of Houston
Constraining NOX and HCHO Emissions Using Satellite NO2 and HCHO Column Measurements over the Southeast Texas

14-020 PI: Xinrong Ren, University of Maryland
Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC4RS

14-022 PI: Richard McNider, University of Alabama-Huntsville
Use of satellite data to improve specifications of land surface parameters

December 2014 – Feb 2015

During this period, the AQRP Project Managers, the AQRP QAPP Manager, and the TCEQ Liaisons reviewed and approved the project Work Plans for the 5 new projects. A Master Agreement was submitted to George Mason University for negotiation and signature. Task Orders were fully executed for 4 of the 5 projects.

March 2015 – May 2015

Project funding was rebudgeted across fiscal years. The funds that were made available when Project 14-023 ended were FY 13 funds. Funding for the 5 new projects is from FY 14 and FY 15 funds, as these projects have an end date of September 30, 2015. Several projects that were previously assigned to FY 14 or FY 15 funds were split between FY 14 or FY 15 and FY 13 in order to ensure the most efficient use of the research funds.

All Master Agreements and Task Orders were fully executed.

The AQRP Workshop was scheduled for June 17 and 18, 2015, in Austin, Texas.

Several projects requested and were granted extensions to their end dates from June 30, 2015 to no later than September 30, 2015.

June 2015 – August 2015

On June 17 and 18, 2015, the AQRP held a Workshop at The University of Texas to disseminate the research findings of the current projects and allow for collaboration between the project investigators. Representatives from each project attended and presented data and results. Members the AQRP and TCEQ were also present for the presentations.

At this time 12 projects have ended and the remaining 9 projects will end on September 30, 2015. Project Managers and TCEQ Liaisons are in the process of reviewing final reports and the Project Administration is closing out contracts and processing final invoices.

An update of the status of each project is listed in the Research Projects section of this report.

RESEARCH PROJECTS

Research projects for FY 2010-2011 and for FY 2012-2013 are complete. All projects have submitted final invoices and those invoices have been paid. The Final Report for each project is posted on the AQRP website at http://aqrp.ceer.utexas.edu/projects.cfm.

The following pages contain a description of the projects approved for funding for FY 2014-2015 and their status. A list of publications resulting from all research projects to date is provided in Appendix D and can also be found on the AQRP website.

FY 2014 – 2015 Projects

Discover AQ

In September of 2013, the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program deployed NASA aircraft to make a series of flights with scientific instruments on board to measure gaseous and particulate pollution in the Houston, Texas area. The purpose, for NASA, of this campaign was to better understand how satellites could be used to monitor air quality for public health and environmental benefit.

To complement the NASA flight-based measurements, and to leverage the extensive measurements being funded by NASA to better understand factors that control air quality in Texas, ground-based air quality measurements were made simultaneously by researchers from collaborating organizations, including research scientists and engineers funded wholly or in part by the AQRP and the TCEQ. Because of the opportunity to leverage NASA measurements, projects related to DISCOVER-AQ were a high priority for the 2012-2013 biennium.

This work continued in the 2014-2015 biennium with several projects dedicated to more in-depth analysis of the data collected during the Discover-AQ field campaign.

Project 14-002 **STATUS: Active – June 6, 2014**

Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC4RS Campaigns

University of Colorado - Boulder – Alan Fried
University of Maryland – Christopher Loughner
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Jim Smith

Funding Amount: $199,895
($150,508 UC-Boulder, $49,387 U of Maryland)

Executive Summary

During summer months the greater Houston-Galveston-Brazoria Metropolitan Area (HGBMA) often experiences elevated levels of ozone exceeding federal standards, particularly during hot and stagnant wind conditions. Although significant progress has been achieved understanding the major causes of these events over the past 10 years, there are still major unanswered questions related to sources of ozone from highly reactive volatile organic compounds (HRVOC's) emitted by large petrochemical facilities throughout the HGBMA. The toxic trace gas formaldehyde (CH_2O) is produced as an intermediate when these HRVOC's breakdown in the atmosphere, and ozone and radicals are formed when CH_2O further breaks down. Therefore a comprehensive understanding of CH_2O emissions, photochemical production rates, and transport processes is needed. Unfortunately, despite extensive efforts and advances from past studies, there are still major gaps in understanding related to the importance of directly emitted CH_2O from sources such as petrochemical flaring operations and automotive emissions relative to secondarily produced CH_2O from HRVOC's produced downwind, affecting large geographic areas far removed from the petrochemical facilities. Updating the emission inventories and temporal trends for CH_2O and its HRVOC precursors are two additional areas requiring attention.

To address these issues, a collaborative team, comprised of scientists from the University of Colorado, the University of Maryland, and the NASA Goddard Space Flight Facility, will analyze ambient measurements of CH_2O they acquired on the NASA P3 and DC-8 aircraft during the 2013 DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) and 2013 SEAC^{4}RS (Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys) studies, respectively.

The analysis will rely on the Community Multiscale Air Quality (CMAQ) model with Process Analysis, in very high-resolution mode (1 km resolution), driven by the WRF (Weather Research and Forecasting) meteorological model. The analysis will begin by identifying favorable time periods, such as Sept. 25, 2013, when sampling large petrochemical and refinery plumes under favorable meteorological conditions as well as other clearly identifiable sources (e.g., ship plumes, etc.) close to their source and downwind. The high resolution WRF-CMAQ model results will be compared with observations downwind at various times to arrive at updated emission rates for CH_2O and to help in validating the model meteorology and chemistry. The CMAQ model will be run in the Process Analysis Mode to quantify the relative importance of the major CH_2O sources. The analysis will conclude with an effort to compare select airborne

CH_2O measurements with 24-hour averaged cartridge measurements acquired by The Texas Commission on Environmental Quality (TCEQ) every 6th day at the Clinton, Deer Park and Channelview sites as a means to further validate and/or provide error bounds, for such long-term CH_2O data in the greater HGBMA.

Project Update

[*Project Management Note:*
The study team of this project notified the AQRP in September 2015 that they recently discovered that CMAQ simulations performed for Projects #14-002 and 14-004 utilized incorrect exit velocities of elevated point source emissions. This may result in artificially high free tropospheric concentrations of various species rather than increased values in the boundary layer.

The study team will correct the exit velocities, re-run CMAQ, and re-do the analyses for these projects. CMAQ will be re-run for all modeling domains (36, 12, 4, and 1 km horizontal resolution domains) and evaluated with observations made during the DISCOVER-AQ field campaign. Additional CMAQ simulations will be performed after the updated base case simulations. For Project #14-002, comparisons between the 1 km CMAQ simulation and NASA P-3B observations will be used to update petrochemical emissions within the 1 km domain. The 1 km CMAQ domain will then be re-run utilizing the process analysis tool and the updated petrochemical emissions. These new results will reveal the relative contribution of formaldehyde concentrations from direct emissions and secondary production and be compared with DNPH cartridge measurements.

The AQRP will provide a no cost extension to Project 14-002 through November 30, 2015, to allow time to re-run the models, analyze the data and revise the final report. No additional funds will be made available for the project.

Please note the project update below was submitted before the error was discovered, thus the analysis is subject to change.]

In the previous Quarterly Report we presented evaluations of the CMAQ CH_2O results by comparing the model run at 1-km spatial resolution with measurements for all the DISCOVER-AQ flights as part of our effort in addressing *Objective 1*. The various objectives can be found in our Project Work Plan. These comparisons were carried out on all daily averages as well as two select days (Sept. 13 and Sept 25, 2013) at higher temporal resolution. In the process, we brought up the topic of petrochemical flaring. This quarterly report summarizes our efforts to: 1) further assess CMAQ CH_2O accuracy; 2) employ various tracers in identifying flaring plume intercepts (*Objectives 2&6***)**; 3) employ the CMAQ model results with P3 CH_2O measurements to assess the accuracy of 24-hour integrated CH_2O results from DNPH sampling at the Clinton, Deer Park and Channelview TCEQ sampling sites (*Objective 5***)**; and 4) employ the CMAQ-modeled-CH_2O output run in the Process Analysis Mode to quantify the relative importance of the three major CH_2O sources: primary emissions, secondary photochemical production, and regional transport (*Objective 4***)**.

Because we employ the CMAQ model to address a number of project objectives involving airmasses in the planetary boundary layer (PBL), it is important to further assess (CMAQ-

Measurement) biases for PBL CH_2O in the absence of: 1) large petrochemical flaring and leakage events; and 2) where fast highly localized airmass changes are not faithfully captured by CMAQ, which employs emission inventories updated each hour. This is accomplished by comparing 1-km resolution CMAQ model results for CH_2O with P3 observations averaged over each sampling day. Figure 1 below shows such plots in the PBL for the entire month of September in 2013. In contrast to our previous report, Fig. 1 below provides more information by showing the CMAQ and P3 observed CH_2O mixing ratios as well as the mean with 1σ daily standard deviations and medians in addition to this same information for the daily biases (CMAQ-P3 Measurement).

As can be seen, the daily mean model and measurement averages overlap within the mutual imprecision limits in the upper plot. However, the bottom plot is the more meaningful plot. Here we display daily (CMAQ-Measurements) biases based upon point-by-point comparisons. As indicated previously, the model is biased low in many cases, most likely because the precursor emission sources in the model input are too low. These emissions sources are from the 2012 emission inventory. However, in 7 of the 9 daily comparisons, the median biases are all within 600 pptv, and in 5 of the 9 cases, median biases are all within 300 pptv. Excluding Sept. 25, which is the major outlier, the overall average of the daily median PBL bias for the remaining 8 flights is -309 ± 322 pptv (11.7% ± 12.9%).

Arising in part from our presentation, the topic of flaring plume intercepts generated a lot of discussion during the AQRP Workshop in June at the University of Texas. We have developed a number of tracers to identify when the P3 intercepted such plumes, and we have identified 37 such events (*Objectives 2&6*). These will be presented in the August monthly report. Figure 2 below shows one of the dominant flaring events observed on Sept. 25 during the 1st P3 Circuit when flying over the Baytown ExxonMobil Complex. This figure shows the temporal profiles for CH_2O, CO, propene, O_3, altitude, CMAQ-modeled boundary layer height, and the NO_x/NO_y ratio and Fig. 3 shows a shot from the P3 forward camera while flying over this complex, revealing a steam-assisted flare. The NO_x/NO_y ratio was introduced into our analysis since it provides an indication of the degree of photochemical processing. Fresh emission plumes, such as from flaring exhibit ratios in the 0.9 to 1.0 range, where nearly all of the nitrogen-oxides are in the form of NO_x ($NO+NO_2$). As the air mass ages, the NO_x undergoes oxidation to form species such as HNO_3, PAN, alkyl nitrates and other species. In addition, in fresh flaring emissions, O_3 is titrated by the emitted NO, resulting in a highly anti-correlated (negative) CH_2O-O_3 slope. The shaded region in Fig. 2 depicts sampling near the Baytown ExxonMobil Complex where CH_2O and CO is highly correlated. A subset of this region (14:47:44 – 14:48:11) in the white inset was further identified where CH_2O, CO, propene, and NO_x/NO_y are all anti-correlated with O_3, indicating the precise location and intercept time of the ExxonMobil flaring plume. The CH_2O/CO and CH_2O/O_3 slopes are 70.5 ± 3.9 ($r^2 = 0.98$) and -263.0 ± 97.4 ($r^2 = 0.51$), respectively for this subset with a NO_x/NO_y range of 0.88 to 1.05. As the measured CH_2O/CO slope is ~ a factor of 6 higher than the 2013 reported normal operating release inventory for the 3 ExxonMobil facilities combined, the large CMAQ model CH_2O under-prediction shown in Fig. 1 is understandable.

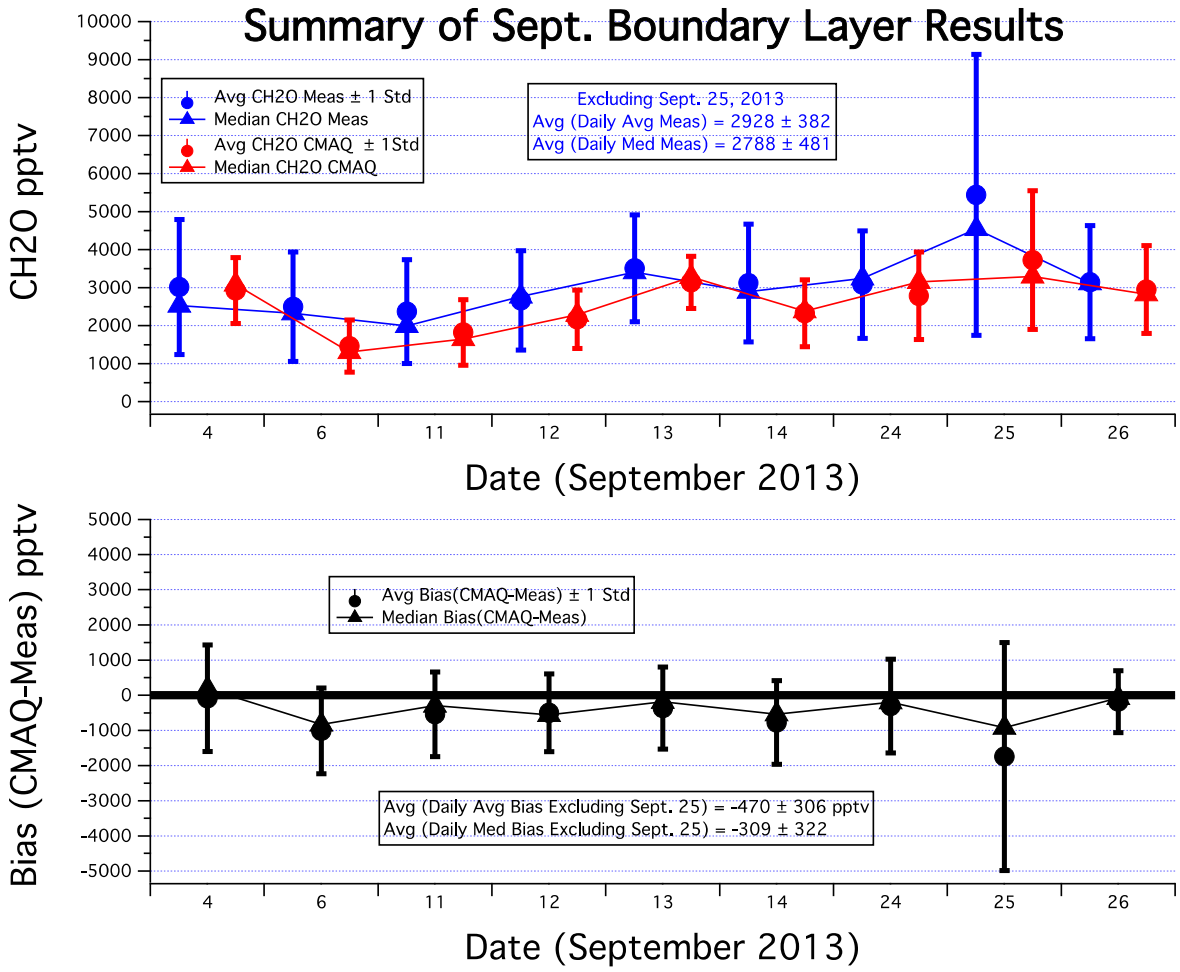

Figure 1: Comparison of daily CH_2O mixing ratios from the P3 observations and the 1km CMAQ model results.

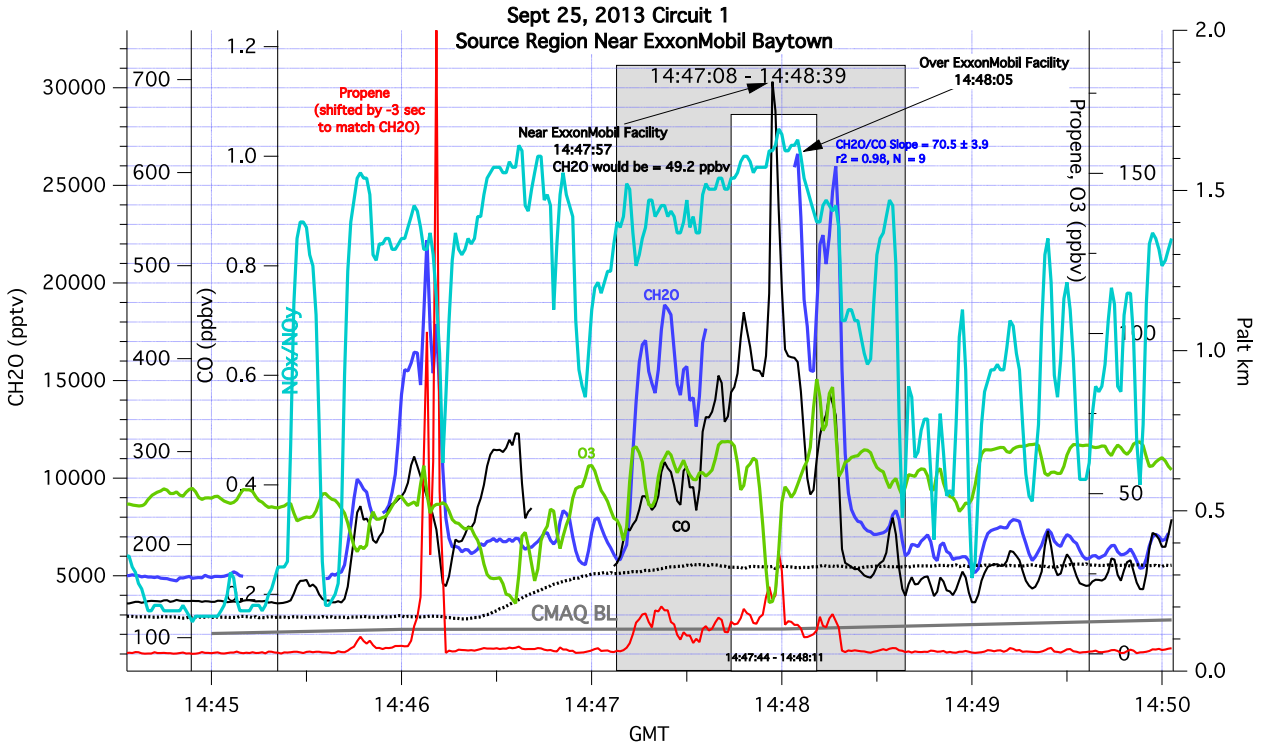

Figure 2: Time series plot of CH_2O, CO, O_3, propene, and NO_x/NO_y ratios during the 1st Circuit of Sept. 25, 2013 near the ExxonMobil Baytown complex**.** The missing CH_2O data at the plume center, unfortunately, occurred when the P3 CH_2O instrument was in an automatic zeroing mode.

Having established the general level of agreement between CMAQ-modeled-CH_2O and P3 measurements in the PBL, we next addressed *Objective 5:* the comparison of *24-hour synthesized integrated airborne measurements*, based upon the temporal dependence calculated from the CMAQ model and the P3 aircraft, with DNPH cartridge sampling measurements from the Clinton, Deer Park and Channelview TCEQ sites. As stated previously, this objective is important since the 24-hour DNPH sampling results have been employed every 6th day over a number of years to collect averaged CH_2O levels at both Deer Park and Clinton, and these data have been used to infer decreasing yearly trends in CH_2O. Unfortunately Sept. 13 at Deer Park was the only day where the DNPH sampling system was operational during a P3 flight day. Fortunately, as shown in Fig. 4 the P3 overflights passed very close to the TCEQ sampling site at low altitudes. Figure 4 shows the P3 flight track, colored by altitude, near the DNPH sampling site. Although this figure only plots the 2nd P3 circuit, each of the 3 circuits passed close to this sampling site over ~ a 6-hour time span.

Figure 3: Forward camera shot on the P3 at 14:47:47 right over the Baytown ExxonMobil Complex revealing a steam assisted flare.

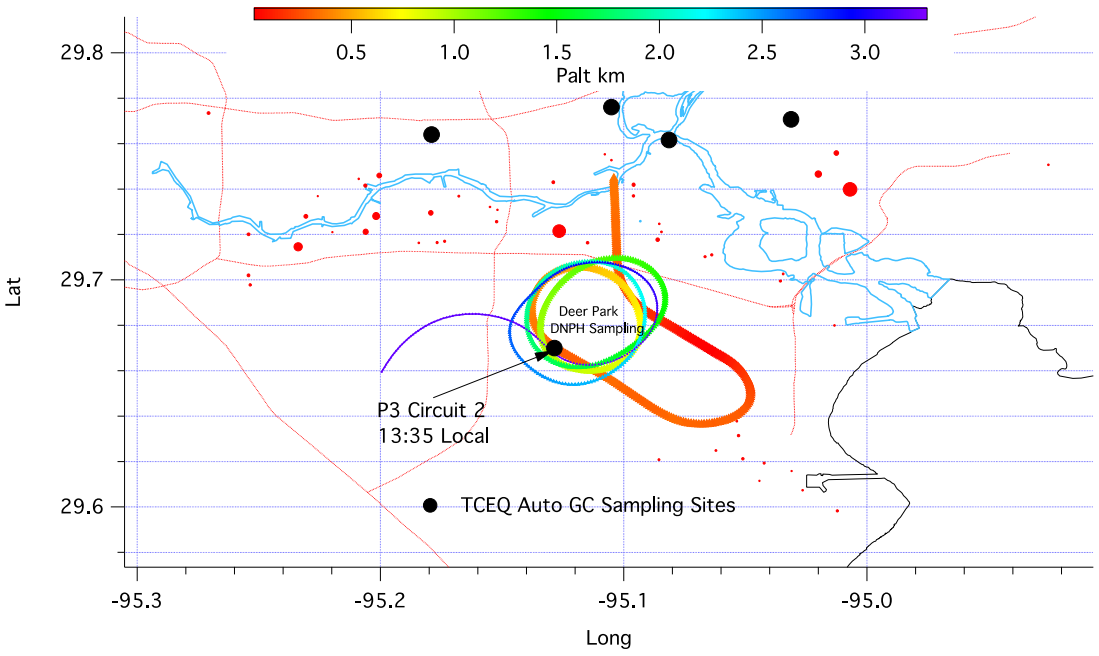

Figure 4: P3 flight track during the 2nd Circuit, colored by altitude over the DNPH TCEQ auto-GC Deer Park sampling site on Sept. 13, 2013.

The traces of Fig. 5 show the results of this comparison. In the top trace, we plot the P3 measurements for both CH_2O (blue points) and propene (red points) at the point of closest approach to the Deer Park sampling site for each of 3 circuits at the indicated local sampling times. The CH_2O measurements also include the total uncertainty (systematic plus random), and we indicate the sampling altitude. The 24-hour averaged DNPH measurements acquired by the

TCEQ system at Deer Park are shown by the solid blue line spanning the 24-hour time period. The agreement in P3 propene measurements from the Wisthaler's group PTRMS instrument with the ground-based TCEQ auto GC measurements collocated with the DNPH sampling system indicate that the P3 and ground sampling site are in the same airmass for all 3 circuits. Without any further information it would be impossible to tell if the significantly elevated propene measured by the auto-GC sampler at around 4 am produces elevated CH_2O. Since there is no significant OH at night to initiate oxidation of propene to CH_2O, one would expect no corresponding CH_2O increase in the dark unless ozone reacts with propene in the dark to produce CH_2O. This would only occur if the elevated propene does not simultaneously occur with simultaneous large emissions of NO from flaring, which would titrate down the O_3.

It is interesting to note that the 24-hour CMAQ temporal profile of CH_2O at the Deer Park surface site shown in the lower trace of Fig. 5 (dashed blue line) indicates a large increase in calculated CH_2O at around 4 am. In fact, the CMAQ temporal CH_2O profile follows the measured auto-GC propene profile. Since CMAQ employs an average emission inventory for each hour for a given season, the apparent coincidence in elevated calculated CH_2O and measured propene on. Sept. 13 in the early morning hours implies that early morning propene spikes at the surface at Deer Park should be a daily occurrence. Throughout the month of September in 2013, the hourly Deer Park auto-GC measurements in fact show such propene spikes on most days between the hours of 4 am and 7am, with typical levels in the 10-30 ppbv range and a maximum value of ~ 90 ppbv. This in turn would imply that elevated surface CH_2O at Deer Park should be a regular occurrence from fugitive emissions and subsequent reactions of O_3 with propene and perhaps ethene in the dark unless O_3 is simultaneously titrated by flares. This latter process, however, would directly release CH_2O. This interesting observation is a subset of *Objective 6***,** which hints at the potential importance of nighttime emissions of CH_2O and/or its precursors, as suggested by Olauger et al. [2009]. Dedicated round the clock ground-based measurements of CH_2O at one or all of the 3 auto-GC sampling sites would be important to carry out in the future to resolve this.

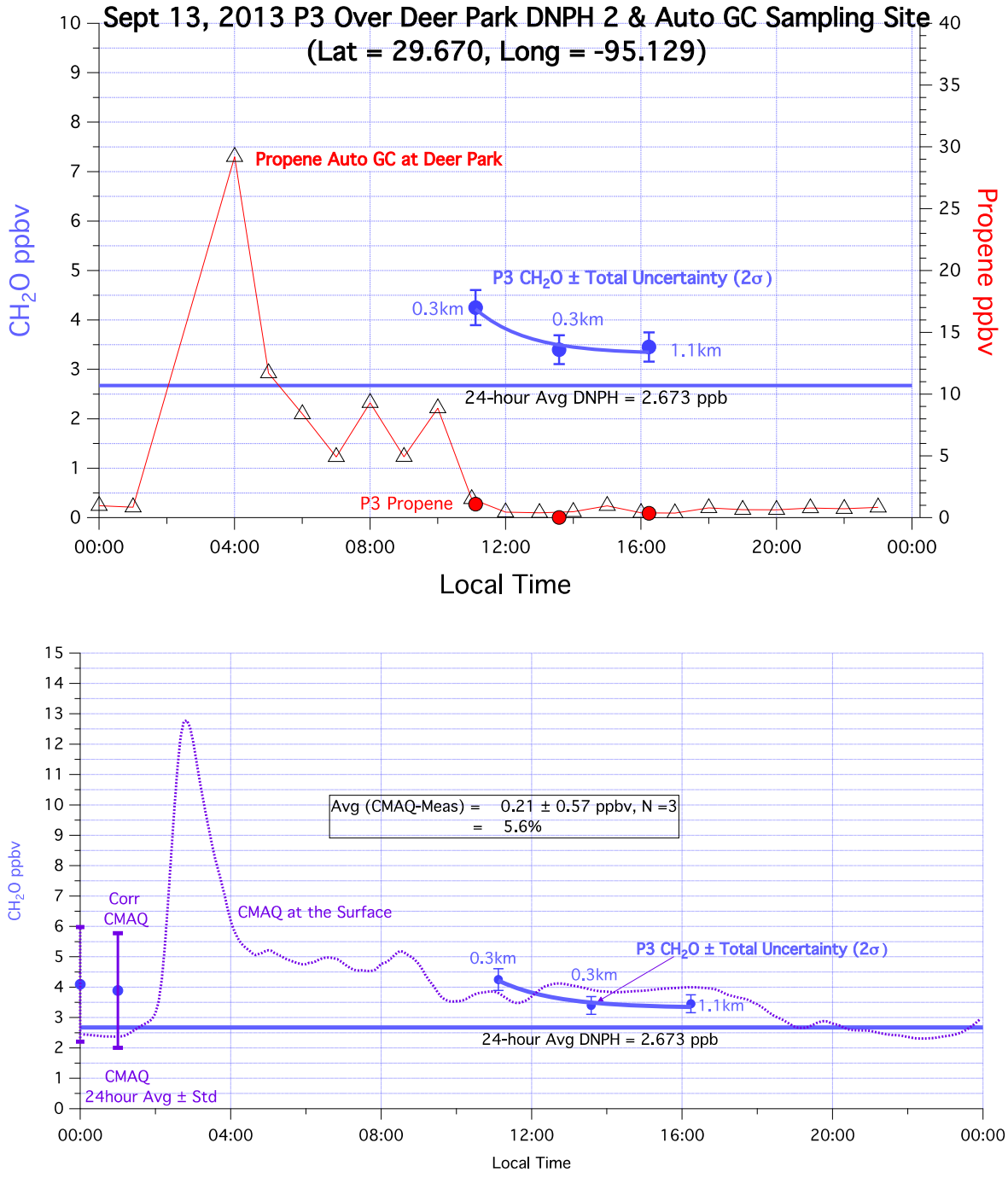

Figure 5: (Top trace) Comparisons of P3 propene measurements with the auto-GC measurements at Deer Park. (Bottom trace) Comparison of P3 measured CH_2O concentrations with CMAQ calculations at the surface of Deer Park and the 24-hour averaged DNPH results as well as the 24-hour integrated CMAQ results (blue points near time 00:00 with error bars)

Aside from the interesting time dependence and associated speculation just discussed, the 24-hour CMAQ surface modeled CH_2O at Deer Park shown in the lower trace of Fig. 5 can be used in conjunction with the P3 CH_2O observations to assess 24-hour DNPH results. As can be seen, the CMAQ model results at the surface at Deer Park agrees with the P3 measurements to within 205 pptv, which is even closer than our previous comparisons. Averaging the CMAQ CH_2O results over the 24-hour DNPH sampling period yields the 4.095 ± 1.9 ppbv value shown at the left on the Y-axis. Applying a small 205-pptv correction to match the CMAQ results with the 3 P3 measurements yields the 3.890 ± 1.9 ppb result shown with the Corr-CMAQ point. This value is in agreement with the averaged DNPH results (2.673 ppbv) within the precision of the CMAQ mean value. The difference is 31%. It is interesting to note that the DNPH value is in line with our averaged daily mean and median CH_2O values of 2.928 ± 0.382 ppbv, and 2.788 ± 0.481 ppbv, respectively, for the composite PBL shown in Fig. 1. It is also interesting to note that this 31% level of agreement is in line with the comparison slopes reported by Gilpin et al. [1997] between diode laser measurements of CH_2O standards and those retrieved by DNPH cartridge sampling methods. *Based on these limited observations, the Deer Park DNPH sampling system should accurately reflect 24-hour integrated surface CH_2O levels at this site (Objective 6).* Clearly more comparisons should be carried if the opportunities arise in the future. In particular, CH_2O measurements with our IR spectrometer located at the Deer Park and Clinton DNPH sites, sampling for at least 1-month each, would provide extremely valuable information. In addition to providing more substantial comparisons with DNPH results, such observations would help to address the nighttime questions just discussed.

The next step in our analysis was to address *Objective 4:* Employ the CMAQ model output runs in Process Analysis Mode to quantify the relative importance of the three major CH_2O sources (primary emissions, secondary photochemical production, and regional transport). This was initially carried out with the existing 2012 emission inventories. Figure 6 below shows the 4 and 1-km domains used in our calculations, however, only the 1-km domain calculations are used in our source attribution assessments. As can be seen, this domain focuses on the Houston-Galveston-Brazoria Metropolitan Area.

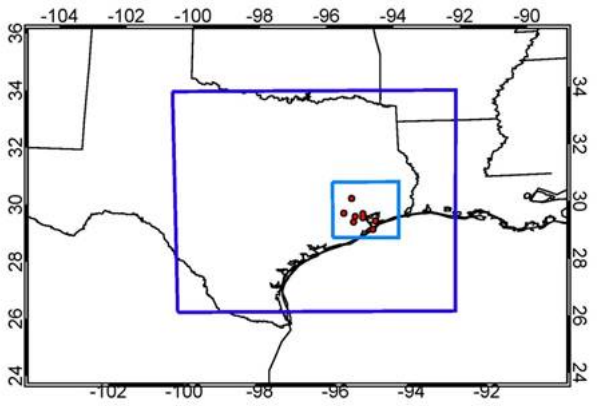

Figure 6: 4 and 1-km domains employed in the CMAQ model

Figure 7 shows the results of our daily average calculations for the entire month of September in 2013 averaged over the entire 1 km domain. As can be seen, CH_2O from secondary production sources (Production – Destruction) is approximately a factor of 5 times higher than direct emission sources in the planetary boundary layer (PBL) over the entire month of September and approximately a factor of 7 to 8 times the direct emission source for the atmosphere over the Houston-Galveston-Brazoria Metropolitan Area up to 5-km altitude. These results are in agreement with our qualitative assessment presented in one of our reports based upon our fast CH_2O-O_3-NO_x/NO_y correlations.

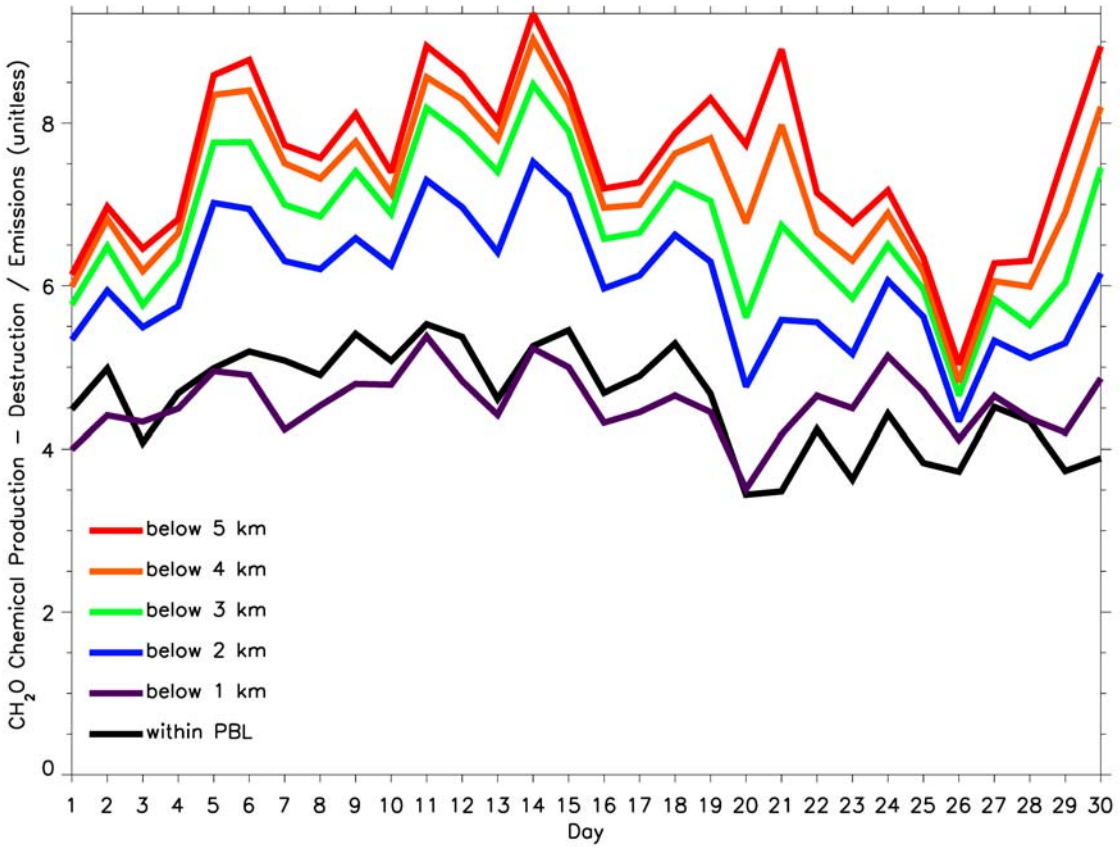

Figure 7: 1-km CMAQ model ratios of CH_2O from secondary production sources (production-destruction) relative to direct emission sources for the entire month of September in 2013 over the Houston-Galveston-Brazoria Metropolitan Area.

Figure 8 below further shows this breakdown as a function of hour for the entire month of September 2013. Over the 7 am – 7 pm daylight hours, the average ratio yields a value of ~ 8/1 within the PBL. This yields a secondary CH_2O contribution of ~ 89% over the daylight hours and this agrees well with the determination from Parrish et al. [2012] of ~ 95% based upon OH reactions of ethene and propene to produce CH_2O during daylight hours. It should be mentioned that our results are based upon present emission inventories for ethene and propene that have not been updated to include possible over-assisted flaring emissions.

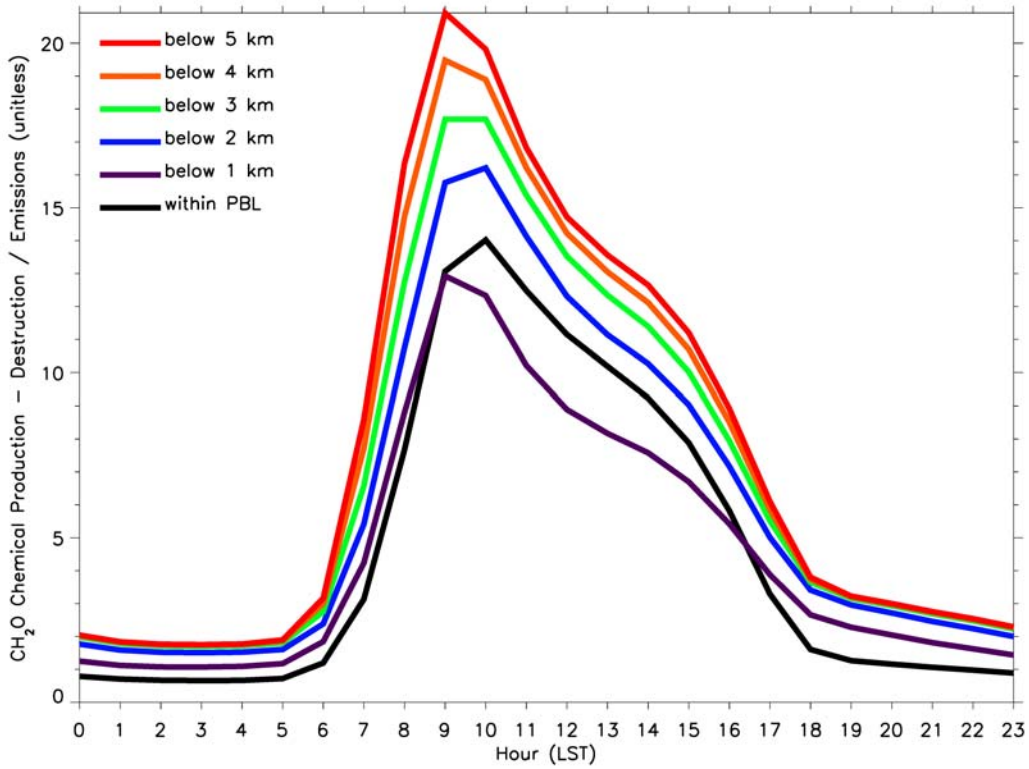

Figure 8: CMAQ model results from Fig. 2 broken out by hour of day for the entire month of September 2013.

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Project 14-003 **STATUS: Active – May 28, 2014**
Completed – June 30, 2015

Update and evaluation of model algorithms needed to predict Particulate Matter from Isoprene

University of North Carolina – Chapel Hill – William Vizuete

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Jim Price

Funding Amount: $200,000 **Expended Amount:** $ TBD

Amount Returned to AQRP: $ TBD

Executive Summary

Terrestrial vegetation emits into the atmosphere large quantities (~500 teragrams C) of the reactive di-olefin isoprene (C_5H_8). Isoprene emissions in eastern Texas and northern Louisiana are some of the largest in the United States. Photochemical oxidation of isoprene leads to significant yields of gas-phase intermediates that contribute to fine particulate matter (PM2.5). The production of isoprene-derived PM2.5 is enhanced when mixed with anthropogenic emissions from urban areas like those found in Houston. To predict PM production from isoprene requires fundamental parameters needed to describe the efficiency with which gas phase intermediates react on the surface of atmospheric particles. Recently, EPA updated a regulatory chemical mechanism to include the formation of these new gas-phase isoprene-derived intermediates. Furthermore, the project investigators recently collaborated with the EPA to update the CMAQ model to predict isoprene-derived PM explicitly across the eastern US. This updated gas- and aerosol-phase framework found in CMAQ remains to be validated against systematically conducted chamber experiments. The goal of this project was to provide new information on these two critical processes. The following four tasks were completed to accomplish this goal:

- Integration of Gas-Phase Epoxide Formation and Subsequent SOA Formation into our smog chamber box model
- Synthesis of Isoprene-derived Epoxides and Known SOA Tracers
- Indoor Chamber Experiments Generating SOA Formation Directly from Isoprene-Derived Epoxides
- Modeling of Isoprene-derived SOA Formation From Environmental Simulation Chambers

Project Update

The final report for this project is under review.

Project 14-004 **STATUS: Active – June 20, 2014**
Completed – July 31, 2015

Emission Source region contributions to a high surface ozone episode during DISCOVER-AQ

University of Maryland – Christopher Loughner
Morgan State University – Melanie Follette-Cook
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Doug Boyer

Funding Amount: $109,111
($55,056 Univ. of Maryland, $54,055 Morgan State Univ.)

Expended Amount: $ TBD
($ TBD Univ. of Maryland, $ TBD Morgan State Univ.)

Amount Returned to AQRP: $ TBD
($ TBD Univ. of Maryland, $TBD Morgan State Univ.)

Executive Summary

The highest ozone air pollution episode in the Houston, TX region in 2013 occurred September 25-26, which coincided with the Deriving Information on Surface Conditions and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) field campaign. The maximum 8-hour average ozone peaked on September 25 at LaPorte Sylvan Beach reaching 124 ppbv, almost 50 ppbv above the current Environmental Protection Agency (EPA) standard of 75 ppbv. We analyzed this air pollution episode and have quantified the contributions of emissions from various anthropogenic source regions.

We used the Weather Research and Forecasting (WRF) and the Community Multi-scale Air Quality (CMAQ) model along with ground and aircraft observations obtained during the DISCOVER-AQ field deployment to evaluate the model simulations. Our first set of simulations did not perform well as compared with observations. The WRF simulation did not accurately capture the sea and bay breeze circulations on September 25, which resulted in an underestimate of surface ozone mixing ratios near the coastline of Galveston Bay. We re-ran WRF using refined model inputs and employing a novel iterative technique developed at the EPA. This new and improved simulation accurately simulated the sea and bay breeze circulations on September 25. This improved WRF simulation was used to drive a new CMAQ simulation. The improved CMAQ run simulated a widespread area that exceeded the EPA ozone standard, which agrees with observations. However, the model still had a low ozone bias downwind of Baytown and Deer Park. This low bias may be due to over-assisted flaring events at petrochemical facilities near Baytown and Deer Park, as is being concurrently investigated in Texas AQRP Project #14-002 to be completed late summer. During over-assisted flaring events, combustion efficiency declines and more VOCs and air toxics are released to the atmosphere. The NASA P-3B aircraft identified possible over-assisted flares by observing high NOx/NOy ratios, low O3 indicating titration taking place, and high formaldehyde as the aircraft flew through the emissions plumes. These high emissions events were not in the CMAQ emissions input files. The model simulated a low bias in ozone downwind of the observed over-assisted flaring emissions over Galveston Bay

and the coastline of Galveston Bay, but the model still simulated ozone exceedances in these areas. This shows that the high emissions events on September 25 that took place near Baytown and Deer Park, possibly from over-assisted flares, made a bad surface ozone episode worse.

We identified possible anthropogenic source regions that impacted Houston during this campaign by calculating back trajectories from our WRF simulation. Houston, Dallas, Beaumont, Lake Charles, marine, and other areas were the anthropogenic source regions tagged for a CMAQ ozone source apportionment simulation based on the back trajectory analysis. Results from the ozone source apportionment model run show that anthropogenic emissions from Houston were the primary contributors during this air pollution episode. In addition, this CMAQ run likely underestimated the contribution of Houston emissions due to the missing over-assisted flare emissions in the model.

Satellite observations were analyzed to determine if they were able to detect the regional transport of air pollution and subsequent buildup in the Houston metropolitan area for this air pollution episode. While satellite observations were not able to detect transport from a specific anthropogenic source region during this episode, tropospheric nitrogen dioxide (NO2) columns and total carbon monoxide (CO) columns as observed from space did show higher pollution over the continent than over the Gulf of Mexico. This suggests that higher air pollution concentrations are transported into Houston when transport is from the continent than from the Gulf of Mexico, which was the case during this air pollution episode.

[*Project Management Note*
The study team of this project notified the AQRP in September 2015 that they recently discovered that CMAQ simulations performed for Projects #14-002 and 14-004 utilized incorrect exit velocities of elevated point source emissions. This may result in artificially high free tropospheric concentrations of various species rather than increased values in the boundary layer.

The study team will correct the exit velocities, re-run CMAQ, and re-do the analyses for these projects. CMAQ will be re-run for all modeling domains (36, 12, 4, and 1 km horizontal resolution domains) and evaluated with observations made during the DISCOVER-AQ field campaign. Additional CMAQ simulations will be performed after the updated base case simulations. For Project #14-004 the 4 km CMAQ domain will be re -run with the ozone source apportionment tool to examine the impact of emissions from several emissions source regions on air quality in the greater Houston metropolitan area.

The AQRP will provide a no cost extension to Project 14-004 through November 30, 2015, to allow time to re-run the models, analyze the data and revise the final report. No additional funds will be made available for the project.]

Project 14-005 **STATUS: Active – February 5, 2015**

Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation

Texas A&M – Sarah Brooks

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Jim Price

Funding Amount: $103,890

Executive Summary

Tropospheric air quality is degraded by local aerosol sources and gas phase precursors as well as aerosol transported over long distances. While the availability of recent satellites such as the Moderate-resolution Imaging Spectroradiometer (MODIS) and the Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) offer improved accuracy and global coverage of aerosol, such measurements still rely on broad assumptions in determination of aerosol source and composition. During the fall of 2013, the Houston area was the site of the 2nd field intensive of the NASA Deriving Information on Surface conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign. During DISCOVER-AQ, this project's research team operated a new scattering instrument, the Cloud and Aerosol Spectrometer with Polarization (CASPOL), which measures the depolarization ratio of individual particles in the aerosol population. The polarization capabilities of CASPOL facilitate an effective approach to validate space-borne aerosol retrieval, particularly CALIOP aerosol type classification. The CASPOL was operated on top of the 60 m tall Moody Tower (MT) on the University of Houston campus, a central urban location and site of many complementary measurements during DISCOVER-AQ. In this study, the CASPOL data set will be analyzed to determine the concentration, size distribution, and optical properties of aerosol from the wide variety of sources, including urban pollution sources from downtown Houston, the industrial Ship Channel, and transported aerosol. Combined with additional measurements of organic carbon, black carbon and ozone, the CASPOL data set provides an opportunity to determine the primary aerosol sources and impacts of aging due to ozone modified aerosol optical properties. These in-situ data will be compared to MODIS and CALIOP aerosol measurements to determine the sensitivity of remote sensing to changes in surface aerosol properties and air quality. Results from the project will improve the linkage between column observations provided by satellite instruments and near-surface atmospheric composition, which is relevant to air quality and human health in the short term and the relationship between future air quality and climate.

Project Update

Project activities are described by task number below.

Task 1. Summary of MODIS aerosol optical depth and CAPSOL aerosol type

In-Situ CASPOL DISCOVER-AQ Aerosol Measurements

As discussed in our previous reports, the Cloud and Aerosol Spectrometer with Polarization (CASPOL) is a new optical particle counter developed by the Droplet Measurement Technology, Inc. (DMT) and calibrated in the laboratory [*Glen and Brooks*, 2013; 2014]. This instrument measures the particle-by-particle optical properties of aerosols. The forward scatter intensity,

measured by the detector in the forward direction, is used to derive the size distribution of particles within 28 bins from 0.68 μm to 30 μm in diameter based on the Mie scattering theory. In addition, two detectors are used measure the parallel and perpendicularly polarized backscatter radiation. The size range covers the cut-off point of ~1 μm that is often adopted to discriminate fine and coarse aerosol particles [*Anderson et al.*, 2005b]. Thus, the ratio of the concentration of particles smaller than the cut-off to the total concentration can characterize the proportion of fine particles. For the purposes of this study, we define this as the CASPOL submicrometer fraction, SMF, following the similar naming by *Anderson et al.* [2005a]. (Specifically, the CASPOL bin boundary closest to 1 μm (1.03 μm) was taken as the cut-off to calculate SMF.)

The 2nd intensive DISCOVER-AQ campaign took place over the Houston area in the late summer and early fall of 2013. One of the missions of the campaign was improved interpretations of satellite observations with regard to air pollutants. During the field campaign, CASPOL was put on the Moody Tower (29.7176° N, 95.3414° W) for measurements from 15 August to 2 October in 2013, providing a chance to compare the CASPOL in-situ aerosol measurements with satellite aerosol retrievals. The Moody tower has been the location of a number of previous field campaigns [*Brooks et al.*, 2010; *Lefer et al.*, 2010; *Rappenglück et al.*, 2010; *Wong et al.*, 2011]. The height of the Moody tower is about 70 meter. It is low enough so that the aerosols being sampled are representative of the aerosols at the surface, but tall enough so that any intermittent point sources will not interfere with the measurements.

Fig. 1 shows a schematic of the experimental setup for CASPOL measurements during the campaign. The CASPOL inlet was specially designed to keep pointing to the upstream wind. The inflow air was first running through a heated stainless-steel pipe (1.5 m in length) wrapped by a non-conductive tubing, where the relative humidity was kept constant to avoid condensation [*Quinn et al.*, 1998]. The sample flow beyond the heated pipe was then split into CASPOL at a rate of 1.2 L min^{-1} and a dump line at a rate of 10 L min^{-1}, controlled by a pair of mass flow controllers and pumps. Behind the CASPOL were two groups of thermocouples (TC1 and TC2) and relative humidity meters (RH1 and RH2) with a high-efficiency particulate arresting (HEPA) filter in between. At least twice a week, the inlet line was changed, and the tubing was changed or dried. If rainfall amounts exceeded three fourths of an inch in six hours, data was removed right before and during the rainy period, because of the possibility of the removal of particles via the wet deposition process.

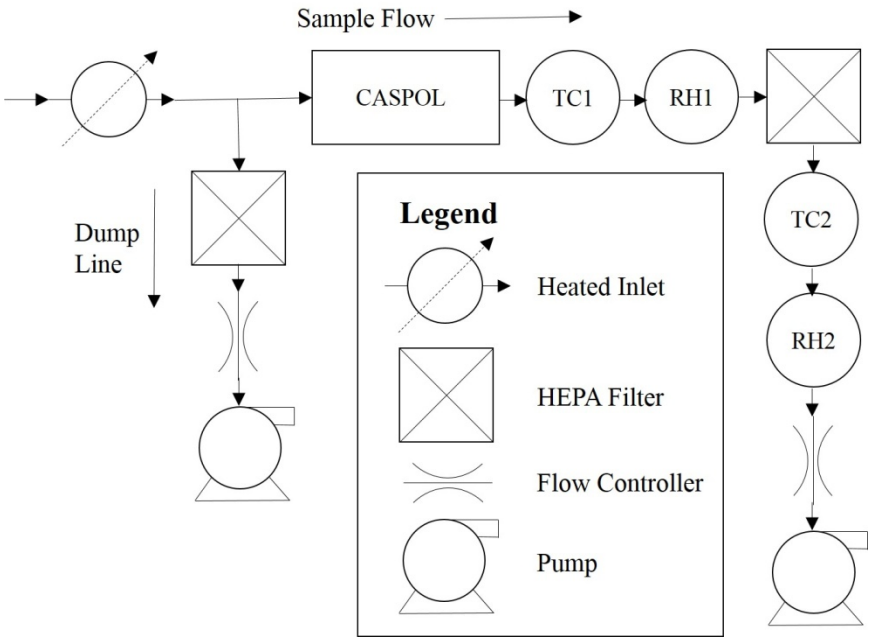

Figure 1. Experimental setup for CASPOL measurements.

DISCOVER-AQ was the first field deployment of CASPOL since it was designed and built by DMT. Following a period of successful data collection, the CASPOL experienced a serious drop in observed concentration on 17 September, 2013. A plausible cause was an (unspecified) instrumental issue in the CASPOL at that time. Hence, we removed the data later than September 17. Recent laboratory calibration indicates that the CASPOL is once again working well and accurately counting and sizing aerosols. Hence, we tentatively conclude that the problem experienced in the field was related to a blockage in the CASPOL inlet tubing, rather than an issue in the instrument itself. As a consequence, only the CASPOL measurements during 5-17 September are included in this study.

How sensitive are MODIS retrievals over the Houston Area to aerosol type?
First, we address the question of whether uncertainty in the MODIS aerosols retrievals over urban areas is due to aerosol assumptions or surface reflectivity. We will use aerosol data available across the full region to give each MODIS retrieval (day and pixel) a predominant aerosol type based on assumptions from each of the MODIS algorithms from Collection 5 and Collection 6 and meteorological condition classification. Then, we will compare the MODIS aerosol optical depth and aerosol type assumptions to AERONET optical depths and CASPOL aerosol typing. Next, we will look specifically at MODIS pixels that include Moody Tower to determine if variability detected by the CASPOL is reflected in the MODIS retrievals. If so, this will enable future use of the CASPOL data to improve MODIS aerosol models.

Table 1. Collocated MODIS (Terra) and CASPOL Data

Date	Time (CDT)	Terra AOD (Aerosol Optical Depth)	AERONET AOD	CASPOL Aerosol Type
6 September	12:30	0.262	0.233	Ship Channel
8 September	12:20	0.278	0.105	Transported
13 September	12:34	0.312	0.203	Urban
22 September	12:29	0.098	0.050	Transported
25 September	11:24	0.152	0.090	Transported
26 September	12:04	0.133	0.060	Transported

Task 1B. Updated Analysis Strategy for MODIS Aerosol Retrievals

In addition to aerosol optical depth, the size parameter (α), and the fine mode fraction, have been used to characterize urban aerosol concentration populations.. In general, anthropogenic aerosols are mostly dominated by fine particles whereas natural aerosols are dominated by coarse particles [e.g. *Deuzé et al.*, 2001; *Kaufman et al.*, 2001; *Tanré et al.*, 2001], and consequently FMF retrievals have been widely used to characterize the anthropogenic component [e.g. *Bellouin et al.*, 2005; *Christopher et al.*, 2006; *Kaufman et al.*, 2005; *Ramachandran*, 2007; *Yu et al.*, 2009].

A number of studies have focused on the validations of MODIS aerosol retrievals since the first-generation MODIS aerosol algorithm [*Chu et al.*, 2002; *Remer et al.*, 2005]. The uncertainties of MODIS aerosol property retrievals stem from the applicability of retrieval assumptions in different environments, including assumed spectral dependence of surface reflectivity and aerosol models. Previous quality assessments of MODIS α and FMF retrievals have been made through comparisons with ground-based or airborne sun-photometer retrievals [e.g. *Anderson et al.*, 2005a; *Chu et al.*, 2005; *Kleidman et al.*, 2005; *Remer et al.*, 2005]. Historically, literature results report a poor correlation between MODIS Collection 5 aerosol size retrievals and sun-photometer FMF retrievals over land. Over oceans, MODIS appears to overestimate low values of FMF and underestimate high values of FMF. Based on these comparison studies, *Levy et al.* [2010] concluded that the MODIS Collection 5 aerosol size retrievals show noteworthy uncertainties and hence have little physical validity in a quantitative sense. However, an updated

MODIS data set, Collection 6, has become available more recently. [*Levy et al.*, 2013]. Also, the spatial resolution of aerosol retrievals in MODIS Collection 6 is km, a major improvement over the previously 10 km resolution. To the best of our knowledge, no study has compared MODIS Collection 6 MODIS FMF retrievals with aerosol size distribution measurements collected in-situ. Here we compare the MODIS FMF retrievals with CASPOL aerosol size distribution measurements in the Houston urban area during DISCOVER-AQ campaign in 2013.

MODIS-CASPOL Size Distribution and Fine Mode Intercomparison

Based on observations of bimodal aerosol size distributions, in the MODIS aerosol algorithm over dark continental surfaces, a combination of fine-dominated and coarse-dominated aerosol models are assumed. Aerosol populations are assumed to be bimodal with a coarse mode assumed to be dust and a fine mode with characteristics defined according to location and season. The fine-dominated model choices include three spherical aerosol models whose absorbance levels are different, representing weakly, moderately, and strongly absorptive aerosols. Consequently, the fine mode was identified as weakly absorptive aerosols for the duration of the DISCOVER-AQ project over the Houston area in September, 2013. Table 2 listed the size parameters of the weakly absorptive fine model and the coarse model in the MODIS aerosol algorithm, where r_v, σ, and V_0 are median radius, standard deviation, and volume concentration, respectively.

Table 2. Size parameters of the weakly absorptive fine model and the coarse model in the MODIS aerosol algorithm [*Levy et al.*, 2009].

	Fine model (weakly absorptive)		Coarse model	
	Accumulated	Coarse	Accumulated	Coarse
Mean Radius, $r_v(\mu m)$	$0.0434\tau+0.1604$	$0.1411\tau+3.3252$	$0.1416\ \tau^{-0.0519}$	2.2
Standard Deviation in radius $\sigma(\mu m)$	$0.1529\tau+0.3642$	$0.1638\tau+0.7595$	$0.7561\tau^{0.148}$	$0.554\ \tau^{-0.0519}$
Volume concentration (V_0)	$0.1718\ \tau^{0.8213}$	$0.0934\ \tau^{0.6394}$	$0.0871\ \tau^{1.026}$	$0.6786\ \tau^{1.0569}$

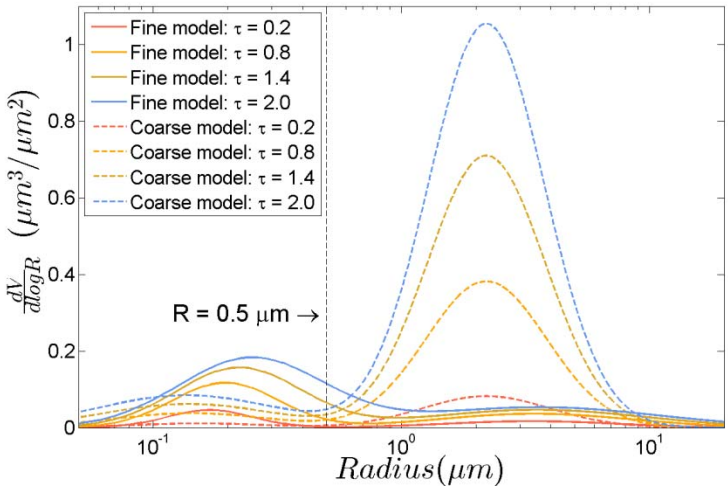

Figure 2. The dynamic volume size distributions of the fine (weakly absorptive) and coarse (dust) models in the conditions of different AODs in the MODIS aerosol algorithm.

Fig. 2 shows the volume size distributions of the fine (weakly absorptive) and coarse models in the conditions of τ = 0.2, 0.8, 1.4, and 2.0, The vertical dashed black line corresponds to a radius of 0.5 μm. The peaks of the coarse model are at a radius 2.2 μm. The peaks of the fine model vary between 0.1 μm and 0.5 μm. Note that ~ 0.5 μm in radius is also a division between the assumed fine and coarse particles in the MODIS aerosol algorithm, in agreement with the CASPOL submicron fraction cut-off chosen above.

MODIS FMF is defined as the proportion of the spectral reflectance contributed by the fine aerosol model [*Levy et al.*, 2010]. We compared MODIS FMF retrievals with CASPOL η measurements during the campaign. Specifically, the 3-km FMF retrievals from the Terra and Aqua MODIS Collection 6 were used in this study. Terra and Aqua, two polar-orbiting satellites, carry MODIS. In the daytime, Terra passes the Houston area around the noon and Aqua passes the same area in the early afternoon.

For example, Fig. 3 shows the monthly mean distributions of FMF retrievals from Terra and Aqua over southeast Texas in September, 2013. In each panel, the red circle is centered at the Moody Tower with a radius of 50 km. We averaged the available FMF retrievals within the circle for the comparisons with CASPOL η measurements. The monthly mean area-averaged FMF from Aqua MODIS outnumbers that from Terra MODIS. They are 0.63 and 0.19, respectively.

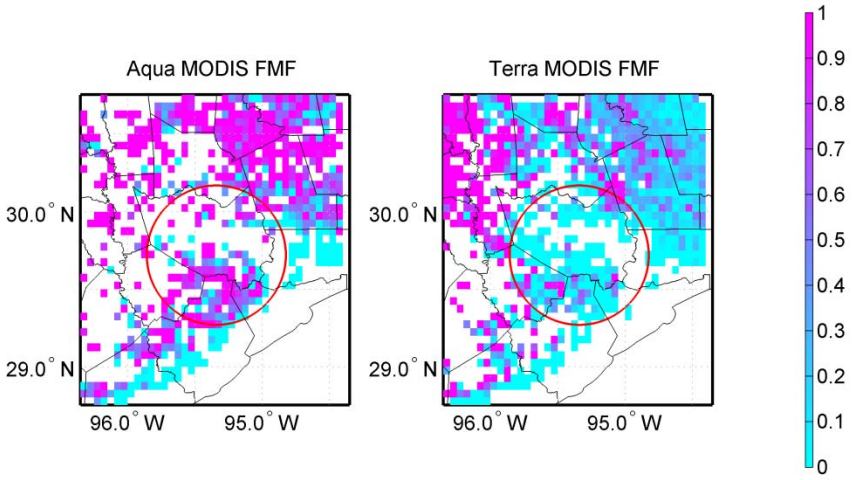

Figure 3. The monthly mean Aqua (left panel) and Terra (right panel) MODIS FMF distributions in September 2013 over an area from 28.75° N to 30.75° N and from 96.35° W to 94.35° W. The red circle in each panel is centered at the Moody Tower with a radius of 50 km. It is not known why the Aqua and Terra monthly average fine mode fractions are remarkably different in the same area.

During the period when CASPOL was sampling, we found 7 Aqua and 6 Terra MODIS FMF retrieval cases. For each case, we counted the particles sampled by CASPOL as to their sizes 30 minutes before and after the satellite overpassing time. Fig. 4 shows the aerosol number size distributions measured by CASPOL for all the 13 cases. The vertical dashed black line marks R = 0.5 μm. As shown in Fig. 4, the proportions of coarse particles for the Terra cases are higher than those for the Aqua cases, suggesting that the concentration of aerosols increased between around noon (when Terra passes over the site) and around 2 pm (when Aqua overpasses the site). This is qualitatively consistent with the differences between the Aqua and Terra monthly averages in Figure 2.

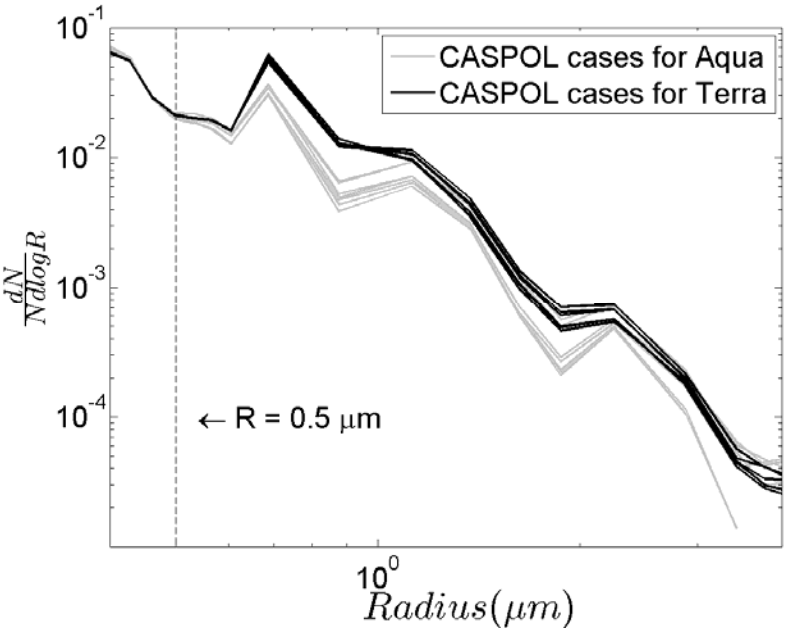

Figure 4. The normalized number size distributions from CASPOL measurements for the 7 Aqua and 6 Terra comparison cases.

We chose a cut-off of 1.03 μm in diameter to calculate the respective SMFs from the number size distribution for each case. Fig. 5 shows the scatterplot of CASPOL η vs. MODIS FMF for the two cut-offs. It appears that CASPOL η measurements are consistent with Aqua MODIS FMF retrievals. They show a correlation coefficient (ρ) and 0.632 for the 1.03 μm cutoff. However, CASPOL η measurements are not consistent with Terra MODIS FMF retrievals which suggest a problem in the Terra MODIS FMF retrievals. Previous studies have shown that the transition of electronics of the Terra MODIS might degrade the quality of its FMF retrievals [*Chu et al.*, 2005; *Remer et al.*, 2005].

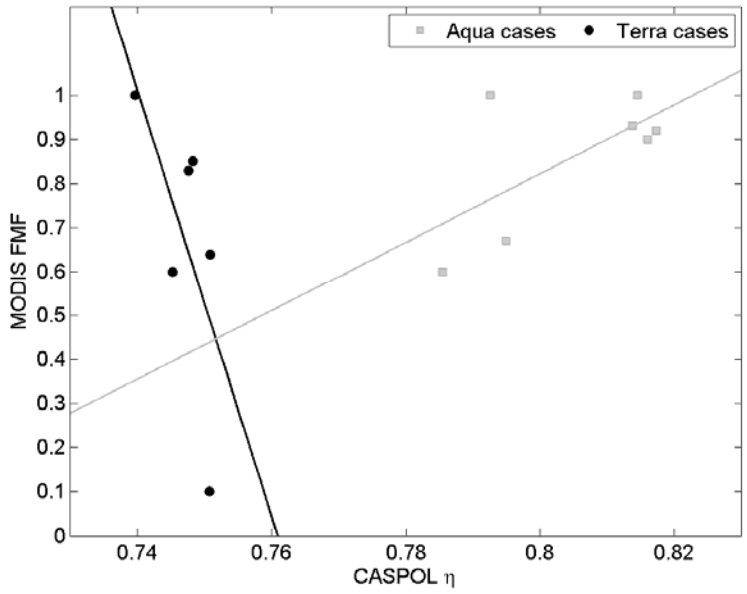

Figure 5. CASPOL Submicron Fraction SMF (η) vs. MODIS Fine Mode Fraction. The lines are the linear regressions.

Task 2. CALIOP remotely sensed optical signature plots for each case identified in the CASPOL data. By inspection of the coordinated data sets, we propose to answer the following questions about MODIS and CALIOP retrievals

How do the CASPOL depolarization ratios and aerosol typing compare with CALIOP? CALIOP data can be processed to produce remotely sensed optical signature plots, which are nearly identical to the CASPOL data. While CASPOL and CALIOP both provide information about aerosol backscatter and depolarization ratio, there are distinct differences between the measurements. For example, CASPOL provides information about individual particles, while CALIOP retrieves averaged information over 5 km horizontally and approximately 30 m vertically. Additionally, the CALIOP retrievals are based on a number of assumptions about aerosol lidar ratio and depolarization ratio for aerosol types. The CASPOL measurements provide us an exciting and novel opportunity to evaluate the CALIOP aerosol assumptions and propose improved aerosol type models.

Table 3. Collocated CALIOP and CASPOL Data

Date	Latitude	Longitude	Distance (km)	CALIOP DPR	CASPOL DPR	CASPOL Backscatter Intensity
11 Sep	29.85	-96.08	73.07	0.014	0.016	64.8
16 Sep	29.81	-94.95	39.33	NA	0.026	40.2
23 Sep	29.51	-96.38	102.89	0.013	0.005	60.1
27 Sep	29.85	-96.04	68.98	0.014	0.007	60.9

*NA is short for not available.

Deliverables Accomplished this Quarter

1A. Originally Planned Deliverable A summary of MODIS aerosol optical depth and aerosol type for each for the cases by the CASPOL.

The results in Table 1 show that MODIS aerosol optical depth (AOD) retrievals over the Houston urban area are overestimated compared to the AERONET in nine of the ten cases (with a 1% significance level). So, while the MODIS treats all cases as weakly absorbing, fine-tuning this would lead to MODIS AODs which are further from, rather than more similar to, AERONET. Our intent was to test whether the agreement between MODIS AOD and AERONET AOD varied between air mass types as determined by the CASPOL. However, in the collocated MODIS-CASPOL data sets in Table 1, there are only 2 Ship Channel cases, and 1 Urban case. Hence a revised approach for comparing CASPOL to MODIS is needed to draw robust conclusions.

An adequate number of cases (10) of collocated MODIS and CASPOL data have been found. Additional analysis will include further analysis of data collected during these time periods, including CASPOL mean backscattering, mean depolarization ratio, particle size distribution, and derived fine mode fraction and MODIS derived fine mode fraction. In contrast, there are not enough cases in which CASPOL data is available for 8 continuous hours centered on the CALIOP overpass. Therefore, no strong conclusions can be drawn from these data. The 8 hour time requirement was chosen to be consistent with the initial MODIS-CASPOL comparisons and is specifically required for the generation of CASPOL optical signatures. However, CASPOL depolarization ratios require less data points than optical scattering signatures. For this reason, we added the comparison of MODIS fine mode fraction and comparison to CASPOL submicron fraction described in Task 1B.

1B. Added Deliverable A summary of MODIS fine mode fraction and comparison to CASPOL submicron fraction.

2. Originally Planned Deliverable CALIOP remotely *sensed optical signature plots for each case identified in the CASPOL data. A report summarizing which variations observed in-situ data can and which cannot be observed in remotely sensed data sets.*

As seen in Table 3 (above), 4 cases of collocated CASPOL and CALIOP are available during DISCOVER-AQ, and in one of these, the CALIOP reports that the value of depolarization ratio is too small to be reported. Based on the low number of data collocated sets available, it is difficult to make a reliable comparison.

Project 14-006 **STATUS: Active – June 12, 2014**
Completed – June 30, 2015

Characterization of Boundary-Layer Meteorology during DISCOVER-AQ Using Radar Wind Profiler and Balloon Sounding Measurements

Sonoma Technology, Inc. – Clinton MacDonald
Valparaiso University – Gary Morris
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Dave Westenbarger

Funding Amount: $65,588
($49,979 Sonoma Technology, $15,609 Valparaiso, $0 St. Edwards Univ.)*

Expended Amount: $ TBD
($ TBD Sonoma Technology, $3,578.11 Valparaiso, $ TBD St. Edwards Univ.)

Amount Returned to AQRP: $ TBD
($ TBD Sonoma Technology, $0.00 Valparaiso, $ TBD St. Edwards Univ.)

Executive Summary

DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) is a National Aeronautics and Space Administration (NASA) Earth Venture program-funded mission that consists of field studies in several locations across the United States, with an overall objective to improve the use of satellites to monitor near-surface air quality, and in turn, to help scientists make better air quality forecasts, more accurately determine pollution sources, and develop successful strategies to reduce pollution and improve public health. The DISCOVER-AQ Houston field study took place in September 2013. During this study, detailed meteorological and air quality observations were taken throughout the Houston area by instruments on the ground, on aircraft, on payloads of balloons (both tethered and free-released), and in Earth orbit. Instrumentation operated during the field campaign included seven radar wind profilers (RWPs) and three ozonesonde sites in and around Houston, Texas. Measurements were taken to provide data to characterize the atmospheric boundary layer conditions during DISCOVER-AQ to support the analysis of chemical data and future air quality modeling by the Texas Commission on Environmental Quality (TCEQ).

This report provides a basis for understanding key meteorological processes that were observed during the 2013 DISCOVER-AQ campaign in the Houston area. Meteorological and air quality data from standard surface monitors, RWPs, ozonesondes, weather satellites and radar, and air parcel trajectory models were analyzed by meteorologists at Sonoma Technology, Inc. (STI) and Gary Morris, PhD (St. Edwards University) to characterize atmospheric boundary layer conditions and relate those findings to observed air quality during the DISCOVER-AQ campaign, as well as on some days with high ozone levels that occurred following the campaign. This analysis stands alone but can also assist other researchers with the interpretation of measurements collected during DISCOVER-AQ and provide context for the results derived from

data collected during DISCOVER-AQ. A summary of key findings from this analysis is provided below.

- Two general meteorological regimes were identified during the DISCOVER-AQ period: (1) deep onshore flow with lower ozone concentrations, and (2) weak large-scale flow and complex local flows with higher ozone concentrations.
- In agreement with previous analyses, the highest ozone concentrations occurred during periods of weak large-scale flow, typically following the passage of a surface cold front. Two days with such events were identified during the time period analyzed in this report: September 25 and October 8, 2013.
- On high-ozone days, mixing heights were typically low (at or below 500 m) at coastal and inland locations during the early- to mid-morning hours, before increasing rapidly to near 2000 m inland during the late-morning and early-afternoon hours while remaining steady at the coast. In contrast, mixing heights on low-ozone days showed less diurnal and spatial variation.
- Surface ozone concentrations were more spatially and diurnally variable on high-ozone days compared to low-ozone days, due to the presence of complex, local flow patterns.
- During both meteorological regimes identified (deep onshore flow with long transport distances or weak offshore/shore-parallel flow with short transport distances), ozone concentrations were typically highest on the downwind side of Houston, illustrating the important impact of local pollution emissions on regional air quality.

* Funding of $15,609 was initially awarded to Valparaiso University. During the term of the project, the Valparaiso University investigator moved to St. Edwards University. The funds remaining unspent at Valparaiso University were transferred to St. Edwards University so that the project could be completed.

Project Update

The final report for this project is under review.

Project 14-007 **STATUS: Active – June 23, 2014**
Completed – June 30, 2015

Improved Analysis of VOC, NO2, SO2 and HCHO data from SOF, mobile DOAS and MW-DOAS during DISCOVER-AQ

Chalmers University – Johan Mellqvist
University of Houston – Barry Lefer

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – John Jolly

Funding Amount: $97,260
($74,179 Chalmers, $23,081 UH)

Expended Amount: $97,260.00
($74,179 Chalmers, $23,081 UH)

Amount Returned to AQRP: $0.00
($0.00 Chalmers, $0.00 UH)

Executive Summary

In a previous project, mobile remote sensing measurements of atmospheric gas column measurements of SO_2, NO_2, HCHO and VOCs were carried out in a box around the Houston Ship channel, in parallel with flights by two aircraft from NASA. In this project the collected data was reanalyzed, improved and compared to other data, as part of the NASA DISCOVER-AQ experiment. The data were obtained using mobile optical remote sensing measurements by the SOF and Mobile DOAS techniques, which were carried out in the Houston area during September 2013.

The DISCOVER-AQ campaign had the objective to demonstrate that geostationary satellites can provide useful environmental data. NASA operated a high altitude aircraft (B200) equipped with optical sensors, measuring columns of SO_2, NO_2, HCHO and aerosol profiles (LIDAR). To validate these measurements they also carried out in situ measurements with a low flying airplane (P3B) that did spirals above two ground stations in the Houston ship channel, equipped with optical (Pandora) and in-situ sensors.

During the 2013 field campaign a new VOC sensor was used to map ratios of the ground concentrations of alkanes and aromatic VOCs downwind of various industries. The sensor is an open path Differential Optical Absorption Spectroscopy (DOAS) system coupled to a custom made multiple-pass cell working in the UV region between 250-280 nm. In this project we have refined the spectral analysis for measurements of aromatic VOCs from this sensor and compared its data to parallel data from a proton transfer mass spectrometer (PTRMS) and canister sampling and subsequent GC-FID. The instrument shows a detection limit of 0.3-1 ppb of for the BTX species. For a number of transects through plumes from real emission sources in the HSC, the ratio of time-integrated benzene concentrations measured by the MW-DOAS and a PTRMS operated by Montana State University was 1.00 on average, indicating very good agreement, while for toluene the PTRMS was 11% lower on average. In a corresponding experiment, canister sampling carried out downwind of several refineries in the Middle East and subsequent GC-FID analysis showed 32 % and 43 % lower values, respectively, for the same species compared to MW-DOAS. This will be further investigated. Ground data measured with MW-DOAS, downwind of a Texas City refinery shows that the BTEX to alkane mass ratios were 0.10±0.04, corresponding to a mass emission 134 kg/h for the 2013 data. Here it is assumed that

the aromatic VOCs and alkanes were well mixed in the emission plume at the measurement position. An additional uncertainty is the few amount of measurements carried out in 2013.

During the campaign, mobile remote sensing by the SOF method and Mobile DOAS were carried out in the Houston area on twenty days in September 2013 together with frequent balloon launches. During ten of these days, column measurements of SO_2, NO_2, HCHO and VOCs in a box around the Houston Ship channel were carried out synchronized with science flights by the NASA aircraft. During the rest of the days more focused industrial measurements were carried out. The weather during the campaign was relatively poor with 4 good clear days, 10 moderate days and the rest rather cloudy.

A small measurement study was carried out in Sweden in September 2014 to investigate the effects of clouds on the Mobile DOAS measurements. During the course of this study, a so far undetected instrumental effect was discovered which was seen to affect the quality of evaluation negatively. A drift in instrumental lineshape was determined to be the cause of this and a method was developed to compensate for it. This method was successfully applied to the measurements during the DISCOVER-AQ campaign and was seen to improve spectral fit quality and give more stable baselines in some cases.

The measurement study also concluded that the changes in evaluated columns experienced due to clouds are most likely real changes in the actual column due to changes in radiative transfer rather than some form of spectral artifacts. Because of this, development of cloud indicator was determined to be the best way to deal with cloud effects. A cloud indicator based on the principle of a color index, a simple ratio between the spectral intensity at two different wavelengths, was developed and applied to the measurement series in order to allow more data to be used for flux calculations.

Multi-angle mobile DOAS measurements performed during the last days of the DISCOVER-AQ campaign were evaluated using a new scheme designed to enable absolute columns to be derived. As part of this scheme radiative transfer simulations were performed using in-situ data from the airborne measurements in order to derive direction dependent differential air mass factors needed to convert the evaluated columns to absolute mixing layer columns. After some averaging and filtering, this data could be used to establish an absolute offset for the relative columns from the standard evaluation and control for baseline drift. This gave a better absolute column product that is suited for comparisons with other data from the DISCOVER-AQ campaign.

Table 1 was shows the final emission rates for the 2013 campaign together with corresponding results from previous studies and reported annual routine emissions from the STARS (State of Texas Air Reporting System) emission inventory for 2013.

Table 1 Emission fluxes (kg/h) measured with SOF and Mobile DOAS for different sites, as reported after the measurement campaign. Results from earlier campaigns and Emission inventory data for 2013 [Johansson, 2014b] are also shown.

Area	Species	2006	2009	2011	2013	Emission Inventories 2013
HSC	Ethene	878 ± 152	614 ± 284	612 ± 168	475 ± 79	53
	Propene	1511 ± 529	642 ± 108	563 ± 294*	394 ± 245	48
	Alkanes	12276 ± 3491	10522 ± 2032	11569 ± 2598	13934 ± 4321	818
	SO_2	2277 ±1056	3364 ± 821	2329 ± 466	1683 ± 223	1153
	NO_2	2460 ± 885	-	1830 ± 330	2242 ± 684	1103
Mont Belvieu	Ethene	443 ± 139	444 ± 174	545 ± 284	271 ± 33	29
	Propene	489 ± 231	303 ± 189	58*	220 ± 115	21
	Alkanes	874	1575 ± 704	1319 ± 280	2854 ± 1212**	146
	NO_2	-	168 ± 39	305 ± 29	245 ± 102	138
Texas City	Ethene	83 ± 12	122 ± 41	177 ± 48	-	2
	Propene	ND	54 ± 22	56 ± 9*	-	4
	Alkanes	3010 ± 572	2422 ± 288	2342 ± 805	1340 ± 140	276
	SO_2	-	834 ± 298	1285 ± 428	414 ± 172	128
	NO_2	460 ± 150	283 ± 30	492 ± 71	408 ± 93	331

* Propene retrievals were of poor quality throughout much of this campaign
** Only a single day of measurements with variable emissions.

Project Update

The final report for this project is under review.

Project 14-008 **STATUS: Active – April 17, 2014**

Completed – July 31, 2015

Investigation of Input Parameters for Biogenic Emissions Modeling in Texas during Drought Years

The University of Texas at Austin – Elena McDonald-Buller

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Barry Exum

Funding Amount: $175,000 **Expended Amount:** $172,784.94

Amount Returned to AQRP: $2,215.06

Executive Summary

The role of isoprene and other biogenic volatile organic compounds (BVOCs) in the formation of tropospheric ozone has been recognized as critical for air quality planning in Texas. In the southwestern United States (U.S.), drought has become a recurring phenomenon and, in addition to other extreme weather events, can impose profound and complex effects on human populations and the environment. Understanding these effects on vegetation and biogenic emissions is important as Texas concurrently faces requirements to achieve and maintain attainment with the National Ambient Air Quality Standard (NAAQS) for ozone in several large metropolitan areas. Previous research has indicated that biogenic emissions estimates are influenced by potentially competing effects in model input parameters during drought, and thatuncertainties surrounding several key input parameters remain high. The primary objective of the project is to evaluate and inform improvements in the representation of one of these key input parameters, soil moisture, through the use of simulated and observational datasets. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) will be used to explore the sensitivity of isoprene emission estimates to alternative soil moisture representations.

Project Note

The final report for this project has been accepted and the PI has transferred a copy of the dataset to the AQRP. All invoices have been paid. This project is complete. A copy of the final report is available on the AQRP website.

Project 14-009 **STATUS: Active – July 1, 2014**
Completed – June 30, 2015

Analysis of Surface Particulate Matter and Trace Gas Data Generated during the Houston Operations of DISCOVER-AQ

Rice University – Robert Griffin
University of Houston – Barry Lefer
AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $219,232
($109,867 Rice, $109,365 UH)
Expended Amount: $ TBD
($106,259.42 Rice, $ TBD UH)

Amount Returned to AQRP: $ TBD
($3,607.58 Rice, $ TBD UH)

Executive Summary

The City of Houston, Harris County, and surrounding areas have a long history of air quality issues because of their large population, extensive industrial activity, and sub-tropical climate. These issues predominantly have been manifested through ozone (O3) mixing ratios that exceed the National Ambient Air Quality Standards (NAAQS) established by the United States Environmental Protection Agency. However, recent measurements indicate that Harris County barely achieves compliance with the NAAQS that have been established for particulate matter (PM), specifically for particles with diameters less than or equal to 2.5 micrometers.

In recent years, the National Aeronautics and Space Administration (NASA) has placed considerable emphasis on the use of satellite remote sensing in the measurement of species such as O3 and PM that constitute air pollution. However, additional data are needed to aid in the development of methods to distinguish between low-level and high-level concentrations in these column measurements. To that end, NASA established a program titled Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ). DISCOVER-AQ began in summer 2011 with work in the Mid-Atlantic Coast region that featured satellite, airborne, and ground-based sampling; similar work was performed in California in 2012. The DISCOVER-AQ program conducted operations in and near Houston in September 2013 and in and near Denver in 2014.

During the Houston operations of DISCOVER-AQ, there was a need for ground-based measurement support. A previous project supported by this program filled that need by providing quantitative measurements of sub-micron particle size and composition and mixing ratios of photochemically relevant gases such as O3 and oxides of nitrogen. The instrumentation for these measurements was deployed using the University of Houston/Rice University mobile air quality laboratory. Data quality assurance/control and preliminary data analyses were performed as part of the original project.

More advanced data analyses have been performed as part of the current project, and results from these analyses are included in this report. These analyses focused on source-specific quantification of PM emissions in a size- and chemically resolved manner, identification of large

but short-lived PM events, assessment of the diurnal and spatial distribution of PM in Houston, estimation of the relative oxidation state of organic PM, investigation of the secondary processes that influence PM in Houston, determination of the roles that biogenic volatile organic compounds play in Houston air quality, comparison of in situ and column nitrogen dioxide measurement techniques, and photochemical zero-dimensional modeling of O3 and radical production.

Project Update
The final report for this project is under review.

Project 14-010 **STATUS: Active – January 26, 2015**

Impact of large-scale circulation patterns on surface ozone concentrations in HGB

Texas A&M Galveston – Yuxuan Wang

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Mark Estes

Funding Amount: $79,325

Executive Summary

The Bermuda High (BH) is a key driver of large-scale circulation patterns in Southeastern Texas in summer. The variations in the location and strength of the Bermuda High are expected to influence surface ozone concentrations and cause high- or low-ozone years in HGB through modulating the southerly flows that bring marine air with lower ozone background from the Gulf of Mexico. This project aims at establishing a statistical relationship from historical observations to quantify the impact of the BH variations on the variability of surface O_3 in HGB during the ozone seasons. Such a relationship will then be used to improve the GEOS-Chem simulation of background ozone inflow from the Gulf of Mexico through development of a bias correction scheme. The more than decade-long observational record of ozone and meteorology (1998 – 2012) during the ozone season (April 1 – October 31) will be analyzed to characterize the complex effects of the BH on surface ozone variations in HGB. The ozone variability will be defined for maximum daily 8-h average (MDA8) at the monthly and interannual time scales (i.e., the timescale of determining air quality attainment or nonattainment). A variety of indices to define the location and strength of the Bermuda High (BH Index; BHI) will be adopted from the literature and new BHI of better relevance to Texas air quality will be proposed. Statistical relationships between the variability of surface ozone concentrations and BHI will be constructed based on observations. The observed relationship will then be used as a mechanistic basis to design a bias correction scheme in the GEOS-Chem global CTM to improve its simulation of background O_3 associated with maritime inflow to HGB. The results will benefit the regulatory models of TCEQ through improved boundary conditions at the Gulf of Mexico model domain.

Project Update

Progress on Project 14-010 is summarized below by Task:

Task 1: In addition to the predictors mentioned in the last report (BH-Lon, BHI (referred to as BHI1) and PDSI), we also adopted another BHI (referred to as BHI2), HGB mean temperature and Arctic Oscillation (AO) as new predictors. BHI2 is defined as the mean sea level pressure (SLP) difference between the northeast Texas (31°-36°N, 91°-96°W) and the Gulf of Mexico (25.3°–29.3°N, 92.5°–87.5°W). BHI1 and BHI2 capture the meridional and zonal wind speed over HGB region respectively. Note that all the BH-related indices are developed on the basis of NCEP reanalysis, while the HGB-mean temperatures are calculated using ERA-Interim reanalysis.

Task 2: We applied a stepwise multiple linear regression (MLR) model to construct the statistical relationship between HGB ozone and the indices selected in Task 1. The candidate predicators in MLR include BH-Lon, BHI1, BHI2, PDSI, AO and HGB-mean temperature. The terms are added and deleted based on Akaike Information Criterion (AIC) statistics to obtain the best

model fit. For an easy comparison, we detrended and normalized all the predictors as well as HGB ozone in the later analysis. The best-fit regression equations for each month are as follows,

$$y_{Jun} = 0.34 \times x_1 - 0.76 \times x_3 + 0.49 \times x_6$$

$$y_{Jul} = 0.77 \times x_1$$

$$y_{Aug} = 0.80 \times x_1 - 0.42 \times x_2 + 0.96 \times x_3 - 1.12 \times x_4$$

$$y_{Sep} = 0.56 \times x_1 - 0.50 \times x_3 + 0.67 \times x_5$$

where y represents detrended mean total ozone; x1 represents BH-Lon; x2 and x3 represent BHI1 and BHI2; x4 represents PDSI; x5 represents AO; x6 represents HGB-mean temperature. Since all the predictors and HGB ozone are normalized, the intercept equals 0 in the MLR equations. BH-Lon is the only predictor selected in the MLR equations for each month, indicating that the westward extension of BH is a key factor influencing HGB ozone during summer months, while the role of other meteorological predictors differs by month.

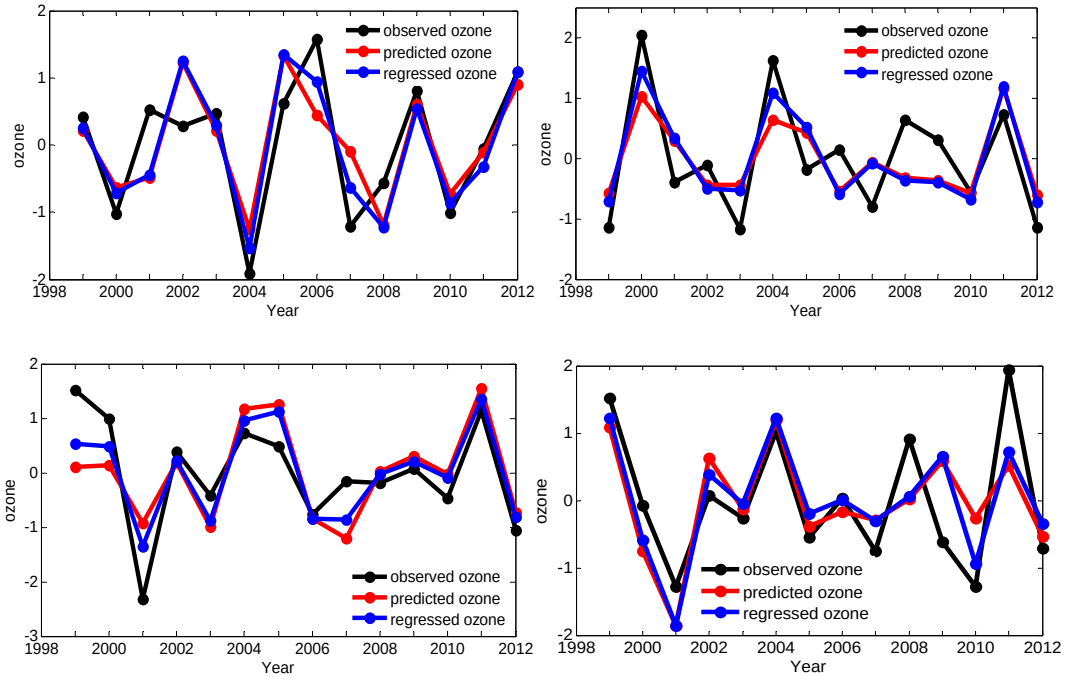

Figure 1. Time series of observed ozone (black line), regressed ozone (blue line) and cross-validation predicted ozone (red line) with the selected indices over the HGB region.

Figure 1 shows the time series of mean HGB MDA8 ozone (black line) and MLR-regressed ozone (blue line) from 1999 to 2012. The correlation coefficients (R^2) for these four months are all higher than 0.55, which indicates that the selected predictors well capture the interannual variability of HGB mean MDA8 ozone. The MLR model captures many of the extremely high and low ozone events in June, July and August. For example, HGB mean MDA8 ozone in June 2004 is the lowest during the studied years, so do the regressed ozone for June 2004. However, in

September, the regressed ozone shows a larger inconsistency with observed ozone in the high ozone year of 2011, which indicates the potential deficiency of the MLR model to predict extreme ozone events in September. The variance inflation factors (VIF) for each month are lower than 10, which is a commonly used VIF threshold to determine collinearity between predictors, indicating that the problem of multicollinearity among the above selected meteorological variables is generally unimportant.

We implemented a cross-validation (CV) method to test the performance of the MLR model. We isolated one month at a time, performed model fitting with the remaining months and validated model performances on the isolated month. The red lines in Figure 1 display the CV-predicted ozone for each month. The correlation coefficients (R^2) between the CV ozone and observed ozone are higher than 0.45. However, some of the extreme values are not very well predicted. With BH-Lon as the single predictor, the CV correlation coefficient in July is the highest among the four months, which verifies our motivating hypothesis of the project that the BH location is a key factor in determining the interannual variations of HGB MDA8 ozone in summer.

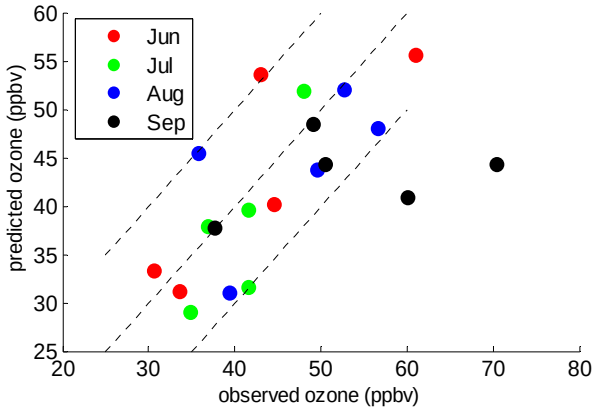

Figure 2. Observed mean total ozone and predicted ozone for June, July, August and September during 1995-1998 and 2014.

To further validate our MLR model, we used the model to predict HGB MDA8 ozone for 1995-1998 and 2014, which are outside of the period (1999-2013) used for the MLR model fitting. The predictors for 1995-1998 and 2014 were obtained and then put in the MLR models to predict HGB ozone for those years by month. Figure 2 shows the observed and MLR-predicted ozone for these 5 years using the obtained MLR equations. 85% of the predicted months are in the category of $y=x\pm10$, indicating the absolute error between the predicted ozone and observed ozone is lower than 10 ppbv.

Task 3: GEOS-Chem simulations have been conducted for June and July from 2004 to 2012 using the GEOS-5 assimilated meteorology and EPA NEI inventory with year-to-year changes of emissions. The model resolution is $0.5^{o}\times0.667^{o}$.

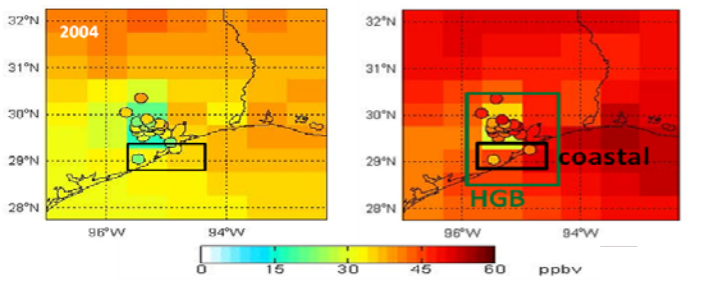

Figure 3. Observed surface ozone (filled circles) and GEOS-Chem simulated surface ozone over HGB region for June (left) and July (right) in 2004.

We used mean ozone at four coastal rural sites (2 over Brazoria region; 2 over Galveston region) as observed background ozone. For simplicity, simulated background ozone is calculated as the mean value over model grids containing these four sites, i.e., the black box shown in Figure 3. The model captures the interannual variations of coastal ozone very well in both June and July (Figure not shown). The mean bias between the simulated and observed surface ozone over the coastal region is 5.17 ppbv for June and 9.54 ppbv for July. The ozone bias is higher in July than in June because the bias is associated with overestimating background ozone with maritime inflow, which peaks in July. Since both observed and simulated coastal ozone over HGB region can be explained by the interannual variations of BH-Lon, the bias between observed and simulated ozone is expected to be correlated with BH-Lon and hence we can use BH-Lon to predict the bias.

The MLR equations for the predicted model bias (y) for June and July are as follows,

$$y_{Jun} = -0.13 \times x + 5.23$$
$$y_{Jul} = -0.34 \times x + 9.59$$

where x indicates the detrended BH-Lon. The negative coefficients in front of the x term (BH-Lon) in June and July both indicate a higher model bias when BH-Lon locates more westward. It in turn testifies that the higher bias in July is due to the stronger maritime inflow coming along with a westward extension of the BH from June to July. The different interannual variations of the bias in June and July support our motivating hypothesis that we need to develop different MLR equations to predict the model bias separately to capture more variance rather than a fixed bias correction.

To correct the simulation results, we then subtracted the predicted bias from simulated background ozone. The time series of corrected simulation is shown in Figure 4 (red line). Compared to the simulation results before the correction (blue line), correlation coefficient between observation and corrected simulation increases from 0.72 to 0.88 and mean bias decreases from 9.54 to 2.36 in July. The correlation coefficient between the observed ozone and simulated ozone after correction is higher in June and the mean bias in June is lower than that in July. This is probably because the stronger maritime inflow brings more clean background air in July which leads to a larger model bias due to the overestimation of background ozone over the Mexican Gulf.

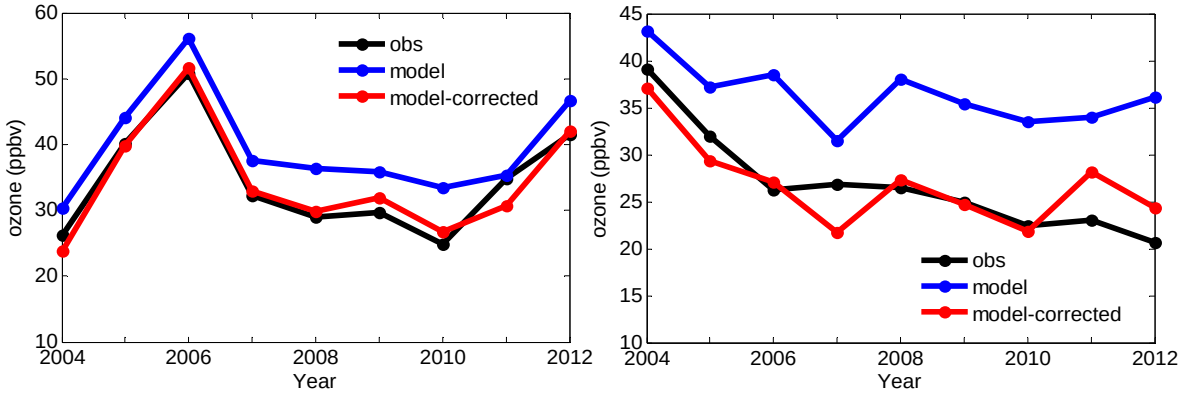

Figure 4. Time series of observation (black line), simulation results (blue line) and corrected simulation results (red line) for June and July.

Project 14-011 **STATUS: Active – June 23, 2014**

Targeted Improvements in the Fire Inventory from NCAR (FINN) Model for Texas Air Quality Planning

The University of Texas at Austin – Elena McDonald-Buller
Environ – Christopher Emery

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Jim MacKay

Funding Amount: $179,586
($151,167 UT-Austin, $28,419 Environ)

Executive Summary

Wildland fires and open burning can be substantial sources of ozone precursors and particulate matter. The influence of fire events on air quality in Texas has been well documented by observational studies. During the 2012-2013 fiscal year of the Air Quality Research Program (AQRP), Dr. Elena McDonald-Buller, Dr. Christine Wiedinmyer, and Mr. Chris Emery led a project (#12-018) that evaluated the sensitivity of emissions estimates from the Fire INventory from NCAR (FINNv1; Wiedinmyer et al. 2011) to the variability in input parameters and the effects on modeled air quality using the Comprehensive Air Quality Model with Extensions (CAMx; ENVIRON, 2011). The project included an analysis of the climatology of fires in Texas and neighboring regions, comparisons of fire emission estimates between the FINN and BlueSky/SmartFire (Larkin 2009; Chinkin et al., 2009) modeling frameworks, evaluation of the sensitivity of FINN emissions estimates to key input parameters and data sources, and assessment of the effects of FINN sensitivities on Texas air quality. Among the many findings of the study were the needs for targeted improvements in land cover characterization, burned area estimation, fuel loadings, and emissions factors. These needs were particularly pronounced in areas with agricultural burning. This project addresses specific improvements in FINN that will support fire emissions estimates for Texas and the next public release of the FINN model. Fire emissions and air quality modeling will focus on 2012 to support TCEQ's air quality planning efforts.

Project Update

Progress on Project 14-011 is summarized below by Task:

Task 1. Regional Land Cover Characterization

Processing of ArcGIS raster files for the land cover datasets in the WGS84 coordinate system has been completed. In addition to the MODIS Land Cover Type Product, these datasets include the Global Land Cover (GLC) - SHARE product from the United Nations Food and Agriculture Organization (FAO), the European Space Agency's (ESA's) Climate Change Initiative Land Cover (CCI-LC) product, the Fuel Characteristic Classification System (FCCS) database and U.S. Department of Agricultural (USDA) National Agricultural Statistical Service (NASS) Cropland Data Layer (CDL) both of which are available for the continental United States, and a high resolution regional land use/land cover database for Texas and surrounding states developed

by Popescu et al. (2011). These land cover products were used alone or in combination in FINN. Seven scenarios were investigated:

Global:
Scenario 1 = MODIS LCT ONLY
Scenario 2 = GLC-SHARE ONLY
Scenario 3 = ESA ONLY

U.S. National:
Scenario 4 = FCCS in the continental US and MODIS LCT elsewhere
Scenario 5 = FCCS_CDL in the continental US and MODIS LCT elsewhere

Texas Regional:
Scenario 6 = TCEQ in the Texas regional domain, FCCS in the continental US, and MODIS LCT elsewhere.
Scenario 7 = TCEQ_CDL in the Texas regional domain, FCCS in the continental US, and MODIS LCT elsewhere.

Annual emissions estimates for carbon monoxide (CO), nitrogen oxides (NO_x), and fine particulate matter ($PM_{2.5}$) associated with fire events during 2012 were generated for each scenario.

Task 2. Mapping of Croplands Data
Cropland data has been obtained from the USDA's CDL as described above. Crop-specific emission factors and fuel loadings have been added to the FINN default configuration. Simulations with (i.e., Scenarios 5 and 7 above) and without the identification of key U.S. crop types were conducted to determine the spatial and seasonal effects of crop identification on FINN emission estimates.

Task 3. Estimation of Burned Area
Development of the algorithms and ArcGIS tools used for processing of the MODIS Rapid Response fire detection records, quantifying burned area, and characterizing the underlying land cover was completed for the new version of FINN.

Task 4. Sub-grid scale Partitioning of NO_x Emissions to NO_z in Fire Plumes
An approach was developed to partition NO_x into aged NO_z forms (HNO_3 and PAN) during EPS3 processing of the FINN emission estimates. A CAMx simulation was conducted using FINN emissions estimates from the TCEQ-CDL land cover scenario with and without the partitioning algorithm in place during EPS3 processing to examine the effects on predicted ozone concentrations.

Task 5. Comprehensive Air Quality Model with Extensions (CAMx) Sensitivity Studies
CAMx simulations with a 2012 episode provided by the TCEQ were conducted using FINN emissions estimates from land cover scenarios 1 (MODIS LCT), Scenario 3 (ESA), and Scenario 7 (TCEQ-CDL). In addition a CAMx simulation was conducted with all fire emissions estimates removed from the input inventory (i.e., no fires). Our team is currently analyzing the results of these simulations.
An initial version of the draft final report was submitted on August 18th and a revised version on August 26th, 2015.

Project 14-014 **STATUS: Active – January 27, 2015**

Constraining NO_X Emissions Using Satellite NO_2 and HCHO Column Measurements over the Southeast Texas

University of Houston – Yunsoo Choi

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Dave Westenbarger

Funding Amount: $84,927

Executive Summary

Ozone production depends not only on availability of Volatile Organic Compounds (VOCs) and Nitrogen Oxides (NO_x) but also on their relative concentrations, which can be expressed as a VOC/NO_x ratio. Over or under prediction of either component in an air quality model changes the VOC/NO_x ratio and limits the capability of an air quality model to predict ozone properly. Additionally, accurate predictions of meteorological variables are crucial to simulate atmospheric chemistry and consequently properly simulate ozone concentrations. In addition to ground and aircraft measurements obtained in Houston during the Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign in September 2013, remote sensing data of NO_2 are available from Aura Ozone Monitoring Instrument (OMI). NO_2 column data products and can be used as a proxy for NO_x and their values in air quality models can be quantified and thus constrained. In this project, an analysis of the archived in-situ aircraft and ground measurements will be performed and satellite measurements of NO_2 will be utilized to improve the bottom-up NO_x emission inventories and study the impact of these improved emissions on ozone predictions. Objective analysis (OA) of meteorological simulations will be applied to improve predictions of meteorological parameters as well as ozone predictions.

The primary objectives of this project are to: (1) utilize satellite measurements of tropospheric NO_2 columns to quantify surface NO_x anthropogenic and soil emissions using inverse modeling; (2) evaluate model-simulated formaldehyde and isoprene concentrations (key drivers for ozone) using in-situ ground and/or aircraft measurements; (3) examine how the ratio of model-simulated NO_2/HCHO in Air Quality Forecasting system at UH (AQF-UH) varies and corresponds to remote sensing NO_2/HCHO column measurements, and (4) perform objective analysis (OA) of meteorological predictions to improve their predictions, and consequently, ozone predictions. The Air Quality Forecasting System will use the Community Multiscale Air Quality (CMAQ) Model with a 4 km resolution for Southeast Texas. The meteorological inputs will be provided by the Weather Research and Forecasting (WRF) model.

Project Update

Previously, we prepared NEI2011 to provide model-ready emissions inventories, conducted inverse modeling to derive posteriori emissions and running CMAQ. We also calculated surface ozone statistics with NEI2011 and compared ozone profile aloft to aircraft measurements.

In the 3rd quarter, we analyzed the surface NO_2, ozone, HCHO/NO_2 ratio sensitivity to emission changes. Using the results of the inverse modeling, we updated NO_x emissions in NEI-2011 and called the updated version NEI-2011n.

1. *The following standard statistics were calculated and used for the comparison:*

1) Correlation (r) between model values and observed values

$$r = \frac{\sum_{t=1}^{n}[(x_t - \bar{x})(y_t - \bar{y})]}{\sqrt{\sum_{t=1}^{n}(x_t - \bar{x})^2 * \sum_{t=1}^{n}(y_t - \bar{y})^2}}$$

n – number of data points, x – observed values, y - model values, over-bar - mean

2) Index of Agreement (IOA) between model values and observed values

$$IOA = 1 - \frac{\sum_{t=1}^{n} e_t^2}{\sum_{t=1}^{n}(|y_t - \bar{x}| + |x_t - \bar{x}|)^2}$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values,

over-bar - mean

3) Root Mean Square Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n} e_t^2}$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

4) Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_{t=1}^{n} |e_t|$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

5) Mean Bias (MB)

$$MB = \frac{1}{n}\sum_{t=1}^{n} e_t$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

2. *Impact on NO_2: surface NO_2, NO_2 aloft, HCHO/NO_2 ratio*

To evaluate the updated NO_x emissions, we performed CMAQ simulations to compare model NO_2 against OMI satellite, aircraft and surface CAMS observations.

Comparison to CAMS

Hourly Surface NO_2 statistics

We also calculated hourly surface NO_2 statistics, which are shown in Table 1.

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
NEI2011	19804	0.65	0.74	6.9	4.5	2.6	5.6	8.2	5.7	8.4
NEI2011n	19804	0.61	0.75	6.0	4.0	1.6	5.6	7.3	5.7	7.1

Table 1. Statistics of hourly surface NO_2**:** N – data points; Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M – Model Mean; SD – Standard Deviation ;Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD: degree ppb

Regional Average Surface NO_2 Time Series in Metro Houston

Figure 1 shows the NO_2 hourly time series averaged using in-situ data from more than 20 CAMS sites. Model consistently over-predicted NO_2 peaks in NEI2011 for most days. With posterior NEI2011n emissions (obtained through inverse modeling), the mean bias and RMSE of NO_2 decreased by 24% and 15% respectively.

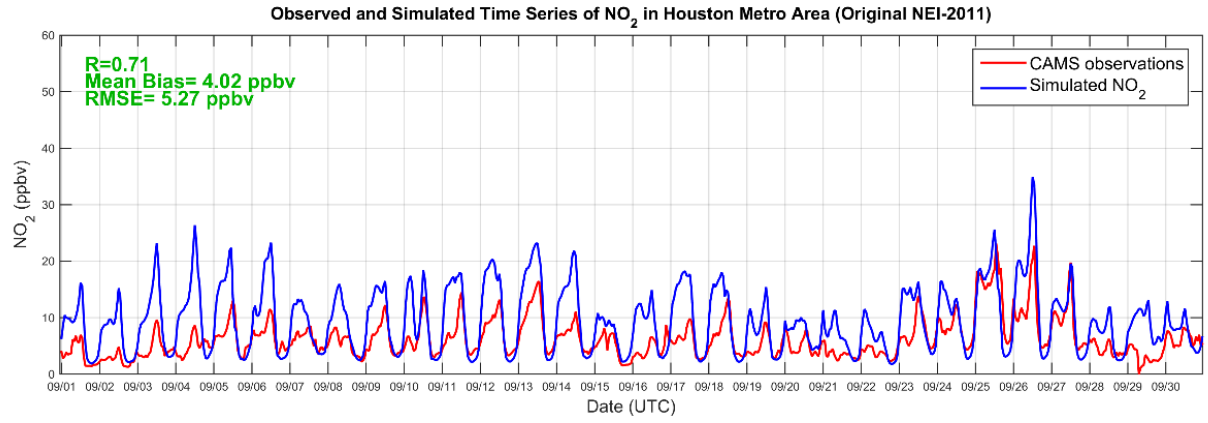

Figure 1(a). Time series of simulated and observed surface NO_2 levels -- NEI2011

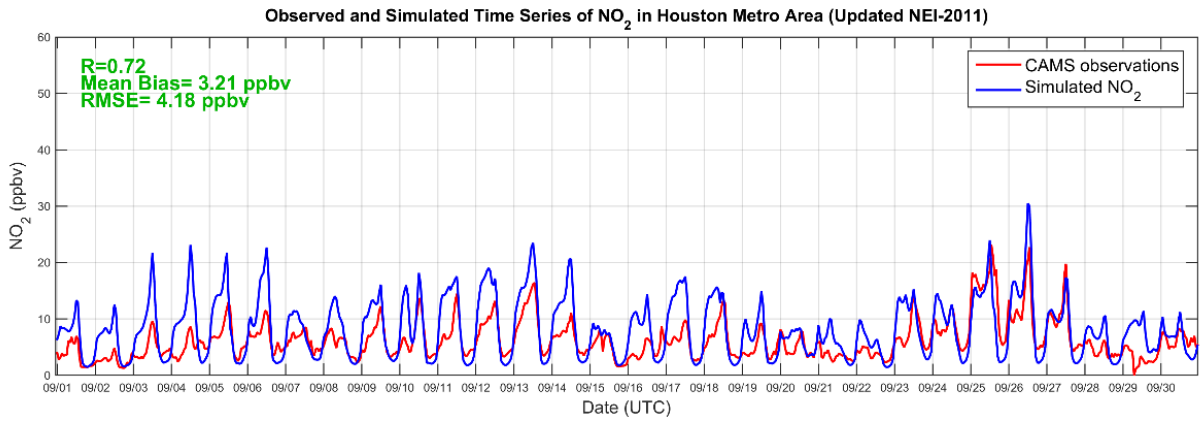

Figure 1(b). Time series of simulated and observed surface NO_2 levels -- NEI2011n

Comparison to Aircraft

NO_2 Vertical Biases for NEI 2011 and NEI 2011n

Figure 2 shows NO_2 vertical biases (against aircraft measurements) for the original and updated emissions. All the 10 days with sufficient observations were plotted. The results are mixed – depending on the individual day and the height level.

When the original simulation (NEI2011) showed a positive bias, the new simulation would reduce the biases. On the other hand, when the old case had a negative bias, the new case would make the bias worse. This is in agreement with the fact that the overall NO_2 emissions in NEI2011n are lower than NEI2011. Above ~1.5 km, NO_2 concentrations fall below 1 ppb for both model and observation. There is usually minimal difference between the two cases.

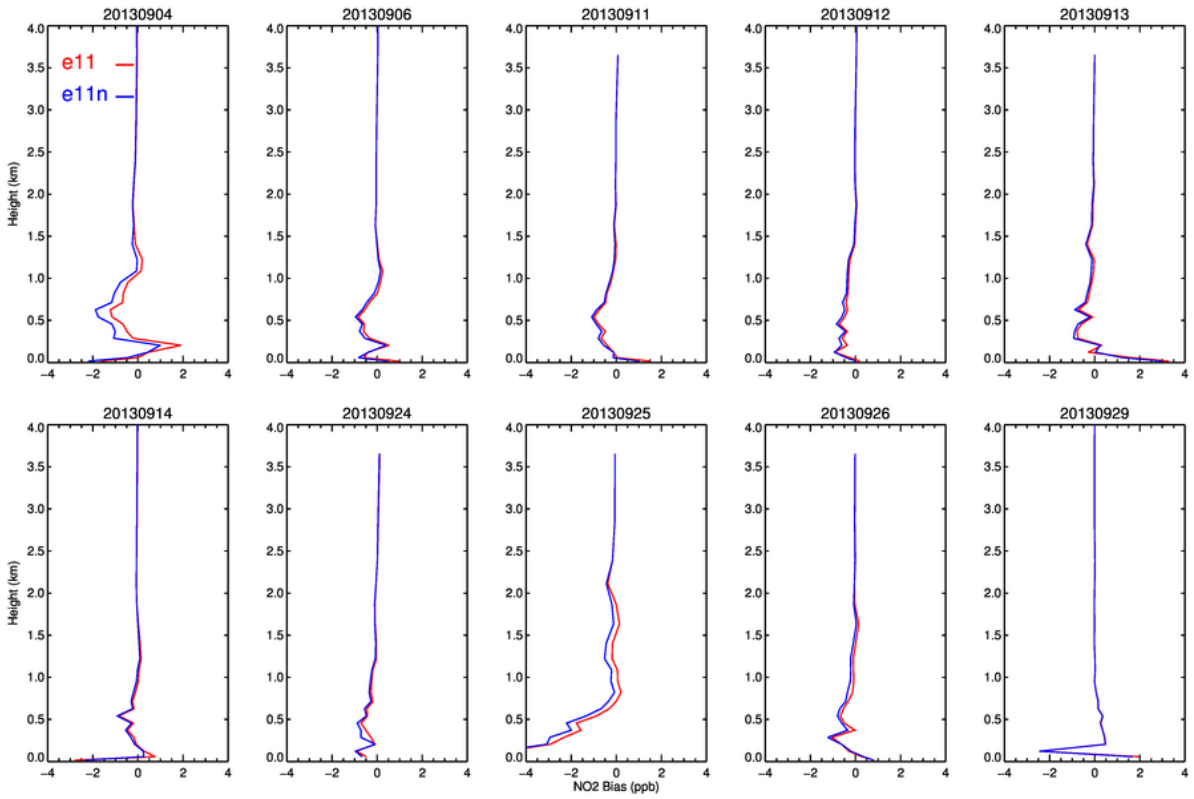

Figure 2. NO_2 vertical biases for NEI2011 ('e11') and NEI2011n ('e11n') for 10 days with available aircraft data, one profile per day. All measurements within one model grid cells and 1hr time period are averaged to one value in order to obtain one-to-one comparison with model.

Impact of Updated Emission Inventory on HCHO/NO_2 Ratio

Due to the fact that both anthropogenic VOC emissions (a source of HCHO) and biogenic ones were constant, only NO_x emissions changes have impacted the ratio before and after adjustment. Figure 3 shows that in urban regions, chemical condition greatly turns into more NO_x-sensitive regime. On the other hand, in remote regions (i.e., rural regions), an opposite trend is seen.

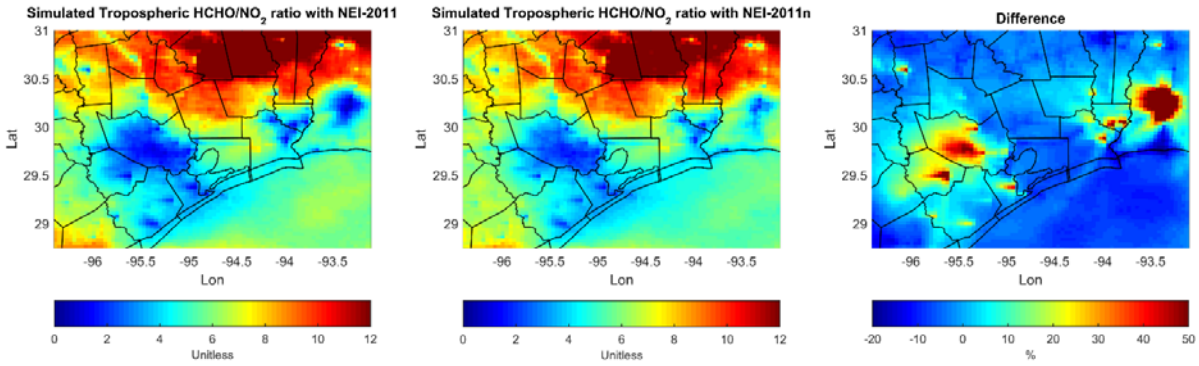

Figure 3. Simulated tropospheric HCHO/NO_2 with NEI-2011 (left panel), NEI-2011n (middle panel) and the difference (right panel). Positive percentage means becoming more NOx-sensitive.

3. *Impact on Ozone: surface O_3, O_3 aloft*

Since the principal pollutant triggering pollution events in Texas are ozone, the ultimate goal of this study is to investigate the impact of updated NO_x emission on ozone. In Texas, the HGB region is assigned a 'non-attainment' status by EPA due to ozone exceeding the National Ambient Air Quality Standards. Here we present the ozone results before and after inverse modeling.

Surface ozone

Hourly Ozone Statistics

Hourly surface ozone statistics are displayed in Table 2 It is based on all available hourly ozone observations. Missing data points are not included. The updated emission slightly improved surface ozone statistics, with correlation increased by 0.02 and IOA by 0.01. The model mean ozone and bias showed minimal change.

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
NEI2011	33308	0.74	0.79	14.6	12.0	9.3	24.4	33.7	16.5	14.2
NEI2011n	33308	0.76	0.80	14.4	11.7	9.2	24.4	33.7	16.5	15.2

Table 2. Statistics of hourly surface ozone: N – data points; Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M – Model Mean; SD – Standard Deviation; Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD: degree ppb

Regional Ozone Average Time Series

Figure 4 shows the time series of daily regional average ozone, averaged over all observed ozone measurements in the modeling domain in the day (24 hours). On most days, the observed average ozone fell below 30 ppb. Since the winds after dawn consistently push the precursors from the industrial area to the southwest of the city, the wind pattern does not favor the local ozone production. The daytime winds also contained persistent easterly component which moved the pollutants away from the metro Houston area. In the first 10-day period, less background ozone coming from the Gulf of Mexico contributed to the low-ozone days. With overcast skies on the 19th and the 20th, ozone values dipped below 20 ppb. The two highest ozone days, characterized by post-frontal ozone events, were the 25th and the 26th.

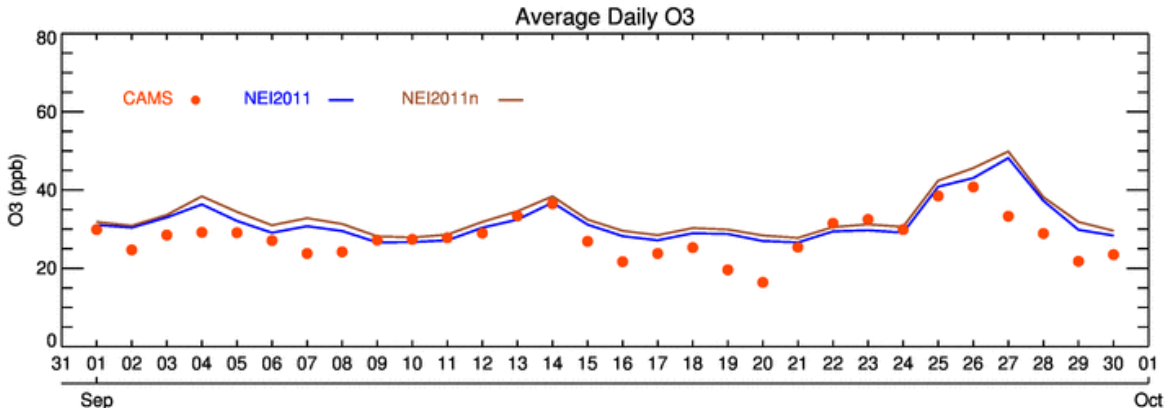

Figure 4. The daily regional averaged ozone over all the sites in the 4 km domain for September 1-30.

In Figure 4, the model ozone generally followed observations reasonably well, although some overestimation by the model are visible, with highest bias on the 20th and the 27th. The overall positive bias, we believe, is largely the result of the static CMAQ lateral boundary conditions. Overall, the updated emission yields slightly better results in regional average ozone.

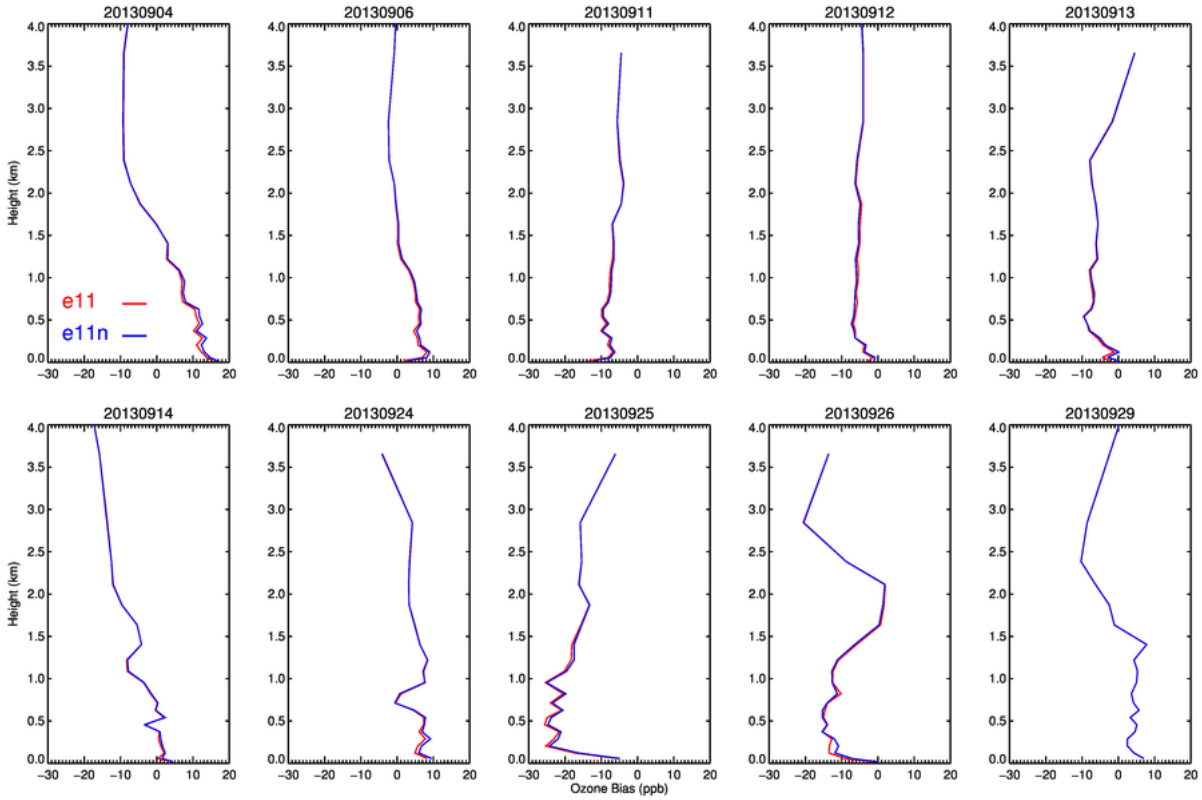

Figure 5. Ozone vertical biases for NEI2011 ('e11') and NEI2011n ('e11n') for 10 days with available aircraft data, one profile per day. All measurements within one model grid cells and 1hr time period are averaged to one value in order to obtain one-to-one comparison with model.

Ozone Aloft

Figure 5 shows ozone vertical biases (against aircraft measurements) for the old and updated emissions. Overall the differences are quite small after emission update. The only day with more visible changes is 09/26, when NEI2011n case showed a smaller negative bias at 200-300 meters level. The ozone profiles display significant swings from day to day, reflecting the varying weather and changing ozone lateral boundary conditions. The actual ozone biases depend on the individual day.

Above 1.5 km, the two cases are virtually the same. This is reasonable as the NO_2 emissions are only adjusted near surface. At higher altitude, NO_2 concentration is quite low and does not affect ozone level.

Project 14-016 **STATUS: Active – June 4, 2014**
Completed – June 30, 2015

Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations

Environ – Greg Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Amount: $271,911 **Expended:** $270,159.38

Amount Returned to AQRP: $1,751.62

Executive Summary

The exchange of gases and aerosols between the Earth's surface and the atmosphere is an important factor in determining atmospheric composition and regional air quality. Accurate quantification of emission fluxes is a necessary step in developing air pollution control strategies. In some cases, emissions can be directly measured (e.g., point sources with continuous emission monitors) or can be estimated with reasonable confidence (e.g., point sources that have well-defined operating parameters). In contrast, large uncertainties are associated with area sources including emissions from vegetation, and in particular, emissions of biogenic volatile organic compounds (BVOCs). Vegetation is the largest source of VOC emissions to the global atmosphere. The oxidation of BVOCs in the atmosphere affects ozone, aerosol and acid deposition. Current BVOC emission estimates are based on measurements for individual plants that must be scaled up to represent landscapes and adjusted for environmental conditions. There is a critical need for independent BVOC emission inputs for air quality models.

AQRP Project 14-016 used aircraft observations from the 2013 Southeast Atmosphere Study (SAS) to assess and reduce uncertainties associated with a widely used BVOC emissions model, namely the Model of Emissions of Gases and Aerosol from Nature (MEGAN; Guenther et al., 2012). The eddy covariance technique was used to directly quantify BVOC emission fluxes for all suitable aircraft observations from the SAS study.

The overall goal of this project is more accurate BVOC emission estimates that can be used in Texas air quality simulations that are critical for scientific understanding and the development of effective regulatory control strategies that will enhance efforts to improve and maintain clean air.

Estimation of Terpenoid Emissions Fluxes from Aircraft Data

Using a wavelet based approach, fluxes of isoprene and total monoterpenes were estimated using turbulence and proton transfer reaction-mass spectrometry (PTR-MS) measurements made onboard the C-130 aircraft during the 2013 SAS field campaign. Uncertainties associated with the estimated fluxes were also quantified. As expected, the highest isoprene fluxes were observed over broadleaf tree dominated woodland areas, while higher monoterpene fluxes were observed over areas such as longleaf pine woodland in Missouri and conifer and hardwood plantations in Louisiana, Texas, Arkansas and Alabama. The forests in these areas generally have higher fractions of high monoterpene emitting trees such as pines. Relatively low isoprene and

monoterpene fluxes were observed over non-forested landscapes. These observations are consistent with a previous aircraft flux study in California (Karl et al., 2013; Misztal et al., 2014).

Subsampling was also performed for select C-130 flight legs to simulate the VOC sampling approach during SAS on the P-3 aircraft, which used a much longer sampling interval (15 s versus 0.6 s on average for the C-130). The increased sampling interval in the P-3 data added significant uncertainty and error to calculated fluxes for sampling intervals greater than a few seconds. Therefore, Fast Fourier Transform and wavelet based approaches were determined to be not suitable for analyzing VOC fluxes from the P-3 aircraft data in heterogeneous regions.

Instead, a mass balance approach was used to estimate isoprene emission fluxes from the NOAA P-3 and C-130 data. In a mass balance approach, it is assumed that the measured BVOC mixing ratio in the boundary layer reflects the equilibrium between emissions, chemical removal by hydroxyl (OH) radicals and entrainment out of the boundary layer (Warneke et al., 2010). The mass balance method requires specification of boundary layer height estimated from the aircraft data, k_{OH} is the rate coefficient for the BVOC+OH reaction, and [OH] is the concentration of OH radicals. The latter parameter was estimated using a parameterization from (Ehhalt and Rohrer, 2000) based on measured NO_2 mixing ratios, and j_{O1D} and j_{NO2} photolysis rates. OH was measured onboard the C-130 during SAS and those data were used here to verify the validity of the OH estimate used for the mass balance approach. While there were significant differences between measured and calculated OH, the calculated OH, on average, agreed within 11% with the measurements.

The emission fluxes derived from the aircraft measurements using the mass balance approach were compared with emissions calculated using the BEIS and MEGAN models. For the purpose of these comparisons, the emissions were calculated along the flight tracks using the temperature and photoactive radiation (PAR) measured onboard the aircraft. The idea behind the approach is to use the aircraft data to constrain all the physical and chemical parameters that determine BVOC concentrations in addition to their emissions.

Isoprene emissions calculated from BEIS3.12, BEIS3.13, MEGAN2.0 and MEGAN 2.1 were compared to those calculated using the mass balance approach with measured isoprene mixing ratios from the following studies: SENEX (the NOAA contribution to the SAS campaign), NOMADSS, TexAQS2000, TexAQS2006, ICARTT2004 and SOS1999. The comparison showed that in general, MEGAN2.1 gives isoprene emissions that are higher than both BEIS3.12 and BEIS3.12 emissions and higher than fluxes inferred from NOMADSS aircraft measurements. The results from the C-130 (NOMADSS) and P-3 (SENEX) measurements during SAS compared very similarly with the emissions inventories. In general, MEGAN2.1 provides results that are higher than the emissions estimated from the measurements, whereas BEIS3.12 and BEIS3.13 estimates are lower. However, the uncertainties in the emissions estimated from the measurements are significant and do not allow a decision to be made as to which emissions model is more accurate. These conclusions are very similar to the observations made in previous NOAA work (Warneke et al., 2010)

<u>Development of High Resolution Land Cover Data for MEGAN Modeling in Texas and the Southeastern US</u>

Land cover characteristics including Leaf Area Index (LAI) and Plant Functional Type (PFT) are key driving variables for the estimation of biogenic VOC emissions by MEGAN and other biogenic emission models. Land cover and emission factor input data sets are considered the major uncertainties associated with BVOC emission estimates. We developed an updated LAI database for all of North America based on the 2013 MODIS (MOderate Resolution Imaging Spectroradiometer) satellite product (MCD15A2.005) and applied maximum green vegetation fraction from USGS (http://landcover.usgs.gov/green_veg.php), which is also based on MODIS remote sensing products. Spatial resolution of the LAIv data is approximately 900 meters. An updated 30-meter resolution PFT database (PFT16v2015) was developed for the continental US based on various ground survey, remote sensing and land surface model data products.

Emission Factor Database Development

The PFT16v2015 PFT database was developed for this project to provide the starting point for development of a high-resolution (30 m) emission factor (EF) database. An initial EF database, EFvE2015, was created using the same enclosure based emissions data used for the EF database, EFvE2011, described by Guenther et al. (2012) but with the new landcover data developed for this project and used for the new PFT database. The resulting EFvE2015 data were then compared with the EFvE2011 data. An additional database, EFvA2015, was created based on aircraft flux measurements and the new landcover and compared with the other EFs.

Compared with the EFvE2011 data, the EFvE2015 data predicts higher isoprene emission factors in some regions in the southeastern US, with the biggest differences in north Florida, central Texas, Oklahoma and Arkansas. Higher broadleaf deciduous tree coverages are also predicted for these areas in the PFT16v2015 database. On the other hand, lower broadleaf deciduous tree coverages were predicted by the PFT16v2015 database for southeast Missouri and northern Minnesota, which also has lower isoprene emission factors in the EFvE2015 database. The differences are mainly due to the incorporation of the LandFire existing vegetation type (EVT) data, which provides more spatial detail than the land cover dataset used to develop the EFvE2011 dataset.

Development of Airborne Emission Factors

Aircraft observations were used to evaluate and constrain MEGAN emission factors following the method of (Karl et al., 2013; Misztal et al., 2014) with some improvements and were used to develop the EFvA2015 emission factor database. The wavelet based approach provides isoprene and monoterpene flux data at high spatial resolution. However, the calculated fluxes are for the altitude at which the aircraft is flying and must be extrapolated to the surface level in order to be used to estimate EFs for biogenic VOCs. We applied a vertical flux divergence approach to perform this task. Surface fluxes of BVOCs were then calculated using a vertical flux divergence correction method (Misztal et al., 2014) that assumes a linear relationship between fluxes at different altitudes.

Converting the surface fluxes into EFs requires accurate estimates of meteorological conditions such as temperature, solar radiation and, to a lesser degree, other factors including soil moisture, wind speed and humidity. The MEGAN model calculates BVOC emissions as the product of an EF and an emission activity factor (EAF) that accounts for the impact of driving variables including canopy environment. We calculated the EAF associated with each aircraft flux

measurement and applied this factor to the extrapolated surface flux to obtain the emission factor for standard conditions.

EAFs were calculated using two different approaches. For one version, EAFs were calculated by executing a single point version of MEGANv2.1 for every flux measurement, using the LAIv and vegetation cover with meteorological fields extracted from the North American Land Data Assimilation System (NLDAS-2) forcing data and soil moisture data extracted from NLDAS-2 model data (VIC model). For the second version, EAFs were calculated using the regional MEGANv2.1 model with EFvE2011 emission factor database and meteorological driving variables derived from the Weather Research and Forecasting Model (WRF) (Skamarock et al., 2008).

The correlation between EFvE2015 and airborne based EF suggest that the land cover data reasonably captures the variations of BVOC emissions among different EVTs. The correlations between airborne EF calculated using different approaches and the landcover based EFvE2015 data range from 0.32 to 0.73.

The airborne EFs calculated using WRF or using NLDAS meteorological data are considerably different. The WRF based EF values are consistently lower due to higher EAF values estimated by WRF. This is likely due to a high bias in solar radiation and temperature due to underestimates of aerosol and clouds. We have used the NLDAS data for our analysis because it includes assimilation of observed meteorology. However, the substantial differences (~37%) between the WRF and NLDAS results demonstrate the importance of having accurate meteorological observations to determine airborne EFs.

Development of MEGAN Biogenic Emission Inventories and Regional Photochemical Modeling

Using the landcover and emission factor databases described above, we prepared three sets of MEGAN v2.1 biogenic emissions for a June 1–July 15, 2013 modeling episode that encompassed the P-3 and C-130 SAS flights. The first inventory was a base-case biogenic emission inventory, which was developed using the MEGANv2.1 default landcover database, PFT16v2011, and default emission factors, EFv2011. This inventory is referred to as EFvE2011 below. Then, a second biogenic emission inventory (denoted by EFvE2015) was derived from updated inputs: the new high-resolution landcover database, PFT16v2015, and the EFvE2015 emission factor database described above. Finally, a third biogenic emission inventory was derived from the new high-resolution landcover database, PFT16v2015, and the EFvA2015 emission factor database; this inventory was used in a sensitivity test described below and is referred to as EFvA2015.

The three MEGAN emissions inventories were developed using temperatures and PAR from a WRF simulation of the June-July 2013 episode performed as part of this study. WRF was run with a new algorithm that accounts for the radiative effects of sub-grid scale cumulus clouds (Alapaty et al., 2012; Herwehe et al., 2014) and has been shown to reduce surface downward shortwave radiation (DSW) and improve the simulation surface temperature and precipitation relative to the unmodified version of WRF.

Comparison of WRF modeled surface downward shortwave radiation (DSW) with visible satellite images for the C-130 flights and solar radiation measured at TCEQ monitoring sites indicated that, despite the additional cloud-radiation feedback, WRF underestimated the

observed cloud field and overestimated DSW. Underestimating clouds and overestimating the available shortwave radiation very likely introduced a high bias in the MEGAN isoprene emissions through a high bias in PAR and affected the partitioning of surface heat and moisture fluxes.

The default (EFvE2011) and updated (EFvE2015) MEGAN biogenic emission inventories were compared against aircraft flux data and then evaluated using a photochemical grid model. The evaluation of the isoprene and monoterpene emissions against aircraft flux data showed that the MEGAN v2.1 isoprene emissions were consistently higher than the aircraft flux data calculated along the C-130 racetrack flight segments. This was true for both the default and updated MEGAN emission inventories. The default and updated MEGAN monoterpene emissions showed closer agreement with the airborne fluxes than the isoprene emissions, but the MEGAN monoterpene emissions were also generally higher than the airborne fluxes. The MEGAN monoterpene emissions had a spatial pattern similar to the airborne fluxes, with high emissions over the Texas-Louisiana border region, Mississippi and Alabama and lower emissions over southern Missouri and western Tennessee. The changes between default and updated inventories varied along the flight tracks, and it is difficult to assess which inventory showed better agreement with the airborne fluxes. The comparison between MEGAN emissions and the airborne fluxes is affected by the use of different meteorological data (WRF and NLDAS) in preparing the emissions flux estimates.

We performed regional photochemical modeling for June 1-July 15, 2013 time period of the C-130 and P-3 aircraft flights using both the default (EFvE2011) and updated (EFvE2015) MEGAN emission inventories. We evaluated modeled concentrations of terpenoid and other species against the aircraft measurements and compared modeled surface layer ozone to ground level ozone measured at rural sites. The CAMx model has a high bias for surface ozone that is most pronounced at coastal sites during periods of onshore flow. This suggests that the model is affected by bias in the model boundary conditions for ozone and/or precursors.

Using both the default (EFvE2011) and updated (EFvE2015) MEGAN inventories, CAMx simulated spatial patterns of high and low isoprene that are similar to those of the aircraft observations. For example, both the modeled and the measured isoprene are relatively high in the region that includes northeast Texas, northwest Louisiana and southwestern Arkansas. Both observed and CAMx isoprene concentrations show hot spots in southeastern Missouri, central Alabama and central Georgia. Areas of low isoprene occur in the model and measurements in northern Indiana, northern Mississippi South Carolina, northeastern Kentucky and central Texas. CAMx generally overestimates isoprene along the aircraft flight tracks with bias of 84% using the default EFvE2011 MEGAN emissions and 104% in the updated case with the EFvE2015 biogenic inventory.

Although the modeled high bias for isoprene relative to aircraft observations increased in the run using the updated EFvE2015 MEGAN emissions, the CAMx model's performance in simulating ground level ozone improved in the Houston area. The updated MEGAN inventory EFvE2015 has a significantly lower isoprene emissions factor and lower isoprene emissions in the Houston area, and this appears to reduce ground level ozone, bringing the model into closer agreement with observations. Kota et al. (2015) compared the gridded MEGAN isoprene emissions factor for the region north of Houston with isoprene emission factor estimates derived from a field

study and found that the MEGAN emission factor was higher. Kota et al. determined that the overestimated isoprene emission factor caused a high bias in modeled isoprene concentrations in their Community Multiscale Air Quality (CMAQ) model simulation, but the isoprene overestimates did not significantly influence modeled ozone; this is in contrast to results of our CAMx simulations, in which changes in Houston area isoprene emissions strongly affected modeled ozone.

In the CAMx simulations, changes in surface ozone due to the change in the MEGAN emission inventory were relatively small outside of the Houston area and monitoring sites near the eastern border of Texas,

In the CAMx runs using default and updated EFvE2015 MEGAN emissions, modeled monoterpene concentrations were generally lower than the observed concentrations along the P-3 and C-130 flight tracks. Values of the coefficient of determination were lower for monoterpenes than for isoprene. In the run with updated EFvE2015 MEGAN emissions, the magnitude of the CAMx model's low bias for monoterpenes was reduced relative to the run with default emissions.

Four additional CAMx sensitivity tests were carried out.

1. We altered the CB6r2 chemical mechanism to increase the production of OH from the breakdown of isoprene following the mechanism of Peeters et al. (2013). The purpose of the test was to gauge the model's response to an isoprene mechanism that represents an upper limit on the production of OH from isoprene. Increasing OH production from isoprene reduces but does not eliminate the high bias in isoprene products.

2. Based on the high bias for isoprene noted in the CAMx run that used default MEGAN emissions, we reduced the MEGAN isoprene emissions by a factor of 2 for all grid cells and times and reran CAMx. For the P-3 data, the CAMx default run high bias for isoprene products (114%) changed to a low bias of -7% in the sensitivity test as a result of the lower isoprene emissions and atmospheric concentrations. For the C-130 data, the CAMx bias for isoprene products changed from 48% to -33%. The reduction in the magnitude of bias for isoprene products in this sensitivity test suggests that the MEGAN isoprene emissions are overestimated in the default EFvE2011 case.

3. In June 2013, Nguyen et al. (2015) measured dry deposition velocities (V_d) for biogenic trace gases in an Alabama forest during the Southern Oxidant and Aerosol Study (SOAS). Comparison of CAMx V_d against the measurements showed Vd was underestimated in the model. We increased CAMx dry deposition of these species to improve agreement with the SOAS measurements. The effects of this test on modeled ozone and isoprene and monoterpenes species were small.
4. We ran CAMx with the EFvA2015 MEGAN emission inventory that used isoprene emission factors developed using SAS aircraft data. In the CAMx run with EFvA2015 MEGAN emissions, the high bias for isoprene decreased from 84%-113% in the default (EFvE2011) run and 104%-132% in the EFvE2015 sensitivity test to the range -5% to -16% in the CAMx EFvA2015 sensitivity test. The use of the EFvA2015 emission factors for isoprene in MEGAN improved the CAMx model's ability to reproduce the isoprene

concentrations measured by the P-3 and C-130 aircraft. Although the high bias seen in the default EFvE2011 and EFvE2015 CAMx runs is reduced in the EFvA2015 sensitivity test, there was no improvement in correlation between observed and modeled values. R^2 values decreased slightly in the EFvA2015 sensitivity test relative to the CAMx runs using the default and EFvE2015 MEGAN emissions.

The best overall performance among all CAMx runs for a subset of species (isoprene, isoprene products, sum of monoterpenes, ozone, OH) occurred in the sensitivity test in which CAMx was run with the EFvA2015 MEGAN emissions that used emissions factors developed using the aircraft data. The CAMx bias for ozone was nearly unchanged across all CAMx runs. In the CAMx run with updated EFvE2015 MEGAN emissions, the CAMx bias for monoterpenes improved, but the overall bias for isoprene, isoprene products and OH increased. These results, taken together with the high bias in MEGAN isoprene emissions compared to the aircraft fluxes, suggest that MEGAN isoprene emissions are overestimated in both the default EFvE2011 and updated EFvE2015 inventories.

Conclusions

Below, we present conclusions drawn from the results of this study.

- Accurate meteorological input data, especially PAR and temperature, are critical for accurate BVOC emission calculations. Bias in weather model simulation of clouds and shortwave radiation introduces bias into the MEGAN emissions. Standard WRF simulations may result in considerable high bias in solar radiation and temperature due to model treatment of clouds. NLDAS appears to be better but also leads to overestimates. It should also be noted that bias in the PAR and temperature used to estimate emission factors from measured emissions will also introduce bias into the calculated emission factors. Data assimilation approaches (satellite and/or in-situ observations) are recommended for improving these inputs and they should be evaluated by comparison to observations.
- Landcover inputs (LAI and vegetation type) are also critical for BVOC emission modelling. LAI can vary considerably between years and we recommend using the provided 2013 LAI data for 2013 simulations and use the provided scripts and approach to calculate LAI for other years. We also recommend using the vegetation type distributions developed for this project.
- Emission factors are another key variable for BVOC emission modelling. We recommend using the new (aircraft based) isoprene emission factors (EFvA2015) developed for this project for BVOC emission modelling since both the eddy covariance and mixed layer approaches indicate this. However, more work still needs to be done to verify these emission factors and reconcile the substantial differences between leaf based, tower based, aircraft based and satellite based emission estimates. There is less evidence that the monoterpenes should be changed so we do not recommend changing the emission factors for monoterpenes from EFvE2015 to EFvA2015 at this time.

Project Update

The final report for this project is under review.

Project 14-017 **STATUS: Active – July 8, 2014**

Incorporating Space-borne Observations to Improve Biogenic Emission Estimates in Texas

University of Alabama - Huntsville – Arastoo Pour Biazar
Rice University – Daniel Cohan

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Amount: $199,982
($137,003 UAH, $62,979 Rice)

Executive Summary

One of the challenges in understanding the Texas air quality has been the uncertainties in estimating the biogenic hydrocarbon emissions. Biogenic volatile organic compounds, BVOCs, play a critical role in atmospheric chemistry, particularly in ozone and particulate matter (PM) formation. In southeast Texas, BVOCs (mostly as isoprene) are the dominant summertime source of reactive hydrocarbon. Despite significant efforts by the State of Texas in improving BVOC estimates, the errors in emission inventories remain a concern. This is partly due to the diversity of the land use/land cover (LU/LC) over southeast Texas coupled with a complex weather pattern, and partly due to the fact that isoprene is highly reactive and relating atmospheric observations of isoprene to the emissions source (vegetation) relies on many meteorological factors that control the emission, chemistry, and atmospheric transport.

BVOC estimates depend on the amount of radiation reaching the canopy (Photosynthetically Active Radiation, PAR), and temperature. However, the treatment of temperature and PAR is not uniform across emissions models and still poses a problem when evaluating the inventories. Recent studies show that the largest uncertainty comes from the model solar radiation estimates and that using satellite-based PAR would be preferable. Emissions from soils also remain as one of the poorly quantified sources of NOx (nitrogen oxides) in most air quality models. Soils can be the largest source of NOx in rural regions where low-NOx conditions make ozone production efficiency especially high, contributing to background ozone levels.

The overall objective of the current activity is to advance our understanding of Texas Air Quality by utilizing satellite observations and the new advances in biogenic emissions modeling to improve biogenic emission estimates. This work specifically addresses a priority area in Texas AQ studies by improving biogenic emission estimates. In particular, the objectives are:

(1) To provide satellite-based PAR estimates for Texas during selected periods of 2006 and the Discover-AQ period (September, 2013).

(2) To produce an improved biogenic emission estimate for Texas and help in the evaluation of biogenic emission inventories over Texas by providing the best model representation of the atmospheric condition during the observations used for evaluation.

(3) To prepare and use a new soil NOx scheme that provides more mechanistic representation of how emissions respond to nitrogen deposition, fertilizer application, and changing meteorology.

The University of Alabama in Huntsville (UAH) currently generates a set of products from the Geostationary Operational Environmental Satellite (GOES) that includes surface incident short-wave radiation as well as cloud albedo and cloud top temperature. Under this activity, UAH will produce the Photosynthetically Active Radiation (PAR) needed in the estimation of biogenic hydrocarbon emissions. Satellite-derived PAR will be evaluated against previous satellite-based products as well as surface observations for the summer of 2006 and also during Texas Discover-AQ campaign. Furthermore, the new PAR retrievals will be used in MEGAN (the Model of Emissions of Gases and Aerosols from Nature) to generate BVOC emissions.

The new soil NOx scheme to be used is an implementation of the Berkeley-Dalhousie Soil NOx Parameterization (BDSNP) within MEGAN. A series of sensitivity simulations will be performed and evaluated against Discover-AQ observations to test the impact of satellite-derived PAR and the new soil NOx emission model on air quality simulations.

Project Update

Overall, the project is on track and all objectives have been achieved. The Study Team is in the process of preparing the data and the model for dissemination and finishing the final report.

Satellite-based PAR estimates

As indicated in the previous reports the evaluation of UAH PAR products for the September 2013 against pyranometer observations and for the summer of 2006 against pyranometer observations as well as PAR data obtained from University of Maryland were satisfactory. Subsequently, the satellite-based PAR product was used within MEGAN for estimates of biogenic emissions.

Biogenic Emissions Estimates

Biogenic emissions estimates for several scenarios in September 2013 were produced and evaluated. These scenarios included two different WRF simulation results as well as utilizing satellite-based PAR in MEGAN. In addition to the control WRF simulation, a WRF simulation with cloud assimilation (from a previous TCEQ project) was also performed. WRF simulation with cloud assimilation improved PAR field over the control simulation when compared to observed pyranometer measurements. Data and the model are being prepared to be shared with other researchers as well as TCEQ. More detail about MEGAN estimates is presented in the following.

MEGAN simulation with satellite PAR during Aug-Sep 2013

Three sets of MEGAN runs over the TCEQ SIP modeling domains (D1 for CONUS 36km domain, D2 for Texas 12km domain and D3 for East Texas 4km domain) during August and September 2013 were performed by using different PAR inputs, namely PAR from control WRF run (cntrl), PAR from WRF cloud assimilation run (analytical), and PAR from GOES satellite retrieval using the new algorithm developed by UAH (UAH). The VOC emissions from biogenic in MEGAN were lumped with CB05 chemical mechanism and were archived in the NetCDF format. The total disk storage of the two months MEGAN runs is 2.9 GB for D1, 5.4

GB for D2 and 16.8 GB for D3. It is ready to share with the CAMx Fortran binary input format using the CMAQ2CAMx interface program provided by Ramboll-Environ (http://www.camx.com/getmedia/a9e648b7-2b2d-487d-9243-2f363a6feea4/cmaq2camx-4sep13.tgz.aspx).

For the ISOP simulations during August 2013, the general emission pattern for the three PAR inputs case is quite similar, with the hot spots over the Texas territory mainly concentrated over the Edwards Plateau and the eastern Texas boundary adjacent with the Louisiana and Arkansas, where the broadleaf evergreen tree or shrub is the dominant plant functional type. In terms of the magnitude, the 'UAH' case is the lowest with the maximum value 54 moles/s, following by the 'analytical' case and 'cntrl' case. For September case, the base ISOP emission is lower than in August 2013 due to the lower mean surface temperature and smaller leaf area index value input from MODIS. For the TERP simulation pattern during the two months in 2013, additional hot spot located near the south Texas boundary adjacent with Mexico is apparent. The overall magnitude of mean TERP emission rate is much smaller than for ISOP, with the range of former 0-6 moles/s and the range of latter 0-68 moles/s.

In order to characterize BVOC emission pattern from different MEGAN simulations over the heterogeneous plant functional type over Texas, the average monthly emission rates over the 10 climate divisions in Texas were calculated separately. The climate classification is based on historical climate analyses (1895-2013) for the monitored drought, temperature, precipitation and heating/cooling degree day values over the continental US

(http://www.ncdc.noaa.gov/monitoring-references/maps/us-climate-divisions.php). An area mask file consistent with the TCEQ domain configurations were generated based on the climate division boundary polygon shapefiles provided by NCAR (

http://www.ncl.ucar.edu/Applications/Data/cdf/climdiv_polygons.nc). The ISOP and TERP results are given as detailed statistics in Table 1. For ISOP, the top 3 highest emission regions in Texas are East Texas (2754 tons/day for case 'UAH'), North Central Texas (2036 tons/day for case 'UAH'), and Edwards Plateau (1199 tons/day for case 'UAH') separately. For TERP, the top 3 highest emission regions are East Texas (1011 tons/day for case 'UAH'), Trans-Pecos (615 tons/day for case 'UAH'), and North Central Texas (562 tons/day for case 'UAH'). To quantify the impact of different PAR inputs on BVOC emission estimation, the case 'UAH' using GOES satellite retrievals on average predict 21% less ISOP than the base WRF case ('cntrl') during August 2013 and -19% during September 2013 (see Table 1). The cloud assimilation WRF case ('analytical') predicts slightly less ISOP than case 'cntrl' with the mean value around -2% during August 2013 and -3% during September 2013. It is expected that not so much impact of TERP emission due to the introduction of more realistic insolation data from satellite, the relative difference between case 'UAH' and case 'cntrl' is on average -5%. The TERP emission algorithm in MEGAN is more directly connected with the surface temperature instead of PAR. At least for the evaluated two months in 2013, the most sensitivity climate region for ISOP emission estimation in Texas due to different PAR inputs is Trans-Pecos, with the relative difference compared to base case -28.8% during August 2013 and -24.7% during September 2013.

Ongoing work includes demonstrating the quantitative ozone impact from different MEGAN BVOC emission estimations by running CMAQ over the TCEQ SIP modeling domains during August and September 2013. The anthropogenic emissions are provided by TCEQ with the base year 2011. Since the boundary condition files from GEOS-Chem are not available during the simulation period, the MOZART outputs with global CO data assimilation will be used as alternative.

Stand-alone soil NO emission simulation with BDSNP scheme

This work has focused on the functionality of the standalone soil NO emission module with BDSNP scheme and the development of a new soil biome map using the 12km resolution CONUS 40-category 2006 NLCD-MODIS land use classification (NLCD40) and Köppen-Geiger climate classification map. With the high efficiency of the standalone version, more sensitivity tests can be carried out by switching the key input parameters for soil NO emission in BDSNP module (e.g. different soil biome, different base emission factors, and different fertilizer pools). Figure 1 provides the spatial pattern difference of soil NO base emission simulated by this standalone model using global GEOS-Chem soil biome (control), updated regional soil biome based on NCLD40 (new Biome), and North American specified emission factors (NA EF) over continental US. Comparing to the 'control' case, the soil NO base emission pattern from case 'new Biome' has much detail texture due to the usage of higher resolution biome map and better representation of geographic locations for cropland over Midwest and evergreen board leaf forest along the South Eastern coastal areas. The original implementation of soil NO BDSNP module used the global average biome type specific emission factors, which is 2-3 times higher than the local US measured values for the category such as cold savannah. The intent of using local emission factors is to provide more realistic results for this project.

The soil NO emission rate is from the default MEGAN model using the Yienger and Levy 1995 (YL95) scheme. Here, the standalone BDSNP module was used to replace the soil NO emission simulation during August and September 2013 over TCEQ SIP simulation domains. All the BDSNP input files including biome type map, fertilizer pool map, arid/non arid map, nitrogen deposition from dry and wet process are re- gridded to the consistent TCEQ modeling domains. At this time, a complete CMAQ run for August and September 2013 is not available. The daily magnitudes of nitrogen deposition pool are assumed from the 2005 CMAQ simulation results. Figure 2 demonstrates the spatial pattern difference for daily mean NO emission rate using YL95 or BDSNP on Augest 1, 2013 over the TCEQ Texas domain (D2). Notice the different color scale, the magnitude of soil NO emission predicted from BDSNP at that day is generally 2-3 times higher than that from YL95, with the maximum value 14.6 gm/s versus 8.4 gm/s. The spatial pattern for the two cases is also quite different due to the combined contributions from different soil biome type, fertilizer implementations and the different response curve for soil temperature and moisture in the two soil NO schemes. The two-month soil NO emission simulated with BDSNP scheme by using the two set of WRF runs (case 'cntrl' and case 'analytical') will be archived separately along with MEGAN results and hand over to TCEQ for further test. The documentation of the user manual for the standalone soil NO BDSNP module is also under way and will be ready to share for the community at the end of this project.

Table 1. Comparison of daily average isoprene (ISOP) and monoterpene (TERP) emission rate (tons/day) over 10 different climate zone at Texas from MEGAN using different PAR inputs

Aug 2013										
			ISOP					TERP		
climate zone	cntrl	analytical	PAR	relative diff. (analytical-cntrl)	relative diff. (PAR-cntrl)	cntrl	analytical	PAR	relative diff. (analytical-cntrl)	relative diff. (PAR-cntrl)
	(tons/day)	(tons/day)	(tons/day)	%	%	(tons/day)	(tons/day)	(tons/day)	%	%
Edwards Plateau	1794.6	1736.4	1374.0	-3.2	-24.2	645.8	640.2	600.9	-0.9	-7.0
East Texas	3876.0	3837.2	3062.0	-1.0	-21.2	1207.4	1196.2	1128.8	-0.9	-6.5
High Plains	600.8	596.9	451.6	-0.6	-25.0	239.2	238.7	222.4	-0.2	-7.0
Low Rolling Plains	1217.1	1199.6	926.4	-1.4	-24.2	423.4	420.6	393.1	-0.7	-7.2
Lower Valley	173.3	171.3	137.8	-1.1	-20.7	80.9	80.3	76.4	-0.7	-5.6
North Central Texas	2887.6	2829.5	2248.1	-2.0	-22.6	673.9	662.7	629.0	-1.7	-6.7
South Central Texas	1203.5	1176.4	955.4	-2.3	-21.1	355.5	351.6	335.3	-1.1	-5.7
South Texas	257.8	248.1	197.7	-3.8	-24.2	110.1	107.3	102.2	-2.6	-7.1
Trans-Pecos	1655.1	1614.4	1189.9	-2.5	-28.8	769.4	758.2	707.6	-1.5	-8.0
Upper Coast	1135.7	1118.2	922.5	-1.5	-19.1	343.7	340.3	326.9	-1.0	-4.9
Sep 2013										
			ISOP					TERP		
climate zone	cntrl	analytical	PAR	relative diff. (analytical-cntrl)	relative diff. (PAR-cntrl)	cntrl	analytical	PAR	relative diff. (analytical-cntrl)	relative diff. (PAR-cntrl)
	(tons/day)	(tons/day)	(tons/day)	%	%	(tons/day)	(tons/day)	(tons/day)	%	%
East Texas	3060.0	3084.5	2445.6	0.8	-19.9	943.5	943.5	892.9	0.0	-5.4
High Plains	411.3	396.6	325.6	-3.6	-21.6	169.6	166.2	161.2	-2.0	-5.0
Low Rolling Plains	905.8	869.0	702.6	-4.1	-23.4	320.1	313.4	302.1	-2.1	-5.6
Lower Valley	137.6	139.0	111.9	1.1	-18.5	68.0	68.5	65.1	0.8	-4.1
North Central Texas	2247.3	2257.1	1823.8	0.4	-18.8	521.2	519.5	495.3	-0.3	-5.0
South Central Texas	908.2	896.0	744.2	-1.3	-18.3	271.3	268.4	259.5	-1.0	-4.3
South Texas	192.4	183.4	149.8	-4.7	-23.2	86.5	84.8	82.0	-1.9	-5.2
Trans-Pecos	1162.8	1089.4	893.5	-6.3	-24.7	553.2	536.9	522.8	-2.9	-5.5
Upper Coast	918.0	942.5	773.6	2.7	-15.3	272.9	274.6	263.4	0.6	-3.5

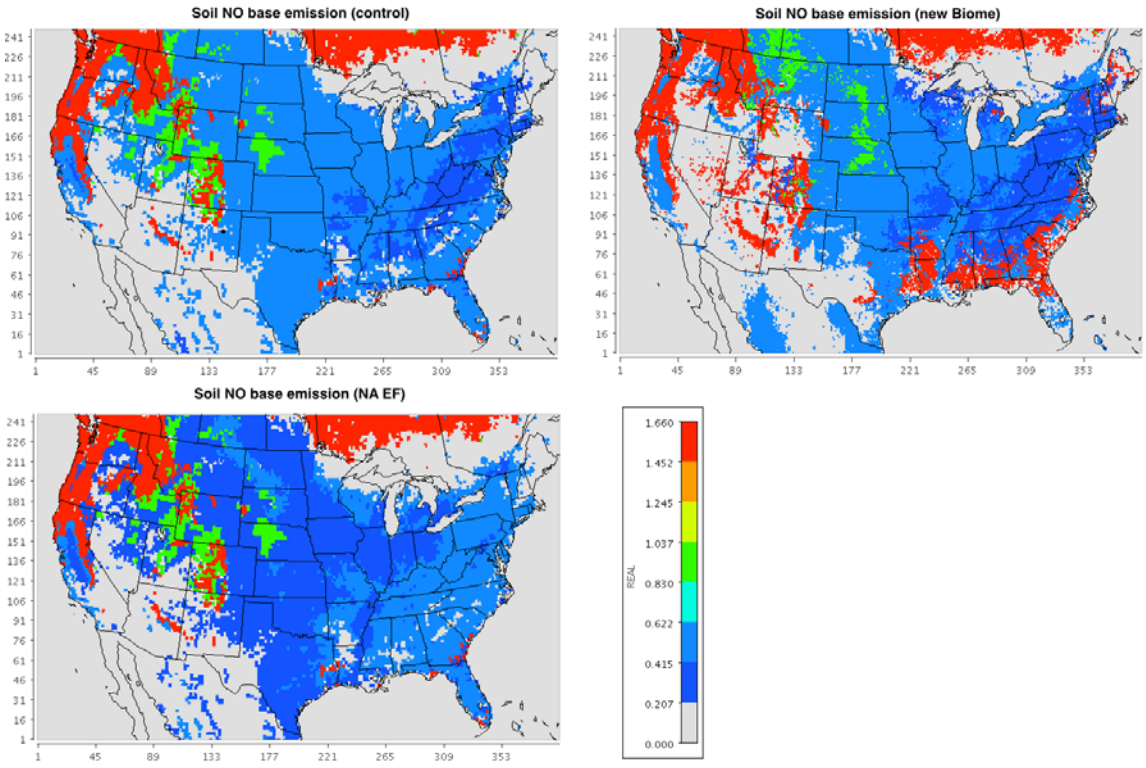

Figure 1. Spatial pattern difference of soil NO base emission simulated from BDSNP module using the global GEOS-Chem soil biome (control), updated regional soil biome based on NCLD40 (new Biome), and North American specified emission factors (NA EF) over the continental US.

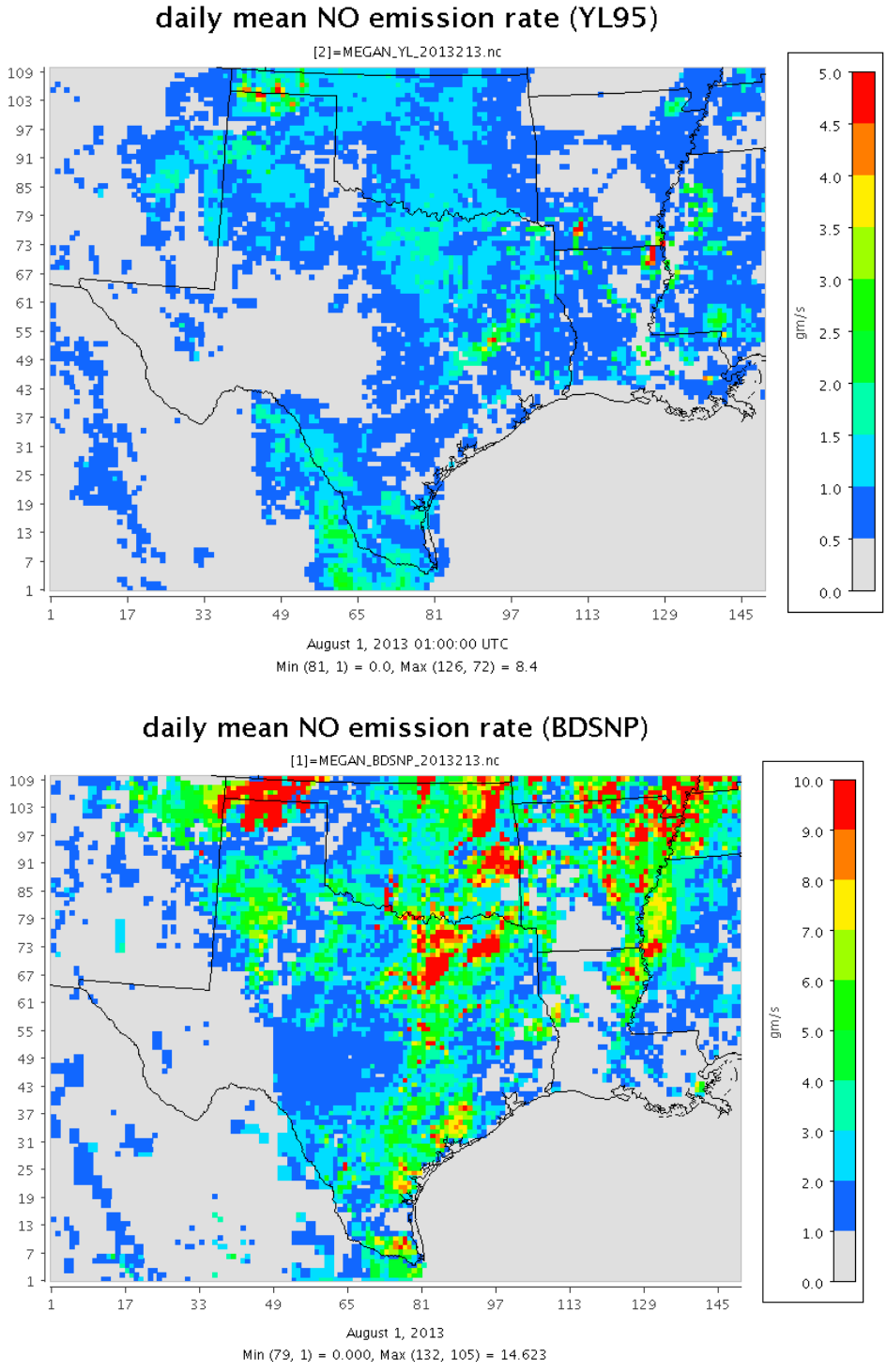

Figure 2. Spatial pattern difference of daily mean soil NO emission rate (g/s) from MEGAN default YL95 scheme (top) and BDSNP scheme (bottom) on August 1, 2013 over the Texas domain.

Project 14-020 **STATUS: Active – February 2, 2015**

Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC4RS

University of Maryland – Xinrong Ren

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Doug Boyer

Funding Amount: $70,000

Executive Summary

Despite great efforts undertaken in the past decades to address the problem of high ozone concentrations, our understanding of the key precursors that control tropospheric ozone production remains incomplete and uncertain. Sensitivity of ozone production to nitrogen oxides (NO_x) and volatile organic compounds (VOCs) represents a major uncertainty for oxidant photochemistry in urban areas and is expected to vary from location to location and from time of day. Understanding of the non-linear relationship between ozone production and its precursors is critical for the development of an effective ozone control strategy.

The DISCOVER-AQ campaign in Houston in August/September 2013 provided rich data sets to examine and improve our understanding of atmospheric photochemical oxidation processes related to the formation of secondary air pollutants like ozone and particulate matter (PM). In this project, an analysis of ozone production and its sensitivity to NO_x and VOCs will be performed. An observation-constrained box model based on Carbon Bond mechanism, Version 5 (CB05) will be used to study the photochemical processes along the NASA P-3B flight track, as well as at eight surface sites where the P-3B conducted spiral profiles. Ozone (O_3) production rates will be calculated at different locations and at different times of day and its sensitivity to NO_x and VOCs will be investigated. Spatially and temporally resolved ozone production and its sensitivity will also be investigated.

This project specifically addresses one of the AQRP priority research areas: Improving the understanding of ozone and particulate matter (PM) formation, and quantifying the characteristics of emissions in Texas through analysis of data collected during the DISCOVER-AQ campaign. The following tasks will be performed in this project:

An investigation of spatial variations of ozone production and its sensitivity to NO_x and VOCs in Houston during DISCOVER-AQ.

(1) An investigation of temporal variations of ozone production and its sensitivity to NO_x and VOCs in Houston during DISCOVER-AQ.

Investigate non-uniform emission reduction of O_3 pollution in Houston using spatial and temporal variations of ozone production and its sensitivity to NO_x and VOCs.

(2) Calculation of ozone production efficiency (OPE) at different locations using the ratio of ozone production rate to the NO_x oxidation rate calculated in the box model.

These activities will strengthen our understanding of O_3 production, which is essential to meet the primary and secondary National Ambient Air Quality Standards (NAAQS) for ozone.

Project Update

[*Project Management Note:*
This project is utilizing the same data as project 14-002 and 14-004. The PI was notified in September 2015 that the CMAQ simulations performed for Projects #14-002 and 14-004 utilized incorrect exit velocities of elevated point source emissions and that it may result in artificially high free tropospheric concentrations of various species rather than increased values in the boundary layer.

The study team will re-do the analyses for this project once the data is made available to them. The AQRP will provide a no cost extension to Project 14-020 through November 30, 2015, to allow time to re-run the models, analyze the data and revise the final report. No additional funds will be made available for the project.

Please note the project update below was submitted before the error was discovered, thus the analysis is subject to change.]

During the period from June 1 to August 31, 2015, the team at University of Maryland College Park has accomplished the following tasks:

(7) Attended the AQRP workshop to report the results of ozone production and its sensitivity to NOx and VOCs during the DISCOVER-AQ in Houston in 2013.

(8) Updated the box model mechanism from CB05 to CB05-TUCL with updated toluene and chlorine chemistry (CB05-TUCL is the mechanism used in the CMAQ model) so that the mechanisms in the box model and CMAQ are now the same.

(9) Prepared the draft final report. Some results from this quarter's data analysis are summarized below.

During the day, the photochemical O_3 production rate is essentially the production rate of NO_2 molecules from HO_2 + NO and RO_2 + NO reactions. The net instantaneous O_3 production rate, $P(O_3)$, can be written approximately as the following equation:

$$P(O_3) = k_{HO_2+NO}[HO_2][NO] + \sum k_{RO_{2i}+NO}[RO_{2i}][NO] - k_{OH+NO_2+M}[OH][NO_2][M] - P(RONO_2)$$
$$-k_{HO_2+O_3}[HO_2][O_3] - k_{OH+O_3}[OH][O_3] - k_{O(^1D)+H_2O}[O(^1D)][H_2O] - L(O_3 + alkenes) \quad (1)$$

where, *k term*s are the reaction rate coefficients. The negative terms in Eq. (1) correspond to the reaction of OH and NO_2 to form nitric acid, the formation of organic nitrates, $P(RONO_2)$, the reactions of OH and HO_2 with O_3, the photolysis of O_3 followed by the reaction of $O(^1D)$ with H_2O, and O_3 reactions with alkenes.

Figure 1 shows net ozone production rate ($P(O_3)$) calculated using the box model results along the P-3B flight track. There are several $P(O_3)$ hot spots over the Houston Ship Channel as well as

its downwind over Galveston Bay. This is expected because of large emissions of ozone precursors (NOx and VOC) from the Houston Ship Channel. The highest $P(O_3)$ up to ~140 ppbv hr^{-1} were observed over Houston Ship Channel. High $P(O_3)$ up to ~80-90 ppbv hr^{-1} were observed over Galveston Bay, mainly on September 25, 2013, consistent with high ozone levels observed cross the Houston area on that day.

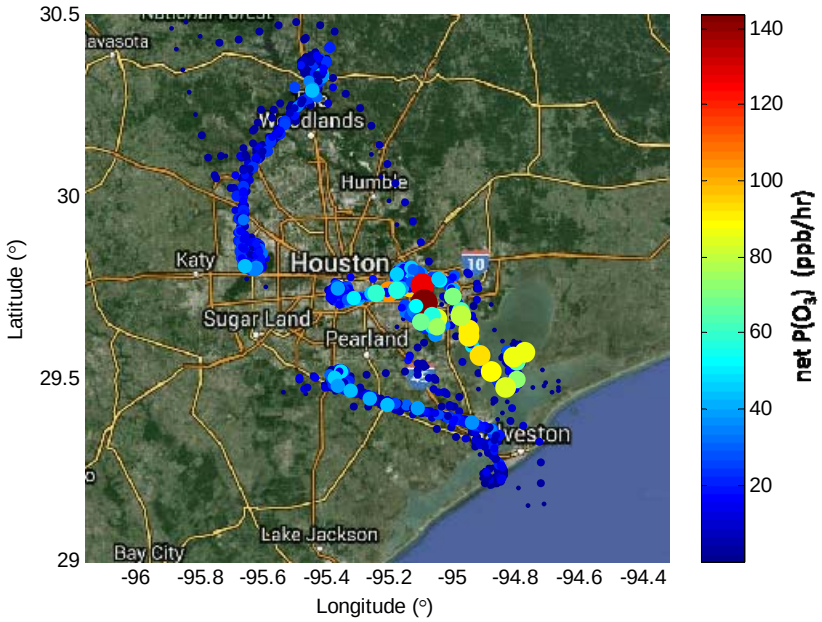

Figure 1. Net ozone production rate ($P(O_3)$) calculated using the box model results along the P-3B flight track. The size of dots is proportional to $P(O_3)$.

A method developed by Larry Kleinman [Kleinman, L. I., The dependence of tropospheric ozone production rate on ozone precursors, Atmos. Environ., 39(3), 575–586, 2005] was used to examine the sensitivity of ozone production to NOx and VOCs. In this method, ozone production is a function of NOx and VOC and the sensitivity of ozone production can be determined by an indicator, L_N/Q, where L_N is radical loss due to NOx, and Q is total primary radical production. Because the radical production rate is about the same as the radical loss rate, this ratio represents the fraction of radical loss due to NOx. It was found that if the ratio > 0.5, $P(O_3)$ is VOC-sensitive. If the ratio < 0.5, $P(O_3)$ is NOx-sensitive.

Figure 2 shows the indicator L_N/Q of ozone production sensitivity along the P-3B flight track. $P(O_3)$ was mainly VOC-sensitive over the Houston Ship Channel and its surrounding urban areas due to large NOx emissions. Over the areas away from the center of the city with relatively low NOx emissions, $P(O_3)$ was usually NOx-sensitive.

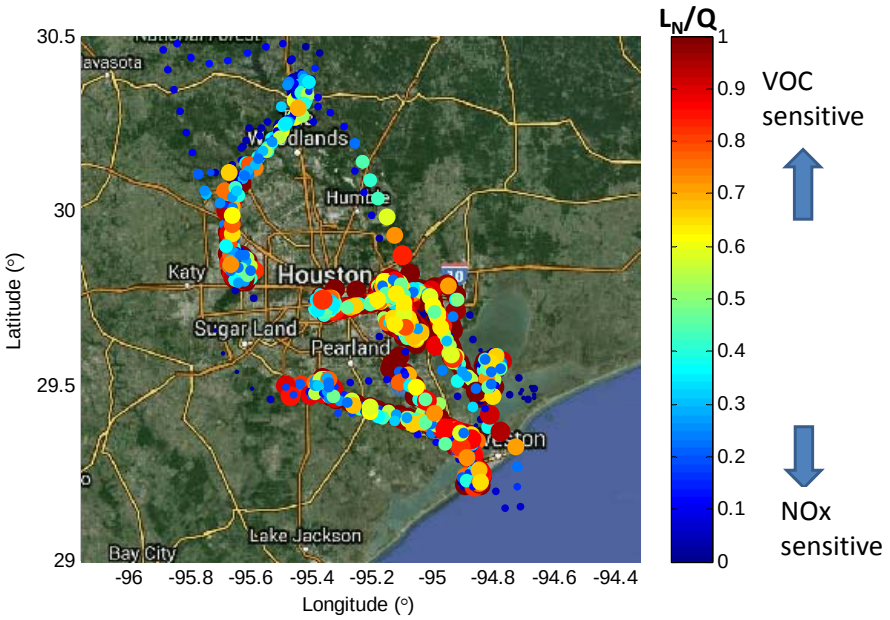

Figure 2. Ozone production sensitivity indicator, L_N/Q, along the P-3B flight track. $P(O_3)$ is VOC-sensitive when $L_N/Q > 0.5$, and NOx-sensitive when $L_N/Q < 0.5$.

In the diurnal variations of $P(O_3)$, a broad $P(O_3)$ peak in the morning with significant $P(O_3)$ in the afternoon was obtained (Figure 3). It is noticed that high $P(O_3)$ mainly occurred with $L_N/Q > 0.5$ (i.e., in the VOC sensitive regime).

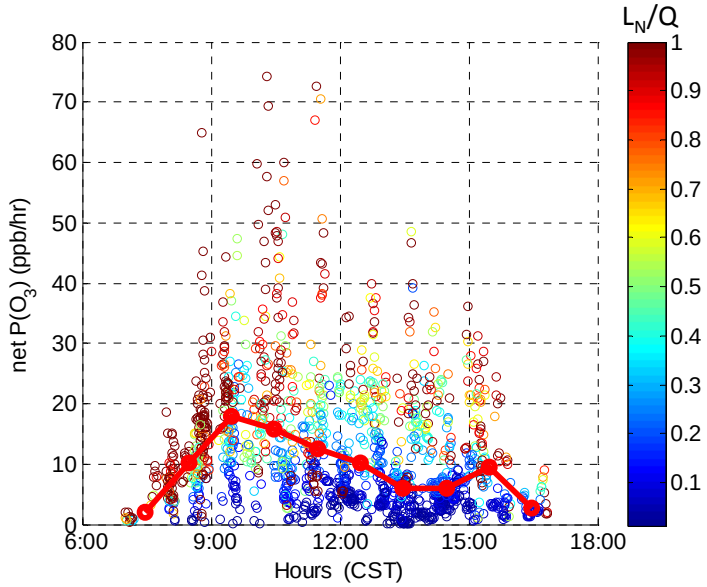

Figure 3. Diurnal variation of ozone production rate colored with the indicator L_N/Q. The solid red circles represent the median values in hourly bins of $P(O_3)$. Data are limited with the pressure altitude less than 1000 m to represent the lowest layer of the atmosphere.

The diurnal variation of L_N/Q indicates that $P(O_3)$ was mainly VOC sensitive in the early morning and then transited towards the NOx sensitive regime later the day (Figure 4). High $P(O_3)$ in the morning was mainly associated with VOC sensitive due to high NOx levels in the morning (points in the red cycle in Figure 4). Even though $P(O_3)$ was mainly NOx sensitive in the afternoon, there were periods when $P(O_3)$ was VOC sensitive.

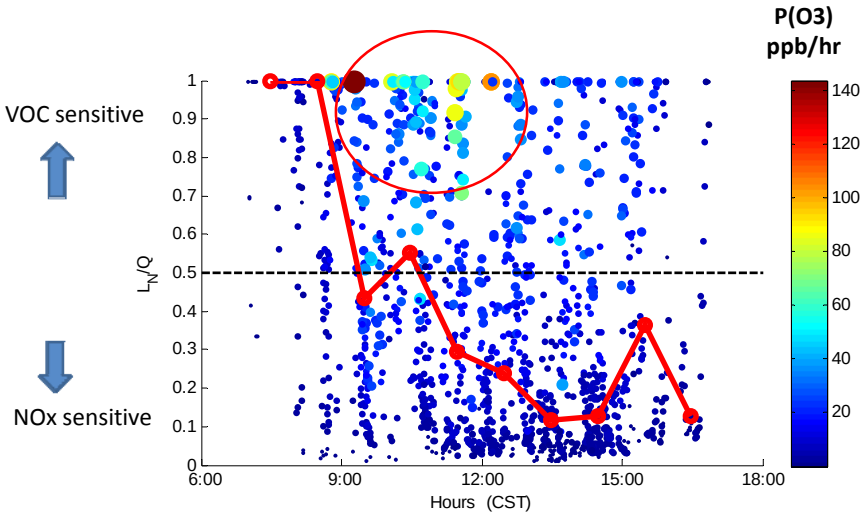

Figure 4. Diurnal variation of the indicator L_N/Q of ozone production rate sensitivity colored with ozone production rate below 1000 m. The solid red circles are the median values in hourly bins of L_N/Q.

The dependence of $P(O_3)$ on NO mixing ratio shows that when NO mixing ratio is less than ~1 ppbv, ozone production increases as [NO] increases, i.e., $P(O_3)$ is in NOx sensitive regime. When NO mixing ratio is great than ~1 ppbv, ozone production levels off as NO mixing ratio further increases, i.e., $P(O_3)$ is in NOx saturated regime (Figure 5). It was also found that at a given NO mixing ratio, higher production rate of HOx results higher ozone production rate, as points shown inside the blue circle in Figure 5.

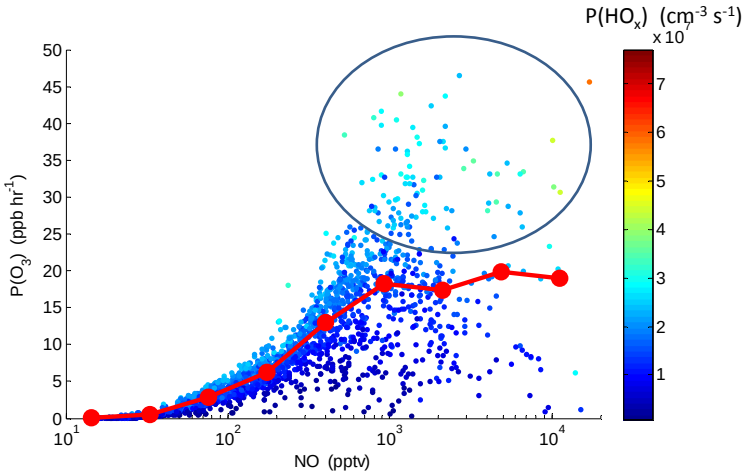

Figure 5. Ozone production as a function of NO mixing ratio. Individual data points are the 1 minute averages and are colored with the production rate of HOx (= OH + HO_2). The linked solid red circles represent the median values in [NO] bins. Note a log scale is used for the x axis.

During the next month before the project ends, the following tasks are anticipated to be accomplished:

(5) Complete remaining data analysis, especially ozone production efficiency (OPE).

(6) Complete the final report.

Project 14-022 **STATUS: Active – February 19, 2015**

Use of satellite data to improve specifications of land surface parameters

University of Alabama-Huntsville – Richard McNider
George Mason University – Daniel Tong
AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Bright Dornblaser

Funding Amount: $116,000
($71,004 UAH, $44,996 GMU)

Executive Summary

Land surface processes play a critical role in air quality model performance. Land surface temperatures impact boundary layer heights and turbulent mixing. Temperature gradients can also produce local wind patterns. For example in Houston the land-sea temperature gradient drives both the daytime sea breeze and nighttime land breeze. This growing temperature contrast in the morning is responsible for physical features such as a dead zone ahead of the sea breeze front, which develops as the land sea pressure gradient force opposes the large scale weather pattern. This dead zone allows the accumulation of precursors that are part of the peak ozone levels later in the day as this dead zone moves northward with the sea breeze front. Surface temperatures also impact air quality levels through temperature dependence of evaporative emissions and biogenic emissions. Temperatures also control the thermal decomposition of nitrogen species, which in turn impacts the efficiency of ozone production per NO molecule emitted. Thus, not only can temperatures affect ozone production, they can impact the efficacy and efficiency of control strategies.

It is the purpose of this project to evaluate and improve the performance of the land surface models used in the meteorological model (WRF) by the use of satellite skin temperatures to better specify physical parameters associated with land use classes. While considerable work has been done by the national community and especially in Texas to develop improved land use classifications, land use classes themselves are not directly used in models. Rather, physical parameters such as heat capacity, thermal resistance, roughness, surface moisture availability, albedo etc. associated with a land use class are actually used in the land surface model. Many of the land use class associated parameters such as surface moisture availability are dynamic and ill-observed depending on antecedent precipitation and evaporation, soil transport, the phenological state of the vegetation, irrigation applications etc. Other parameters such as heat capacity, thermal resistance or deep soil temperature are not only difficult to observe they are often unknowable *a priori.* This project will use satellite data to retrieve or adjust these critical land surface parameters.

The project will first develop skin temperature data sets from geostationary satellites and polar orbiting platforms and make direct comparisons to the skin temperatures from the WRF land surface model. This will be done for intensive field programs such as the recent DISCOVER-AQ and SEAC4RS campaigns. Second, techniques to use satellite observed skin temperatures to adjust land surface parameters such as surface moisture and surface thermal resistance will be tested to improve WRF skin and air temperatures. Extensive evaluation of model performance will be made against standard National Weather Service observations, special observations made during the DISCOVERY-AQ field campaign in September 2013 and other independent satellite observations.

Project Update

This report describes the second aspect of the project which is the use of satellite skin temperatures to adjust soil moisture in a new version of the Pleim-Xiu (PX) scheme in a similar way that observed surface air temperatures are used to adjust moisture in the current PX scheme.

Description of Skin Temperature Nudging Within The Pleim-Xiu Scheme

The previous quarterly report described the skin temperature products and their evaluation. As noted in that report, an alternative skin temperature which is a single channel retrieval by NOAA NESDIS that supports the ALEXI suite of products will be used in the land surface adjustment process (Anderson et al. 2007a and Anderson et al. 2007b).

Xiu and Pleim 2001 noted that since surface moisture is not a direct observable that use of auxiliary information is needed. They have used observed NWS surface temperatures to nudge moisture. Here they adjust surface layer moisture w_G using the difference between model daytime temperatures (T^F) and analyses of observed temperatures (T^A) and model and observed relative humidity.

$$\Delta w_G = \alpha_1 \left(T^A - T^F \right) + \alpha_2 \left(RH^A - RH^F \right)_{Daytime} \quad (1)$$

The Pleim-Xiu approach has been widely used and in recent California inter-comparisons performed better than the NOAH complex land surface scheme (Fovell 2013). Because observed NWS observations are coarse we proposed to replace the observed temperatures with satellite skin temperatures, i.e.

$$\Delta w_G = \beta_1 (T_s^{Sat} - T_s^{Mod})_{Morning} \quad (2)$$

where the nudging will be applied in the morning time frame. While the nudging in the original assimilation in (2) was applied throughout the day, here we believe it best to only nudge moisture during the morning hours for two reasons. The first is that skin temperature response is most sensitive to moisture in the morning hours (Carlson 1986). Second, because of afternoon cumulus clouds there is also a greater chance that undetected clouds may contaminate the surface skin temperature satellite retrieval.

Differences Between Satellite and Model Skin Temperatures

The assumption in the skin temperature assimilation process in (2) is that where model temperatures are cooler than observed temperatures then moisture will be reduced so that more energy will go to sensible heating rather than evaporation. On the other hand where model skin temperatures are warmer than observed skin temperatures then moisture will be increased. This is similar to the original PX moisture nudging by air temperatures. In order to see what differences exist in skin temperatures between model and satellite and the potential for changing surface moisture, figure 1 shows the mean difference between model and observed satellite data for the month of September 2013.

In the Eastern and Midwestern U.S. it can be seen that there are subtle differences between the model and satellite skin temperatures in corn growing regions in Iowa, Illinois and Indiana. Here the model is too cool. This is likely due to the fact that by September corn has senesced. That is, it has completed its kernel filling stage and leaves have browned up. Thus, it is no longer transpiring. Thus, model moisture may be too high causing the model to under predict

temperatures. The senescence would also cause an increased albedo over that of actively growing corn which would produce a cooler surface. However, in this case the lack of transpiration is likely overcoming the cooling due to albedo change as McNider et al. 1994 found for winter wheat in Oklahoma. Thus, the differences seen here and which seem physical give hope that the model can be nudged to a drier state and warmer solution more consistent with observations.

Looking at the figure the biggest areas of disagreement are in the West. Here the model is greatly underestimating the skin temperatures compared to the satellite observations. Based on the adjustment paradigm, it would be expected that the model may have moisture values that are too high or heat capacity values that or too low.

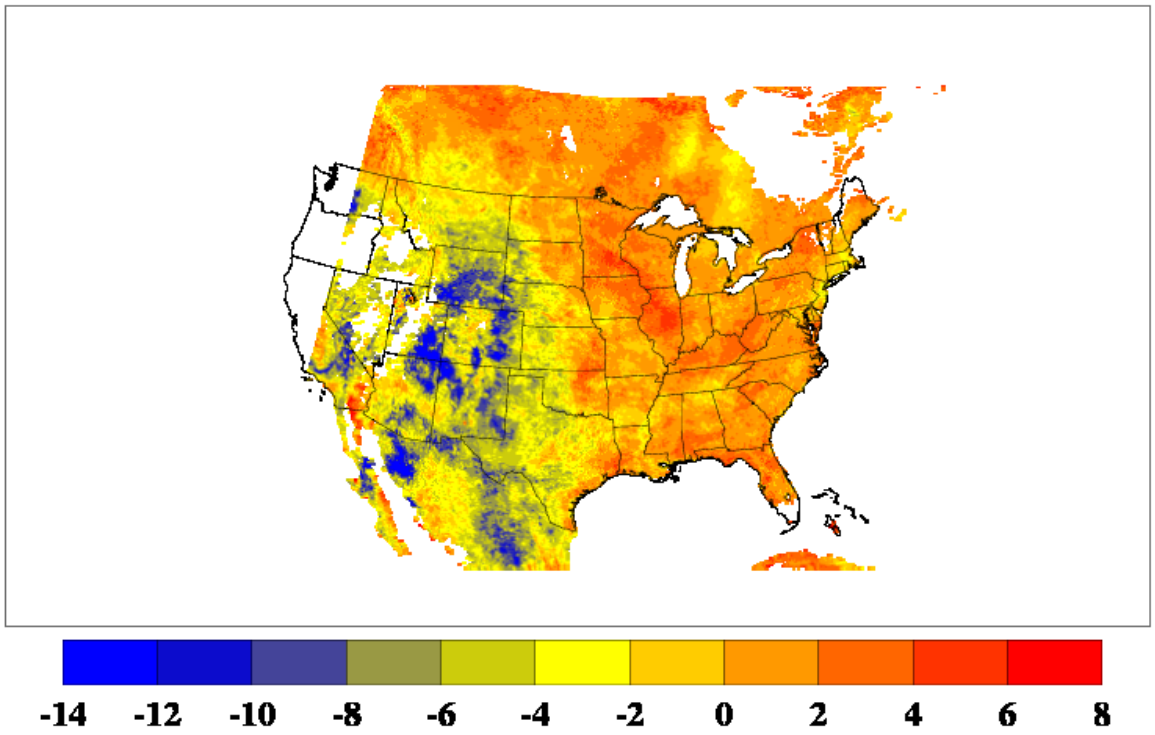

Fig. 1. Average daytime difference of the WRF diagnosed skin temperature minus the NOAA ALEXI observed skin temperature for the period 0000 UTC 1 September 2013 through 0000 UTC 6 September 2013. The NOAA ALEXI observed skin temperatures are the most recent version with aggressive cloud screening. Simulation is the insolation replacement run with the old (Pleim) vegetation fraction. Values truncated between -14 and +8 K.

In preliminary runs of the assimilation technique, one of the disappointing features is that the areas in the West which showed large differences between model and observed skin temperatures showed little difference after the moisture nudging. In starting our investigation it was found, however, that a least part of the issue was that in those areas where temperature was drastically under-predicted, there were large fractions of vegetation used in the model in contrast with what can be seen in visible images. In examining the PX code it was found that they used a seasonal growth algorithm to attempt to correct vegetation fraction in which temperature is used to adjust the vegetation fraction. It appears based on the USGS vegetative fractions and visible

images that the seasonal adjustment is erroneously (at least for September) producing unrealistic vegetative fractions. In the examples that follow the USGS vegetation fraction is used without seasonal adjustment.

Figure 2 provides difference between the new WRF CONTR and the observed satellite skin temperature. This is same information as figure 1 except it includes the changes in the control run (USGS vegetation fraction and no NWS nudging). As can be seen the use of the raw USGS vegetation fraction rather than the default PX seasonally adjusted vegetation fraction has reduced the area and magnitude of the disagreement especially in the western part of the domain. It is noted that in personal communication with Jon Pleim that they also are looking at changing their vegetation fraction calculation and perhaps moving to a MODIS vegetation fraction (Ran et al 2014). Figure 2 provides the WRF-CONTR to be used in assessing the impact of moisture nudging by skin temperatures.

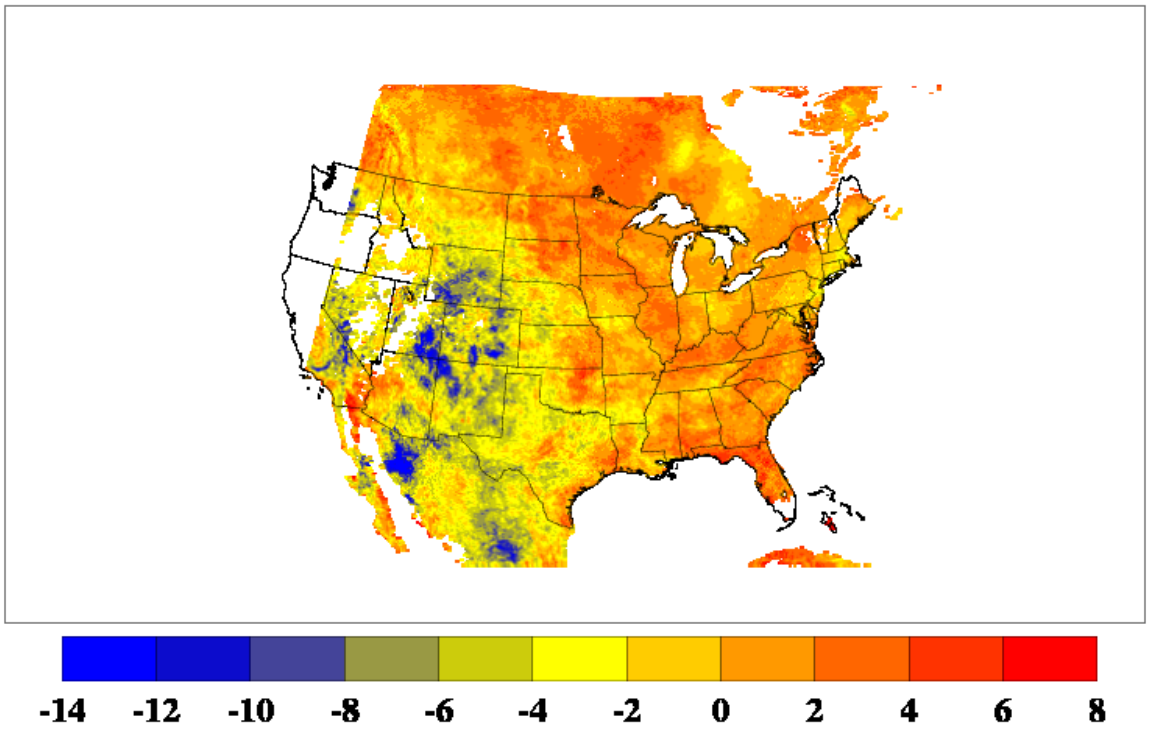

Fig. 2. Average daytime difference of the WRF diagnosed skin temperature minus the NOAA ALEXI observed skin temperature for the period 0000 UTC 1 September 2013 through 0000 UTC 6 September 2013. The NOAA ALEXI observed skin temperatures are the most recent version with aggressive cloud screening. Simulation is the insolation replacement run with the new (USGS) vegetation fraction and without any nudging. Values truncated between -14 and +8 K. This is the WRF –CONTR simulation.

Defining Statistical Measures for Assessing Impact of Skin Temperature Nudging

After the first set of runs using the skin temperature it was decided to make some changes in the model and protocols. The nudging coefficient, β_1 was set to a time scale of a few minutes which provides for a fairly fast assimilation. First, it was felt that with the short time available in the morning for assimilation that a stronger nudging coefficient be used than was employed in the original PX form which continuously assimilated the NWS observations.

Second, because in the PX scheme ET from vegetation is only impacted by deep layer moisture (W_2) it was decided to nudge the deep soil moisture in a similar fashion to the first layer moisture given in (2), i.e.

$$\Delta W_2(x,y,t) = \beta_1 (T_{SO}(x,y,t) - T_{SM}(x,y,t))_{morning} \quad . \quad (3)$$

In order to make comparisons of the impact of the assimilation it was felt that the control run that did not include the 2-m NWS nudging was a more appropriate control. With this WRF control run a pure comparison of the impact of the skin temperature can be seen. In the end a comparison with the PX 2-m nudging will be made but to understand the impact of the satellite skin temperature nudging this is a better control. The control run included the satellite insolation forcing. The WRF control will be referred to as WRF-CONTR and seen in Figure 4.

The WRF skin temperature nudging run (hereafter referred to as WRF-TS) was run in the same configuration.

Three statistics are used to evaluate whether the case with skin temperature nudging (WRF-TS) was providing an improvement over the control case (WRF-CONTR). These are defined below.

$$B_I = \left| \frac{1}{n} \sum_{t=1}^{n} (T_{WI} - T_{OBS}) \right| \quad (5)$$

$$B_N = \left| \frac{1}{n} \sum_{t=1}^{n} (T_{WN} - T_{OBS}) \right| \quad (6)$$

$$P = \frac{100(B_N - B_I)}{B_I} \quad (7)$$

B_I is the magnitude of the skin temperature bias for the insolation replacement run as in equation (5), where n is the total number of comparisons pairs, T_{WI} is the WRF diagnosed skin temperature for the WRF-CONTR, and T_{OBS} is the NOAA-Alexi GOES-derived skin temperature. In a similar manner B_N is the magnitude of the skin temperature bias for the insolation replacement plus soil nudging run as in equation (6), where T_{WN} is the WRF-TS diagnosed skin temperature for the run. BN can be defined for a simulation where only the top soil layer was nudged, or for simulation where both top and bottom soil layers were nudged. The comparison statistic is then provided by (7) which gives the percentage change in bias between the insolation and nudging runs.

Model Impact Using Skin Temperature Differences to Nudge Surface Soil Moisture

The soil moisture nudging as given is now tested using the statistical measures discussed above. Figure 3 gives the difference between the case WRF-TC (with moisture nudging) and the observed satellite skin temperature. As can be seen in comparison to Figure 2 there is improvement with the soil moisture adjustment. There are still some significant discrepancies in the west. In examination of visible imagery these areas are very sparsely vegetated areas and maybe due to errors in thermal resistance. This will be discussed later below.

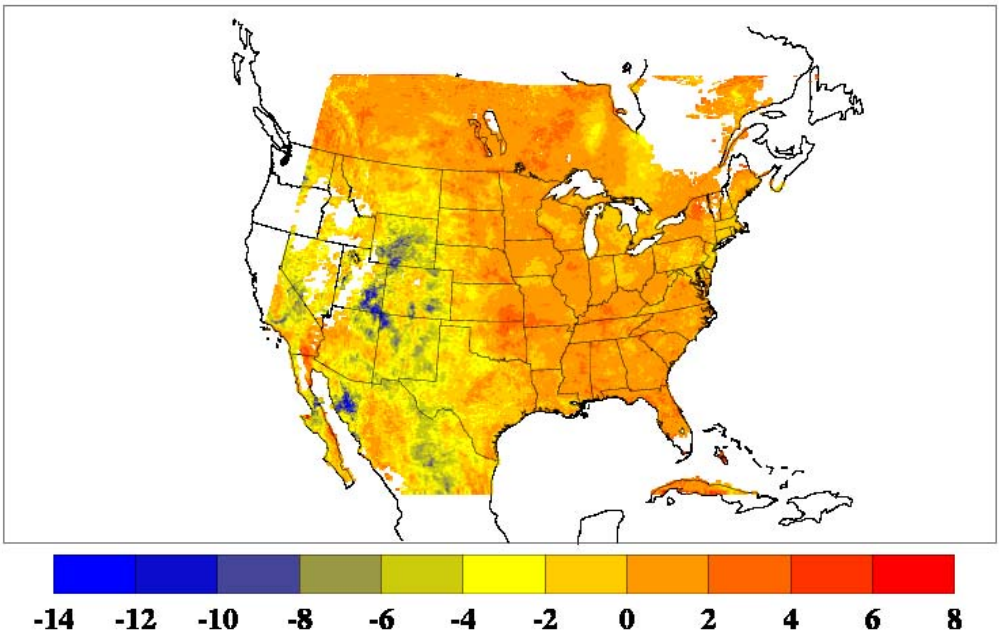

Fig. 3. Average daytime difference of the WRF diagnosed skin temperature minus the NOAA ALEXI observed skin temperature for the period 0000 UTC 1 September 2013 through 0000 UTC 6 September 2013. The NOAA ALEXI observed skin temperatures are the most recent version with aggressive cloud screening. Simulation is the insolation replacement run with the new (USGS) vegetation fraction with soil nudging (shallow and deep) with a nudging time scale of 600 s.

Figure 4 provides a measure of the improvement in model performance with nudging (WRF-TC) over the control (WRF-CONTR). This is the P statistic given by (7). It shows that over most of the domain there is improvement over large part of the domain. The scaling of the P statistic by the B_I (the bias in the control) may accentuate the percentage error where B_I is small. Figure 5 gives the raw difference in bias – that is in without normalization by B_I in (7). This gives a measure of the improvement or degradation in degrees K.

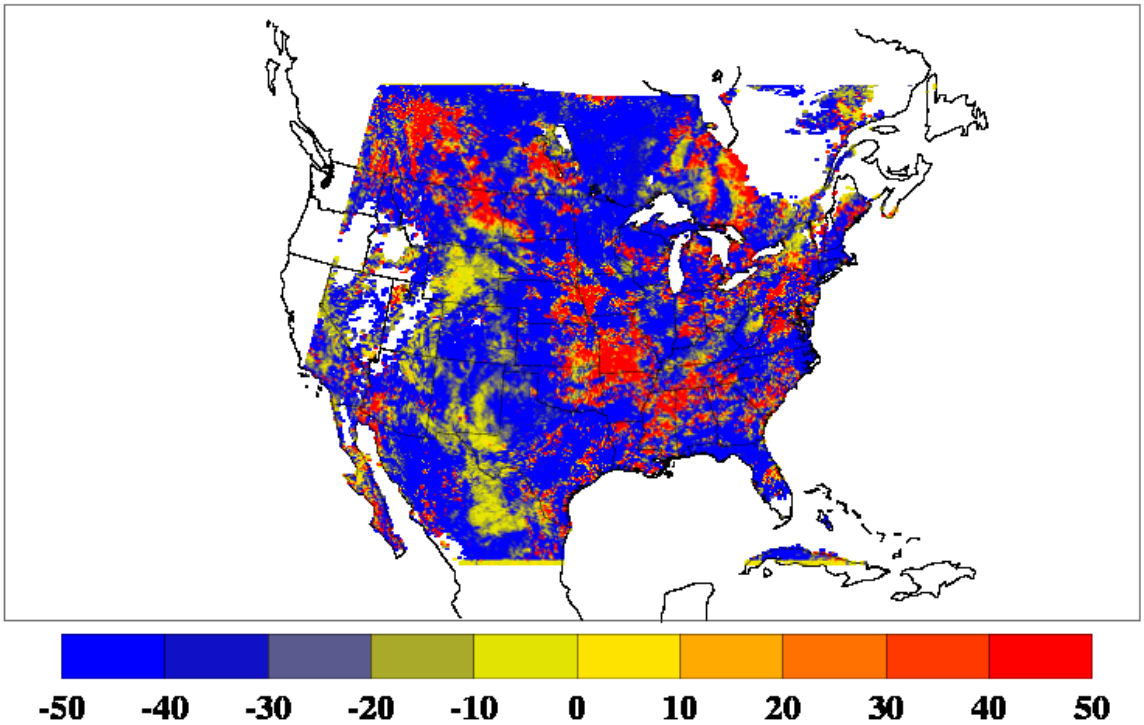

Fig. 4. Percentage change of the magnitude of the soil nudging bias (BN, absolute value of bias) relative to the magnitude of the insolation bias (BI, absolute value of bias) as given by 100 (BN – BI) / BI. This is the P statistic given by equation (7). Values truncated to ± 50 %. Both simulations used the USGS vegetation fraction. The NOAA ALEXI observed skin temperatures are the most recent version with aggressive cloud screening. Both simulations are for the period 0000 UTC 1 September 2013 through 0000 UTC 6 September 2013. Bias values are daytime only.

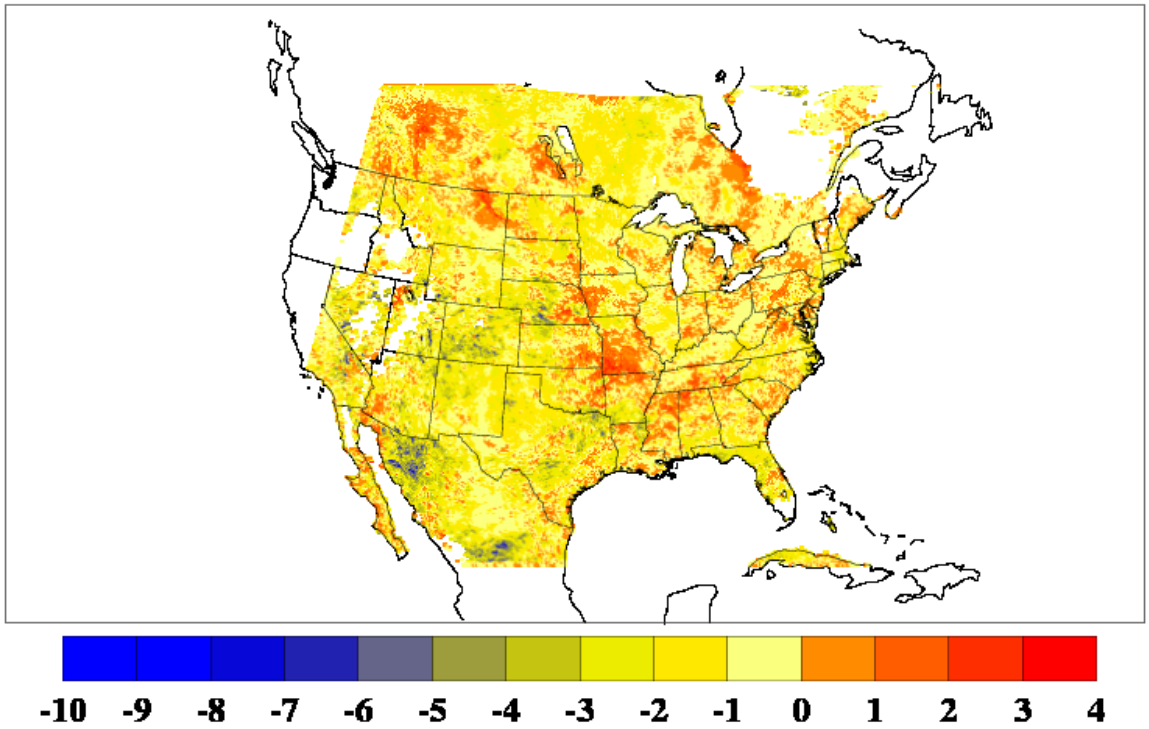

Fig. 5 Difference between the magnitude of the soil nudging bias (BN, absolute value of bias) and the magnitude of the insolation bias (BI, absolute value of bias) as given by BN – BI in units of K. This is an unscaled version of the P statistic given in (7) - i.e. without the division of by B_I. The NOAA ALEXI observed skin temperatures are the most recent version with aggressive cloud screening. Both simulations are for the period 0000 UTC 1 September 2013 through 0000 UTC 6 September 2013. Bias values are daytime only. Same information as in Fig. 6.6 but not normalized with respect to the insolation bias. Negative values (cool colors) correspond to a reduction in the magnitude of the bias, and positive values (warm colors) correspond to an increase in bias

Finally, figure 6 shows the sign of the change in bias over the domain negative areas (blue) show improvement due to the moisture nudging while positive values (red) indicate a degradation in performance. As can be seen there is improvement over most of the domain but some areas such as in Missouri there is degradation.

Additional point by point analyses will be provided in the final report to try to understand both the improvement and degradation. This will be accomplished by examining time series at the points identified in Figure 6.

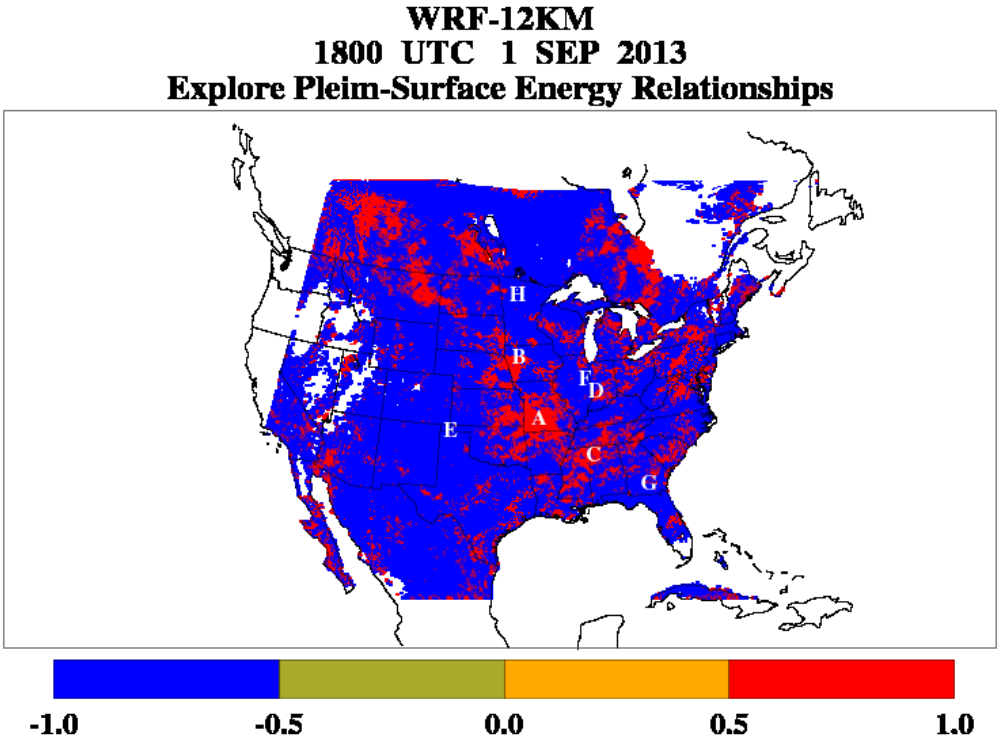

Fig. 6 Sign of the percentage change in bias from Fig.5. Negative areas indicate a reduction in bias whereas positive areas indicate an increase in bias. Key and locations used in the following time series plots are as follow: A- southwestern Missouri, B-western Iowa, C- northwestern Alabama, D-southern Indiana, E- northern Texas, F-eastern Illinois, G-southwestern Georgia, and H-northern Minnesota. Locations A-D correspond to locations with bias degradation, and locations E-H correspond to locations with bias improvement.

Summary and Conclusions

Under this activity a technique was developed which diagnoses a skin temperature consistent with the surface fluxes in the PX scheme. This skin temperature is then used in a technique to nudge soil moisture (see equations (2) and (3). Fundamentally, if the model temperatures are lower than the observed temperature then soil moisture is decreased. If the model temperatures are greater than the observed temperature then soil moisture is increased. This is consistent with that of Pleim and Xiu in that they argued that soil moisture is ill observed and thus needs an indirect observational adjustment. Techniques within the WRF framework allow us to bring in satellite skin temperature data to carry out the nudging of soil moisture using satellite skin temperatures as opposed the NWS soil moisture nudging in the original PX scheme.

A control simulation was carried (WRF-CONTR) which did not include the skin temperature nudging. Bias statistics were developed for this control. Second, a new WRF run was made using the skin temperature nudging technique. The results showed that over most of the domain that the model was improved (i.e. the bias was decreased compared to the control run).

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Project 14-023 **STATUS: Active – May 23, 2014**
Ended – August 31, 2014

Assessment of Two Remote Sensing Technologies to Control Flare Performance

The University of Texas at Austin – Vincent Torres
Aerodyne Research, Inc. – Scott Herndon
Leak Surveys, Inc. – Joshua Furry
Providence Photonics, LLC – Yongshen Zeng

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Russell Nettles

Original Funding Amount: $480,741
($239,773 UT-Austin, $157,066 Aerodyne, $26,716 Leak Survey, $57,186 Providence Photonics)

Final Funding Amount: $36,587.11 ($25,874.37 UT-Austin, $10,712.74 Aerodyne)

Executive Summary
Industrial flares are devices used at industrial facilities to safely dispose of relief gases in an environmentally compliant manner through the use of combustion. Recent studies of industrial air- and steam-assisted flares have shown that merely complying with federal regulations like the Environmental Protection Agency's 40CFR § 60.18 and 40CFR § 63.11, do not ensure the flare will operate with at high combustion efficiency when combusting hydrocarbons over the entire range of operating scenarios for dual service flares. For vent gas streams containing hydrocarbons, the combustion efficiency (CE) is the percentage of the total hydrocarbon stream entering the flare that burns completely to form only carbon dioxide and water. It is desirable to have high combustion efficiency at all times to maximize flare performance.

The purpose of the proposed project was to conduct a series of field tests using an operational, full-scale industrial flare at a Petrologistics, LLC plant in Houston, Texas, to determine the technical, economic and operational feasibility of two approaches designed to maximize flare performance. These approaches continuously measure or determine the flare's combustion efficiency and would use this information to adjust the steam assist to the flare to adjust the flare's performance. To assess the technical performance of the approaches, the combustion efficiency measurements of each approach will be compared to an independent direct sampling measurement (the reference measurement) of the flare's combustion efficiency to determine the accuracy and completeness of the measurements obtained from the two approaches. For the field tests, the performance of the flare will not be controlled by either of the two approaches so that the prescribed test plan can be conducted with the flare. After the test series, the economic and operational feasibility will be evaluated based on the operational and safety characteristics observed during the tests and the estimated cost to implement each approach.

Project Update
On August 15, 2014, notice was sent to the AQRP Project Manager that the project would need to be ended and all unspent funds returned to the AQRP due to the plant where the testing was to be done no longer being able to participate.

No further work will be performed or costs incurred on this project.

Project 14-024 **STATUS: Active – June 18, 2014**
Completed – August 31, 2015

Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ Data, Modeling and Experiments

The University of Texas at Austin – Lea Hildebrandt Ruiz
Environ – Greg Yarwood
University of California – Riverside – Gookyoung Heo

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $300,000
($163,282 UT-Austin, $101,404 Environ, $35,314 UC – Riverside)

Expended Amount: $ TBD
($ TBD UT-Austin, $101,404 Environ, $30,875.39 UC – Riverside)

Amount Returned to AQRP: $ TBD
($ TBD UT-Austin, $0.00 Environ, $4,438.61 UC – Riverside)

Executive Summary

The new annual National Ambient Air Quality Standard (NAAQS) for particulate matter smaller than 2.5 micrometers in diameter ($PM_{2.5}$) brings the Houston region to near non-attainment for $PM_{2.5}$, underlining the importance of understanding the composition and sources of $PM_{2.5}$ in Houston. Over half of fine PM in the Houston region is composed of organic material including primary organic aerosol (POA), which are compounds that are emitted as particles and have not reacted in the atmosphere and secondary organic aerosol (SOA), which is formed when gas-phase compounds undergo one or more chemical transformations in the gas phase, forming less volatile compounds that then partition between the gas and particle phases. Understanding the sources and formation of organic aerosol is therefore very complex, and significant uncertainties remain. In this work laboratory experiments, ambient measurements and a photochemical model were combined to better understand the sources of organic particulate matter in the Houston region.

Sixteen laboratory chamber experiments were conducted to form SOA from the oxidation of different intermediate volatility organic compounds (IVOCs). Out of the six IVOCs studied (n-pentadecane, 2,6,10-trimethyldodecane, 2-methylnapthalene, butyl CARBITOL™, Texanol™, and mineral spirits), all but Texanol™ formed secondary organic aerosol. SOA mass yields of 2-methylnapthalene measured in this study agreed well with literature data. A novel contribution of this work is quantification of the SOA yield from butyl CARBITOL™, a glycol ether used in surface coatings. The SOA yields from this compound were similar to yields from 2-

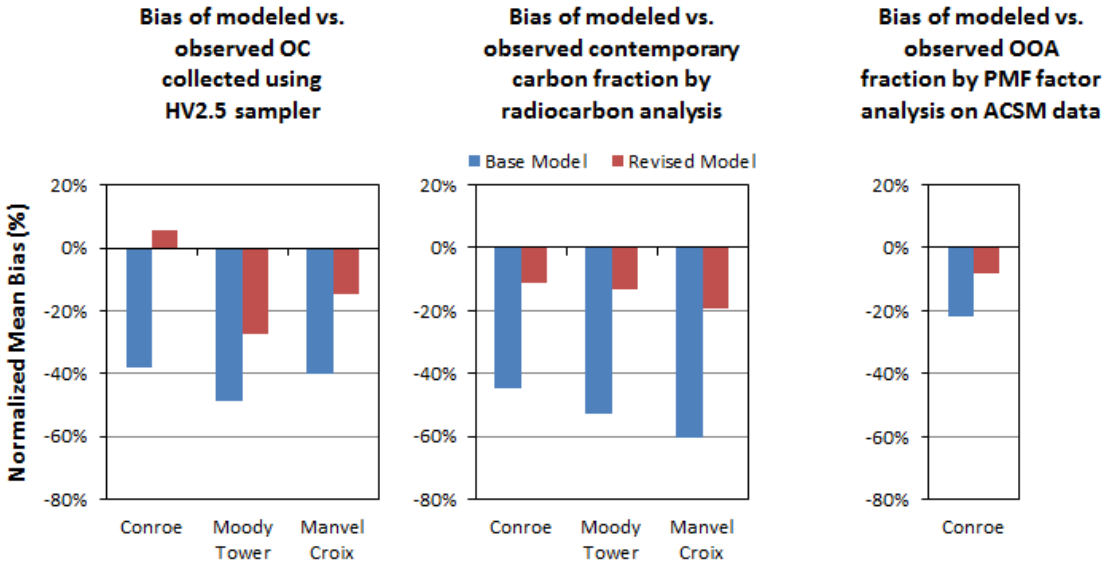
methylnapthalene. The vapor pressure of SOA formed from n-pentadecane, 2,6,10-trimethyldodecane and mineral spirits was analyzed using a thermodenuder developed as part of this work. The SOA formed from mineral spirits was more volatile than the SOA formed from n- pentadecane and 2,6,10-trimethyldodecane (a branched pentadecane).

Ambient data collected during an ambient measurement campaign in Houston, TX termed Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ, http://discover-aq.larc.nasa.gov/) were analyzed focusing on the concentrations and composition of fine particulate matter. The data were obtained at an air quality monitoring ground site in Conroe, TX (30.350278°N, 95.425000°W) located approximately 60 km north-northwest from the Houston, TX urban center and approximately 125 km northwest of the nearest coastline. On average 65% of the mass of non-refractory particulate matter smaller than 1 micrometer in diameter (PM_1) was due to organic material (including organic nitrates), highlighting the importance of organics in controlling fine PM mass in the Houston region. Positive matrix factorization analysis (PMF) was applied to the organic aerosol mass spectra measured by aerosol chemical speciation monitor (ACSM). The data were best represented by two factors of oxygenated organic aerosol (OOA), a more oxidized OOA (MO- OOA) and a less oxidized OOA (LO-OOA), as well as a fresher factor representative of hydrocarbon like organic aerosol (HOA) and biomass burning organic aerosol (BBOA). According to this analysis on average 85% of the organic aerosol sampled at Conroe consisted of oxygenated organic aerosol, highlighting the importance of atmospheric processing in influencing concentrations of organic particulate matter in the Houston region.

The Comprehensive Air quality Model with Extensions (CAMx) utilizing the 1.5 dimensional volatility basis set (1.5-D VBS) was applied to simulate organic aerosol formation in the Houston region during the 2013 DISCOVER-AQ campaign. Emissions of IVOC from major combustion sources were added using IVOC fractions of total non-methane organic gas (NMOG) emissions estimated from environmental chamber studies. The model results were evaluated against $PM_{2.5}$ filter measurements at Conroe, Moody Tower and Manvel Croix and PM_1 ACSM measurements at Conroe. The base model generally underpredicts the observed total organic carbon (OC) concentrations and PMF-estimated OOA fractions. The radio carbon analysis indicates that the base model underestimates contemporary carbon fractions while the modeled fossil carbon mass is comparable to observations.

Several improvements were made to the base model: a basis set for cooking-influenced organic aerosol was added, the organic aerosol mass yields from the reactions of monoterpenes and NO_3 were updated, the organic aerosol mass yields of IVOC precursors were adjusted, an error in the emissions of primary organic aerosol from biomass burning area sources was corrected and the formation of secondary organic aerosol from long alkane precursors (8-11 carbons) was added. The base case scenario was simulated again with the revised model. The results show that the

revised model gives much better agreement than the base model with the measured OC concentrations, PMF-based OOA fractions, and contemporary carbon fractions by radiocarbon analysis.



The supplemental measurements in the evaluation database (including filter OC and radiocarbon analysis data, ACSM measurements and PMF analysis) were very useful in guiding model improvements and providing a more informative evaluation. This project greatly benefited from the AQRP projects 14-024 and 14-029 that collected these data.

Project Update

The final report for this project is under review.

Project 14-025 **STATUS: Active – May 21, 2014**
Completed – July 31, 2015

Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model

Environ – Christopher Emery
Texas A&M University – John Nielson-Gammon
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Khalid Al-Wali

Funding Amount: $256,261
($135,735 Environ, $120,526 TAMU)
Expended Amount: $ TBD
($135,603.98 Environ, $ TBD TAMU)

Amount Returned to AQRP: $ TBD
($131.02 Environ, $ TBD TAMU)

Executive Summary

Under Texas Air Quality Research Program (AQRP) Project 14-025, Ramboll Environ and collaborators at Texas A&M University (TAMU) incorporated an explicit sub-grid cloud model into the Comprehensive Air quality Model with extensions (CAMx) and evaluated its effects against aircraft measurements logged during two field study campaigns. This report documents the approach, implementation, and testing of the cloud model system. We are providing the new model to the Texas Commission on Environmental Quality (TCEQ); this update will be combined with other modifications and publicly released in a future version of CAMx.

The US Environmental Protection Agency (EPA) requires the use of photochemical grid models to demonstrate how local emission control plans will achieve the federal air quality standard for ground-level ozone in nonattainment areas designated as moderate or higher (EPA, 2014). There are currently two ozone nonattainment areas in the State of Texas but this number will likely increase with the promulgation of a stricter ozone standard in late 2015. TCEQ uses CAMx for both regulatory and research applications.

Daily convective cloudiness and rainfall are common occurrences throughout much of Texas and the southern US during the ozone season (typically April through October). Such convection most often occurs at small scales, and its ubiquity and abundance provide important mechanisms for exchanging boundary layer air with the free troposphere, for chemical processing, and for wet removal. Up to this point CAMx has not explicitly treated cloud processes at scales smaller than the grid resolution (1-10 km). While diagnosed sub-grid cloud fields have been used to parametrically influence grid-scale photolysis rates, wet deposition, and aqueous chemistry, CAMx has not included cloud convective transport.

The new "Cloud-in-Grid" (CiG) treatment includes a new vertical convective transport component for both in-cloud and ambient fractions of the grid column, as well as explicit aqueous chemistry and wet scavenging within the sub-grid cloud compartment. The CAMx/CiG is linked to updates to the Weather Research and Forecasting (WRF) meteorological model's Kain-Fritsch (K-F) sub-grid cumulus scheme that has been recently improved by EPA's National Exposure Research Laboratory (NERL). The new algorithm has been thoroughly quality assured, and process testing in serial and parallel modes indicates no substantial impact to overall model speed. The CiG offers

two advantages over approaches employed in other off-line photochemical grid models: (1) a direct and consistent link between WRF and CAMx models that removes the need to independently re-diagnose convection location, depth, intensity, and water contents; and (2) the inclusion of both in-cloud convective fluxes and compensating vertical motions in the ambient portion of the cell.

CAMx/CiG was evaluated by applying the model to multi-day episodes in 2008 and 2013 when ozone and precursor concentration measurements were available from aircraft measurement campaigns during the 2008 Stratosphere-Troposphere Analyses of Regional Transport (START08) and the 2013 Deriving Information on Surface conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ), respectively. Specific days during each episode were selected for the presence of various convective modes. The consequences of convective mixing on the horizontal and vertical distribution of key gas-phase constituents (ozone, nitrogen oxides and carbon monoxide) were qualitatively assessed for plausibility and were compared to aircraft observations in nearby locations and similar times.

We confirm that the convective mixing parameterization produces substantial changes in constituent mixing ratio in areas of model-simulated convection, with smaller yet potentially widespread contributions from regional convection. The CiG generally improves boundary layer simulations of ozone and nitrogen oxides when compared to aircraft-derived profiles. A relative lack of impact at aircraft-sampled locations in the 2008 episode is a consequence of insufficient model-simulated convection rather than any deficiency in the convective mixing parameterization. Based on the project results summarized in this report, we recommend follow-on projects that address additional evaluation and necessary extensions to other areas of the model.

Project Update
The final report for this project is under review.

Project 14-026 **STATUS: Active – May 21, 2014**

Quantifying ozone production from light alkenes using novel measurements of hydroxynitrate reaction products in Houston during the NASA SEAC4RS project

Environ – Thomas Ryerson

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Chris Kite

Original Funding Amount: $231,182
($135,782 Environ, $95,400 CalTech)

Revised Funding Amount: $165,562
(Environ only)

Executive Summary

The objective of this project is to improve and quantify our understanding of ozone (O_3) and formaldehyde (HCHO) production from industrial emissions of Highly Reactive Volatile Organic Compounds (HRVOCs) in the Houston area. Aircraft flights during the National Aeronautics and Space Administration (NASA) Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC^{4}RS) project encountered plumes with enhanced O_3 downwind of petrochemical facilities in Houston. For example, on 25 September 2013, ground monitoring downwind of the Ship Channel showed 5-minute average O_3 values peaking at 165 ppb and are associated with elevated concentrations of the oxidation products of HRVOCs. HRVOCs, specifically ethene, propene, butenes and 1,3-butadiene, have been implicated in these types of high ozone events but quantifying the relative contributions of individual HRVOCs to O_3 formation has been difficult.

The project objective will be accomplished by a combination of data analysis and reactive plume modeling. Data taken aboard the NASA DC-8 research aircraft during the 2013 SEAC^{4}RS project in Houston will be analyzed. Chemical compounds called β-hydroxynitrates are formed when HRVOCs react in the atmosphere in the presence of nitrogen oxides (NOx). Measurements of the C_2-C_4 hydroxynitrates aboard the DC-8 provide a novel means to link observed enhancements of O_3 and HCHO to reactions of specific HRVOCs. Analyzing the data will provide a robust first-order attribution of observed O_3 and HCHO enhancements to the oxidation of individual HRVOCs emitted from the Houston Ship Channel. The plumes of HRVOCs and O_3 that the DC-8 intercepted will be analyzed further to estimate what emissions of HRVOCs and NOx gave rise to each plume. A reactive plume model (SCICHEM) will be used to model these plumes and test chemical reaction mechanisms for individual HRVOCs. The model sensitivity to plume expansion rates will be evaluated to test how plume dilution influences chemical processing and therefore how grid model resolution can influence assessments for HRVOC sources. The benefits of this project to the TCEQ will be a data-driven assessment of the contributions of individual HRVOCs to O_3 and HCHO enhancements downwind of the Houston ship channel and improved modeling tools for assessing the air quality impacts of HRVOC emissions in the Texas State Implementation Plan (SIP).

Project Update
This AQRP project is being performed by Ramboll Environ, NOAA, and Dr. David Parrish. Both NOAA and Dr. Parrish are conducting their tasks under subcontract to Ramboll Environ.

Data Analysis
Dr. Parrish completed the initial data analysis and prepared a report on the analysis for inclusion in the preliminary draft final report submitted to AQRP on August 18, 2015. Dr. Parrish met with scientists from Ramboll Environ on August 25, 2015 to discuss and compare initial modeling results with those from the observational analysis. Subsequent to this meeting, Dr. Parrish conducted additional analysis for inclusion in the final draft final report.

Photochemical plume modeling
The CB6r2 mechanism and simplified kinetics scheme for the HRVOC chemistry implemented in the beta version of SCICHEM 3.0 were ported to the final release version of SCICHEM 3.0 (released June 19, 2015). Dr. Greg Yarwood presented data analysis and preliminary results from the modeling of the 18 September 2013 Ship Channel plume at the AQRP Workshop at UT Austin on June 17 and 18, 2015. Results from the initial base case simulation were documented in the preliminary draft final report submitted to AQRP on August 18, 2015. Additional SCICHEM base case and sensitivity simulations were conducted after a meeting between Ramboll Environ scientists and Dr. David Parrish on August 25, 2015. The results from these simulations are being incorporated in the final draft report.

Final Report
A preliminary draft report describing the data analysis and initial modelling results was submitted to AQRP on August 18, 2015. This report will be finalized in September 2015.

Project 14-029 **STATUS: Active – July 10, 2014**
Completed – June 30, 2015

Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ

Baylor University – Rebecca Sheesley

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $178,679 **Expended Amount:** $ TBD

Amount Returned to AQRP: $ TBD

Executive Summary

This project builds on a previously-funded Air Quality Research Program (AQRP) project which characterized initial elemental carbon (EC) and organic carbon (OC) particulate matter (PM) during DISCOVER-AQ (Deriving Information on Surface conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality) Houston Texas 2013 (AQRP 12-032). The overall goals of the current project were to quantify the strength of PM formation and PM emission sources across the Houston metropolitan area. This was accomplished using samples collected over the DISCOVER-AQ sampling period at two primary sites in Houston: Moody Tower (downtown; urban) and Manvel Croix (southern; suburb); and two auxiliary sites: Conroe (far north; suburb) and La Porte (east; urban industrial). The detailed chemical characterization included elemental carbon and organic carbon, radiocarbon, water-soluble organic carbon, organic and elemental tracers and inorganic ions. A majority of the analysis focused on samples collected during 9/21/13-9/28/13. Source apportionment methods utilized for this project included radiocarbon source apportionment and chemical mass balance modeling using organic and elemental tracers.

The radiocarbon apportionment effectively constrained chemical mass balance source apportionment results to provide estimation of anthropogenic and biogenic, primary and secondary contributions to carbonaceous aerosol. The results indicated that Moody Tower (a site indicative of urban Houston) had a consistent primary motor vehicle exhaust contribution (18-27%) and a fossil secondary organic aerosol (SOA) contribution that varied from 5-33% depending on atmospheric condition. Conroe (a site indicative of aged urban aerosol combined with biogenic contributions) had a lower contribution of motor vehicle exhaust (5-10%) and a similarly variable fraction of fossil SOA (4-25%). Manvel Croix (a site indicative of residential Houston area) had an intermediate motor vehicle contribution (9-15%) with variable fossil SOA (5-30%). There was minimal wood smoke contribution during the examined week (0-9% at all sites) except one La Porte sample which had 16% wood smoke contribution. This indicates that wood smoke is an event-based contribution for summer in Houston at the urban sites. In contrast, the biogenic SOA was a large contributor at all sites; this ranged from 40-75% at Moody Tower, 56-81% at Manvel Croix to 60-79% at Conroe. In summary, the motor vehicle contribution was consistent at each site during the analysis week, while the biogenic SOA was consistently high, while the fossil SOA showed the most variability and dependence on atmospheric conditions.

Project Update
The final report for this project is under review.

Project 14-030 **STATUS: Active – June 25, 2014**
Completed – June 30, 2015

Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation

Texas A&M University – Qi Ying

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Mark Estes

Funding Amount: $176,109 **Expended Amount:** $ TBD

Amount Returned to TCEQ: $ TBD

Executive Summary

Emissions of isoprene in a three-level nested air quality modeling domain (Continental United States (CONUS), Texas and surrounding states, and east Texas) during a severe drought year (2011) and a non-drought year (2007) were estimated using the most recent version (v2.10) of the Model of Emissions of Gases and Aerosols from Nature (MEGAN). Regional soil moisture field needed for MEGAN was estimated using the Weather Research and Forecasting (WRF) model (v3.6) with the Noah land surface scheme initialized with the soil moisture field from North American Land Data Assimilation Systems (NLDAS)-2 with Noah-2.8. Wilting point data needed for the drought parametrization in the MEGAN model was estimated using the Penn State CONUS-Soil database and the soil-related hydraulic parameters from Table 2 of Chen and Dudhia. While the predicted soil moisture generally agrees with observations at limited number of sites (mostly in Oklahoma), field measurements of soil moisture and isoprene emission at three field sites in east Texas in 2011 indicated that root zone soil moistures may not be adequately represented in the model because (i) the model may over- or under-predict grid average rainfall and/or evapotranspiration, and (ii) it does not consider differences in rooting depth between isoprene emitters. Greenhouse measurements on potted oak species revealed that there does not appear to be major physiological differences between species and that the current factor scaling isoprene emissions to drought stress adequately represents observed responses. When those are applied to the field data, differences between isoprene emitting oak species do emerge, but are more likely be related to root structure (and depth) and physiology than to average soil moisture.

Using the default MEGAN model without considering drought effects led to CMAQ predicted isoprene concentrations that are significantly higher than observations (by a factor of 2-5) at most observation sites in both drought and non-drought years, suggesting an over-prediction of isoprene emissions by MEGAN v2.10 in Texas. Using the default drought parameterization reduces isoprene emissions but does not solve the isoprene over-prediction problem, suggesting that other factors might play a more important role than soil moisture. The exact cause of this over-prediction needs to be explored in future studies. Simulated ozone concentrations generally agree with observations but peak concentrations are constantly over-predicted in 2011. Lower isoprene emissions due to drought lead to lower ozone peak concentrations which in some cases agree better with the observations, and better peak ozone performance statistics. However, the overall 1-h ozone performance does not show significant improvement. While it is obvious that isoprene emissions could affect ozone predictions under drought conditions quite significantly

(~5-15% reduction in average ozone concentrations), uncertainty in base case isoprene emissions needs to be constrained to better understand the drought effect on air quality in future studies.

Project Update
The final report for this project is under review.

FINANCIAL STATUS REPORT

Initial funding for fiscal year 2010 was established at $2,732,071.00. In late May 2010 an amendment was issued increasing the budget by $40,000. Funding for fiscal year 2011 was established at $2,106,071, for a total award of $4,878,142 for the FY 2010/2011 biennium. FY 2010 funds were fully expended in early 2012 and the FY 2011 funds expired on June 30, 2013 with a remaining balance of $0.11.

In February 2012, funding of $1,000,000 was awarded for FY 2012. In June 2012, an additional $160,000 was awarded in FY 2012 funds and $1,000,000 was awarded in FY 2013 funds, for a total of $2,160,000 in funding for the FY 2012/2013 biennium.

In April 2013, the grant was amended to reduce the FY 2012 funds by $133,693.60 and increase the FY 2011 funds by the same amount.

In June 2013, the grant was amended to increase the FY 2013 funds by $2,500,000.

In October 2013, the grant was amended to award FY 2014 funds of $1,000,000 and FY 2015 funds of $1,000,000. The budget for each fiscal year can be found in Appendix C.

FY 2012 funds were fully expended at the end of April 2014. FY 2013 funds were fully expended at the end of June 2015.

For each biennium (and fiscal year) the funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

Program Administration – limited to 10% of the overall funding (per Fiscal Year)
This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC
These funds are to cover the costs, largely travel expenses, for the ITAC meetings.

Project Management – limited to 8.5% of the funds allocated for Research Projects
Each research project will be assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual
These are the funds available to support the research projects that are selected for funding.

Program Administration

Program Administration includes salaries and fringe benefits for those overseeing the program as a whole, as well as, materials and supplies, travel, equipment, and other expenses. This category allows indirect costs in the amount of 10% of salaries and wages.

During the reporting period several staff members were involved, part time, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. James Thomas, AQRP Manager, is responsible for assisting

Dr. Allen in the program administration. Maria Stanzione, AQRP Grant Manager, with Rachael Bushn, Melanie Allbritton, and Susan McCoy each provided assistance with program organization and financial management. This included assisting with the contracting process. Denzil Smith is responsible for the AQRP Web Page development and for data management.

Fringe benefits for the administration of the AQRP were initially budgeted to be 22% of salaries and wages across the term of the project. It should be noted that this was an estimate, and actual fringe benefit expenses have been reported for each month. The fringe benefit amount and percentage fluctuate each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. For example, the amount of fringe benefits is greater for a person with family medical insurance versus a person with individual medical insurance. Actual fringe benefit expenses to date are included in the spreadsheets above.

As discussed in previous Quarterly Reports, the AQRP Administration requested and received permission to utilize funds in future fiscal years. This is for all classes of funds including Administration, ITAC, Project Management, and Contractual. As of the writing of this report, the FY 2010, FY 2011, FY 2012, and FY 2013 funds have been fully expended. This same procedure will be followed for the FY 2014 and FY 2015 funds.

In May 2014, UT-Austin received a Contract Extension for the AQRP. This extension will continue the program through April 27, 2016.

Table 1: AQRP Administration Budget

Administration Budget (includes Council Expenses)
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$202,816.67	$172,702.06	$375,518.73	$375,518.73	$0.00	$0.00
Fringe Benefits		$38,665.65	$33,902.95	$72,568.60	$72,568.60	$0.00	$0.00
Travel		$346.85	$0	$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$101.25	$15,197.39	$15,197.39	$0.00	$0.00
Equipment		$0	$0	$0			$0.00
Total Direct Costs		$256,925.31	$206,706.26	$463,631.57	$463,631.57	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$17,270.20	$37,551.89	$37,551.89	$0.00	$0.00
10% of Salaries and Wages							
Total Costs		**$277,207.00**	**$223,976.46**	**$501,183.46**	**$501,183.46**	**$0.00**	**$0.00**
Fringe Rate		22%	22%		19%		

Administration Budget (includes Council Expenses)
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$74,238.65	$256,154.46	$330,393.11	$330,393.11	$0.00	$0.00
Fringe Benefits		$17,068.38	$59,405.87	$76,474.25	$76,474.25	$0.00	$0.00
Travel		$339.13	$0.00	$339.13	$339.13		$0.00
Supplies		$3,560.62	$8,824.23	$12,384.85	$12,384.85	$0.00	$0.00
Equipment							
Total Direct Costs		$95,206.78	$324,384.56	$419,591.34	$419,591.34	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$25,615.44	$33,039.30	$33,039.30	$0.00	$0.00
10% of Salaries and Wages							
Total Costs		**$102,630.64**	**$350,000.00**	**$452,630.64**	**$452,630.64**	**$0.00**	**$0.00**
Fringe Rate		22%	22%		23%		

Administration Budget (includes Council Expenses)
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$70,000.00	$70,000.00	$140,000.00	$45,664.64	$0.00	$94,335.36
Fringe Benefits		$15,150.00	$15,150.00	$30,300.00	$10,870.30	$0.00	$19,429.70
Travel		$350.00	$350.00	$700.00	$0.00	$0.00	$700.00
Supplies		$7,500.00	$7,500.00	$15,000.00	$670.56	$0.00	$14,329.44
Equipment							
Total Direct Costs		$93,000.00	$93,000.00	$186,000.00	$57,205.50	$0.00	$128,794.50
Authorized Indirect Costs		$7,000.00	$7,000.00	$14,000.00	$4,566.47	$0.00	$9,433.53
10% of Salaries and Wages							
Total Costs		**$100,000.00**	**$100,000.00**	**$200,000.00**	**$61,771.97**	**$0.00**	**$138,228.03**
Fringe Rate		22%	22%		23.8%		

ITAC

No ITAC activities requiring travel occurred during this period and none are planned through the end of the AQRP Grant period. In June 2015, the program administration was granted permission to transfer the FY 14 and FY 15 ITAC funds to the Research Projects.

Table 2: ITAC Budget

ITAC Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$16,378.86	$6,292.97	$22,671.83	$22,671.83	$0.00	$0.00
Supplies		$1,039.95	$284.67	$1,324.62	$1,324.62	$0.00	0
Total Direct Costs		$17,418.81	$6,577.64	$23,996.45	$23,996.45	$0.00	$0.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$17,418.81**	**$6,577.64**	**$23,996.45**	**$23,996.45**	**$0.00**	**$0.00**

ITAC Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$5,323.31	$0.00	$5,323.31	$5,323.31	$0	$0.00
Supplies		$231.86	$0.00	$231.86	$231.86		$0.00
Total Direct Costs		$5,555.17	$0.00	$5,555.17	$5,555.17	$0	$0.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$5,555.17**	**$0.00**	**$5,555.17**	**$5,555.17**	**$0**	**$0.00**

ITAC Budget
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$0.00	$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$0.00	$0.00	$0.00	$0.00	$0.00	$0.00
Total Direct Costs		$0.00	$0.00	$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management

During the first three quarters of FY 2014-2015, Project Managers assisted with project questions, reporting requirements, and budget amendment requests as projects drew to a close. Project Managers also reviewed draft final reports and provided feedback. Activity transitioned to reviewing final project reports for the FY 2014-2015 research cycle as projects closed at the end of June, July, and August 2015, including a thorough review of each project against its Quality Assurance Project Plan (QAPP). As final reports are approved they will be posted on the AQRP web page.

Table 3: Project Management Budget

Project Management Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$145,337.70	$121,326.64	$266,664.34	$266,664.34	$0	$0
Fringe Benefits		$28,967.49	$23,102.60	$52,070.09	$52,070.26	$0	($0.17)
Travel		$0	$0	$0	$0		$0
Supplies		$778.30	$207.98	$986.28	$986.22	$0	$0.06
Total Direct Costs		$175,083.49	$144,637.22	$319,720.71	$319,720.82	$0	($0.11)
Authorized Indirect Costs		$14,533.77	$12,132.66	$26,666.43	$26,666.32	$0	$0.11
10% of Salaries and Wages							
Total Costs		**$189,617.26**	**$156,769.88**	**$346,387.14**	**$346,387.14**	**$0**	**$0.00**

FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$53,384.46	$123,279.85	$176,664.31	$176,664.31	$0.00	$0.00
Fringe Benefits		$10,991.04	$23,666.75	$34,657.79	$34,657.79	$0.00	$0.00
Travel		$0.00	$0	$0.00	$0.00		$0.00
Supplies		$967.98	$699.40	$1,667.38	$1,667.38		$0.00
Total Direct Costs		$65,343.48	$147,646.00	$212,989.48	$212,989.48	$0.00	$0.00
Authorized Indirect Costs		$5,338.44	$12,328.00	$17,666.44	$17,666.44	$0.00	$0.00
10% of Salaries and Wages							
Total Costs		**$70,681.92**	**$159,974.00**	**$230,655.92**	**$230,655.92**	**$0.00**	**$0.00**

Project Management Budget
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$52,000.00	$52,000.00	$104,000.00	$57,217.24	$0.00	$46,782.76
Fringe Benefits		$9,300.00	$9,300.00	$18,600.00	$11,821.76	$0.00	$6,778.24
Travel							
Supplies		$1,000.00	$1,000.00	$2,000.00	$542.39	$0.00	$1,457.61
Total Direct Costs		$62,300.00	$62,300.00	$124,600.00	$69,581.39	$0.00	$55,018.61
Authorized Indirect Costs		$5,200.00	$5,200.00	$10,400.00	$5,721.72	$0.00	$4,678.28
10% of Salaries and Wages							
Total Costs		**$67,500.00**	**$67,500.00**	**$135,000.00**	**$75,303.11**	**$0.00**	**$59,696.89**

Research Projects

FY 2010-2011

The FY 2010 Research/Contractual budget was originally funded at $2,286,000. After all transfers, it was increased by $1,827.93. The FY 2011 Research/Contractual budget was originally funded at $1,736,063. After all transfers, it was increased by $377.62, plus an additional $116,000 from FY 2012 funds that were changed to FY 2011 funds. This is an overall net increase of $13,205.55 to the Research/Contractual funds (and net reduction in Project Management/ITAC funds). ($105,000 in FY 2012 research funds were transferred to FY 2011, the remaining $11,000 were transfers from Project Management funds.)

All FY 2010 Research Project funding was fully expensed before the expiration of FY 2010 funds in June 2012. The FY 2011 Research Project funding that remained after all FY 2011 research projects were completed was allocated to FY 2012-2013 projects. This included the funds that were reallocated from FY 2012 to FY 2011. The funds were allocated to project 13-016 Valparaiso and project 13-004 Discover AQ Infrastructure. Both projects utilized their FY 2011 funds (project 13-004 $116,000 and project 13-016 $20,168.90) by June 30, 2013. A remaining balance of $0.11 was returned to TCEQ.

Table 4 on the following 2 pages illustrates the 2010-2011 Research Projects, including the funding awarded to each project and the total expenses reported on each project through the expiration of the FY 2011 funds on June 30, 2013.

FY 2012-2013

The FY 2012 Research/Contractual budget was originally funded at $815,000. Transfers to date have increased the budget by $32,438.67. These funds were fully expended as of April 2014. The FY 2013 Research Contractual budget was originally funded at $835,000. In June 2013, Amendment 9 increased this budget by $2,100,000. (The remaining $400,000 was allocated to Admin and Project Management.) Transfers to date have increased that by an additional $55,026 for a total FY 2013 Research Contractual budget of $2,990,026. This includes funds transferred from the FY 13 Project Management budget to the Research Projects budget, in order to fund as many research projects as possible, and the return of $53,974 to FY 13 Project Management to cover the additional Project Manager needed for the additional 5 projects.

Funds that were not expended by the FY 2012 – 2013 research projects totaling $1,716,863.39 (including an April 2015 refund of $18.40 to a project that ended in March 2014) were allocated to projects from the FY 2014-2015 RFP, with $53,974 of the funds allocated to Project Management, as noted above. Table 5 illustrates the 2012-2013 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of June 30, 2015. This includes Research Projects awarded in the FY 2014-2015 call for proposals, but funded with FY 2013 funds. FY 2013 funding was fully expended on June 30, 2015.

FY 2014-2015

The FY 2014 and 2015 Research/Contractual budgets were originally funded at $825,000 each. This was increased by $7500 each when the unused ITAC funds were transferred in June 2015. Research projects were awarded to FY 2013, 2014, and 2015 funds. As of June 2015, all FY 2013 funds were expended and all remaining expenditures on the Research Projects will post to FY 2014 or 2015 funds.

The TCEQ and the Advisory Council has approved a State of the Science assessment project which will review and summarize the impact of the research performed under the AQRP during the 2014 – 2015 biennium. This will be funded from the remaining Research/Contractual funds and unspent funds that are returned from research projects as they are completed.

Table 6 illustrates the portion of the Research Projects funded with FY 2014 – 2015 funds. This includes the funding awarded to each project (from this source of funding) and the total expenses reported on each project as of August 31, 2015.

Table 7 shows the distribution of funding for each FY 2014-2015 RFP project across the combination of FY 2013 funds and either FY 2014 or FY 2015 funds. In order to expend all FY 2013 funding by June 30, 2015, adjustments were made to the amount of FY 2013 funding allocated to specific projects, and project expenses that were originally charged to the FY 2014 or FY 2015 portion of the project funds were transferred to the FY 2013 portion.

Table 4: 2010/2011 Contractual Expenses

Contractual Expenses

FY 10 Contractual Funding	$2,286,000
FY 10 Contractual Funding Transfers	$1,827.93
FY 10 Total Contractual Funding	**$2,287,827.93**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-008	Rice University	$128,851	$126,622.32	$2,228.68
10-008	Environ International	$49,945	$49,944.78	$0.22
10-009	UT-Austin	$591,332	$591,306.66	$25.34
10-021	UT-Austin	$248,786	$248,786.41	-$0.41
10-022	Lamar University	$150,000	$132,790.80	$17,209.20
10-032	University of Houston	$176,314	$176,314	$0
10-032	University of New Hampshire	$23,054	$18,850.65	$4,203.35
10-032	UCLA	$49,284	$47,171.32	$2,112.68
10-034	University of Houston	$195,054	$186,657.54	$8,396.46
10-042	Environ International	$237,481	$237,479.31	$1.69
10-045	UCLA	$149,773	$142,930.28	$6,842.72
10-045	UNC - Chapel Hill	$33,281	$33,281	$0
10-045	Aerodyne Research Inc.	$164,988	$164,988.10	-$0.10
10-045	Washington State University	$50,000	$50,000	$0
10-DFW	UT-Austin	$37,857	$37,689.42	$167.58
FY 10 Total Contractual Funding Awarded		$2,286,000		
FY 10 Contractual Funding Expended (Init. Projects)			$2,244,812.59	
FY 10 Contractual Funds Remaining Unspent after Project Completion				$41,187.41
FY 10 Additional Projects				
	Data Storage	$7,015.34	$7,015.34	$0
10-SOS	State of the Science	$36,000.00	$36,000.00	$0
FY 10 Contractual Funds Expended to Date*			$2,287,827.93	
FY 10 Contractual Funds Remaining to be Spent				$0

FY 11 Contractual Funding		$1,736,063.00		
FY 11 Contractual Funding Transfers		$116,377.62		
FY 11 Total Contractual Funding		**$1,852,440.62**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179	$262,179	$0
10-006	University of Houston	$222,483	$217,949.11	$4,533.89
10-015	Environ International	$201,280	$201,278.63	$1.37
10-020	Environ International	$202,498	$202,493.48	$4.52
10-024	Rice University	$225,662	$223,769.99	$1,892.01
10-024	University of New Hampshire	$70,747	$70,719.78	$27.22
10-024	University of Michigan	$64,414	$60,597.51	$3,816.49
10-024	University of Houston	$98,134	$88,914.46	$9,219.54
10-029	Texas A&M University	$80,108	$78,276.97	$1,831.03
10-044	University of Houston	$279,642	$277,846.38	$1,795.62
11-DFW	UT-Austin	$50,952	$29,261.75	$21,690.25
FY 11 Total Contractual Funding Awarded		$1,758,099		
FY 11 Contractual Funds Expended (Init. Projects)			$1,713,287.06	
FY 11 Contractual Funds Remaining Unspent after Project Completion				$44,811.94
FY 11 Additional Projects				
	Data Storage	$2,984.66	$2,984.66	$0.00
	12-016 Valparaiso	$20,168.90	$0.00	$21,168.90
	12-004 Discover AQ Infrastructure	$116,000.00	$115,999.89	$0.11
FY 11 Contractual Funds Expended to Date*			$1,852,440.51	
FY 11 Contractual Funds Remaining to be Spent				$0.11
Total Contractual Funding		$4,022,063.00		
Total Contractual Funding Transfers		$118,205.55		
Total Contractual Funding Available		$4,140,268.55		
Total Contractual Funds Expended to Date			$4,140,268.44	
Total Contractual Funds Remaining				$0.11

Table 5. 2012/2013 Contractual Expenses

Contractual Expenses

FY 12 Contractual Funding	$815,000.00
FY 12 Contractual Funding Transfers	$32,438.67
FY 12 Total Contractual Funding	**$847,438.67**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
12-004	UT-Austin (Torres)	$20,174.10	$20,174.10	$0.00
12-006	UC-Riverside	$101,765.00	$101,765.00	$0.00
12-006	TAMU/TEES	$44,494.00	$42,134.22	$2,359.78
12-011	Environ International	$77,420.00	$77,410.16	$9.84
12-012	UT-Austin (Hildebrandt)	$79,463.00	$79,173.94	$289.06
12-012	Environ International	$69,374.00	$69,372.64	$1.36
12-013	Environ International	$59,974.00	$59,960.93	$13.07
12-018	UT-Austin (McDonald-Buller)	$85,282.00	$85,197.80	$84.20
12-018	Environ International	$21,688.00	$21,686.26	$1.74
12-028	University of Houston	$19,599.00	$16,586.51	$3,012.49
12-028	UCLA	$17,944.00	$17,709.51	$234.49
12-028	Environ International	$44,496.00	$44,496.00	$0.00
12-028	UNC - Chapel Hill	$35,230.00	$35,230.00	$0.00
12-032	Baylor	$45,972.00	$43,642.21	$2,329.79
12-TN1	Maryland	$64,994.00	$64,537.12	$456.88
12-TN2	Maryland	$69,985.00	$68,362.27	$1,622.73
FY 12 Total Contractual Funding Awarded		$847,438.67		
FY 12 Contractual Funds Expended to Date			$847,438.67	
FY 12 Contractual Funds Remaining to be Spent				$0.00

Note:
Project 12-004 on this page and Project 13-004 on the following page were the same project, with funding split across fiscal years. After all FY12 projects were completed and fully invoiced, the remaining FY12 funds were transferred to 12-004 and 13-004 was reduced by the same amount, so that the total project budget remained the same, but all FY12 funds could be expended.

FY 13 Contractual Funding	$835,000
FY 13 Contractual Funding Transfers	$2,209,000

FY 13 Total Contractual Funding		**$3,044,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
13-004	UT-Austin (Torres)	$1,555,770	$805,209.66	$750,560.24
13-005	Chalmers University of Tech	$129,047	$129,047.00	$0.00
13-005	University of Houston	$48,506	$44,928.24	$3,577.76
13-016	Valparaiso	$46,652	$46,652.10	$0.00
13-016	University of Houston	$19,846	$14,101.40	$5,744.60
13-022	Rice University	$89,912	$75,881.86	$14,030.14
13-022	University of Houston	$116,903	$116,122.47	$780.53
13-024	Maryland	$90,444	$89,658.88	$785.12
FY 13 Total Contractual Funding Awarded		$2,097,080		
FY 13 Contractual Funds Expended (Init. Projects)			$1,321,601.61	
FY 13 Contractual Funds Remaining Unspent				$1,722,398.39
FY 13 Additional Expenditures				
	DATA Storage	$5,535	$5,535	$0.00
FY 13 Contractual Funds Expended			$1,327,136.61	
FY 13 Contractual Funds Remaining Unspent				$1,716,863.39

Note:
After all FY13 projects were completed contractual funds in the amount of $1,716,844.99 remained. In April 2015, a refund of an expense totaling $18.40 was reimbursed to project 13-004, increasing the remaining funds to $1,716,863.39. The funds will be utilized for FY14 projects and will be accounted for on the following page.

FY 13 Remaining Contractual Funding		**$1,716,863.39**		
FY 13 Remaining Contractual Funding Transfers		**($53,974.00)**		
FY 13 Total Remaining Contractual Funding		**$1,662,889.39**		
Awarded to FY 2014-2015 Projects				
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-002	University of CO - Boulder	$136,818.02	$136,818.02	$0.00
14-003	UNC Chapel Hill	$80,632.41	$80,632.41	$0.00
14-006	Sonoma Technology	$41,235.05	$41,235.05	$0.00
14-006	Valparaiso	$3,578.11	$3,578.11	$0.00
14-006	St. Edwards University	$0.00	$0.00	$0.00
14-007	Chalmers Univ.	$64,584.00	$64,548.00	$0.00
14-007	Univ. of Houston	$23,081.00	$23,081.00	$0.00
14-008	UT-Austin (McDonald-Buller)	$155,378.82	$155,378.82	$0.00
14-009	Rice University	$60,000.00	$60,000.00	$0.00
14-011	UT-Austin (McDonald-Buller)	$111,426.21	$111,426.21	$0.00
14-011	Environ	$6,000.00	$6,000.00	$0.00
14-016	Environ	$240,000.00	$240,000.00	$0.00
14-017	University of Alabama - Huntsville	$25,000.00	$25,000.00	$0.00
14-017	Rice University	$18,152.98	$18,152.98	$0.00
14-023	UT-Austin (Torres)	$25,874.37	$25,874.37	$0.00
14-023	Aerodyne	$10,712.74	$10,712.74	$0.00
14-024	UT-Austin (Hildebrandt Ruiz)	$138,585.78	$138,585.78	$0.00
14-024	Environ	$25,000.00	$25,000.00	$0.00
14-024	UC Riverside	$30,875.39	$30,875.39	$0.00
14-025	Environ	$89,000.00	$89,000.00	$0.00
14-025	TAMU	$47,970.84	$47,970.84	$0.00
14-029	Baylor University	$109,650.32	$109,650.32	$0.00
14-030	TEES	$112,056.23	$112,056.23	$0.00
FY 13 Total Remaining Contractual Funding Awarded		$1,62,889.39		

FY 13 Remaining Contractual Funds Expended		$1,662,889.32	
FY 13 Remaining Contractual Funds Unspent			$0.00
Total Contractual Funding	$3,837,465		
Total Contractual Funding Awarded	$3,837,465		
Total Contractual Funding Remaining to be Awarded	$0.00		
Total Contractual Funds Expended to Date		$3,837,464.67	
Total Contractual Funds Remaining to be Spent			$0.00

Table 6. 2014/2015 Contractual Expenses

Contractual Expenses

FY 14 Contractual Funding	**$825,000**
FY 14 Contractual Funding Transfers	**$7,500**
FY 14 Total Contractual Funding	**$832,500**

Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-002	University of CO - Boulder	$13,689.98	$0.01	$13,689.97
14-002	Univ. of Maryland	$49,387.00	$44,918.62	$4,468.38
14-003	UNC Chapel Hill	$119,367.59	$13,089.21	$106,278.38
14-004	Univ. of Maryland	$55,056.00	$48,578.50	$6,477.50
14-004	Morgan State Univ.	$54,055.00	$33,627.19	$20,427.81
14-006	St. Edwards University	$11,025.00	$0.00	$11,025.00
14-009	Rice Univ.	$49,867.00	$46,259.42	$3,607.58
14-009	Univ. of Houston	$109,635.00	$66,492.40	$43,142.60
14-014	Univ. of Houston	$84,927.00	$51,384.41	$33,542.59
14-022	Univ. of Alabama – Huntsville	$71,004.00	$24,311.35	$46,692.65
14-022	George Mason Univ.	$44,996.00	$0.00	$44,996.00
14-026	Environ	$58,284.88	$25,245.59	$33,039.29
14-030	TAMU/TEES	$64,052.77	$0.00	$64,052.77
FY 14 Total Contractual Funding Awarded		$785,347.22		
FY 14 Contractual Funding Remaining to be Awarded		$47,152.78		
FY 14 Contractual Funds Expended to Date			$353,906.70	
FY 14 Contractual Funds Remaining to be Spent				$478,593.30

FY 15 Contractual Funding		**$825,000**		
FY 15 Contractual Funding Transfers		**$7,500**		
FY 15 Total Contractual Funding		**$825,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-005	TAMU	$103,890.00	$16,080.85	$87,809.15
14-006	Sonoma Technology	$9,749.95	$4,858.00	$4,891.00
14-007	Chalmers University	$9,595.00	$0.00	$9,595.00
14-007	Univ. of Houston	$0.00	$0.00	$0.00
14-008	Univ. of Texas – Austin	$19,621.18	$17,406.12	$2,215.06
14-010	TAMU	$79,325.00	$30,129.77	$49,195.23
14-011	Univ. of Texas - Austin	$39,740.79	$23,074.78	$16,666.01
14-011	Environ	$22,419.00	$7,973.16	$14,445.84
14-016	Environ	$31,911.00	$16,748.27	$15,162.73
14-017	Univ. of Alabama - Huntsville	$112,003.00	$77,469.16	$34,533.84
14-017	Rice University	$44,826.02	$30,548.09	$14,277.93
14-020	Univ. of Maryland	$70,000.00	$3,444.69	$66,555.31
14-023	Aerodyne Research	$0.00	$0.00	$0.00
14-024	Univ. of Texas - Austin	$24,696.22	$23,459.45	$1,236.77
14-024	Environ	$76,404.00	$26,199.38	$50,204.62
14-025	Environ	$46,735.00	$30,709.89	$16,025.11
14-025	TAMU	$72,555.16	$64,919.99	$7,635.17
14-029	Baylor University	$69,028.68	$0.00	$69,028.68

FY 15 Total Contractual Funding Awarded	$832,500.00		
FY 15 Contractual Funding Remaining to be Awarded	$0.00		
FY 15 Contractual Funds Expended to Date		$373,021.60	
FY 15 Contractual Funds Remaining to be Spent			$459,478.40
Total Contractual Funding	$1,665,000		
Total Contractual Funding Awarded	$1,617,847		
Total Contractual Funding Remaining to be Awarded	$47,153*		
Total Contractual Funds Expended to Date		$726,928.30	
Total Contractual Funds Remaining to be Spent			$938,072

*The State of the Science Project (with a budget of $50,000) will be added to the list of projects once any funds remaining from the projects that closed on June 30, 2015, are released.

Table 7. Breakdown of Project Funding Across Fiscal Years

Project	Final Approved Budget by Entity		FY 13	FY 14	FY 15		
14-002 - UC Boulder	150,508.00		136,818.02	13,689.98			$150,508.00
14-002 - Maryland	49,387.00			49,387.00			$49,387.00
14-003 - UNC - CH	200,000.00		80,632.41	119,367.59			$200,000.00
14-004 - Maryland	55,056.00			55,056.00			$55,056.00
14-004 - Morgan State	54,055.00			54,055.00			$54,055.00
14-005 - TAMU	103,890.00				103,890.00		$103,890.00
14-006 - Sonoma Tech	50,985.00		48,985.00		2,000.00		$50,985.00
14-006 - Valpo	3,578.11		3,578.11				$3,578.11
14-006 - St. Edwards	11,025.00		0.00	11,025.00			$11,025.00
14-007 - Chalmers	74,179.00		65,233.00		8,946.00		$74,179.00
14-007 - UH	23,081.00		23,081.00		0.00		$23,081.00
14-008 - UT Austin	175,000.00		156,500.00		18,500.00		$175,000.00
14-009 - Rice	109,867.00		60,000.00	49,867.00			$109,867.00
14-009 - UH	109,635.00			109,635.00			$109,635.00
14-010 - TAMU	79,325.00				79,325.00		$79,325.00
14-011 - UT	151,167.00		131,166.00		20,001.00		$151,167.00
14-011 - Environ	28,419.00		6,000.00		22,419.00		$28,419.00
14-014 - UH	84,927.00			84,927.00			$84,927.00
14-016 - Environ	271,911.00		240,000.00		31,911.00		$271,911.00
14-017 - UA - Huntsville	137,003.00		25,000.00		112,003.00		$137,003.00
14-017 - Rice	62,979.00		25,000.00		37,979.00		$62,979.00
14-020 - Maryland	70,000.00				70,000.00		$70,000.00
14-022 - UA - Huntsville	71,004.00			71,004.00			$71,004.00
14-022 - GMU	44,996.00			44,996.00			$44,996.00
14-023 - UT	25,874.37		25,874.37		0.00		$25,874.37
14-023 - ARI	10,712.74		10,712.74		0.00		$10,712.74
14-023 - Leak Sys	0.00						$0.00
14-023 - Provid	0.00						$0.00
14-024 - UT	163,282.00		143,282.00		20,000.00		$163,282.00
14-024 - Environ	101,404.00		25,000.00		76,404.00		$101,404.00
14-024 - UC-Riverside	30,875.39		30,875.39				$30,875.39
14-025 - Environ	135,735.00		89,000.00		46,735.00		$135,735.00
14-025 - TAMU	120,526.00		20,000.00		100,526.00		$120,526.00
14-026 - Environ	165,562.00		80,000.00	85,562.00			$165,562.00
14-026 - CalTech	0.00			0.00			$0.00
14-029 - Baylor	178,679.00		109,650.32		69,028.68		$178,679.00
14-030 - TAMU	176,109.00		112,056.23	64,052.77			$176,109.00
Amt in Projects	3,280,736.61		1,648,444.59	812,624.34	819,667.68		
Available Funding			1,662,889.39	825,000.00	825,000.00		
Funding Remaining			14,444.80	12,375.66	5,332.32		

Appendix A

Financial Reports by Fiscal Year

FY 10 and 11

(Expenditures reported as of August 31, 2015.)

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67		$0
Fringe Benefits		$38,665.65	$38,665.65		$0
Travel		$346.85	$346.85		$0
Supplies		$15,096.14	$15,096.14		$0
Equipment		$0.00			$0
Other					
Contractual					
Total Direct Costs		$256,925.31	$256,925.31		$0
Authorized Indirect Costs		$20,281.69	$20,281.69		$0
10% of Salaries and Wages					
Total Costs		**$277,207.00**	**$277,207.00**	**$0**	**$0**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00		$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment					
Other		$0.00			$0.00
Contractual					
Total Direct Costs		$206,706.26	$206,706.26	$0.00	$0.00
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$223,976.46**	**$223,976.46**	**0.00**	**$0.00**

ITAC Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$16,378.86	$16,378.86	$0	$0
Supplies		$1039.95	$1,039.95		$0
Equipment					
Other					
Total Direct Costs		$17,418.81	$17,418.81	$0	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$17,418.81**	**$17,418.81**	**$0**	**$0**

ITAC Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$6,292.97	$6,292.97	$0.00	$0
Supplies		$284.67	$284.67	$0.00	$0
Equipment					
Other					
Total Direct Costs		$6,577.64	$6,577.64	$0.00	$0
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$6,577.64**	**$6,577.64**	**$0.00**	**$0**

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$145,337.70	$145,337.70		$0
Fringe Benefits		$28,967.49	$28,967.49		$0
Travel		$0	$0		$0
Supplies		$778.30	$778.30		$0
Equipment					
Other					
Total Direct Costs		$175,083.49	$175,083.49	$0	$0
Authorized Indirect Costs		$14,533.77	$14,533.77		$0
10% of Salaries and Wages					
Total Costs		**$189,617.26**	**$189,617.26**	**$0**	**$0**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$121,326.64	$121,326.64	$0	$0
Fringe Benefits		$23,102.60	$23,102.77	$0	($0.17)
Travel		$0			$0
Supplies		$207.98	$207.92	$0	$0.06
Equipment					
Other					
Total Direct Costs		$144,637.22	$144,637.33	$0	($0.11)
Authorized Indirect Costs		$12,132.66	$12,132.55	$0	$0.11
10% of Salaries and Wages					
Total Costs		**$156,769.88**	**$156,769.88**	**$0**	**$0.00**

AQRP Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$202,816.67	$202,816.67	$0.00	$0.00
Fringe Benefits		$38,665.65	$38,665.65	$0.00	$0.00
Travel		$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$15,096.14	$0.00	$0.00
Equipment		$0	$0.00	$0.00	$0.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,287,827.93	$2,287,827.93	$0.00	$0.00
ITAC		$17,418.81	$17,418.81	$0.00	$0.00
Project Management		$189,617.26	$189,617.26	$0.00	$0.00
Total Direct Costs		$2,751,789.31	$2,751,789.31	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$20,281.69	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,772,071.00**	**$2,772,071.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$172,702.06	$172,702.06	$0.00	$0.00
Fringe Benefits		$33,902.95	$33,902.95	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$101.25	$101.25	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$1,852,440.62	$1,852,440.51	$0.00	$0.11
ITAC		$6,577.64	$6,577.64	$0.00	($0.00)
Project Management		$156,769.88	$156,769.88	$0.00	$0.00
Total Direct Costs		$2,222,494.40	$2,222,494.29	$0.00	$0.11
Authorized Indirect Costs		$17,270.20	$17,270.20	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$2,239,764.60**	**$2,239,764.49**	**$0.00**	**$0.11**

Appendix B

Financial Reports by Fiscal Year

FY 12 and 13

(Expenditures reported as of August 31, 2015.)

Administration Budget (includes Council Expenses)

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$74,238.65	$74,238.65	$0.00	$0.00
Fringe Benefits		$17,068.38	$17,068.38	$0.00	$0.00
Travel		$339.13	$339.13		$0.00
Supplies		$3,560.62	$3,560.62	$0.00	$0.00
Equipment		$0.00			$0.00
Other					
Total Direct Costs		$95,206.78	$95,206.78	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$7,423.86	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$102,630.64**	**$102,630.64**	**$0.00**	**$0.00**

Administration Budget (includes Council Expenses)

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$256,154.46	$256,154.46		$0.00
Fringe Benefits		$59,405.87	$59,405.87		$0.00
Travel		$0.00	$0.00		$0.00
Supplies		$8,824.23	$8,824.23		$0.00
Equipment					
Other		$0.00			
Total Direct Costs		$324,384.56	$324,384.56	$0.00	$0.00
Authorized Indirect Costs		$25,615.44	$25,615.44		$0.00
10% of Salaries and Wages					
Total Costs		**$350,000.00**	**$350,000.00**	**$0.00**	**$0.00**

ITAC Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$5,323.31	$5,323.31		$0.00
Supplies		$231.86	$231.86		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$5,555.17	$5,555.17	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$5,555.17**	**$5,555.17**	**$0.00**	**$0.00**

ITAC Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00		$0.00
Supplies		$0.00	$0.00		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$53,384.46	$53,384.46	$0.00	$0.00
Fringe Benefits		$10,991.04	$10,991.04	$0.00	$0.00
Travel		$0.00	$0.00		$0.00
Supplies		$967.98	$967.98		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$65,343.48	$65,343.48	$0.00	$0.00
Authorized Indirect Costs		$5,338.44	$5,338.44	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$70,681.92**	**$70,681.92**	**$0.00**	**$0.00**

Project Management Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$123,279.85	$123,279.85		$0.00
Fringe Benefits		$23,666.75	$23,666.75		$0.00
Travel					
Supplies		$699.40	$699.40		$0.00
Equipment					
Other					
Contractual					
Total Direct Costs		$147,646.00	$147,646.00	$0	$0.00
Authorized Indirect Costs		$12,328.00	$12,328.00		$0.00
10% of Salaries and Wages					
Total Costs		**$159,974.00**	**$159,974.00**	**$0.00**	**$0.00**

AQRP Budget

FY 2012

Budget Category		FY12 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$74,238.65	$74,238.65	$0.00	$0.00
Fringe Benefits		$17,068.38	$17,068.38	$0.00	$0.00
Travel		$339.13	$339.13	$0.00	$0.00
Supplies		$3,560.62	$3,560.62	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$847,438.67	$847,438.67	$0.00	$0.00
ITAC		$5,555.17	$5,555.17	$0.00	$0.00
Project Management		$70,681.92	$70,681.92	$0.00	$0.00
Total Direct Costs		$1,018,882.54	$1,018,882.54	$0.00	$0.00
Authorized Indirect Costs		$7,423.86	$7,423.86	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$1,026,306.40**	**$1,026,306.40**	**$0.00**	**$0.00**

AQRP Budget

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$256,154.46	$256,154.46	$0.00	$0.00
Fringe Benefits		$59,405.87	$59,405.87	$0.00	$0.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$8,824.23	$8,824.23	$0.00	$0.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$2,990,026.00	$2,990,026.00	$0.00	$0.00
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$159,974.00	$159,974.00	$0.00	$0.00
Total Direct Costs		$3,474,384.56	$3,474,384.56	$0.00	$0.00
Authorized Indirect Costs		$25,615.44	$25,615.44	$0.00	$0.00
10% of Salaries and Wages					
Total Costs		**$3,500,000.00**	**$3,500,000.00**	**$0.00**	**$0.00**

Appendix C

Financial Reports by Fiscal Year

FY 14 and 15

(Expenditures reported as of August 31, 2015.)

Administration Budget (includes Council Expenses)

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$45,664.64	$0.00	$24,335.36
Fringe Benefits		$15,150.00	$10,870.30	$0.00	$4,279.70
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$541.56	$0.00	$6,958.44
Equipment					
Other					
Total Direct Costs		$93,000.00	$57,076.50	$0.00	$35,923.50
Authorized Indirect Costs		$7,000.00	$4,566.47	$0.00	$2,433.53
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$61,642.97**	**$0.00**	**$38,357.03**

Administration Budget (includes Council Expenses)

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$129.00	$0.00	$7,371.00
Equipment					
Other					
Total Direct Costs		$93,000.00	$129.00	$0.00	$92,871.00
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$129.00**	**$0.00**	**$99,871.00**

ITAC Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$0.00	$0.00	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

ITAC Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary					
Fringe Benefits					
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$0.00	$0.00	$0.00	$0.00
Equipment					
Other					
Total Direct Costs		$0.00	$0.00	$0.00	$0.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$0.00**	**$0.00**	**$0.00**	**$0.00**

Project Management Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$52,000.00	$45,956.02	$0.00	$6,043.98
Fringe Benefits		$9,300.00	$9,601.94	$0.00	($301.94)
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$1,000.00	$20.00	$0.00	$980.00
Equipment					
Other					
Total Direct Costs		$62,300.00	$55,577.96	$0.00	$6,722.04
Authorized Indirect Costs		$5,200.00	$4,595.60	$0.00	$604.40
10% of Salaries and Wages					
Total Costs		**$67,500.00**	**$60173.56**	**$0.00**	**$7,326.44**

Project Management Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$52,000.00	$11,261.22	$0.00	$40,738.78
Fringe Benefits		$9,300.00	$2,219.82	$0.00	$7,080.18
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$1,000.00	$522.39	$0.00	$477.61
Equipment					
Other					
Total Direct Costs		$62,300.00	$14,003.43	$0.00	$48,296.57
Authorized Indirect Costs		$5,200.00	$1,126.12	$0.00	$4,073.88
10% of Salaries and Wages					
Total Costs		**$67,500.00**	**$15,129.55**	**$0.00**	**$52,370.45**

AQRP Budget

FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$45,664.64	$0.00	$24,335.36
Fringe Benefits		$15,150.00	$10,870.30	$0.00	$4,279.70
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$541.56	$0.00	$6,958.44
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$832,500.00	$353,906.70	$0.00	$478,593.30
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$67,500.00	$60,173.56	$0.00	$7,326.44
Total Direct Costs		$993,000.00	$471,156.76	$0.00	$521,843.24
Authorized Indirect Costs		$7,000.00	$4,566.47	$0.00	$2,433.53
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$475,723.23**	**$0.00**	**$524,276.77**

AQRP Budget

FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$129.00	$0.00	$7,371.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$832,500.00	$373,021.60	$0.00	$459,478.40
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$67,500.00	$15,129.55	$0.00	$52,370.45
Total Direct Costs		$993,000.00	$388,280.15	$0.00	$604,719.85
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$388,280.15**	**$0.00**	**$611,719.85**

Appendix D

AQRP Publications and Presentations

FY 10-11

10-006

Johansson, J., Johan Mellqvist, Jerker Samuelsson, Brian Offerle, Jana Moldanova , Bernhard Rappenglück, Barry Lefer, and James Flynn (2014) , Formaldehyde Quantitative Measurements and Modeling of Industrial Formaldehyde Emissions in the Greater Houston Area during Campaigns in 2009 and 2011, Journal of Geophysical Research: Atmospheres, 119, DOI: 10.1002/2013JD020159

Johansson, J. K. E., J. Mellqvist, J. Samuelsson, B. Offerle, B. Lefer, B. Rappenglück, J. Flynn, and G. Yarwood(2014), Emission measurements of alkenes, alkanes, SO2, and NO2 from stationary sources in Southeast Texas over a 5 year period using SOF and mobile DOAS, J. Geophys. Res. Atmos., 119, doi:10.1002/2013JD020485.

10-008

Digar, A., D.S. Cohan, X. Xiao, K.M. Foley, B. Koo, and G. Yarwood (2013). Constraining ozone-precursor responsiveness using ambient measurements. *Journal of Geophysical Research*, 118(2), 1005-1019, doi:10.1029/2012JD018100.

Daniel S. Cohan and Antara Digar, "Observation-constrained probabilistic evaluation of modeled concentrations and sensitivities." CMAS Annual Conference, Chapel Hill, NC, October 2012.

10-009

The following papers were published in the journal Industrial & Engineering Chemistry Research in a Special Issue on Industrial Flaring:

Torres, V.M., Herndon, S., Wood, E., Al-Fadhli, F.M., Allen, D.T., Emissions of Nitrogen Oxides from Flares Operating at Low Flow Conditions, *Industrial & Engineering Chemistry Research,* 51, 12600-12605, DOI: 10.1021/ie300179x (2012)

Pavlovic, R.T., Al-Fadhli, Kimura, Y., Allen, D.T., and McDonald-Buller, E.C. Impacts of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area, *Industrial & Engineering Chemistry Research,* 51, 12593-12599, DOI: 10.1021/ie203052w (2012).

Knighton, W.B., Herndon, S.C., Franklin, J.F., Wood, E.C., Wormhoudt, J., Brooks, W., Fortner, E.C., and Allen, D.T. Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy, *Industrial & Engineering Chemistry Research,* 51, 12674-12684, DOI: 10.1021/ie202695v (2012)

Torres, V.M., Herndon, S., Kodesh, Z., Nettles, R., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research,* 51, 12559-12568, DOI: 10.1021/ie202674t (2012).

Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research,* 51, 12569-12576, DOI: 10.1021/ie202675f (2012)

Herndon, S.C., Nelson, D.D., Wood, E.C., Knighton, W.B., Kolb, C.E., Kodesh, Z., Torres, V.M., and Allen, D.T., Application of the carbon balance method to flare emissions characteristics, *Industrial & Engineering Chemistry Research,* 51, 12577-12585, DOI: 10.1021/ie202676b (2012)

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research,* 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

The following presentations were given at the Air& Waste Management Association June 2012 Conference, and papers were published in the Conference Proceedings:

Torres, V.M., Allen, D.T., Herndon, S. and Kodesh, Z., Overview of the Texas Commission on Environmental Quality 2010 Flare Study, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-437-AWMA, San Antonio, June, 2012.

Torres, V.M., Al-Fadhli, F.M., Allen, D.T., Herndon, S., and Wood, E., NOx Emissions from Industrial Flaring, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-315-AWMA, San Antonio, June, 2012.

10-015
The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models
J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride
J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

10-020
Brown, S. S., et al. (2012), Effects of NO_xcontrol and plume mixing on nighttime chemical processing of plumes from coal-fired power plants, J. Geophys. Res., 117, D07304, doi:10.1029/2011JD016954.

Brown, S. S., Dubé, W. P., Bahreini, R., Middlebrook, A. M., Brock, C. A., Warneke, C., de Gouw, J. A., Washenfelder, R. A., Atlas, E., Peischl, J., Ryerson, T. B., Holloway, J. S., Schwarz, J. P., Spackman, R., Trainer, M., Parrish, D. D., Fehshenfeld, F. C., and Ravishankara, A. R.: Biogenic VOC oxidation and organic aerosol formation in an urban nocturnal boundary layer: aircraft vertical profiles in Houston, TX, Atmos. Chem. Phys., 13, 11317-11337, doi:10.5194/acp-13-11317-2013, 2013.

In preparation for Atmosphere:
Reactive Plume Modeling to Investigate NOx Reactions and Transport at Night
Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:
Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique
Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021
The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the submitted abstract was *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022
Kanwar Devesh Singh, Tanaji Dabade, Hitesh Vaid, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, Kuyen Li, and Christopher B. Martin "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Model," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12611-12620

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, " Parametric Study of Ethylene Flare Operations and Validation of a Reduced Combustion Mechanism," Engineering Applications of Computational Fluid Mechanics, Vol. 8, No. 2, pp. 211–228 (2014).

Hitesh S. Vaid, Kanwar Devesh Singh, Helen H. Lou, Daniel Chen, Peyton Richmond, "A Run Time Combustion Zoning Technique towards the EDC Approach in Large-Scale CFD Simulations," International Journal of Numerical Methods for Heat and Fluid Flow, Vol. 24 No. 1, 2014, pp. 21-35.

K. Singh, T. Dabade, H. Vaid, P. Gangadharan, D. Chen, H. Lou, X. Li, K. Li, C. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Ind. & Eng. Chem. Research, 51 (39), 12611-12620, October, 2012.

H. Lou, D. Chen, C. Martin, X. Li, K. Li, H. Vaid, K. Singh, P. Gangadharan, "Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, " Industrial &

Engineering Chemistry Research, Industrial flares special issue, 51 (39), 12697-12705, October, 2012.

H. Lou, C. Martin, D. Chen, X. Li, K. Li, H. Vaid, A. Tula, K. Singh,"Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, Volume 14, Issue 4, pp 737-748, August 2012, DOI 10.1007/s10098-011-0441-6.

Helen H. Lou, Christopher B. Martin, Daniel Chen, Xianchang Li, Kyuen Li, Hitesh Vaid, Anjan Tula Kumar, Kanwar Devesh Singh, & Doyle P. Bean, "A reduced reaction mechanism for the simulation in ethylene flare combustion," Clean Technologies and Environmental Policy, Volume 14, Issue 2, pp 229-239, April 2012, doi:10.1007/s10098-011-0394-9.

10-024
Kim, S.; Guenther, A.; Lefer, B.; Flynn, J.;Griffin, R.; Rutter, A.P.; Gong, L.W.; Cevik, B.K.; "Potential Role of Stabilized Criegee Radicals in Sulfuric Acid Production in a High Biogenic VOC Environment," ENVIRONMENTAL SCIENCE & TECHNOLOGY, Volume 49, Issue: 6, Pages: 3383-3391, doi: 10.1021/es505793

The Project Investigators have submitted articles to the following journals:
Atmospheric Environment (one in revision and one in review)
ES&T (one in review)

10-032
Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhan, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappengluck, K. W. Wong. C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke and P. Kelley (2013), Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *Journal of Geophysical Research-Atmospheres,118*,5770-5780,doi:10.1002/jgrd.50342.

10-042
Heo, G., McDonald-Buller, E.C., Carter, W.P.L., Yarwood, G., Whitten, G.Z. and Allen, D.T. "Modeling Ozone Formation from Alkene Reactions using the Carbon Bond Chemical Mechanism, *Atmospheric Environment*, 59, 141-150, DOI: 10.1016/j.atmosenv.2012.05.042 (2012).

Heo, G. Y. Kimura, E. McDonald-Buller, D. T. Allen, G. Yarwood, G. Z. Whitten Evaluation of a New Toluene Mechanism For Carbon Bond 05 Using Environmental Chamber Data and Ambient Data, Air and Waste Management Association Annual Meeting, Paper #154, Detroit, June 2009

In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate NOx removal and recycling represented in atmospheric mechanisms for air quality modeling* Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen
In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial NOx* Gookyoung Heo, William Carter, Greg Yarwood

10-045
Olga Pikelnaya, James H. Flynn, Catalina Tsai, and Jochen Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, Journal of Geophysical Reserch, Volume 118, Issue 15, pages 8716–8728, 16 August 2013, DOI: 10.1002/jgrd.50643

The following papers were published in Industrial & Engineering Chemistry Research Special Issue on Industrial Flaring. The paper edition of this special edition came out in Fall 2012.

W. Berk Knighton, Scott C. Herndon, Ezra C. Wood, Edward C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Detecting Fugitive Emissions of 1,3-Butadiene and Styrene from a Petrochemical Facility: An Application of a Mobile Laboratory and a Modified Proton Transfer Reaction Mass Spectrometer," *Industrial & Engineering Chemistry Research* **2012** *51* (39), 12706-12711

Ezra C. Wood, Scott C. Herndon, Ed C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, W. Berk Knighton, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Combustion and Destruction/Removal Efficiencies of In-Use Chemical Flares in the Greater Houston Area," *Industrial & Engineering Chemistry Research* **2012** *51* (39), 12685-12696

Pikelnaya, O., J. H. Flynn, C. Tsai, and J. Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, J. Geophys. Res. Atmos., 118,8716–8728, doi:10.1002/jgrd.50643.

This project has also resulted in the following publications:
Olga Pikelnaya, Jochen Stutz, Scott Herndon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuete, Evan Couzo, "*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview",* in preparation for Journal of Geophysical Research

Olga Pikelnaya, Scott Herndon, Ezra Wood, and Jochen Stutz, "*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign,"* under development.

Presentation
Stutz, Jochen; 2011, Aerosols in Urban and Rural Environments: Sources, Transformations, Properties, and Atmospheric Effects, presented at 2011 Fall Meeting, AGU, San Francisco, CA 5-9 Dec.

FY 12-13

12-006

Journal Papers:

Gookyoung Heo, Peng Wang, Qi Ying, Ron Thomas, William P.L. Carter. Using chemically detailed emissions data to test assumptions used in developing chemical mechanisms: a case study for southeast Texas, USA. [To be submitted to Atmospheric Environment in Summer 2015]

Peng Wang, Gookyoung Heo, William P.L. Carter, Qi Ying. Comparison of a detailed and a lumped version of SAPRC-11 photochemical mechanism during a summer ozone episode. [To be submitted to Atmospheric Environment in Summer 2015]

Gookyoung Heo, Chia-Li Chen, Ping Tang, William P.L. Carter. Evaluation of mechanisms for major terminal and internal alkenes with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2015]

Gookyoung Heo, Shunsuke Nakao, William P.L. Carter. Evaluation of mechanisms for 1,3-butadiene with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2015]

Conference Paper:

Heo, G., Carter, W.P.L., Wang, P., Ying, Q., Thomas, R. (2013). Evaluating and improving atmospheric chemical mechanisms used for modeling ozone formation from alkenes. Presented at the 12th Annual CMAS Conference, Chapel Hill, NC, October 28-30, 2013.

12-012

Conference presentations:

C. Faxon, J. Bean, L. Hildebrandt Ruiz. Evidence of atmospheric chlorine chemistry in Conroe, TX: Regional implications. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

J. Bean, C. Faxon, L. Hildebrandt Ruiz. Atmospheric processing of pollutants in the Houston Region: First insights from DISCOVER-AQ. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

L. Hildebrandt Ruiz, J. Bean, G. Yarwood, B. Koo, U. Nopmongcol. Formation and Gas-Particle Partitioning of Organic Nitrates: Influence on Ozone Production. American Association for Aerosol Research Annual Meeting, October 2013, Portland, OR.

J. Bean and L. Hildebrandt Ruiz. Hydrolysis and gas-particle partitioning of organic nitrates formed in environmental chamber experiments. American Association for Aerosol Research Annual Meeting, October 2014, Orlando, FL.

Submitted publications:
J.K. Bean and L. Hildebrandt Ruiz. Hydrolysis and Gas-particle Partitioning of Organic Nitrates Formed from the Oxidation of α-Pinene in Environmental Chamber Experiments. *Atmospheric Chemistry and Physics Discussions*, in press, 2015.

Planned Presentations:
J. Bean and L. Hildebrandt Ruiz. Sources and composition of aerosol measured near Houston, TX: anthropogenic-biogenic interactions. American Association for Aerosol Research Annual Meeting, October 2015, Minneapolis, MN.

D. Wang, Surya V. Dhulipala and L. Hildebrandt Ruiz. Secondary Organic Aerosol from Chlorine-Radical Initiated Oxidation of Volatile Organic Compounds: Organic Aerosol Mass Yields, Composition, and Gas-Phase Products. American Association for Aerosol Research Annual Meeting, October 2015, Minneapolis, MN.

B. Koo, L. Hildebrandt Ruiz, R. Sheesley and G. Yarwood. Evaluation of Modeled Organic Aerosol Formation in the Houston Region Using Measurements from the 2013 DISCOVER-AQ Campaign. American Association for Aerosol Research Annual Meeting, October 2015, Minneapolis, MN.

13-016
Morris, G.A., An Overview of the Tropospheric Ozone Pollution Project (TOPP): Ozone and SO2 sondes from 2004 – 2014, Texas Air Quality Symposium, University of Texas – Pickle Center, 10 April 2015.

Morris, G.A., B.L. Lefer, A.M. Thompson, A.J. Weinheimer, H.B. Selkirk, D.K. Martins, and A. Kotsakis, Urban-scale boundary layer and lower free tropospheric ozone variability in Houston during DISCOVER-AQ (September 2013), 2014 Fall Meeting, AGU, San Francisco, CA, 15 – 19 December 2014.

Kotsakis, A., B.L. Lefer, G.A. Morris, A.M. Thompson, D.K. Martins, A.J. Weinheimer, and R.E. Orville, Sources of Ozone in the Free Troposphere in Houston During DISCOVER-AQ 2013, 2014 Fall Meeting, AGU, San Francisco, CA, 15 – 19 December 2014.

13-024
NASA AQAST meeting at Rice University in Houston, TX (Jan. 14-16, 2014), where Xinrong Ren gave a talk titled: "Measurements of trace gases at the Manvel Croix and Galveston sites during DISCOVER-AQ."

NASA DISCOVER-AQ science meeting at NASA Langley in Hampton, VA, where Winston Luke gave a talk titled: "NOAA/Air Resources Laboratory Surface Observations at Galveston and Manvel-Croix: Summary and Comparison with Aircraft Data."

A paper is in preparation with the intent to submit to Atmospheric Chemistry and Physics within about 3 months.

12-028
Implementation and Refinement of a Surface Model for HONO formation in a 3-D Chemical Transport Model. Prakash Karamchandani[1], Chris Emery[1], Greg Yarwood[1], Barry Lefer[2], Jochen Stutz[3], Evan Couzo[4], and William Vizuete[5]. ([1]ENVIRON, [2]University of Houston, [3]University of California-Los Angeles, [4]University of North Carolina-Asheville, and [5]University of North Carolina-Chapel Hill.)

Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas. Evan Couzo[1], Barry Lefer[2], Jochen Stutz[3], Greg Yarwood[4], Prakash Karamchandani[4], Barron Henderson[5], and William Vizuete[1]. ([1]University of North Carolina-Asheville, [2]University of Houston, [3]University of California-Los Angeles, [4]ENVIRON, [5]University of Florida.)

12-032
Poster at the American Geophysical Union national meeting (Dec 2013) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Poster at the DISCOVER-AQ Science Working Group meeting (Feb 2014) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Clark, A. E.; Yoon, S.; **Sheesley, R. J.; Usenko, S.,** Pressurized liquid extraction technique for the analysis of pesticides, PCBs, PBDEs, OPEs, PAHs, alkanes, hopanes, and steranes in atmospheric particulate matter. *Chemosphere* 2015, *137*, 33-44.
Manuscript in preparation. Submission planned to Atmospheric Environment in summer 2014. Draft title: "*Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX*."

12-TN1
Presentation:
"A regional chemical reanalysis prototype" Pius Lee , Greg Carmichael, Tianfeng Chai, Rick Saylor, Li Pan, Hyuncheol Kim, Daniel Tong, and Ariel Stein

Poster:
"Preliminary analyses of flight measurements and CMAQ simulation during Southeast Nexus (SENEX) field experiment" Li Pan, Pius Lee , Hyun Cheol Kim, Daniel Tong ,Rick Saylor and Tianfeng Chai

Publication:
Pius Lee, Fantine Ngan, Hang Lei, Barry Baker, Bright Dornblaser, Gary McGauhey,and Daniel Tong. An Application for Improving Air Quality: a Houston Case Study, Earthzine 2014 [available at: http://www.earthzine.org/2014/03/29/an-application-for-improving-air-quality-a-houston-case-study/?shareadraft=baba698217_53330c8eab882]

12-TN2
The project team presented at the Community Modeling and Analysis System (CMAS) Conference in October 2013.

Presentations:
"HCHO and NO2 column comparisons between OMI, GOME-2 and CMAQ during 2013 SENEX campaign (21 slides)" Hyun Cheol Kim, Li Pan, Pius Lee, Rick Saylor, and Daniel Tong
Posters:
Fine-scale comparison of GOME-2, OMI and CMAQ NO2 columns over Southern California in 2008" Hyun Cheol Kim, Sang-Mi Lee, Fong Ngan, and Pius Lee

FY 14- 15

14-003
Chen, Y.Z., et al., Assessment of SAPRC07 with updated isoprene chemistry against outdoor chamber experiments. Atmospheric Environment, 2015. **105**: p. 109-120.

Riedel, T.P., et al., Heterogeneous Reactions of Isoprene-Derived Epoxides: Reaction Probabilities and Molar Secondary Organic Aerosol Yield Estimates. Environmental Science & Technology Letters, 2015. **2**(2): p. 38-42.

Riedel, T. P., Z. Zhang, K. chu, J. Thornton, W. Vizuete, A. Gold and j. d. Surratt, Constraining Condensed-Phase Formation Kinetics of Secondary Organic Aerosol Components from Isoprene Epoxydiols. Atmospheric Chemistry and Physics, **in preparation** 2015.

Additional publications and presentations will be added to this list and to the AQRP website as PIs notify the AQRP.

Appendix E

State of the Science Assessments

State of the Science of Air Quality in Texas:

Scientific Findings from the Air Quality Research Program (AQRP) and Recommendations for Future Research

Prepared by:

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With input from:
Mark Estes and members of the Air Quality Division
Texas Commission on Environmental Quality

Air Quality Research Program Independent Technical Advisory Committee

April 30, 2012

Executive Summary

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,
(ii) to integrate AQRP research with the work of other organizations, and
(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

Beginning with the 2010-2011 biennium, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. During the 2010-2011 biennium, the AQRP funded 16 projects, which have now been completed. The purpose of this State of the Science document is to describe the current state of scientific understanding on key issues addressed by the AQRP, to summarize key findings from 2010-2011 AQRP projects and to identify high priority topics for AQRP funded research in the 2012-2013 biennium.

Current scientific understanding of emissions, chemistry, meteorology and modeling of the transport of air pollutants is described through sets of key findings; citations to the scientific literature provide additional details. Because many of the measurements on which findings are based emerge from air quality field programs, a separate section provides a summary of recent field studies conducted in Texas, including studies sponsored by AQRP and studies sponsored by other organizations.

AQRP projects funded in the 2010-2011 biennium made significant contributions to improved scientific understanding of air quality in Texas. Highlights include continuing improvement in characterizing emission sources from industrial operations, deployment of advanced measurement instruments in natural gas production regions near Fort Worth (Barnett Shale), studies of industrial flares, both in production operations and in controlled burn situations, and a variety of improvements to air quality modeling tools.

In 2012-2013, priorities for the AQRP research program will include continuing data analyses for measurements conducted during the 2010-2011 biennium:

- Analysis of data collected in the Dallas-Fort Worth (Barnett Shale) field campaign
- Analysis of flare operating regimes that provide both high combustion efficiency and minimal smoke formation

In addition, several new initiatives will have a high priority:

- Deployment of supplementary measurements in a large field measurement campaign planned by NASA for the summer of 2013
- Analysis of prior Texas field study data and modeling tools to investigate transformation of gas-phase pollutants to aerosol phase
- Investigation of how the temporal resolution of meso-scale meteorology and photochemical grid models must be altered for high spatial resolution modeling; investigation of mesoscale modeling of cloud formation and the effects of clouds upon ozone and PM chemistry;
- Analysis of radical chemistry in Texas cities, especially HONO formation, ozone removal and production by halogen chemistry, and atmospheric chemistry within industrial plumes.
- Analysis of the impact of global and regional transport of air pollutants on Texas

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1. Overview of Air Quality Research in Texas

1.1 Issues

Exposure to air pollutants remains a significant public health issue around the world. In Texas, the state's two largest urban areas exceed the National Ambient Air Quality Standard (NAAQS) for ozone and concentrations of air toxics remain a health concern in many communities. Reducing emissions and improving air quality, while supporting economic growth and an increasing population, is challenging, yet over the past decade, substantial improvements in air quality have been made in Texas. Over the decade from 2000 to 2010, average design values of ozone concentrations* at regulatory monitors decreased by 27% in Texas, roughly double the national average rate (Hildebrandt, 2011). The Houston metropolitan area went from, in 1999, having the highest number of days exceeding the NAAQS for ozone of any US city and one of the highest ozone design values*, to meeting the then current NAAQS in 2009 and 2010.

*An ozone design value is the fourth highest daily maximum, 8-hr averaged concentration over the course of a year, averaged over three years. The design value is used to compare measurements at regulatory monitors to the NAAQS.

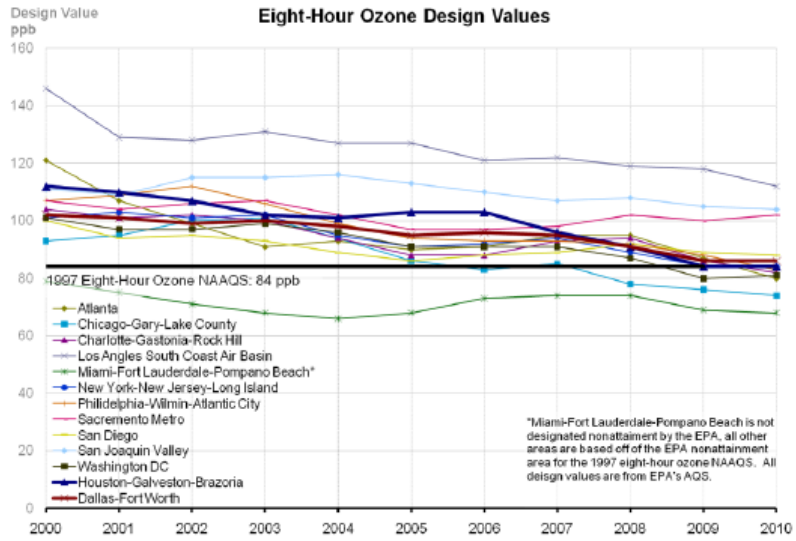


Figure 1.1.1 Comparison of ozone reductions in the Houston and Dallas-Fort Worth areas to other US cities, 2000-2010.

Source: TCEQ (http://www.tceq.texas.gov/airquality/airsuccess/others)

Identifying the most effective and efficient approaches to improving air quality in Texas requires a sound understanding of the emissions and atmospheric processes that lead to air pollution. One reason for the success that the State has had in reducing ozone concentrations is its investments in air quality research, which have helped to identify focused strategies for emission reductions, designed to be most effective for conditions in the State.

While progress in air quality over the past decade has been impressive, challenges remain as air quality standards become more stringent. More than 10 million Texans live in cities that do not meet new air quality standards for ozone. Continuing to make improvements in air quality will require new strategies which, in turn will require continuing improvements in scientific understanding. For example, it is becoming increasingly recognized that regional, continental and even global factors now have a significant influence on air quality in some parts of Texas

(McDonald-Buller, et al, 2011). Identifying the most effective and efficient balance between local, regional and national air quality improvement actions will require a new body of scientific information. In addition, driven by advances in drilling technology, oil and gas production activities in Texas have seen a substantial resurgence over the past 5 years. These activities have the potential to impact air quality in complex ways. Direct emissions associated with the production activities include ozone precursors and some air toxics. Indirectly, the availability of relatively inexpensive natural gas and natural gas liquids could change emissions associated with electricity generation and chemical manufacturing. Again, identifying the most effective and efficient approaches to reducing emissions, while promoting energy development, will require new scientific information.

These are just a few of the examples of the types of challenges Texas will face as the State strives to continue to improve air quality. This document summarizes the current state of scientific understanding of air quality in Texas. It draws on and builds on previous State of the Science assessments (Allen, et al., 2004). Findings from recent work, particularly work funded by the Texas Air Quality Research Program (AQRP) are summarized and priority topics for additional research are identified.

KEY CITATIONS:

Allen, D.T., Olaguer, E., Nielsen-Gammon, J., Estes, M., Carmichael, G., Carter, W., Sattler, M., Scire, J. State of the Science of Air Quality in Eastern Texas: Major Scientific Findings and Recommendations, July, 2004.

McDonald-Buller, E.C., Allen, D.T., Brown, N., Jacob, D.J., Jaffe, D., Kolb, C. Lefohn, A., Oltmans, S., Parrish, D., and Yarwood, G., "Establishing Policy Relevant Background (PRB) Ozone Concentrations in the United States", *Environmental Science & Technology,* 45, 9484-9497 DOI: 10.1021/es2022818 (2011).

Update of Air Quality in Texas Susana M. Hildebrand, P.E. Chief Engineer http://www.tceq.texas.gov/agency/air_main.html, May 20, 2010.

1.2 Field Measurement Campaigns

Air pollutant formation and accumulation depends on emissions, meteorology, atmospheric chemistry and other inter-dependent phenomena. Because of the complexity and interdependence of atmospheric processes, experimental studies often involve simultaneous measurements of many chemical and physical features of the atmosphere. These coordinated measurement efforts are referred to as field measurement campaigns.

1.2.1. Field Measurement Campaigns

- Texas Air Quality Study (TexAQS 2000)
- Texas Air Quality Study II (TexAQS 2005-2006)
- Study of Houston Atmospheric Radical Precursors (SHARP, 2009)
- Formaldehyde and Olefin from Large Industrial Sources (FLAIR) measurements (Houston and Texas City, 2009)
- 2010 Flare Study (Controlled, full scale flare tests)
- 2010-date Dallas-Fort Worth Barnett Shale field measurements
- DISCOVER AQ 2013
- Near-road Monitoring 2013

Since 2000, multiple field measurement campaigns have been conducted in Texas (Box 1.2.1), and these measurement campaigns have generally been a focal point for both measurements and modeling done to improve the scientific understanding of air quality in Texas. The campaigns have ranged greatly in size and scope, with the smallest programs involving approximately a dozen investigators, and the largest involving several hundred. One of the largest campaigns was conducted in southeastern Texas in the summer of 2000 and focused on air pollutant formation, accumulation and transport. Known as the Texas Air Quality Study, or TexAQS, this field campaign involved approximately 300 researchers drawn from around the world. TexAQS led to the identification of the role of Highly Reactive Volatile Organic Compounds (HRVOCs, ethene, propene, butenes, 1,3-butadiene) in ozone formation in southeast Texas. Based on the results of TexAQS, the TCEQ substantially revised the air quality management plan (State Implementation Plan, or SIP) for the Houston-Galveston-Brazoria region. A follow-up field campaign was conducted in 2005 and 2006 (TexAQS II) and involved many of the same investigators. This field campaign documented substantial reductions in HRVOC concentrations, relative to the measurements made in 2000. In addition, TexAQS II identified new mechanisms for activation of chlorine in sea salt particles and made measurements to quantify inter-city transport of ozone.

Since 2006, more focused field studies, involving smaller numbers of investigators, have been conducted. Many of these field campaigns focused on issues associated with HRVOCs initially raised during the 2000 TexAQS campaign. For example, two campaigns in 2009 (SHARP and FLAIR) sought better characterization of olefin, formaldehyde and free radical sources in southeast Texas. A series of full scale flare tests conducted in 2010 at an industrial research facility in Tulsa, Oklahoma examined the emissions of flares operating at low flow rates and with low heating value gases as a potential source of HRVOC emissions. All of these studies have provided insights that will be useful in developing plans for reducing ozone formation in southeast Texas.

Beginning in 2010, the focus of field campaigns shifted from the industrial regions of southeast Texas to measurements made in regions with recently expanded oil and gas production activity, particularly production involving hydraulic fracturing of shale formations. The majority of these measurements have been made in the Barnett Shale natural gas production region near

Fort Worth. These measurements are continuing and analysis of data from the campaigns is on-going.

In addition to continuing measurements associated with expanded oil and gas production, future plans for field studies include a joint effort with the National Aeronautics and Space Administration (NASA). A 2013 field campaign titled DISCOVER AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) will use southeast Texas as a test bed for the use of satellite measurements in characterizing air quality. Sub-orbital (aircraft and ground station) measurements will be compared to satellite measurements to assess the limits of current and the needs for future satellite measurement capabilities. In addition, the US EPA has recently required states to deploy near-road monitors in cities with populations larger than 500,000. These near-road monitors will be used to assess compliance with a new National Ambient Air Quality Standard for NO_2. These near-road measurements may have significant air quality management implications for Texas and enhancing scientific understanding of near-road environments could help inform air quality planning.

These field programs are described in more detail in Sections 1.2.1-1.2.8.

KEY CITATIONS:

Web sites describing TexAQS and its principal findings have been maintained by the University of Texas, www.utexas.edu/research/ceer/texaqs www.utexas.edu/research/ceer/texaqsarchive

Summary of TexAQS II: Parrish, D.D., D.T. Allen, T.S. Bates, M. Estes, F.C. Fehsenfeld, G. Feingold, R. Ferrare, R.M. Hardesty, J.F. Meagher, J.W. Nielsen-Gammon, R.B.Pierce, T.B. Ryerson, J.H. Seinfeld, E.J. Williams "Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS)", *Journal of Geophysical Research – Atmospheres*, 114, D00F13, doi:10.1029/2009JD011842 (2009).

Reports describing the FLAIR, SHARP, Controlled Industrial Flare, and Barnett Shale field studies are available at the AQRP web site: http://aqrp.ceer.utexas.edu/projects.cfm ; the controlled industrial flare study is also described at: Torres, V.M., Herndon, S., Kodesh, Z., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research* DOI: 10.1021/ie202674t (2012); Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research* DOI: 10.1021/ie202675f (2012).

The DISCOVER-AQ program is described at the NASA web site: http://discover-aq.larc.nasa.gov/

The EPA mandated near-road measurement program is described at http://www.epa.gov/ttnamti1/nearroad.html

1.2.1 Texas Air Quality Study (TexAQS 2000)

In August and September of 2000, an international team of more than 300 researchers, drawn from nearly two dozen universities, the National Oceanic and Atmospheric Administration, Brookhaven National Laboratory, Pacific Northwest National Laboratory, and the Environmental Protection Agency, undertook the largest air quality study ever conducted in the State of Texas. The study was designed to improve understanding of the formation, transport and accumulation of air pollutants along the Gulf Coast of southeastern Texas. Measurements were made at approximately 20 ground stations, shown in Figure 1.2.1. Additional sampling was carried out with aircraft that flew over broad regions of eastern Texas.

Figure 1.2.1. Ground sampling sites operated during the Texas Air Quality Study during the summer of 2000.

TexAQS led to the identification of the role of Highly Reactive Volatile Organic Compounds (HRVOCs, ethene, propene, butenes, 1,3-butadiene) in ozone formation in southeast Texas. Key scientific findings were summarized in an Accelerated Science Evaluation (see citation below), and based on these findings, the TCEQ substantially revised the air quality management plan (State Implementation Plan, or SIP) for the Houston-Galveston-Brazoria region. Understanding the sources of HRVOC emissions, which were not well quantified in emission inventories, and reducing HRVOC emissions, became a priority that has continued for more than a decade.

KEY CITATIONS:

Daum, P.H., J. Meagher, D. Allen, and C. Durrenberger. 2002. Accelerated Science Evaluation of Ozone Formation in the Houston-Galveston Area. Summary. 6 pp. http://www.utexas.edu/research/ceer/texaqsarchive/accelerated.htm

Web sites describing TexAQS and its principal findings have been maintained by the University of Texas, www.utexas.edu/research/ceer/texaqs www.utexas.edu/research/ceer/texaqsarchive

1.2.2 Texas Air Quality Study II (TexAQS 2005-2006)

The first Texas Air Quality Study, conducted in the summer of 2000 (Section 1.2.1), was focused primarily on southeast Texas, and helped inform state decisions concerning how to meet then current air quality standards for southeast Texas. After 2000, however, regulations for ozone shifted in emphasis, from concentrations averaged over short periods of time (i.e., the ozone standard with ozone concentrations averaged over one-hour), to concentrations averaged over longer time periods (e.g., ozone concentrations averaged over eight hours). Longer averaging times mean broader geographical regions influence air pollutant concentrations. A second Texas Air Quality Study (TexAQS II) was conducted in 2005 and 2006 to characterize pollutant transport over regional (~100-1000 km) scales. The study also characterized progress that had been made in improving air quality in Houston since 2000.

Among the most significant findings emerging from TexAQS II was the magnitude of ozone transported into Texas. Background ozone in concentrations in eastern Texas, which represent the minimum ozone concentration that is likely achievable through only local controls, can approach or exceed 75 ppbv for an 8 hour average, which is the level of the current National Ambient Air Quality Standard (see Parrish, et al, 2009, cited below).

A second set of major findings were associated with concentrations of Highly Reactive Volatile Organic Compounds (HRVOCs, identified as critical to ozone formation in Houston during TexAQS 2000). Observed concentrations of HRVOCs in southeast Texas were lower in 2006 than in 2000, however, despite improvements in inventory estimates since the TexAQS 2000 study, significant discrepancies were still observed between reported emissions and observed concentrations (see Parrish, et al, 2009, cited below). This finding led to additional field programs related to potential sources of HRVOCs (FLAIR and the 2010 Controlled, full-scale industrial flare study)

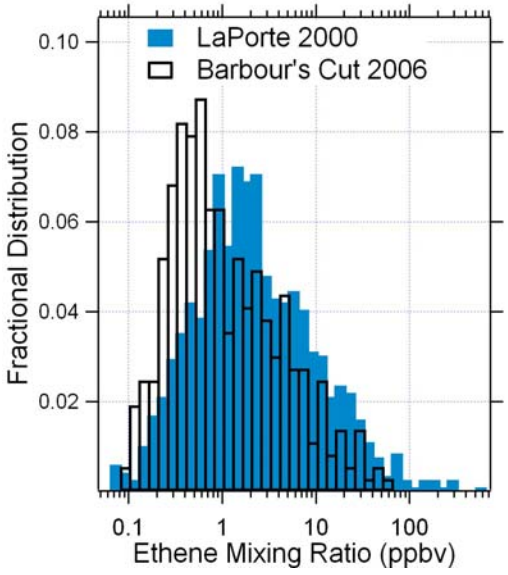


Figure 1.2.2. Comparison of ethylene concentrations made at similar locations in the Houston Ship Channel region in 2000 (LaPorte) and 2006 (Barbour's Cut). A significant decrease in average and extreme ethylene concentrations was observed

KEY CITATION:

Parrish, D.D., D.T. Allen, T.S. Bates, M. Estes, F.C. Fehsenfeld, G. Feingold, R. Ferrare, R.M. Hardesty, J.F. Meagher, J.W. Nielsen-Gammon, R.B.Pierce, T.B. Ryerson, J.H. Seinfeld, E.J. Williams "Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS)", *Journal of Geophysical Research – Atmospheres*, 114, D00F13, doi:10.1029/2009JD011842 (2009).

1.2.3 Study of Houston Atmospheric Radical Precursors (SHARP)

The chemistry of atmospheric radicals, especially the hydroxyl radical (OH) and hydroperoxyl radical (HO_2), together called HOx, is deeply involved in the formation of ozone and other photochemical air pollutants. Radical precursors, such as nitrous acid (HONO) and formaldehyde (HCHO), significantly affect the HOx budget in urban environments such as Houston. The Study of Houston Atmospheric Radical Precursors (SHARP), in the spring of 2009, examined sources and sinks for free radicals and the impact of radical sources and sinks on the sensitivity of ozone formation to emissions of oxides of nitrogen (NOx) and volatile organic compounds (VOCs). Both measurements and modeling were performed and reconciling model predictions and observations has been a major focus of the study.

Among the HONO formation mechanisms that have been considered are gas-phase photolysis of nitrophenols, heterogeneous conversion of NO_2 on fresh and aged soot particles and soil surfaces, photolysis of surface adsorbed nitric acid, and heterogeneous conversion of HNO_3 on the surface of primary organic aerosol. HO_x production during the SHARP campaign in Houston was dominated by the photolysis of HONO in the early morning and by photolysis of O_3 in the midday; at night, OH production occurred mainly via O_3 reactions with alkenes. On average, the daily HO_x production rate was 23.8 ppbv day^{-1} in the region, of which 31% was from O_3 photolysis, 23% from HONO photolysis, 12% from HCHO photolysis, and 14% from O_3 reactions with alkenes (Lefer et al., 2011).

Daytime observed HONO mixing ratios are often far larger than expected. Statistically significant vertical gradients of HONO throughout the day, with smaller mixing ratios aloft, have suggested that a likely source of daytime HONO could be photocatalytic conversion of NO_2 on the ground surfaces in Houston. Although daytime mechanisms for HONO formation have been a subject of exploration, it is evident that uncertainty remains and further studies are needed.

KEY CITATIONS:

Lefer, B.L., W.H. Brune, D.R. Collins, J.E. Dibb, R.J. Griffin, S.C. Herndon, L.G. Huey, B.T. Jobson, W.T. Luke, J. Mellqvist, G.A. Morris, G.H. Mount, S.W. North, E.P. Olaguer, B. Rappenglück, X. Ren, J. Stutz, X. Yu, R. Zhang, Overview and Major Findings of the Study of Houston Atmospheric Radical Precursors (SHARP) Campaign. American Geophysical Union, Fall Meeting 2010b, abstract #A34C-05.

Lefer, B., J. Stutz, X. Ren, W. Brune, J. Dibb, Study of Houston Atmospheric Radical Precursors (SHARP) data analysis. Air Quality Research Program, TCEQ Grant No. 582-10-94300, November 2011.

1.2.4 Formaldehyde and Olefin from Large Industrial Sources (FLAIR) measurements (Houston and Texas City, 2009)

The goal of the FLAIR program was to use a variety of remote sensing and direct field measurements to assess the strength of industrial sources of formaldehyde and olefins. Measurements were made in Texas City, and the Houston Ship Channel region. The study was motivated by a variety of divergent analyses of the relative contribution of primary sources and secondary chemical production to ambient formaldehyde concentrations and fluxes in Houston.

Among the sources examined in the study were flares. Consistent with controlled flare studies done in 2010 (described in Section 1.2.5), a variety of measurement techniques used in the FLAIR study found that formaldehyde is not directly emitted by un-ignited flare stacks, but burning flares emit formaldehyde at the flare tip. Emission rates of burning flares observed during FLAIR varied between 0.3-2.5 kg/h. Also consistent with results from controlled flare studies, combustion efficiencies were found to vary from 0 (unlit) to 0.7 (over-assisted) to 0.999 (presumably operating as intended).

The FLAIR study also identified a large source of primary formaldehyde emissions in the Texas City refinery complex with a strength of 18 ± 5 kg/h. Analysis of the $HCHO/SO_2$ ratio revealed that during most of the time this source(s) co-emitted with a ratio of roughly 0.1. However, some of the formaldehyde emissions were not correlated with SO_2. Analysis of the emission inventory in Texas City, as well as triangulation and wind field analysis revealed that the most likely source of HCHO is a Fluid Catalytic Cracking Unit (FCCU) regeneration unit.

While the measurements made during the FLAIR study in 2009 indicate that some formaldehyde is directly emitted from flares and from FCCU catalyst regeneration units, most of the formaldehyde observed in Houston (~92%) is associated with secondary formation from the oxidation of VOCs (Parrish et al., 2012). Photochemical modeling studies indicate that directly-emitted formaldehyde associated with over-assisted flares does not accentuate ozone formation as greatly as originally hypothesized.

The olefin measurements made during the FLAIR campaign continued to show discrepancies between reported emissions and observations with observations exceeding levels expected from inventories by a factor of 2 orders of magnitude or more at many sites.

KEY CITATIONS:

Parrish, D.D., T.B. Ryerson, J. Mellqvist, J. Johansson, A. Fried, D. Richter, J.G. Walega, R.A. Washenfelder, J.A. de Gouw, J. Peischl, K.C. Aikin, S.A. McKeen, G.J. Frost, F.C. Fehsenfeld, S.C. Herndon, Primary and secondary sources of formaldehyde in urban atmospheres: Houston Texas region. Atmospheric Chemistry and Physics 12 (2012), doi:10.5194/acp-12-3273-2012.

Stutz, J. O. Pikelnaya, G. Mount, E. Spinei, S. Herndon, E. Wood, O. Oluwole, W. Vizuette, E. Causo, Quantification of hydrocarbon NOx and SO2 emissions from petrochemical facilities in Houston: Interpretation of the 2009 FLAIR dataset, Quality Research Program, TCEQ Grant No. 582-10-94300, November 2011.

1.2.5 Flare Study (2010, Controlled, full scale flare tests)

One of the potential sources of HRVOCs in the Houston area is industrial flaring operations. Flares are safety devices that must be able to combust large emergency releases of hydrocarbons. These emergency events are rare, however, and most flare operations occur at flow rates much lower than the maximum flare capacity. Achieving complete combustion at low flow rates, particularly with low heating value gases, can be challenging, but little data existed on flare combustion efficiencies at these conditions. In response to this, the TCEQ contracted with the University of Texas to perform a series of full scale flare tests at low flow conditions with low heating value gases. A 24" diameter air-assisted flare with a flow capacity of 144,000 lb/hr and a 36" steam-assisted flare with a flow capacity of 937,000 lb/hr were employed in the testing. The range of flared gas flow rates was 0.1% to 0.25% of the flare's design capacity and heating values of the flared gases were in the range of 300-600 BTU/scf.

Figure 1.2.2 Full scale flare tests

Destruction/removal efficiencies (DRE, fraction of vent gas reacted) for steam-assisted flares dropped rapidly when combustion zone heating values fell below 250 BTU/scf. Air-assisted flares showed a linear drop in DRE as a function of air flow. While DREs of 98-99% were observed in some experiments, many operating conditions produced DREs of substantially less than 99%. Since standard methods for estimating emissions would have allowed a 98-99% DRE for all the tests, some test conditions resulted in the production of flare emissions multiple times the value that would be calculated using the standard methods. (from Torres, et al., 2012a, cited below) Air quality modeling of theoretical scenarios associated with low flaring destruction efficiencies have shown that the majority of the ozone formation associated with low destruction efficiency flares is due to the unburned gases sent to the flare, rather than products of incomplete combustion (e.g., formaldehyde).

KEY CITATIONS:

Torres, V.M., Herndon, S., Kodesh, Z., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Indus. Eng. Chem.Res.* DOI: 10.1021/ie202674t (2012a);

Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Indus. Eng. Chem. Res.* DOI: 10.1021/ie202675f (2012b).

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research*, DOI: 10.1021/ie201400z (2011).

1.2.6 Dallas-Fort Worth Barnett Shale field measurements (2010-date)

Driven by advances in drilling technology, oil and gas production activities in Texas have seen a substantial resurgence over the past 5 years. The use of hydraulic fracturing and other technologies has enabled significantly expanded oil and gas production in the Barnett Shale formation near Fort Worth, the Eagle Ford formation south of San Antonio, the Haynesville formation in east Texas, and in other formations throughout the state. These activities have the potential to impact air quality in complex ways. Direct emissions associated with the production activities include ozone precursors (nitrogen oxides, volatile organic compounds), and some air toxics (e.g., benzene). Indirectly, the availability of relatively inexpensive natural gas and natural gas liquids could change emissions associated with electricity generation and chemical manufacturing.

A series of field campaigns have been undertaken since 2010, primarily to characterize direct emissions of volatile organic compounds and air toxics in the Barnett Shale formation. With funding provided by the TCEQ and cities in the Barnett Shale region, hourly and daily measurements of concentrations of volatile organic compounds were made at multiple sites. In addition, the Texas Air Quality Research Program funded the deployment of an augmented set of measurements in and around Eagle Mountain Lake in the summer of 2011. These measurements assessed emissions from individual well and processing sites and examined, in detail, the ozone formation chemistry in the Barnett Shale region.

Results from the studies are just becoming available, but should help to clarify the role of direct emissions associated with renewed oil and gas production activities on ozone formation.

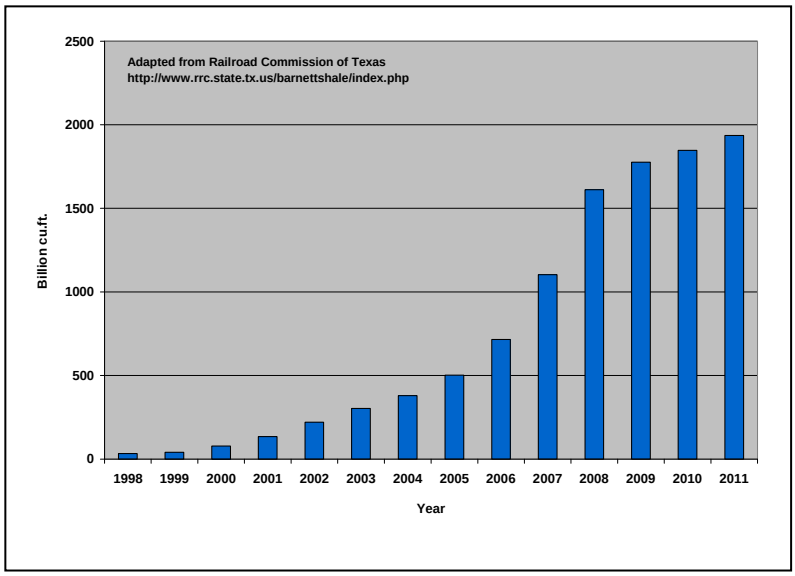


Figure 1.2.4. Natural gas production in the Barnett Shale region near Fort Worth. Significant expansion in production activities has occurred over the past 5-10 years

KEY CITATIONS:

Eastern Research Group and Sage Environmental Consulting, Final Report, City of Fort Worth Natural Gas Air Quality Study, prepared for the City of Fort Worth, July 13, 2011.

Final Reports of AQRP funded projects for the DFW field campaign are available at: http://aqrp.ceer.utexas.edu/projects.cfm

1.2.7 DISCOVER AQ 2013

"DISCOVER-AQ, a NASA Earth Venture program funded mission, stands for Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality.

In recent years, progress in reaching air quality goals has begun to plateau for many locations. Furthermore, near-surface pollution is one of the most challenging problems for Earth observations from space. However, with an improved ability to monitor pollution from satellites from DISCOVER-AQ, scientists could make better air quality forecasts, more accurately determine the sources of pollutants in the air and more closely determine the fluctuations in emissions levels. In short, the more accurate data scientists have at hand, the better society is able to deal effectively with lingering pollution problems.

The campaign will employ NASA aircraft to make a series of flights, with scientific instruments on board to measure gaseous and particulate pollution, beginning in 2011. The series of flights -- which will be made by NASA Langley's King Air and NASA's P-3B – will commence over Baltimore-Washington, D.C. in 2011. Other future flights may include Houston (2013); Sacramento (2013); and a final site in 2014 to be determined. The measurements will be taken in concert with ground observations in order to shed light on how satellites could be used to make similar, consistent measurements over time, with the ultimate goal of putting better data in the hands of policymakers and elected officials." (From NASA Discover AQ web site: http://discover-aq.larc.nasa.gov/science.php)

The State of Texas, through the TCEQ and the Air Quality Research Program, is working with NASA to develop sampling strategies for the 2013 field measurement campaign in Houston. The field campaign will involve coordinating ground measurements and instrumented aircraft flights with satellite overpasses. The field measurements have the potential to benefit the State both through improved capabilities for the use of satellite measurements and through availability of a new set of measurements that can assess progress in southeast Texas air quality since TexAQS II in 2006.

KEY CITATION:

The DISCOVER-AQ program is described at the NASA web site: http://discover-aq.larc.nasa.gov

1.2.8 Near-road sampling for NO_2 NAAQS compliance

The U.S. Environmental Protection Agency (EPA) recently established a new National Ambient Air Quality Standard for NO_2 (100 ppb, 1 hour averaged concentrations, 98th percentile averaged over 3 years). It is anticipated that the highest concentrations of NO_2 will be observed in near-roadway environments, therefore the EPA has also mandated the deployment of a national near-roadway monitoring network for NO_2. The network is to be deployed by January of 2013. Every city with a population greater than 500,000 will have at least one monitor that will be located at positions anticipated (e.g., due to traffic volume and type) to lead to high NO_2 concentrations.

The TCEQ has supported a series of pilot studies designed to characterize near-roadway concentrations of NO_2 and other traffic related air pollutants, and to determine the rate at which pollutant concentrations decrease with distance from roadways. These studies have indicated that near-roadway emissions and chemistry are complex, especially for NO_2.

In current vehicles, most NOx is emitted as NO. New generation diesel control technologies reduce NOx emissions, but may increase the NO_2/NO ratio, suggesting that fleet mix and age will have complex impacts on near-road NO_2 emissions. Studies near Texas roadways have further demonstrated that within tens of meters of a roadway, ozone reactions with NO can significantly increase NO_2 concentrations, making the positioning of monitors and ambient ozone concentrations potentially critical factors in NAAQS compliance.

Currently only NO_2 and CO measurements are mandated in the near-road monitoring requirements due to be implemented in 2013, however, the draft Technical Assistance document developed by the EPA suggests a variety of additional measurements that could be added to the network. These include meteorological variables, traffic counts and vehicle types, ozone concentrations, and other measurements that can improve understanding of NO_2 sources.

Should Texas near-road monitors detect exceedances of the NAAQS, additional near-road measurements could help inform appropriate responses.

KEY CITATIONS:

EPA near roadway monitoring program website: (http://www.epa.gov/ttnamti1/nearroad.html) and technical assitance document (http://www.epa.gov/ttnamti1/files/nearroad/20111221tad.pdf)

Zhu, Y., J. Pudota, D. Collins, D. Allen, A. Clements, A. Denbleyker, M. Fraser, Y. Jia, E. McDonald-Buller, E, Michel "Air pollutant Concentrations near 3 Texas Roadways, Part 1: Ultrafine Particles, *Atmospheric Environment,* 43, 4513-4522 (2009).

Jia, Y., A. Denbleyker, E. McDonald-Buller, M. Fraser, D. T. Allen, E, Michel, D.R. Collins, J. Pudota, Y. Zhu "Air pollutant Concentrations near 3 Texas Roadways, Part 2: Chemical Characterization and Transformation of Pollutants, *Atmospheric Environment,* 43, 4523-4534, doi:10.1016/j.atmosenv.2009.06.044 (2009).

Wang, Y.J., DenBleyker, A., McDonald-Buller, E., Allen, D., and Zhang, K.M. "Modeling the chemical evolution of nitrogen oxides near roadways", Atmospheric Environment, 45, 43-52 (2011).

2. State of the Science: Emissions, Chemistry, and Meteorology and Transport/Modeling

2.1 Overview and methods for developing state of the science findings

Scientific findings emerging from large field campaigns and data analysis programs, of the type that have occurred in Texas over the past decade, are multifaceted. Many of the scientific findings have direct and immediate policy relevance. For example, scientific findings from TexAQS were used to guide the development of the approaches used to attain the National Ambient Air Quality Standard for ozone in Houston. Other scientific findings have longer-term policy relevance. For example, scientific findings that improve understanding of emissions and chemistry associated with natural gas production may help inform the direction of air quality policies in regions such as the Dallas-Fort Worth area. Better understanding of how flare operating practices influence emissions can guide emission reduction strategies. This document summarizes the scientific findings emerging from air quality studies performed in Texas. Findings with both immediate and longer-term relevance are summarized.

Scientific findings have varying degrees of certainty. The findings reported in this document are not limited to those for which there is a high degree of certainty; in many cases highlighting critical areas where uncertainty exists can be important in determining the likelihood that a policy will be effective, and identifying areas where uncertainty exists is critical to continued progress in scientific understanding. However, when uncertainty or areas of disagreement concerning the implications of scientific findings exist, this document clearly characterizes the uncertainties.

Initial drafts of this report were written by AQRP staff (David Allen, Elena McDonald-Buller and Gary McGaughey of the University of Texas). The draft findings and recommendations for future work were reviewed by both the Texas Commission on Environmental Quality.

The findings are divided into four sections corresponding to the areas where the AQRP performs research: emissions, chemistry, and atmospheric transport/modeling. In each section, there is a brief statement of major findings; citations to the scientific literature provide additional details.

2.2 Ozone Precursor Emissions

2.2.1 Overview of Emission Inventories

Emission inventories are used for a variety of purposes and at a variety of spatial and temporal scales. Inventories are used at state and national spatial scales and at annual and multi-year temporal scales to establish trends in air quality. They are also used as inputs to air quality models that require kilometer-level spatial resolution and hourly temporal resolution. These variable applications of emission inventories lead to very different information needs. This State of the Science assessment focuses on emission inventories that are used in air quality models that are used to evaluate air quality management plans for ozone. These models must predict atmospheric processes on days when extreme ozone concentrations have been observed, therefore emission inventories resolved at kilometer-level spatial scales and at hourly temporal scales are of greatest interest. Findings are reported for motor vehicle emissions, point source emissions, and emissions associated with oil and natural gas production. Biogenic emissions are discussed in the section on atmospheric chemistry. Other categories of emissions (e.g., off-road equipment) are significant sources but have not been the focus of AQRP research activities and therefore are not summarized here, but have been described in previous scientific assessments (Allen and Durrenberger, 2003).

Data summarized in this assessment indicate that emissions of ozone precursors from some sources can vary significantly on a daily, even an hourly basis (Murphy and Allen, 2005). Consequently, both the magnitude and the variability in ozone precursor emissions are reported.

KEY CITATIONS:

Allen, D., Durrenberger, C. and Texas Commission on Environmental Quality, Technical Analysis Division. 2003. Accelerated Science Evaluation of Ozone Formation in the Houston-Galveston Area: Emission Inventories Version 3, February, 2003, available at http://www.utexas.edu/research/ceer/texaqsarchive/accelerated.htm

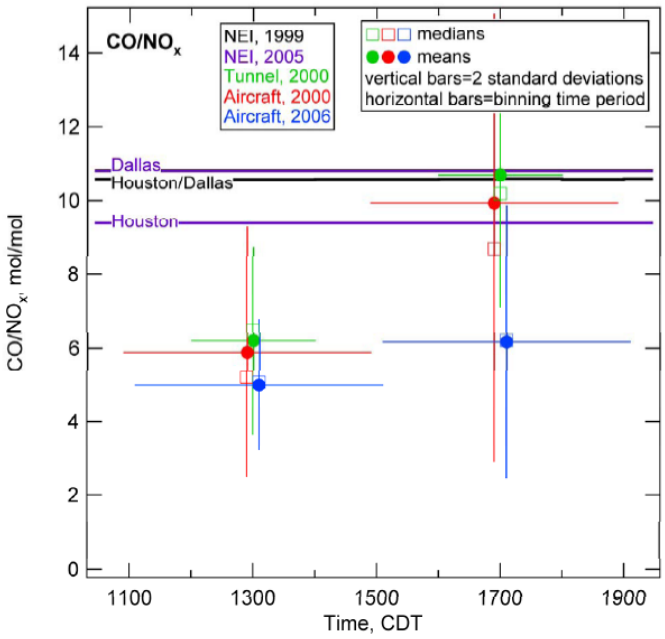
Murphy, C. F. and D. T. Allen "Hydrocarbon Emissions from Industrial Release Events in the Houston-Galveston Area and their Impact on Ozone Formation," *Atmospheric Environment*, 39, 3785 – 3798 (2005).

2.2.2 Motor Vehicle Emissions

1. On-road mobile source emissions have historically been obtained using the MOBILE model, which overestimates CO/NO_x ratios in eastern Texas urban areas.

Observational evaluation of CO/NOx ratios from airborne sampling and tunnel studies during TexAQS II has indicated that emissions inventories based on the MOBILE6 model overestimate CO/NO_x ratios in eastern Texas urban areas. Figure 2.2.1 (Frost et al., 2008) compares measured CO/NO_x ratios during the morning and evening rush hours obtained from airborne sampling and tunnel studies during TexAQS and TexAQS II with those obtained from the 1999 and 2005 National Emissions Inventories (NEIs). In addition, CO/NOx emission ratios of 5.81 ±0.94 were observed during the morning rush hour from the Moody Tower supersite (Luke et al., 2010) during the 2006 TexAQS-II Radical and Aerosol Measurement Project (TRAMP). Discrepancies between observed and MOBILE predicted CO/NOx ratios have become more pronounced over time and have been attributed to a factor of 2-3 overestimate in CO emissions (Parrish, 2006; Frost et al., 2008) and an underestimate of NO_x emissions (Parrish, 2006) in the more recent emissions inventories. The Texas Roadway Study (Denbleyker et al., 2007; Zhu et al., 2009; Clements et al., 2009) characterized ambient concentrations of CO and NO_x, as well as other vehicular emitted pollutants, and chemical processes in the microenvironments of three Austin roadways. Comparisons between MOBILE6 predictions and observations from the Texas Roadway Study suggested that MOBILE6 overpredicts CO/NO_x ratios, but is generally within a factor of three of observed ratios.

Figure 2.2.1. Mobile source CO/NO_x emission ratios from airborne and tunnel studies during TexAQS and TexAQS II and from the 1999 and 2005 National Emissions Inventories (ref. Frost et al., 2008).



2. Estimates of vehicular emitted pollutants in Texas will change with the transition from the MOBILE model to MOVES.

The U.S. EPA (2003) and the TCEQ have utilized versions of the MOBILE model to obtain estimates of vehicular emitted pollutants since 1978. The Motor Vehicle Emissions Simulator (MOVES) was released as a replacement to the MOBILE model in March 2010 with a minor update (MOVES2010a) in September 2010 (EPA, 2010a). MOVES2010b is the most recent version and was released in April 2012. MOVES offers a substantially improved understanding of the relationship between vehicle activity, environmental variables and emissions and includes new emissions test data, while accounting for recent changes in vehicle technology and regulations. Preliminary analyses with MOVES have indicated that PM, NO_x, and CO_2 emissions rates are higher than MOBILE6.2, while VOC and especially CO emissions rates are lower (Bai et al., 2008, Beardsley, 2009). Tables 2.2.1 and 2.2.2 present summaries of 2006 and 2018 HGB area on-road emissions inventories developed by the Texas Transportation Institute under contract to the TCEQ using local area travel demand model (TDM) output coupled with emission rates from MOBILE6.2, MOVES2010, and MOVES2010a. Relative to MOBILE6.2 estimates, MOVES predictions are substantially greater for NO_x, slightly higher for VOC, and slightly lower for CO.

Table 2.2.1 Comparison of 2006 Summer Weekday On-Road Emission Inventory Estimates for the HGB Area Using MOBILE6.2, MOVES2010, and MOVES2010a

Model Version and Level of Effort	**Development Date**	**Daily VMT**	**2006 Summer Weekday Emissions** (tpd)		
			NOx	**VOC**	**CO**
MOBILE6.2 SIP-Quality	Summer 2007	133,868,661	206.74	90.71	1,115.28
MOVES2010 Sensitivity	Summer 2010	133,868,661	292.65	107.57	1,013.21
MOVES2010a SIP-Quality	Summer 2011	143,408,584	270.00	104.74	1,024.03

Table 2.2.2. Comparison of 2018 Summer Weekday On-Road Emission Inventory Estimates for the HGB Area Using MOBILE6.2, MOVES2010, and MOVES2010a

Model Version and Level of Effort	**Development Date**	**Daily VMT**	**2018 Summer Weekday Emissions** (tpd)		
			NOx	**VOC**	**CO**
MOBILE6.2 SIP-Quality	Spring 2009	180,993,087	52.55	45.97	733.18
MOVES2010 Sensitivity	Summer 2010	180,993,087	109.07	48.10	617.79
MOVES2010a SIP-Quality	Winter 2012	180,955,402	103.34	50.13	656.24

For any future studies involving ambient measurements near roadways, careful attention must be paid to the mix of vehicle types being monitored. Many on-road emission inventories are based on either daily or annual average vehicle miles traveled (VMT) distributions by vehicle category. However, these distributions can vary significantly by individual roadway segment, time-of-day, day-of-week, etc. If VOC and/or CO were the only pollutants of concern, then the focus of a study could be primarily limited to the light-duty gasoline fleet, which dominates both VMT and emissions of these two pollutants. However, NO_x emission totals are heavily dependent on the VMT split between the light-duty gasoline passenger fleet and "eighteen-wheeler" heavy-duty diesel trucks. Comparisons between ambient measurements and emission inventory estimates must pay special attention to this split if CO/NO_x ratios are being evaluated.

3. In-use characterization of heavy-duty diesel vehicle (HDDV) exhaust emissions suggests variability in MOVES performance among classes and model years.

Johnson et al. (2012) conducted driving and idling emission testing on 30 selected HDDV from the City of Houston fleet to characterize their emissions with respect to vehicle classes, types (high emitting or non-high emitting), and model years. Measurements were compared with MOVES2010a (refer to p.27 in Johnson et al. 2012) estimates, as well as among vehicle classes and types. CO and NO_x emissions from potential high emitting vehicles, which were generally older, were highly consistent with MOVES estimates. Randomly selected vehicles, which were of newer model years (2003 and 2006), exhibited greater variability with respect to divergence from MOVES estimates. These results may be associated with the limited field data used in MOVES for HDDVs. Total hydrocarbon (THC) emissions from potential high emitting Class 8 vehicles, i.e., heavy duty trucks with a gross vehicle weight rating (GVWR) above 33,000 pounds, were generally higher than MOVES estimates, but were lower than MOVES for all other vehicle types. Observed PM emissions for all test vehicles were significantly lower than MOVES estimates, which could have been associated with differences in measurement methods between the study of Johnson et al. (2012) and those used for the development of MOVES.

4. Strong spatial gradients in concentrations exist and chemical processing of vehicular emitted air pollutants occurs in the near-roadway microenvironment. Characterization of near-roadway processes is required to respond to new ambient monitoring requirements and to assess human exposure patterns.

The Texas Roadway study (Denbleyker et al., 2007; Zhu et al., 2009; Clements et al., 2009; Wang et al., 2011) measured the spatial gradients of vehicular emitted air pollutants in the vicinity of three roadways, with varying traffic volume counts and fractions of heavy-duty vehicles, near Austin, Texas. Regardless of roadway type or wind direction, ultrafine particulate (UFP; number, surface, and volume), CO, NO, and NO_x concentrations increased between the upwind and downwind side of the roadways with return to background levels within a few hundred meters of the roadway. The behavior of particle-bound organic species was complex. $PM_{2.5}$ mass concentrations, PAHs, hopanes, and EC concentrations generally exhibited concentrations that decreased with distance downwind. Relative to upwind concentrations, concentrations of OC increased immediately downwind and continued to increase further downwind, which may have resulted from the condensation of vehicular emitted semi-volatile organic species. The decay rate for NO was more than a factor of two greater than for CO, and it comprised a larger fraction of NO_x closer to the roadways than further downwind suggesting the potential significance of near roadway chemical processing, as well as atmospheric dilution. Wang et al. (2011) suggested that the chemical evolution of NO_2 and NO may not be well simulated by historically utilized Gaussian dispersion models, such as CALINE4. Comparisons of the performance of CALINE4 with a computational fluid dynamics model, CFD-VIT-RIT, that couples a standard k - ε turbulence model for turbulent mixing and the Finite-Rate model for chemical reactions, with observations from the Texas Roadway Study indicated that CFD-VIT-RIT was capable of predicting both NO_x and NO_2 profiles downwind. Although CALINE4 captured near-roadway NO_x profiles, it underpredicted NO_2 concentrations under high wind velocities. In addition, Wang et al. (2011) found that initial NO_2/NO_x ratios must be carefully selected based on traffic conditions in order to assess NO_2 concentrations near roadways. Commonly assumed NO_2/NO_x ratios by volume of 5% or 10% may not be suitable for most roadways, especially those with a high fraction of heavy-duty truck traffic. Recognition that the majority of ambient exposures to peak NO_2 concentrations (EPA, 2011) are associated with roadways has led to the requirement for near-road monitoring in U.S. metropolitan areas. Understanding near-roadway spatial gradients in NO_2 concentrations and chemical processes and atmospheric modeling capabilities will be critical as Texas responds to forthcoming deadlines for site selection and configuration.

Unlike MOBILE6.2 that only estimated total NO_X, the MOVES2010a model estimates NO and NO_2 emission rates separately. The NO_2 portion of total NO_X can be as low as 1% for some gasoline vehicles in the cold start mode, and as high as 40% for newer technology diesel vehicles in the hot stabilized running mode. For the on-road emission inventories developed to date with MOVES2010a, the TCEQ has been estimating and processing NO and NO_2 separately when preparing air quality modeling inputs. The recently released MOVES2010b version of the model has added nitrous acid (HONO) emissions as a subset of NO_X, so that NO + NO_2 + HONO = NO_X. MOVES2010b currently assumes that HONO comprises 0.8% of total NO_X for all combinations of vehicle type, fuel type, and mode of engine operation. Until an updated version of MOVES is released, TCEQ will be using MOVES2010b for all future on-road inventory

development, and will estimate NO, NO_2, and HONO separately for air quality modeling purposes.

5. The use of catalyzed Diesel Particulate Filters (DPFs) and Diesel Oxidation Catalysts (DOCs) in on-road and off-road diesel equipment have the potential to increase NO_2 emissions.

Modern diesel engines are increasingly incorporating DOC and catalyzed DPF, which have the potential to form additional NO_2 emissions, in on-road and off-road vehicles, to meet PM emissions standards (Bar-Ilan et al., 2009; Carslaw, 2005). Bar-Ilan et al. (2009) examined the potential impacts of these additional NO_2 emissions on ozone formation in the DFW area for two scenarios. One scenario assumed a maximum penetration, in which there was significant turnover to newer model year on-road vehicles and higher Tier non-road equipment, and a second scenario, which is more realistic, considered the fractional usage of DOC/DPF devices in the 2009 fleet of heavy-duty on-road trucks, buses and some construction equipment. In order to achieve the maximum penetration scenario, highly accelerated turnover of the fleet to newer vehicles and equipment was required, that resulted in decreases in total NO_x emissions. Air quality modeling showed that the maximum penetration scenario resulted in a decrease in ozone due primarily to reductions in total NO_x emissions, despite increase in NO_2. The realistic scenario analysis, which did not consider equipment turnover, resulted in a modest increase in total NO_2 emissions and ozone increases within the DFW area of less than 1ppb. Bar-Ilan et al. (2009) noted that manufacturers of these devices are investigating strategies to mitigate the excess NO_2 formation. Future studies are needed to consider the impacts of these devices on NO_2 concentrations and human exposure patterns in near-road microenvironments in Texas.

6. Retrofit devices aimed at reducing tailpipe and crankcase emissions from diesel vehicles may also improve cabin air quality by reducing vehicle self-pollution.

Rim et al. (2008) examined the effects of a staged installation of a Spiracle Crankcase Filtration System followed by a DOC, on cabin pollutant concentrations in Central Texas school buses. Following installation of the Spiracle Crankcase Filtration System, in-cabin concentration decreases ranged from 24 to 37% for NO_x and 26 to 62% and 6.6 to 43% for $PM_{2.5}$ and ultrafine PM, respectively. Following installation of the Spiracle, the DOC provided negligible or only small additional reductions of in-cabin pollutant levels.

7. The air quality benefits of increasing the penetration of plug-in hybrid electric vehicles (PHEVs) in the Texas fleet will be influenced by the temporal pattern of battery charging.

Thomson et al. (2011) examined the air quality impacts of replacing approximately 20% of the gasoline-powered light duty vehicle miles traveled (VMT) with electric VMT by the year 2018 for four major cities in Texas: Dallas/Ft Worth, Houston, Austin, and San Antonio. Three charging scenarios, occurring on the Electricity Reliability Council of Texas (ERCOT) grid, were compared: nighttime charging, charging to maximize battery life, and charging to maximize driver convenience. Net impacts of PHEVs included an increase in NO_x emissions from EGUs during times of day when the vehicle was charging, and a decrease in NO_x from mobile emissions. In general, PHEVs were predicted to lead to an increase in ozone during nighttime hours and a decrease in ozone during daytime hours. Larger increases in ozone for the convenience charging scenario relative to the other scenarios were predicted at the locations of a

few ambient monitoring sites. Nighttime charging was found to most likely reduce a measure of ozone exposure potential versus the other two scenarios.

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2.2.3 Point Sources

1. Emissions of highly reactive VOCs (HRVOCs) and nitrogen oxides (NOx) declined between the time periods of the TexAQS2000 and TexAQS II studies, but discrepancies between observations and reported emissions inventories remain.

Observational evidence has indicated substantial reductions in emissions of ozone precursors in the Houston area during the time period between the TexAQS 2000 and TexAQS II field campaigns,. Washenfelder et al. (2010) measured reductions of 29% ± 20% in NO_x emissions between August 2000 and September 2006 in the Houston industrial area that were consistent with reductions in NO_x emissions at larger point sources throughout the southeastern United States that have implemented controls. Temporal trends in the ratios of the HRVOCs, ethene and propene, respectively, to oxides of nitrogen (i.e., C_2H_4/NO_x and C_3H_6/NO_x) over the same time period indicated decreases by 30% ± 30%; median ambient concentrations of ethene and propene within the Houston urban area decreased by 52% and 48%, respectively.

However, even with declines in emissions and ambient concentrations, this study and others conducted during TexAQS II have suggested that discrepancies between reported VOC emissions inventories and observations remain. Washenfelder et al. (2010) found that measured ratios of C_2H_4/NO_x and C_3H_6/NO_x exceeded emission inventory values by factors of 1.4–20 and 1–24, respectively. Mellqvist et al. (2010) found that emission flux estimates from Solar Occultation Flux (SOF) measurements in the Houston area were, in some locations, an order of magnitude larger than a 2006 daily emission inventory from the TCEQ, which are similar to the findings of de Gouw et al. (2009). Mellqvist et al. (2010) also found large variability in alkene emission flux estimates, especially propene, downwind of petrochemical plants. These facilities reported highly variable emissions from flaring during August and September of 2006 that periodically dominated their alkene emissions.

2. Temporal variability in industrial emissions can affect ozone formation in the Houston-Galveston-Brazoria (HGB) area and should be characterized for air quality models.

Studies performed in the HGB area indicate that some industrial emissions sources exhibit high temporal emissions variability, with emissions changing by orders of magnitude over hourly to daily time periods (Murphy and Allen, 2005; Nam et al., 2006; Webster et al., 2007; Nam et al., 2008). These temporal variations in emissions can lead to very rapid ozone formation, especially when emissions are composed of highly reactive volatile organic compounds (HRVOCs, defined as ethene, propylene, 1,3-butadiene, and butenes), and consequently, may have a significant impact on ozone generation in the HGB region (Kleinman et al., 2003; Allen et al., 2004; Vizuete et al., 2008; Olaguer et al., 2009; Henderson et al., 2010).

Recognition of the importance of industrial emission variability motivated the collection of hourly emissions data from 141 industrial locations in the HGB area over 32 days during the time period of TexAQS II (August 15 through September 15, 2006). This emissions database, which is the largest collection of hourly industrial emissions in a single area of the United States, was incorporated into the 2006 Special Inventory (2006 SI) by the Texas Commission on Environmental Quality (2008). Flares constituted 45% of all VOC and 77% of all HRVOC emissions in the SI, followed by stacks and cooling towers (41% VOC and 18% HRVOC), and finally fugitives (14% VOC and 5% HRVOC).

Pavlovic et al. (2009; 2012a) categorized emissions from refinery and olefin production flares, the largest sources of VOC in the 2006 SI. Flares were categorized by industrial process, chemical composition, and the temporal patterns of their emissions. Stochastic representations

of emissions were developed using a Markov process model for each flare subcategory based on the earlier work of Nam et al. (2006) and Webster et al. (2007). Industrial flare emission temporal patterns were comprised of multiple components, including as nearly constant, routinely variable or episodic emissions. The stochastic models provided a representation of flare emissions that were used to explore the effects of the variable emissions inventory, relative to a typical ozone season day inventory, on ozone formation using the Comprehensive Air Quality Model with extensions (CAMx). The temporal variability in flare emissions from the 2006 SI was found to lead to localized differences in ozone concentrations of as much as 27 ppb in the HGB area relative to the ozone season daily inventory (Pavlovic et al., 2010; Pavlovic et al., 2012b). The ozone impacts associated with the temporal variability in emissions typically lasted a few hours, consistent with the length of large flaring events (Pavlovic et al., 2012b). This finding was consistent with those of an earlier study by Nam et al. (2008), which indicated that strategies that eliminate the infrequent largest emissions are more effective at reducing the highest localized ozone concentrations than changes in nearly constant emissions. Use of a fine model horizontal grid resolution (2 km x 2km) was necessary to capture the impacts on ozone predictions.

3. Ensuring high destruction removal efficiencies (DREs) during flaring operations can be important for regional air quality.

Most flares are designed to have destruction removal efficiencies (DREs), defined as the percentage of waste gas fed to the flare that is destroyed by complete or partial combustion, of 98% or 99%. Flares are also designed to operate over a very large range of flow rates. Recent observations have indicated that DRE can fall substantially below the target range of 98-99% under low flows and high steam or air assist rates, for some types of flares (Strosher, 2000; Mellqvist, 2001; Allen and Torres, 2011; Torres et al., 2012a; Torres et al., 2012b). In addition, recent measurements have characterized products of incomplete combustion (PICs) in flares, which include both highly reactive gases, such as formaldehyde and acetaldehyde, and less reactive gases, such as CO (Allen and Torres, 2010; Herndon, 2011). Al-Fadhli et al. (2011) examined the impacts of flare DRE (95, 90, 75 and 50% versus a base case with 98% or 99%) and PICs (a scenario that accounted for PICs, consistent with Allen and Torres (2011) versus a base case that did not consider PICs) on predicted ozone formation in southeastern Texas using CAMx. Of the five flares examined in the study, two flares showed predicted increases in ozone concentrations in excess of 15 ppb when the DRE was reduced, while the others showed more modest effects on predicted ozone concentrations. The flare DRE impact on ozone concentrations depended on the amount of flare emissions and chemical composition of the emissions. Accounting for the PICs had a relatively modest impact on ozone concentration because most of the mass was carbon monoxide which had a low chemical reactivity to form ozone. The analyses were intended to represent upper bounds on the ozone formation potential of flare emissions. Overall, the results indicated the potential effects of flare DRE on regional air quality.

4. Field tests in a semi-controlled environment indicate that the most efficient flare operation, as measured by the DRE and combustion efficiency (CE), are achieved at or near the incipient smoke point (ISP). Minimum levels of steam or air assist that comply with the flare manufacturer's recommendations should be used when possible.

Recent studies, sponsored by the TCEQ and led by the University of Texas at Austin with Aerodyne Research, Inc. and other collaborators, have focused on the measurement of emissions and the collection of process and operational data from full-scale industrial design flares in a semi-controlled environment at John Zink, LLC in Tulsa, Oklahoma, in order to determine the relationship between flare design, operation, vent gas lower heating value (LHV), flow rate, destruction and removal efficiency (DRE), and combustion efficiency (CE; percentage of the total hydrocarbon stream entering the flare that burns completely to form only carbon dioxide and water) (Allen and Torres, 2011). A key assumption has been that flares operating over the range of requirements stated in Title 40 Code of Federal Regulations (CFR) § 60.18 achieve the assumed hydrocarbon DRE of 98-99 percent at varying vent gas flow rate turndown, assist ratios and vent gas heat content, although limited observational evidence in southeastern Texas has suggested that HRVOC flares routinely do not meet the assumption of 99% DRE (Herndon et al., 2011). Given the significance of flaring emission to the total VOC and HRVOC inventories in the region, these recent studies have led to new insights regarding efficient flare operational conditions that potentially minimize emissions.

As an example, at low vent gas flow rates (nominally 937 lb/hr and 2,342 lb/hr) and low LHVs (nominally 350 Btu/scf and 600 Btu/scf), the flare performance curve of DRE versus steam assist had a very short to non-existent "shelf" before the DRE fell off to less than 98%. Beyond this point, the DRE and CE decrease as steam assist increases. For nominal LHVs of 350 Btu/scf and 600 Btu/scf and vent gas flow rates of 359 lb/hr and 937 lb/hr, air flare test data showed that an air assist quantity of up to 6 times the stoichiometric air-to-fuel ratio (lb/lb) produced a DRE > 99%. Higher levels of air assist produced lower DREs.

The most efficient flare operation, as measured by the DRE and CE, for the flare operating conditions tested, was achieved at or near the incipient smoke point. Higher efficiencies could have been achieved with steam or air assist slightly less than the ISP assist value but this condition, i.e., a smoking flare, would not have been in compliance with 40 CFR § 60.18.(f) Therefore, no more than the minimum levels of steam or air assist that comply with the flare manufacturer's recommendations should be used when possible. Further development of remote sensing technologies, such as Passive and Active Fourier Transform Infrared (PFTIR, AFTIR) Spectroscopy (Allen and Torres, 2011), and modeling techniques, such as Multivariate Image Analysis (MIA; Rawlings et al., 2011), may offer approaches for improving the detection, monitoring, and evaluation of flare operational conditions in the future.

Options for controlling routine emissions using methods other than flaring must be addressed on a case-by-case basis. However, Pavlovic et al. (2009) describe that several approaches have been utilized in the Houston area, including implementation of process and operating changes that eliminate flows to the flare; use of higher efficiency control devices during normal operating conditions; and/or flare gas recovery for reprocessing or use as a fuel. Individually or in combination, these techniques could potentially be used to effectively eliminate emissions from flaring during normal or routine operations.

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2.2.4 Oil and Gas Production Emissions

1. Texas oil and gas production is associated with substantial emissions of NOx and VOC that impact predicted ozone concentrations.

NOx (and VOC) emissions occur from compressor stations that produce and move natural gas in pipelines as well as during drilling, hydraulic fracturing, and well completions; VOC is emitted from additional processes such as dehydration of natural gas, venting from oil and condensate tanks, and production and transmission fugitives (Armendariz, 2009; Grant et al., 2009). Emissions from individual oil and gas production sites are typically small, but collectively may become a significant source of emissions (Pring et al., 2010). As shown in Figure 2.2.2, there were over 400,000 active oil and gas wells in Texas during 2011 (http://www.dallascityhall.com/pdf/GasDrilling/ DallasGasDrillingTaskForce_TCEQ.pdf). With recent advancements in exploration and production technology such as the hydraulic fracturing and horizontal drilling of natural gas wells (ERG and SAGE, 2011), oil and gas exploration and production is increasingly taking place in populated areas, including the DFW nonattainment and Tyler-Longview-Marshall (TLM) near nonattainment areas. For example, Figure 2.2.3 shows that Barnett Shale (North Texas) natural gas production increased 540% during 2003 - 2011 (http://www.rrc.state.tx.us/barnettshale/ NewarkEastField_1993-2011.pdf).

In 2012, NOx and VOC emissions in the 9-county DFW area are predicted to be 19 tons/day and 114 tons/day, respectively (TCEQ, 2011a). Although shale gas is projected to play an increasingly important role in meeting US energy needs, studies of the ozone impacts associated with shale gas development are uncommon (Kemball-Cook et al., 2010). Ozone analysis using Anthropogenic Precursor Culpability Assessment (APCA) in support of the DFW SIP suggested that oil and gas emissions during 2012 may contribute up to 3.5 ppb to 8-hour ozone concentrations at some monitoring locations on some days (TCEQ, 2011b). High ozone days in Tyler-Longview-Marshall are often characterized by stagnant winds (Kemball-Cook et al., 2008; Stoeckenius and Yarwood, 2004), which would tend to keep Haynesville ozone precursor emissions near TLM (Grant et al., 2009). Ozone studies for 2012 predicted that increases in the 8-hour ozone design values of up to 5 ppb occurred over some portions of Northeast Texas and Northwest Louisiana resulting from development in the Haynesville Shale (Kemball-Cook et al., 2010).

2. Emissions from oil and gas production have substantial uncertainty.

The oil and gas exploration and production industry in Texas is extensive with many potential sources of emissions. Emissions sources at the larger "downstream" transmission/distribution stations, processing plants, and refineries are reported as major point sources to the TCEQ so they are generally well-handled in annual inventories (ERG, 2007). With the recent advancements in hydraulic fracturing of shale rock, the amount of oil and gas drilling is increasing rapidly in portions of the US including Texas. Emissions from these "upstream" shale oil and gas production sites are subject to substantial uncertainty (Thoma, 2009). Recently, TCEQ has expended significant resources to improve emissions inventories for the predominant oil and gas exploration and production NOx sources such as drilling rigs (ERG, 2009; ERG, 2011) and other internal combustion engines such as natural gas compressor stations and pumpjacks (Grant et al., 2009; Pring et al., 2010). The accuracy of the emission inventories is limited by the availability of county-specific data and the absence of sufficient data often requires substantial assumptions. For example, since the Haynesville Shale is in the initial stages of development and site-specific data were not yet available from many gas producers, historical

data for the Barnett Shale were utilized to estimate current and future activity in the Haynesville Shale (Grant et al., 2009).

Figure 2.2.2. Locations of active oil and gas wells in Texas (Source: TCEQ, http://www.tceq.state.tx.us/assets/public/implementation/barnett_shale/bs_images/txOilGasWells.png)

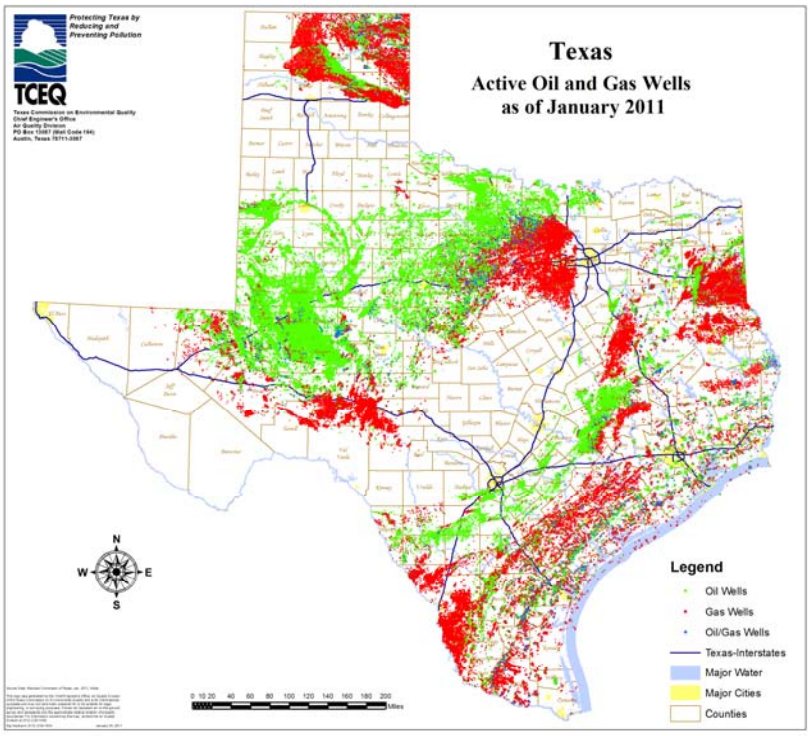
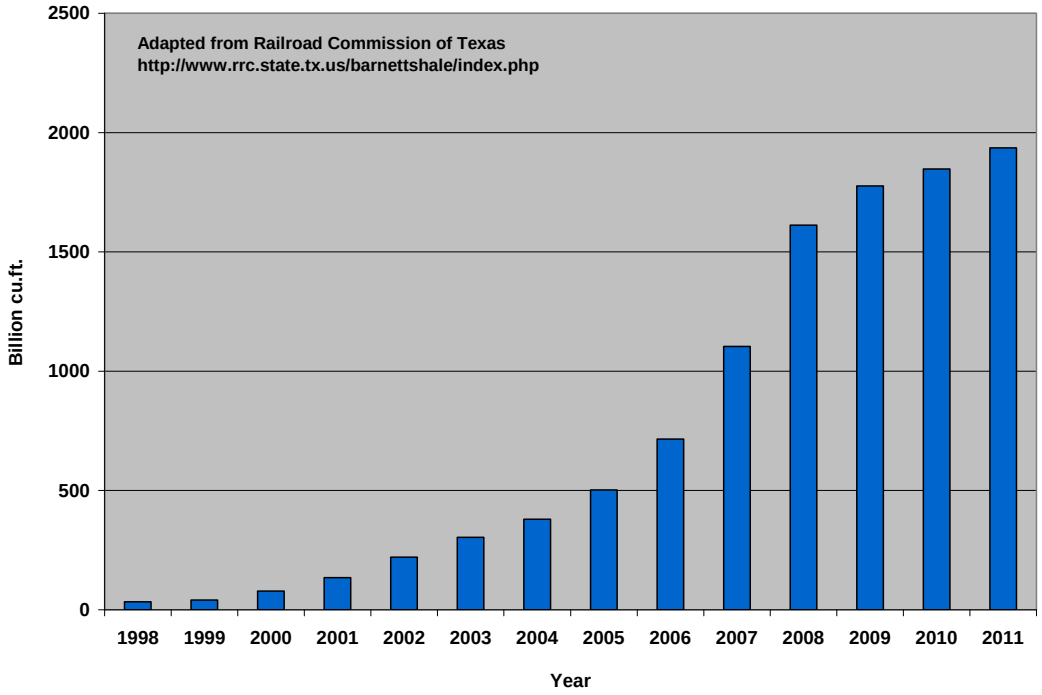


Figure 2.2.3. Barnett Shale natural gas production (billion cubic feet) for 1998 – 2011. Adapted from Railroad Commission of Texas (http://www.rrc.state.tx.us/ barnettshale/index.php).



Emissions inventories show that VOC is primarily associated with oil and condensate storage tanks and production/transmission fugitives in the Barnett Shale (Pring, 2010) and engine exhaust, pneumatic devices, and completion venting in the Haynesville Shale (Grant et al., 2009). An intensive study of oil and gas sources in the Forth Worth area found that the majority of VOC emissions occur at well pads and that compressor engines can be a significant contributor to emissions at natural gas-related facilities (ERG and SAGE, 2011). Important sources of emissions included faulty tank thief hatches and pneumatic valve controllers, both of which could be controlled under an appropriate maintenance program. Emission factors for VOC components are often not available or are associated with substantial uncertainty since the site-specific composition of the gas production stream is often unknown (Grant et al., 2009; Pring et al., 2010). Over the past few years, TCEQ has supported a number of field studies that have investigated emissions rates for specific VOC source types. These studies have included sampling of emissions from oil and condensate storage tanks (Hendler et al., 2009; Gidney and Pena, 2009; ENVIRON, 2010a), water storage tanks (ENVIRONb, 2010), fuel oil tanks (Boczek et al., 2010), and pipelines (ERG, 2010). The results of these recent Texas field studies are often limited in scope and large variability in results is sometimes indicated even at a single site. As such, additional work is necessary to evaluate the general applicability of these studies to other locations (e.g., ENVIRON, 2010c).

3. Recent field studies in the Barnett Shale have focused on the measurement of speciated hydrocarbon compounds associated with oil and gas production.

Several studies were conducted in the Fort Worth area during 2010 – 2011 that included the measurement of speciated hydrocarbons from natural gas production. The City of Fort Worth, City of Arlington and the Barnett Shale Energy Education Council (BSEEC) engaged TITAN

Engineering, Inc. to collect ambient air samples in the vicinity of two compressor stations and eight completed well pads projected to have the relatively high emissions rates of compounds such as benzene and formaldehyde as well as sulfur compounds (TITAN, 2010). Concentrations of compounds such as isopentane, xylene, and toluene were elevated downwind of one completed well site, including a maximum 24-hour average benzene concentration of 1.96 ppbv; however, the study concluded that natural gas operations at most sampling locations made a negligible contribution to downwind concentrations. A second study in Fort Worth focused on a number of potential sampling locations such as compressor stations, condensate tanks, and well pads (Zielinska et al., 2010). For a representative condensate tank adjacent to gas wells, the most abundant non-methane hydrocarbon species were ethane, propane, butanes, and pentanes; aromatic compounds such as benzene, toluene, and xylenes accounted for approximately 0.1-0.2% of non-methane emissions. There was no evidence suggesting that emissions from any natural gas facilities contributed to measured carbonyl compounds such as formaldehyde and acetaldehyde.

A third study performed in Forth Worth included the collection of more than 15,000 ambient air samples at eight different locations (ERG and SAGE, 2011). It was estimated that 98% of the associated hydrocarbon emissions were methane, ethane, propane, and butane, with the majority (75%) occurring at well pads. Individual compounds such as benzene, toluene, and propene were measured at most locations and times at concentrations above the detection limit; however, benzene concentrations were clearly elevated at a location nearby to a well pad and compressor station (average of 0.686 ppbv) compared to concentrations measured at the other sites (0.1 – 0.3 ppbv). Overall, the measurements demonstrated that carbonyl compounds such as formaldehyde (0.70 – 1.14 ppbv) were not unusually elevated when compared to levels measured by TCEQ elsewhere in Texas; however, results from dispersion modeling using measured and/or estimated emissions rates suggested that formaldehyde concentrations could be significant downwind of large (>1500 Hp) compressor engines so that further study was warranted.

During summer 2011, the University of Houston (UH) flew five complete low-level flights over the Barnett Shale to investigate the potential contribution of emissions associated with natural gas production to ozone concentrations (Alvarez et al., 2011). The results of the aircraft measurements did not indicate enhancements in ozone concentrations clearly associated with oil and gas emissions, but the UH team noted that the persistent southerly winds (~10 mph) may not have favored localized ozone production. On some occasions, elevated concentrations of reactive alkenes and formaldehyde (4-6 ppbv compared to background concentrations of 2-3 ppbv) were measured over the Barnett Shale, such as immediately downwind of a large compressor station in the Eagle Mountain Lake area. A FTIR and canister sampling analysis performed in the Barnett Shale by Johansson, et al. (2011) estimated significant rates of ethene emissions from large compressor stations (0.4 kg/hr) and from flash venting from a single condensate tank (2 kg/hr). High ethene concentrations have not been observed in other recent mobile sampling studies (e.g., Sullivan, 2010); however, given the large numbers of oil and condensate tanks and the potential importance of ethene in ozone formation, Johansson et al. (2011) suggested that additional studies to verify these results are warranted since flash venting is an important but intermittent emissions activity.

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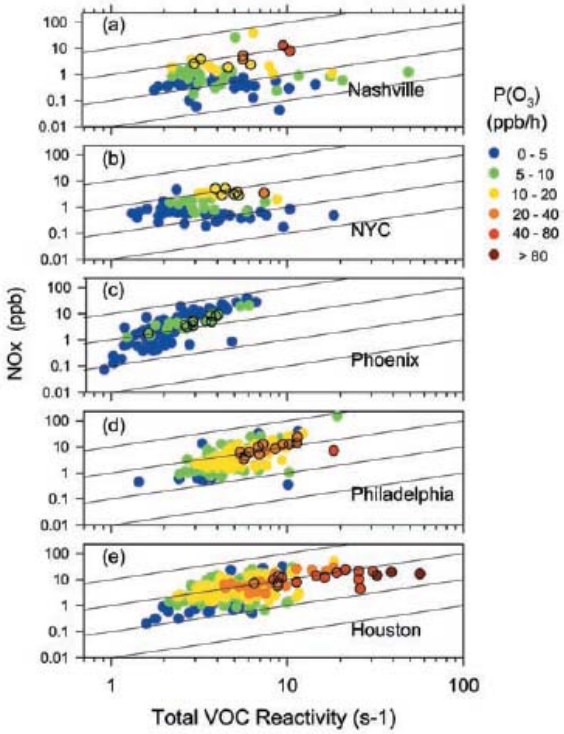
2.3 Tropospheric Chemistry

1. Ozone production rates and efficiencies in the Houston area are similar between the Texas 2000 and TexAQS II studies and indicate the continued importance of co-located emissions of highly reactive VOCs and NO_x in the Houston Ship Channel.

The proximity of NO_x and reactive VOC- rich plumes in Houston's extensive petrochemical complex lead to conditions that favor rapid ozone formation. During TexAQS2000, ozone production rates and ozone production efficiencies (OPE; the integrated number of O_3 molecules formed for each NO_x or observed ($\Delta O_3/\Delta(NO_y - NO_x)$), in plumes originating from the Houston Ship Channel industrial complex were found to be greater than those for the Houston urban core and others areas of the United States (Ryerson et al., 2003; Daum et al., 2003; Berkowitz et al., 2004; Kleinman et al., 2005). For example, comparison of ozone production rates for five U.S. cities by Kleinman et al. (2005), shown in Figure 2.3.1, indicates that the top 10% of the distribution of ozone production rates for Houston are substantially higher than those in Philadelphia, Phoenix, New York City, and Nashville.

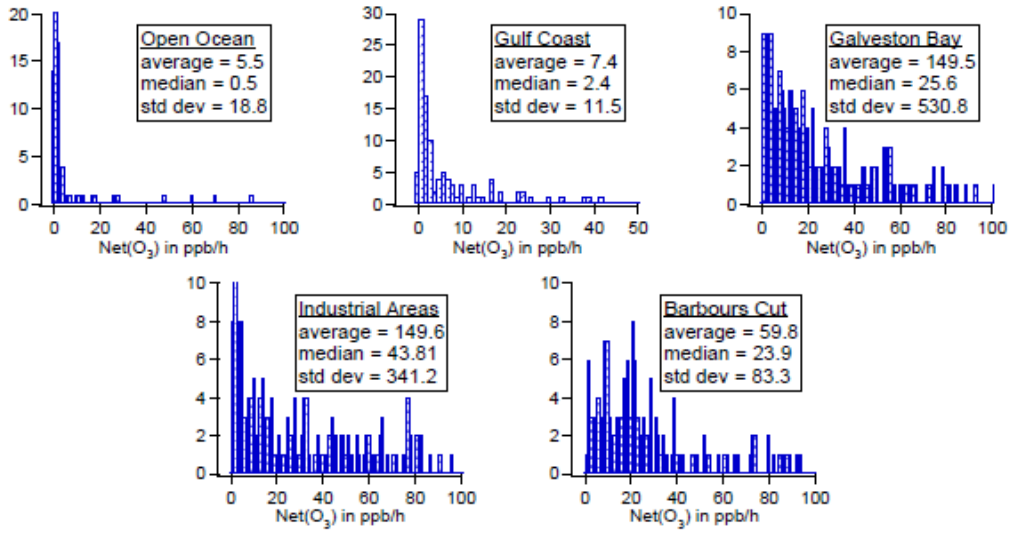
Figure 2.3.1. Ozone production rates for five U.S. cities in the style of an ozone isopleths diagram from Kleinman et al. (2005). Samples comprising the top 10% of the distribution in each city are outlined in bold.



During TexAQS 2000, strong spatial gradients in the rates of ozone formation were found across the Houston area (Berkowitz et al., 2005) with levels between 3 and 18 ppb h^{-1} over downtown Houston and 3 and 80 ppb h^{-1} in the eastern industrial plume (Daum et al., 2003). Net ozone production rates by Sommariva et al. (2011), shown in Figure 2.3.2, during TexAQS II varied spatially throughout the Houston/Galveston region and Gulf Coast. Ozone production

efficiencies from Neuman et al. (2009) and Cowling et al. (2007) obtained during TexAQS II were similar to those during TexAQS 2000, although maximum observed ozone concentrations and concentrations of highly reactive VOCs in Houston area have decreased over the same time period (Cowling et al., 2007). Similar to TexAQS 2000, ozone production during TexAQS II was found to be NO_x- limited with the influence of reactive hydrocarbons, especially alkenes and their oxidation products, to be of continued importance (Sommariva et al., 2011).

Figure 2.3.2. Frequency distributions of *Net*(O3) at locations during the NOAA R/V Brown cruise in the summer of 2006 as part of TexAQS II from Sommariva et al. (2011). The bin size is 0.1 ppb h-1 for the open ocean and 1 ppb/h for all other locations. Values on the y-axis are the number of data points in each bin.



2. Formaldehyde (HCHO) and nitrous acid (HONO) are radical precursors and their characterization is important for understanding atmospheric radical budgets.

Formaldehyde (HCHO) and nitrous acid (HONO) represent critical precursors for the formation of hydroxyl radical (OH). Atmospheric radicals, notably OH and hydroperoxyl radical (HO_2), which collectively are known as HO_x, have important roles in the formation of ozone and fine particulate matter. Over the past decade, field campaigns, such as the Second Texas Air Quality Study (TexAQS II) and 2006 TexAQS-II Radical and Aerosol Measurement Project (TRAMP), the Study of Houston Atmospheric Radical Precursors (SHARP) in 2009, and Formaldehyde and Olefins from Large Industrial Releases (FLAIR), have sought to improve the characterization of HCHO and HONO and the understanding of their influence on radical budgets, primarily in the Houston-Galveston-Brazoria airshed.

As described in detail by Seinfeld and Pandis (1998) and others (e.g., Parrish et al., 2012), formaldehyde originates from primary emissions sources as well as from secondary chemical production through the oxidation of biogenic and anthropogenic volatile organic compounds (VOCs), including alkenes, alkanes, and aromatic compounds. Secondary production of formaldehyde occurs via photochemical oxidation of precursor VOCs initiated by OH during the day; while at night, oxidation of precursor VOCs occurs via ozone and nitrate radical. Atmospheric loss of formaldehyde can occur by photolysis, reaction with OH, and deposition.

The relative contribution of primary sources and secondary chemical production to ambient formaldehyde concentrations and fluxes in Houston has been a topic of focus and divergent analysis during the past several years (Olaguer et al., 2009a; Olaguer et al., 2009b; Olaguer, 2010; Lefer et al, 2010a; Cowling et al., 2007; Parrish et al., 2012). Nonetheless, there is recognition by air quality stakeholders that understanding formaldehyde sources is critical to defining effective ozone control strategies in the Houston area. During TexAQS II, formaldehyde concentrations in excess of 50 ppb were observed in the Houston Ship Channel (Eom et al., 2008). In addition to vehicular emissions, which are common to many urban areas, industrial emissions from Houston's petrochemical complex are expected to have an important contribution to measured formaldehyde concentrations that may be atypical relative to other urban areas. Most recently, Parrish et al. (2012) undertook a reanalysis of the quantification of primary and secondary sources of formaldehyde in the Houston area using archived data from airborne, mobile, and elevated surface (i.e., Moody Tower) studies collected during 2000-2009 and a measurement constrained inventory based upon the 2005 National Emissions Inventory (NEI). In contrast to earlier studies, their analysis indicated that secondary production of formaldehyde from alkenes emitted by petrochemical facilities and on-road vehicles is the major source of formaldehyde in the Houston-Galveston-Brazoria area, as shown in Table 2.3.1 below; primary emissions from these sources represent a much smaller amount of formaldehyde in the region and are well represented by current emissions inventories. The authors argue that although there are cases where targeted reductions of primary formaldehyde emissions may be warranted, for example from the Texas City area where a single primary formaldehyde source was identified (Stutz et al., 2011), on-going efforts to reduce highly reactive VOC (HRVOC) emissions from Houston industrial facilities and VOCs from on-road vehicles should result in control of secondary formaldehyde formation in the region.

Table 2.3.1. Rates of secondary production and primary emissions (kmol h^{-1}) of formaldehyde in the Houston-Galveston-Brazoria area as 24-hour averages from Parrish et al. (2012). Uncertainties of primary emissions are estimated as ±30%.

Source	Secondary	Primary
Point sources	220 ± 90 (92 %)	10.6 (4 %)
On-road vehicles	6.5 ± 2.6 (3 %)	2.5 (1 %)
Total	227 ± 90	13.1
Percent total	95 ± 3 %	5 ± 3 %

As described by Lefer et al. (2011), the calculated HO_x production during SHARP was dominated by the photolysis of HONO in the early morning and by photolysis of O_3 in the midday; at night, OH production occurred mainly via O_3 reactions with alkenes. On average, the daily HO_x production rate was 23.8 ppbv day^{-1} in the region, of which 31% was from O_3 photolysis, 23% from HONO photolysis, 12% from HCHO photolysis, and 14% from O_3 reactions with alkenes (Lefer et al., 2011). Finlayson-Pitts (2003) and others (e.g. Wong et al., 2011) describe that HONO formation in the nocturnal boundary layer is thought to occur via heterogeneous conversion of NO_2 on humid surfaces. Accumulation of HONO in the nocturnal boundary layer and rapid photolysis at sunrise drives morning OH production. Recent measurements have indicated though that daytime observed HONO mixing ratios are often far

larger than the expected photostationary state with OH and NO in locations throughout the world (Wong et al., 2012; Acker et al., 2006a; Acker et al., 2006b, Zhou et al., 2007; Carter and Seinfeld, 2012). For example, HONO concentrations in Houston can exceed 2 ppb close to sunrise, and remain at several hundred ppt during much of the day with winds from the Houston Ship Channel (Olaguer et al., 2009b; Wong et al., 2012). During the SHARP campaign, Wong et al. (2012) found that observed HONO mixing ratios were often ten times larger than expected from the photostationary state with OH and NO.

Daytime formation mechanisms that account for enhanced HONO formation have been a focal point of studies over the past several years (e.g., Olaguer et al., 2009b; Wong et al., 2012). Both gas-phase and heterogeneous mechanisms on aerosol surfaces have been investigated, including gas-phase photolysis of ortho-nitrophenols (Bejan et al., 2006), heterogeneous conversion of NO_2 on fresh and aged soot particles (Zhang et al., 2009, Lefer et al., 2010b), humic acids, and soil surfaces (Stemmler et al., 2006), photolysis of surface adsorbed nitric acid (Zhou et al, 2011), and heterogeneous conversion of HNO_3 on the surface of primary organic aerosol (Ziemba et al., 2010). In the Houston area during SHARP, Wong et al. (2012) and Lefer et al (2011) found statistically significant vertical gradients of HONO throughout the day, with smaller mixing ratios aloft, and suggested that a likely source of daytime HONO could be photocatalytic conversion of NO_2 on the ground.

Although daytime mechanisms for HONO formation have been a subject of exploration, it is evident that uncertainty remains and further studies are needed. As further progress is made, incorporation into air quality models will be important. For example, comparisons of CAMx predictions by the TCEQ with radical budgets obtained by Mao et al. (2009) and Chen et al. (2009) during the TRAMP study indicated good agreement in HOx radical production from HCHO photolysis, but poor agreement in HOx formation from HONO photolysis (http://www.tceq.state.tx.us/assets/public/implementation/air/sip/hgb/hgb_sip_2009/09017SIP_ado_Appendix_I.pdf). Czader et al. (2010) found the incorporation of HONO formation via heterogeneous chemistry in CMAQ simulations improved the correlation with measured values in the Houston area.

3. Nitryl chloride ($ClNO_2$) can affect tropospheric oxidation capacity and ozone formation in coastal and inland regions.

Dinitrogen pentoxide (N_2O_5) is a nocturnal reservoir of NO_x, formed from the reaction of nitrate radical (NO_3^-) and NO_2. Heterogeneous reaction of N_2O_5 can proceed via two pathways: (1) hydrolysis to form soluble nitrate, the rate of which depends on the availability of aerosol surface area and on the heterogeneous uptake coefficient of N_2O_5 to aerosol (Brown et al., 2009; Parrish et al., 2009), or (2) reaction with chloride to form nitryl chloride and nitrate, which depends on, among other factors, particulate chloride (PCl) availability (Finlayson-Pitts et al., 1989; Behnke et al., 1997; Kercher et al., 2009; Osthoff et al., 2008; Thornton et al., 2010). At sunrise, $ClNO_2$ photolysis can affect the cycling of oxidants by providing a source of chlorine atoms that enhance VOC oxidation (Osthoff et al., 2008; Knipping and Dabdub, 2003; Tanaka et al., 2003). During the past several years, the presence of nitryl chloride has been characterized in the coastal environment of Houston during the 2006 TexAQS/Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS) (Osthoff et al., 2008), as well as for the inland region of Boulder, Colorado (Thornton et al., 2010).

Simon et al. (2009) used the Comprehensive Air Quality Model with extensions (CAMx) to examine the effects of observed nitryl chloride concentrations on ozone chemistry in southeast

Texas. Predicted $ClNO_2$ increased total reactive chlorine mass by 20–40%. Modest increases in predicted ozone concentrations (up to 1.0–1.5 ppb when baseline 1-h average ozone concentrations were between 60 and 85 ppb) were found to be affected by vertical dispersion and local VOC and NO_x mixtures. These results suggested the potential importance of NO_x emissions reductions on chlorine cycling.

Recently, Koo et al. (2012) undertook an analysis of nitryl chloride formation in Houston, using data from TexAQS II and SHARP (on the top of Moody Tower), and in Los Angeles, using data from the CalNex study in 2010. In addition, the authors implemented the chemistry in CAMx and conducted simulations that included reactive and particulate chloride emissions inventories. Overall, CAMx simulated, but underpredicted, $ClNO_2$ formation, and underpredicted HCl and PCl, which was thought to be due to missing sea salt aerosols in the model. Further CAMx studies suggested that reaction of a fraction of coarse mode sea salts in addition to fine mode sea salts, in combination with a reduced dry deposition velocity for HCl, would improve model performance. The study suggested the need for additional measurements of nitryl chloride and related chlorine species in coastal and inland areas, better estimation of the HCl dry deposition velocity, and inclusion of other chlorine/chloride emission sources in the inventory.

4. NO_x sink and recycling reactions should be represented in atmospheric chemical mechanisms for photochemical modeling of ozone.

As described by Yarwood et al. (2012a), most VOCs can remove NO_x by forming NO_x sink compounds, including organic nitrates, peroxy nitrates, or nitro compounds, that reduce the availability of NO_x for ozone formation. These NO_x sink species may eventually react to return NO_x back to the atmosphere, known as NO_x recycling, potentially causing additional ozone production in NO_x-limited regions. Reactions of NO_x-sink compounds that return sequestered NO_x to an active form are referred to as NO_x-source reactions.

Using novel environmental chamber experiments performed at the University of California at Riverside, Yarwood et al. (2012a) demonstrated the importance of NO_x sinks for toluene and isoprene. The product o-cresol and furan (a precursor to 2-butenedial, which is a major ring-opening product of toluene) had an important influence in producing the observed NO_x sink for toluene. Experimental data were used to test and to improve the mechanisms for isoprene and aromatics in version 6 of the Carbon Bond mechanism (CB6), resulting in the creation of a revised mechanism known as CB6r1. Although CB6r1 performed better than CB6 in simulating experiments for toluene, xylenes and mixtures combining aromatics with other VOCs, aspects of the aromatics chemistry are still not fully understood. Experiments strongly supported the occurrence of NO_x-recycling in the photolysis reactions of the NO_x-source compounds isopropyl nitrate, isobutyl nitrate and 2-nitrophenol; CB6r1 includes NO_x-recycling from photolysis of alkyl nitrates and nitrocresols. Additional experiments are needed to test for the occurrence of NO_x recycling from alkyl nitrates larger than isopropyl and isobutyl.

5. Biogenic VOCs have an important contribution to regional atmospheric chemistry in eastern Texas. Ambient measurements, characterization of land use and land cover, and modeling of biogenic emissions have continued to evolve over the past decade.

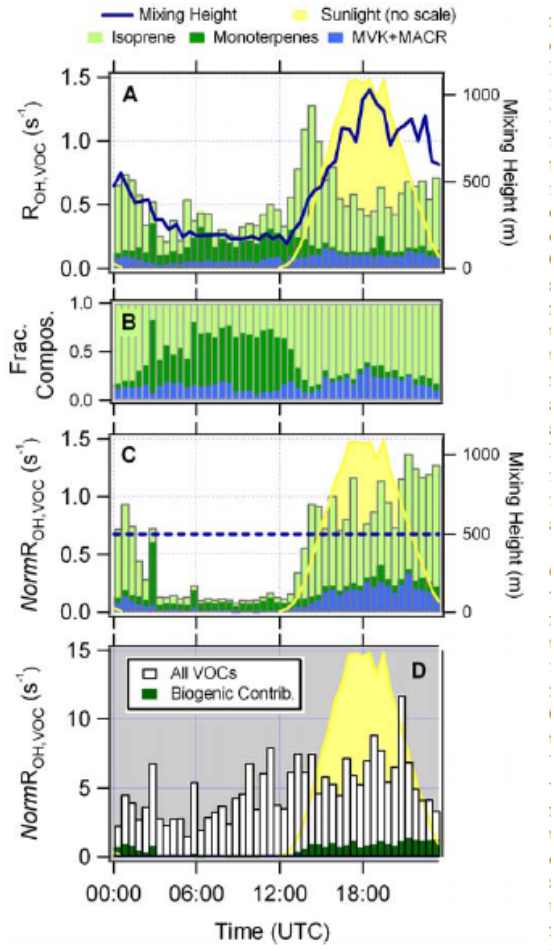
Biogenic VOCs, including isoprene and monoterpenes, and their oxidation products have important influences on the formation of ozone and secondary organic aerosol. Emissions of biogenic VOCs exhibit strong diurnal variability with temperature and sunlight and spatial gradients due to differences in land use/land cover. Figure 2.3.3 from measurements by Gilman

et al. (2009) aboard the NOAA R/V Brown during TexAQS II/GoMACCS, shows the relative fraction and diurnal profiles of isoprene, its oxidation products (methyl vinyl ketone and methacrolein), and monoterpenes (alpha-pinene, beta-pinene, and limonene), as well as the hydroxyl radical reactivity (R_{OH}) as a quantification of the contribution to potential ozone formation in the Houston-Galveston-Brazoria area. Similar to observation during TexAQS 2000, isoprene had the largest overall contribution to biogenic $R_{OH, VOC}$; during the afternoon, biogenic VOCs accounted for up to 20% of the VOC reactivity (Gilman et al., 2009).

Using a regional chemical transport model with emissions during an eight day period of TexAQS 2000, Li et al. (2007) found that isoprene emissions had an important role in ozone formation when the ozone plume occurred in the afternoon over the urban Houston area. When isoprene emissions were decreased or increased by 50%, predicted ozone concentrations decreased or increased by 5–25 ppb over the urban Houston area, but less than 5–10 ppb over the Houston Ship Channel industrial area. Differences in ozone concentrations were primarily attributed to local emissions of isoprene, but transport from regions north of Houston were important on selected episode days (Li et al., 2007).

Accurate local and regional characterizations of land use/land cover data are essential for estimating biogenic emissions and have been an area of research for the State of Texas for the past 10 – 15 years (e.g., Wiedinmyer et al., 2001; Feldman et al., 2010; Popescu, 2010). In recent revisions to the State Implementation Plans for the Dallas Fort Worth and Houston-Galveston-Brazoria area, the TCEQ has utilized the Global Biosphere Emissions and Interactions System (GloBEIS3.1), available from http://www.globeis.com/, for estimating biogenic emissions (http://www.tceq.texas.gov/assets/public/implementation/air/sip/dfw/ad_2011/AppB_EI_ado.pdf ;http://www.tceq.state.tx.us/assets/public/implementation/air/sip/hgb/hgb_sip_2009/09017SIP_ado_Appendix_B.pdf.). Comparisons of predicted emissions estimates from GloBEIS, the EPA's Biogenic Emissions Inventory System 3 (BEIS3), and the Model of Emissions of Gases and Aerosols from Nature version 2 (MEGAN2), with measurements of isoprene and monoterpenes have generally shown agreement within a factor of two (Song et al., 2008; Warneke et al., 2010). Drought, the influence of inter-annual variability in emissions, and evaluation of inventories over large spatial scales (Warneke et al., 2010) remain areas for further research.

Figure 2.3.3. (a) Average diurnal profiles of mixing height, sunlight, and $R_{OH,VOC}$ for all biogenic VOCs for the Houston-Galveston-Brazoria area; (b) the fractional contribution of isoprene, monoterpenes, and methyl vinyl ketone (MVK) and methacrolein (MACR) to $R_{OH,VOC}$; (c) the average diurnal profile of *Norm*$R_{OH,VOC}$ for the biogenics; (d) a comparison of the average diurnal profile of *Norm*$R_{OH,VOC}$ for all VOCs (biogenic + anthropogenic + oxygenated VOCs) and the contribution solely from biogenic VOCs from Gilman et al. (2009). *Norm*$R_{OH;VOC}$ is the normalized OH reactivity for which the dependence of VOC mixing ratios on mixing heights is considered by normalization with a constant mixing height of 500 m.



6. Characteristics of fine particulate matter composition and sources between the time periods of the TexAQSII, GoMACCS, and SHARP campaigns and TexAQS 2000 have remained consistent. Houston's industrial complex contributes to the formation of organic-rich aerosols at levels above that typical of urban areas and have been associated with emissions of hydrocarbons with high SOA-forming potential, such as aromatics.

Understanding particulate matter composition and concentrations is of concern not only due to direct human health impacts and visibility impacts, but also because chemical reactions at aerosol surfaces influence ozone formation, and these reactions depend on particle surface area

(particle size) and particle composition. A variety of studies have been conducted to better characterize particulate matter size, composition and concentrations in Texas. TexAQS 2000 coincided with Gulf Coast Aerosol Research and Characterization Program (GC-ARCH) or the Houston Supersite which had the aim of improving the understanding of the concentrations, spatial and temporal variability, composition, and sources of fine particulate matter in southeastern Texas (Allen, 2005). A number of findings emerged from these studies. Daily average fine particulate matter concentrations ($PM_{2.5}$) were remarkably consistent spatially and seasonally in southeast Texas, ranging between 10 and 15 $\mu g/m^3$. However, extreme values of $PM_{2.5}$ mass concentrations showed more variability with a number of instances when localized, high concentrations were observed. Sulfate, ammonium, organic carbon (OC), and elemental carbon (EC) were the major constituents of $PM_{2.5}$ in southeast Texas, and relative concentrations of these components were, on average, also spatially homogeneous. Sulfate accounted for approximately 40% and OC for approximately 25% of the fine particulate mass. OC to EC ratios in southeast Texas were generally well above the value assumed for primary emissions, suggesting that much of the OC may be due to secondary organic aerosol (SOA) formation. Primary sources of $PM_{2.5}$ were associated with mobile sources, cooking, burning, dust, and industrial sources. Sources of secondary $PM_{2.5}$ precursors associated with inorganic sulfate and ammonium were transported from the interior continental United States, SO_2 from electricity generation, and livestock and domestic activities, respectively, and those associated with secondary organic aerosol included industrial point sources, mobile sources, area/non-road sources, and biogenic sources (notably in forested areas north and southwest of Houston urban core). Particle size distributions were not spatially homogeneous; industrial sites have higher concentrations of ultrafine particles than more residential sites, even on a seasonal basis.

Since the 2000 study, other studies have sought to further the characterization of particulate matter in southeastern Texas and/or to examine differences over time. Yu and Cowin (2009) found that the averages and ranges of OC, EC, and total carbon (TC) during SHARP were comparable to observations in the early 2000s (Allen, 2004; 2005). The average OC to EC ratio of Yu and Cowin (2009) was 6.9, indicating that secondary organic aerosols were a component in the carbonaceous aerosols observed in Houston; OC generally peaked concurrently with an ozone event (defined as concentrations > 75 ppb). Average EC was fairly low during SHARP similar to the findings of Allen (2004). Five types of particles were observed including 1) sulfate (primary and secondary); 2) mineral dust; 3) soot; 4) sea salt; and 5) mixed sulfate and sea salt, which varied in composition, size, shape, morphology, and mixing state.

Bahreini et al. (2009) measured organic aerosol (OA) in urban plumes from Houston and Dallas/Fort Worth as well as in industrial plumes in the Houston area during TexAQS II. Consistent with the TexAQS-2000 study, observations showed a greater amount of aerosol mass downwind of the industrial centers compared to urban area. Bahreini et al. (2009) found that observed ratios of the enhancement above background in OA, ΔOA, to the enhancement above background in carbon monoxide (CO), ΔCO, downwind of urban centers of Houston and Dallas/Fort Worth were within a factor of two of the same values in plumes from urban areas in the northeastern United States by de Gouw (2008) indicating similar concentrations of precursors and chemical processes. In Houston Ship Channel plumes, $\Delta OA/\Delta CO$ exceeded that in the urban areas by factors ranging from 1.5 to 7. Initial carbon mixing ratios of aromatics in the urban plumes were approximately a factor of two *lower* than those in the Houston Ship Channel plumes, which Bahreini et al. (2009) noted had at least twice the potential for SOA formation from these precursors under similar NO_x conditions.

Bates et al. (2008) examined aerosol sources and transformation processes in the Houston-Galveston-Gulf of Mexico region, aboard the NOAA R/V Ronald H. Brown during TexAQS II/GoMACCS 2006. Aerosol measured in the Gulf of Mexico during onshore flow was highly impacted by Saharan dust and possibly ship emissions (acidic sulfate and nitrate). Mean and median mass concentrations of the total submicrometer and supermicrometer aerosol were higher than expected for marine atmospheres. As the background aerosol moved onshore, local urban and industrial sources added an organic rich submicrometer component (66% particulate organic matter, 20% sulfate, 14% elemental carbon) but no significant supermicrometer aerosol. Bates et al. (2008) found that these air masses, with minimal processing of urban emissions contained the highest $SO_2/(SO_2 + SO_4^{=})$ ratios and the highest hydrocarbon-like organic aerosol (i.e., non-oxygenated) to total organic aerosol ratios. In contrast, during periods of offshore flow, the aerosol was more processed and much richer in oxygenated organic aerosol.

7. The overnight transport of plumes from urban, petrochemical, and coal-fired power plants can potentially affect the air quality in regions several hundred kilometers downwind the next day.

Atmospheric chemical processes and transport that occur at night can influence next day ozone and fine particulate matter formation on urban and regional scales. Studies during TexAQS II and more recently have sought to further the understanding of nighttime plume chemistry and transport and the impacts of emissions sources and controls.

Two such studies utilized nighttime flights of the NOAA WP-3D aircraft during TexAQS II to investigate nocturnal VOC oxidation by NO_3. Brown et al. (2011) conducted a regional analysis to quantify loss rates and budgets for both NO_3 and highly reactive VOC downwind of Houston industrial, urban, and rural areas. Net NO_3 radical productions rates were large (1–2 ppbv h^{-1}) within NO_x-containing plumes of industrial origin, but generally smaller in rural plumes and plumes that originated from urban Houston and were transported downwind. NO_3 was lost primarily to reaction with VOCs, with the sum of anthropogenic VOCs (30–54%) and isoprene (10–50%) as the largest contribution; alkenes, and to a lesser extent, aromatics, were the most significant anthropogenic VOC contribution. NO_3 was 3 to 5 times more important than O_3 as a nighttime oxidant of VOCs for the flights in the Houston area. Yarwood et al. (2012b) analyzed nighttime vertical profiles during missed approaches, takeoffs and landings at airfields in and around the Houston urban area. Nocturnal boundary layer depths varied between 100 – 400 m, with overlying residual layer depths of 0.8 – 1.5 km. Ozone was never titrated to zero by surface level NO_x emissions during these aircraft measurements, and nighttime oxidative and heterogeneous chemistry was active. Findings regarding nocturnal VOC oxidation and nitrate radical production were consistent with those reported by Brown et al. (2011). Both studies found nighttime NO_x loss through N_2O_5 heterogeneous uptake to be modest, but subject to uncertainty due to the uptake coefficient for N_2O_5. In previous analyses of the P-3 flights, Brown et al. (2009) determined reactive uptake coefficients for N_2O_5, $\gamma(N2O5)$, were generally in the range $0.5–6 \times 10^{-3}$ and were substantially smaller than current parameterizations used for atmospheric modeling; N_2O_5 uptake represented a significant, but not dominant, fraction of the NO_3 loss budget (Brown et al., 2011). Brown et al. (2011) found that loss of NO_3 to nighttime reactions with peroxy radicals was small, but also subject to uncertainty due to the lack of peroxy radical measurements.

Zaveri et al. (2010) examined the transport and chemical processing of a photochemically aged plume that contained a mixture of urban and petrochemical industrial emissions located north of Houston metropolitan area under southerly flow conditions across the state on July 26, 2005 using measurements from a Twin Otter aircraft. Enhanced levels of olefins and acetaldehyde of petrochemical industrial origin were observed in this plume at sunset and 8 hours later. A constrained plume modeling analysis indicated that small amounts of NO_x (<1 ppbv) were present in the photochemically aged plume at sunset and were converted to nitric acid, organic nitrates, and peroxy acyl nitrates via reactions of NO_3 radicals with olefins and aldehydes and subsequent radical chemistry at night. Predicted NO_3 and N_2O_5 mixing ratios were small, indicating fast loss of NO_3 due to its reactions with VOCs. The N_2O_5 heterogeneous uptake coefficient was likely on the order of 0.001 for Houston urban/industrial aerosol, but direct measurements of NO_3, N_2O_5, and HNO_3 were not made.

In addition to plumes that originate from urban and industrial areas, plumes from coal-fired power plants, which are frequently located in relatively rural areas, are also subject to nocturnal transport and chemical processing that may affect air quality downwind. Federal regulations, such as the recent Cross-State Air Pollution Rule (CSAPR), have aimed to reduce emissions of NO_x and SO_2 from power plants that contribute to ozone and fine particulate matter formation. Recently, Yarwood et al (2012b) analyzed the nighttime NOAA WP-3D aircraft intercepts, described above, of the plumes from two different Texas power plants, Oklaunion near Wichita Falls and W. A. Parish near Houston. The plants have different NO_x emissions due to their control technologies. In 2006, the Oklaunion plant had low NO_x burner technology, but not selective catalytic reduction (SCR). In contrast, the W. A. Parish plant coal-fired units had both technologies, resulting in lower NO_x emissions. Yarwood et al. (2012b) found that these differences in NO_x emissions led to differences in the titration of ambient ozone. The plume from Oklaunion had full titration of ozone through 74 km/2.4 hours of downwind transport that suppressed nighttime oxidation of NO_2 to higher oxides of nitrogen across the majority of the plume. The plume from W.A. Parrish did not have sufficient NO_x to titrate background ozone, which led to rapid nighttime oxidation of NO_2 during downwind transport. Empirical plume modeling suggested that NO_x controls may not only reduce emissions directly, but may also lead to an additional overnight NO_x loss of up to 73% for the sample conditions. Ambient ozone concentrations coincident with the Parrish plume, on the night that the measurements were collected were relatively high, which likely added to the production of NO_3 and the additional overnight NO_x loss. The results implied that power plant NOx emissions controls may have larger than expected impacts on next-day downwind ozone production following nighttime transport.

The findings from the study of Yarwood et al. (2012b) resulted in improvements to the Plume-in-Grid (PiG) formulation in CAMx Version 5.40, released in October 2011. These modifications will likely improve, although not completely, replicate the measured nighttime plume spread, which was minimal. PiG puff growth rates were modified to ignore growth contributions from horizontal and vertical shear during stable/nighttime conditions. Shear effects remain during neutral/unstable/daytime conditions. Minimum limits on vertical diffusivity, turbulent flux moments, and nighttime planetary boundary layer (PBL) depths were reduced. With these improvements, PiG puff behavior will change potentially significantly at night and above the boundary layer, usually leading to longer lifetimes.

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2.4 Meteorology

1. Regionally high ozone episodes in Texas most commonly occur during synoptic (i.e., large-scale) weather patterns that are consistent with the long-range transport of elevated background concentrations of ozone and/or its precursors into Texas.

Nielsen-Gammon (2005) showed that background ozone concentrations have a strong seasonality with peaks during the spring and late summer/early fall. This strong seasonality is associated with the frequency of occurrence, strength, and location of anticyclones that impact Texas weather. Cluster analyses of synoptic weather conditions showed that a center or ridge of high pressure in the lower troposphere is commonly located to the west or north of Houston during high ozone episodes (Rappenglück et al. (2008); Ngan and Byun (2011)). These weather patterns are associated with long-range northerly or easterly transport of continental air, which is often characterized by elevated ozone and/or its precursors, into Texas (e.g., Olaguer et al., 2009; McGaughey et al., 2010). These large-scale high pressure systems are sometimes associated with fair weather and light wind speeds that enhance the amount of locally-formed ozone as well. High ozone days during September most often occur in a postfrontal environment (Tobin and Nielsen-Gammon, 2010), which can increase background ozone in Houston from 30 ppbv to 60-70 ppbv (Rappenglück et al. (2008)). Ozone contributions associated with regional as well as local (e.g., sea breeze, nocturnal low-level jets, urban) circulation features must be correctly simulated in air quality models to accurately predict the magnitude and spatial extent of high ozone concentrations (Olaguer et al., 2009).

2. Mesoscale (i.e., local-scale) atmospheric circulation features play an important role during high ozone episodes in Texas.

The evolution and development of the sea breeze plays a dominant role in high ozone episodes along the Texas coast. Based on findings from TexAQS I, the worst ozone exceedances in HGB were associated with local stagnation associated with reversals of the wind direction along the sea-breeze front (Nielsen-Gammon et al., 2005; Banta et al., 2005; Darby, 2005). Analysis of TexAQS II data found the sea breeze reversal combines with the larger-scale circulation to form a wind pattern known as the coastal oscillation (Olaguer et al., 2009) and the interaction of the mesoscale sea-breeze circulation and synoptic-scale flows determine where ozone and its precursors are accumulated or diluted. A second complex coastal circulation is the nocturnal sea-breeze low level jet, which typically forms a few hundred meters above the surface. Ship-based Doppler measurements during TexAQS II found that strong jets were associated with low ozone concentrations the following afternoon in Houston while weaker jets during periods of northerly or easterly large-scale flow were associated with higher next-day ozone concentrations (Tucker et al., 2010). Observations at an instrumented tower in Moody, Texas found evidence of inland nighttime jets that only occasionally brought high ozone concentrations into the area during the summer but were associated with high ozone pulses more frequently during other seasons (Andrews et al., 2010; Oltmans et al., 2010). A third important local circulation feature associated with high ozone concentrations in Texas are stagnation zones along stationary fronts. Data collected in the vicinity of DFW during TexAQS I/II found that local pollution accumulated in zones of light winds and subsidence along the frontal trough (McNider, et al., 2009). The local circulation features in these “dead zones” may also be associated with re-entrainment of aged pollution aloft that may have originated from distant sources (Olaguer et al., 2009).

3. The evolution and development of the nighttime and daytime planetary boundary layer (PBL) influences the diurnal variability in surface ozone concentrations.

The PBL height effectively establishes a cap to near-surface vertical atmospheric mixing and defines the volume of air into which emissions from surface sources are well-mixed compared to the overlying free troposphere. A number of studies have demonstrated that afternoon mixing heights on high ozone days in Texas tend to be relatively high (Cowling et al., 2007; Rappenglück et al., 2008; Nielsen-Gammon, 2008) suggesting that the impact of concurrent meteorological conditions (such as light wind speeds) offset the diluting effect of increased near-surface dilution volume. In addition, the afternoon vertical growth of the PBL may mix to the surface relatively high concentrations of ozone and/or its precursor compounds aloft that were transported into Texas from other continental areas (Olaguer et al., 2009; Schade et al., 2011). Although rapid growth of the morning PBL causes dilution of freshly-emitted precursors and also alters chemical pathways (Olaguer et al., 2009), near-surface pollutants from the previous day trapped above the nocturnal boundary layer have been shown to explain 60-70% of the variability in afternoon mixed layer ozone concentrations (Morris, et al., 2010). The PBL in coastal areas is especially spatially and temporally complex, impacted by differences associated with both land and marine environments (e.g., Banta et al., 2005; Darby, 2005). Emissions that flow offshore into the shallow near-surface layer can result in very high ozone concentrations that return inland with little initial dilution (Banta et al., 2005).

4. Observations and results from TexAQS I/II have guided modeling and sensitivity studies designed to improve the performance of meteorological modeling applications in Texas.

The accurate simulation of the temporal and spatial evolution of important atmospheric features such as the boundary layer and sea breeze circulations require that vertical mixing and land surface processes be properly represented in meteorological models. Numerous studies have evaluated treatments of vertical diffusion and convective mixing in support of Texas air quality modeling applications in recent years (Emery et al., 2009; Hu et al., 2010a; ENVIRON, 2011) and have indicated that model performance is sensitive to the choice of PBL scheme. One of the most successful efforts to reduce uncertainties in the simulation of daytime lower-tropospheric winds and PBL heights is the assimilation of radar wind profiler data (e.g., Nielsen-Gammon et al., 2007; Zhang et al., 2007; Stuart et al., 2007) that remains essential for good meteorological modeling performance (TCEQ, 2011). Using a TexAQS II episode and a technique known as the Ensemble Kalman Filter, better agreement was obtained between observations and predictions of near-surface temperatures and wind profiles suggesting that additional experiments were warranted (Hu et al., 2010b).

Land-surface modeling (LSM), which fully simulates the energy exchange between the land/water surface and atmosphere, presents challenges in Texas areas. Studies by Misenis and Zhang (2010) using WRF/Chem found that meteorological predictions showed stronger sensitivity to the choice of LSM than to PBL schemes. Results also indicated that using more physically-complex model configurations (such as 2-way nesting or reduced horizontal grid spacing) did not necessarily provide more accurate results. Cheng et al. (2008) modified the LSM and PBL schemes in MM5 to utilize the Texas Forest Service land use and land cover dataset. Improvements in boundary layer mixing conditions and local wind patterns in the Houston Ship Channel demonstrated the importance of high resolution observational datasets to model performance. Using a single-layer urban canopy model (UCM), Lee et al. (2011) found

that more realistic prediction of sensible and latent heat fluxes was associated with improved replication of diurnal profiles of temperature and PBL height over the Houston area. Although wind field performance was not substantially different between UCM, LSM, and modified LSM simulations, the results suggested that more accurate representation of the surface and explicit parameterization of physical processes is necessary for improvements in atmospheric modeling over urban areas.

5. The greatest differences in observed and predicted ozone concentrations in SIP modeling tend to occur when clouds are under-predicted (TCEQ DFW SIP, 2011).

Photochemistry is strongly influenced by clouds, which can both attenuate and enhance the actinic flux of ultraviolet (UV) radiation (e.g., Emery et al., 2010). Accurate simulation of cloud cover is necessary to simulate photolysis rates, and ozone predictions are very sensitive to photolysis rates (Byun et al., 2007; TCEQ, 2011). In addition, clouds impact the rate and depth of vertical mixing in the lower troposphere (e.g., Langford et al., 2010) as well as the chemical composition of the atmosphere (e.g., Flynn et al., 2010). The vertical depth and spatial/temporal distribution of clouds are some of the most difficult meteorological phenomena to accurately simulate (Pour-Biazar et al., 2007; Emery et al., 2010). Spurious thunderstorms and clouds are also common in air quality modeling (Olaguer et al., 2009), suggesting the need for flexibility in the selection of modeling parameterizations (TCEQ, 2011).

Pour-Biazar et al. (2007) used GOES satellite data to correct the photolysis rates in CMAQ for a TexAQS I episode. The results demonstrated that clouds increased the lifetime of ozone precursors leading to increased ozone production and improvements in model performance. A study by ENVIRON (2010) found that surface ozone predictions in CAMx were more responsive to the placement of sub-grid clouds than how photolysis rates were applied (TCEQ, 2011). Efforts by Pour-Biazar et al. (2011) to develop a GOES cloud assimilation technique in WRF relied on adjustments to the modeled vertical velocities to force better agreement between predicted and satellite-observed cloudiness. Although the study showed improvements of 7-10% in cloud prediction, additional work is needed.

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2.5 Transport of Ozone and Its Precursors/Modeling

1. The long-range transport of ozone is an important contributor during periods of high ozone concentrations throughout the eastern half of Texas.

Using a subset of monitoring stations surrounding the metropolitan area, Nielsen-Gammon (2005) found that background ozone concentrations in Houston have a double peak, with high levels in the spring and late summer/early fall, and estimated that the background and local contributions during summer were roughly equal. For Dallas, Tobin and Nielsen-Gammon (2010) found that average background contributions during summer were greater than the average local contributions. Kemball-Cook et al. (2009) noted that ozone transported into Houston and Dallas was 55-60 ppb on many study days during the TexAQS I and II programs. Using ozonesonde data, Rappenglück et al. (2008) estimated that background ozone levels in Houston ranged from 30 ppbv during maritime (e.g., southerly) flow to 60-70 ppb during continental (e.g., northerly or easterly) flow. Langford et al. (2009) found that nearly 84% of the variance in daily maximum 8-hour ozone concentrations among 30 monitors in Houston was attributed to changes in the regional background due to long-range transport. Regional transport may play an even larger role during high ozone episodes in other areas of Texas. For example, McGaughey et al. (2010) estimated that background ozone in Austin accounted for approximately 85% of the maximum monitored levels. Schade et al. (2011) showed that elevated ozone coincided with northerly flow following the passage of cold fronts through College Station and background ozone concentrations were estimated to be as high as 80 ppb.

Aircraft studies are generally consistent with the background ozone results based on ground monitoring data. Kemball-Cook et al. (2009) found that background ozone into Houston contributed, on average, 50% and 66% of the total ozone on 8-hour exceedance days during 2000 and 2006, respectively. In DFW, background ozone accounted for up to 72% of the maximum downwind ozone concentration. Based on data obtained by Alvarez et al. (2011) on five sampling days in the DFW area during summer 2011, background ozone varied between 40% and 66%. The use of satellite data to investigate long-range transport has been demonstrated by studies such as McMillan, et al. (2010). Retrievals of tropospheric CO from NASA's Atmospheric InfraRed Sounder (AIRS) tracked smoke from fires in the Pacific Northwest to Houston and additional analyses suggested these smoke emissions contributed to increases in observed Houston ozone concentrations.

Numerous modeling and source apportionment techniques have been used to estimate the contributions of Texas ozone from specific source regions. Pierce et al. (2009) quantified the contributions of background ozone production in Houston and Dallas by combining modeling and satellite observations. The majority of high ozone events occurred during periods of elevated background ozone production owing to NOy enhancements from emissions in the Southern Great Lakes for Houston and from within Chicago and Houston for Dallas. Average ozone production in excess of 15 ppbv/day could occur during continental-scale transport. Kim et al. (2009) using CAMQ and HDDM found that long-range east-northeasterly winds favored interstate transport into Dallas during two 2005 episode periods. The CAMx and HDDM modeling indicated that NOx emissions in neighboring states (e.g., Oklahoma, Arkansas, Louisiana, and Mississippi) contributed approximately 10 ppb, on average, while VOC emissions from upwind states had a negligible impact. Using CAMx and APCA, Kemball-Cook et al. (2009) found similar results in terms of the frequently identified upwind states. Zhang and Ying (2011) found that local emissions had the largest contribution to Houston ozone but that ozone

from upwind sources could account for 20-50% of the overall average daytime ozone concentration in HGB and BPA. Southeastern states were important upwind source regions, and even northeastern states could have 20-25 ppb contributions during favorable transport conditions.

2. The amount of ozone transport between Texas metropolitan areas can be significant on some days.

The results of photochemical modeling studies have supported the importance of intrastate transport between Texas areas. Zhang and Ying (2011) used an episode from 2000 to investigate source attribution of ozone concentrations in HGB/BPA. They showed that contributions from other counties in Texas accounted for 7-36% of HGB/BPA predicted ozone. Zero-out studies that quantified the impact of Houston emissions on other Texas areas found that transported Houston ozone could increase predicted concentrations in Austin or DFW by 10-20 ppbv (Dionisio, 2010). DFW SIP modeling (TCEQ, 2011) results for six representative high ozone days demonstrated that non-DFW Texas emissions contributed approximately 18%, on average, to simulated ozone concentrations at the Denton monitor, with daily contributions ranging between 4 ppb and 26 ppb. Kim et al. (2009) found that interstate and within-Texas contributions dominated the ozone concentrations accounting for about half of the ozone at the DFW-area Kaufman monitor. The intra-state (local and other Texas areas) contribution from NOx emissions sources could exceed 15 ppbv.

High ozone episodes in Texas are often characterized by large-scale flow patterns with northerly or easterly winds in the lower troposphere that are associated with high background concentrations of ozone and/or its precursors into Texas (e.g., Olaguer et al., 2009; Tobin and Nielsen-Gammon, 2010). Similarly, large-scale flow patterns are sometimes conducive to the transport of the Houston urban plume into adjacent Texas areas as well. Senff et al. (2010) used data collected on six flights in the Houston area to investigate the impact of the Houston urban plume on east Texas ozone concentrations. The study found that daily ozone exported from the Houston area raised regional background ozone by about 10 ppbv over a 40,000 km^2 geographic area. The potential importance of Houston transport to downwind areas was supported by an observational study by Schade et al. (2011). On five study days in College Station, Texas, during August 2006, background ozone increases of 20 – 50 ppbv during periods of southeasterly winds were attributed to the Houston urban plume. In general, back-trajectories nearer to the center of Houston were associated with the largest enhancements in ozone concentrations.

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3. Findings from the Air Quality Research Program (AQRP, 2010-2012)

Fourteen research projects, one field study support project and one synthesis project were funded by the AQRP during the 2010-2012 biennium. The 14 research projects are listed, by category, in Table 3-1. Full project reports are available at the AQRP web site (http://aqrp.ceer.utexas.edu/reports.cfm). Key findings from the research projects, organized into the topical areas of emissions, chemistry, and transport/modeling are summarized below.

Table 3-1. AQRP Research Projects 2010-2012

Project Number	Title
Dallas-Fort Worth Area Studies	
10-024	Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area
10-034	Dallas Measurements of Ozone Production
10-044	Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season
Houston Area Studies	
10-032	SHARP Data Analysis: Radical Budget and Ozone Production
10-045	Quantification of Hydrocarbon, NOx and SO2 Emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR Dataset
Flares and Emission Inventories	
10-006	Quantification of Industrial Emissions of VOCs, NO2 and SO2 by SOF and Mobile DOAS
10-009	Additional Flare Test Days for TCEQ Comprehensive Flare Study
10-022	Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas
Modeling and Atmospheric Chemistry	
10-008	Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling
10-015	An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-Attainment Areas in Texas
10-020	NOx Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone
10-021	Dry Deposition of Ozone to Built Environment Surfaces
10-029	Wind Modeling Improvements with the Ensemble Kalman Filter
10-042	Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms

Emissions:

Despite improvements in inventory estimates over the past decade, significant discrepancies are still observed between annual average reported emissions and instantaneous emission estimates inferred from observed concentrations. Some of these discrepancies can be resolved through refinement of the temporal resolution of emissions; other discrepancies may be due to missing or under-estimated sources.

The AQRP projects related to industrial flaring have provided information about both temporal variability and potential underestimation of emissions. The studies of flares under controlled operating conditions demonstrated that at low flow rates, and with low heating value gases, standard emission estimation methods may understate emissions if excess steam or air-assist is used. Subsequent air quality modeling demonstrated that these emissions, coupled with the temporal variability in the emissions, can lead to additional ozone formation both locally and over large spatial scales. Field observations in the FLAIR project support these findings. Specifically:

- Field tests in a semi-controlled environment indicate that the most efficient industrial flare operation, as measured by the destruction and removal efficiency and combustion efficiency, are achieved at or near the incipient smoke point. Minimum levels of steam or air assist that comply with the flare manufacturer's recommendations should be used when possible.

- Further development of remote sensing technologies, such as Passive and Active Fourier Transform Infrared Spectroscopy, and modeling techniques, such as Multivariate Image Analysis, may offer approaches for improving the detection, monitoring, and evaluation of flare operational conditions in the future.

A variety of additional studies have involved field measurements to resolve emission inventories. A particular focus has been on alkenes and aldehydes.

- Remote sensing measurements in the Houston Ship Channel and Texas City indicated that alkane and ethene emissions were similar in 2006, 2009, and 2011, while propene emissions decreased. Formaldehyde emissions in the Houston Ship Channel and Texas City were similar between 2009 and 2011, and many sources were associated with industries also emitting alkenes. In the Houston Ship Channel, Beaumont/Port Arthur, and Longview areas, comparison of the 2011 measurements with the 2009 TCEQ inventory showed primarily good agreement for NO_x and SO_2 but large discrepancies in VOC with observations at certain locations, such as Mont Belvieu, exceeding reported emissions by 400-1500% for alkanes, 300-1500% for ethene, and 170-800% for alkenes.

- The strength of industrial emissions sources of formaldehyde and olefins were assessed in Texas City and the Houston Ship Channel region during the 2009 FLAIR study. Consistent with previous studies, computed ethene, propene, benzene, and 1,3-butadiene emission rates significantly exceeded levels reported in emissions inventories (by more than 2 orders of magnitude in some cases). Ignited flares emitted formaldehyde at the tip at rates between 0.3-2.5 kg/h. Combustion efficiencies were found to vary from 0 (unlit) to 0.7 (steaming) to 0.999. A large source of primary formaldehyde emissions was identified in a Texas City refinery complex with a strength of 18 ± 5 kg/h, which may be associated with a FCCU regeneration unit.

Chemistry

Atmospheric chemistry in Texas has a number of unique features. The combinations of industrial and urban emissions, and forested and coastal environments lead certain chemical pathways to become more significant in Texas than in other regions. Specific findings arising from the AQRP program that address ozone and radical formation under Texas conditions include:

- Nitryl chloride can affect tropospheric oxidation capacity and ozone formation in coastal and inland regions. Representation of the chemistry of nitryl chloride formation in CAMx has been implemented and chlorine/chloride sources have been characterized for Texas emissions inventories.

- Volatile organic compounds can remove NO_x by forming NO_x sink compounds that reduce the availability of NO_x for ozone formation. These NO_x sink species may eventually react to return NO_x back to the atmosphere, known as NO_x recycling, potentially causing additional ozone production in NO_x-limited regions. Novel experimental data, describing the NO_x sinks for aromatics and isoprene and NO_x-recycling from photolysis of alkyl nitrates and nitrocresols, have been obtained and used to develop a revised version of the Carbon Bond mechanism (CB6) known as CB6r1.

- Calculated HO_x production during the SHARP campaign in Houston was dominated by the photolysis of HONO in the early morning and by photolysis of O_3 in the midday; at night, OH production occurred mainly via O_3 reactions with alkenes. On average, the daily HO_x production rate was 23.8 ppbv day^{-1} in the region, of which 31% was from O_3 photolysis, 23% from HONO photolysis, 12% from HCHO photolysis, and 14% from O_3 reactions with alkenes.

- Recent measurements have indicated that daytime observed HONO mixing ratios are often far larger than the expected photostationary state with OH and NO in Houston and other locations throughout the world. Statistically significant vertical gradients of HONO throughout the day, with smaller mixing ratios aloft, have suggested that a likely source of daytime HONO could be photocatalytic conversion of NO_2 on the ground in Houston. Although daytime mechanisms for HONO formation have been a subject of exploration, it is evident that uncertainty remains and further studies are needed. As further progress is made, incorporation into air quality models will be important.

Transport/Modeling

One of the ways in which air quality models are improved is by collecting detailed field measurements that can be used to evaluate the performance of the air quality models. Previous field measurement campaigns in the state were primarily focused on southeast Texas. In 2010-2012, a field measurement program in the Dallas-Fort Worth area was funded by AQRP. The measurements led to a number of significant findings and future comparisons with modeling results are expected to lead to additional insights.

- Aircraft measurements downwind of the Dallas-Fort Worth area indicated enhancements in maximum ozone concentrations by factors ranging from 1.5-2.5 relative to upwind concentrations. Downwind concentrations of NO, NO_2, and reactive alkenes were modest indicating a photochemically aged air mass.

- Aircraft flights over portions of the Barnett Shale did not find enhancements in ozone concentrations clearly associated with oil and gas emissions, but persistent southerly winds (~10 mph) may not have favored mixing of urban DFW and Barnett Shale emissions that would change the VOC/NOx ratio towards a regime favoring ozone production. On some occasions, elevated concentrations of reactive alkenes (up to 10 ppbv) and formaldehyde (4-6 ppbv compared to background concentrations of 2-3 ppbv) were measured over the Barnett Shale, such as immediately downwind of a large compressor station in the Eagle Mountain Lake area.

- Preliminary results from deployment of the Measurement of Ozone Production Sensor (MOPS) during August – October 2011 at the Meacham site near Dallas-Fort Worth showed that ozone production on sunny days peaked at 40-60 ppbv/h in the mid-mornings, which suggested that Meacham may be an ozone source region. Preliminary ozone production rates at Eagle Mountain Lake were generally lower, with peak ozone productivities of 40 ppbv/h in the late mornings on only a few days.

- Preliminary analyses of surface measurements during May 30 – June 30, 2011 indicated that Eagle Mountain Lake was most often affected by aged and processed air from the Dallas-Fort Worth metropolitan area and intermittently by emissions from nearby oil and gas operations in the Barnett Shale.

- The largest sources of methane and other hydrocarbon species at oil and gas locations near Fort Worth were gas treatment facilities combined with large compressor stations. Emissions were an order of magnitude lower from smaller compressor stations and well pads; however, flashing emissions on one occasion from a condensate tank were estimated at 140 kg/h methane and 10 kg/h ethane (and other species) suggesting further study for this potentially important intermittent source.

In addition to the field measurement program, AQRP projects also included data analysis of previously conducted field programs. Among these were flights examining the long range transport, overnight, of urban, industrial and power plant plumes. Results from laboratory and field studies of pollutant loss mechanisms (dry deposition) were also incorporated into air quality models.

- Overnight transport of plumes from urban, petrochemical, and coal-fired power plant plumes can affect regional air quality the following day. Aircraft flights in the Houston area have shown NO_3 to be 3 to 5 times more important than O_3 as a nighttime oxidant of VOCs. Net NO_3 radical productions rates can be large (1–2 ppbv h^{-1}) within NO_x-containing plumes of industrial origin from Houston. Nighttime NO_x loss through N_2O_5 heterogeneous uptake is modest, but should be an area of continued study.

- Analysis of nighttime aircraft intercepts from two different Texas power plants resulted in improvements to the plume-in-grid formulation in CAMx version 5.40, released in October 2011. Plume-in-grid puff growth rates were modified to ignore growth contributions from horizontal and vertical shear during stable/nighttime conditions. Shear effects remain during neutral/unstable/daytime conditions. Minimum limits on vertical diffusivity, turbulent flux moments, and nighttime planetary boundary layer depths were reduced. With these improvements, plume-in-grid puff behavior will change potentially significantly at night and above the boundary layer, usually leading to longer lifetime.

- The heterogeneity of the urban environment is typically not represented in the dry deposition algorithms used for photochemical modeling. Refined characterization of the urban built environment on the dry deposition of ozone in Austin, Texas resulted in decreases in predicted daily maximum 8-hour average ozone concentrations of 0.2 to 1.3 ppb. The results were primarily attributed to deposition to urban vegetation and highlighted the importance of characterizing Texas urban landscapes undergoing rapid development.

4. Recommendations for AQRP Research, 2012-2013

A primary goal of the State of Texas Air Quality Research Program (AQRP) is to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling. As outlined in this State of the Science document, the research needs in these areas are significant and continuing. Because AQRP resources are limited, proposed research projects should focus on high priority, targeted areas.

For the 2012-2013 biennium, the targeted areas for AQRP research are:

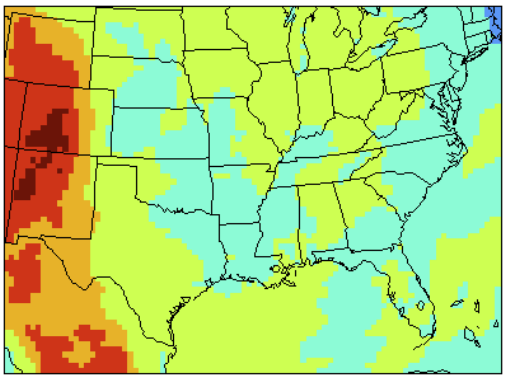
- Analysis of data collected in the Dallas-Fort Worth (Barnett Shale) field campaign
- Analysis of flare operating regimes that provide both high combustion efficiency and minimal smoke formation
- Deployment of supplementary measurements in a large field measurement campaign planned by NASA for the summer of 2013
- Analysis of prior Texas field study data and modeling tools to investigate transformation of gas-phase pollutants to aerosol phase
- Investigation of how the temporal resolution of meso-scale meteorology and photochemical grid models must be altered for high spatial resolution modeling; investigation of mesoscale modeling of cloud formation and the effects of clouds upon ozone and PM chemistry;
- Analysis of radical chemistry in Texas cities, especially HONO formation, ozone removal and production by halogen chemistry, and atmospheric chemistry within industrial plumes.
- Analysis of the impact of global and regional transport of air pollutants on Texas

State of the Science of Air Quality in Texas:

Scientific Findings from the Air Quality Research Program (AQRP)

Report for the period 2010-2015

February 15, 2016



Prepared by:
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University of Texas at Austin

With input from:
Members of the Air Quality Division
Texas Commission on Environmental Quality

Air Quality Research Program Independent Technical Advisory Committee

Executive Summary

The goals of the State of Texas Air Quality Research Program (AQRP) are:

> (i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,
> (ii) to integrate AQRP research with the work of other organizations, and
> (iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

Beginning with the 2010-2011 biennium, and continuing through the 2012-2013 and 2014-2015 biennia, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. During this period, the AQRP funded more than 50 projects, which have now been completed. The purpose of this State of the Science document is to describe the current state of scientific understanding on key issues addressed by the AQRP, and to summarize key findings from 2010-2015 AQRP projects.

The contributions of the AQRP program to the scientific understanding of air quality in Texas is grouped into major sections on emissions (Section 2.2), tropospheric chemistry (Section 2.3), and atmospheric physical processes (Section 2.4). Most of the research of the AQRP program has been focused on improving the understanding of emissions, chemistry and atmospheric physical processes that lead to ozone formation and accumulation. This is because ozone is the air pollutant for which the State has the greatest number of regions that do not meet National Ambient Air Quality Standards (NAAQS). With the recent tightening of the NAAQS for fine particulate matter, however, some regions in Texas are approaching non-attainment for fine particulate matter NAAQS; a number of AQRP projects have been funded to specifically address particulate matter. These projects are summarized in Section 2.5.

On the topic of emissions, AQRP projects over the past 6 years have focused on reducing uncertainties in emissions from industrial flaring, industrial sources of highly reactive volatile organic compounds (HRVOCs; ethene, propene, butenes and 1,3-butadiene), aldehyde emissions, fires, and biogenic volatile organic compounds. On the topic of tropospheric chemistry, AQRP projects have improved understanding of and models for the atmospheric chemistry of HRVOCs, biogenic hydrocarbons, and the cycling of nitrogen oxides in the atmosphere. On the topic of atmospheric physical processes, AQRP projects have improved models of physical pollutant loss mechanisms, and have made improvements in cloud characterizations, cloud processes, and models of wind fields. Further, multiple studies have examined how inter-state and global transport of pollutants impacts air quality in Texas. On the topic of fine particulate matter, AQRP projects have provided information regarding the chemical make-up of atmospheric particles in Texas and how atmospheric particles influence the cycling of gas phase air pollutants. Finally, multiple AQRP projects on the topics of emissions, tropospheric chemistry, atmospheric physical processes and particulate matter have been coordinated around large air quality field studies, in which many teams of investigators make measurements simultaneously. This coordination has provided scientific insights that are greater than would have been possible for projects performed in isolation.

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1. Overview of Air Quality Research in Texas

1.1 Issues

Exposure to air pollutants remains a significant public health issue around the world. In Texas, several of the state's largest urban areas exceed the National Ambient Air Quality Standard (NAAQS) for ozone, and concentrations of particulate matter and air toxics remain a health concern in many communities. Reducing emissions and improving air quality, while supporting economic growth and an increasing population, is challenging, yet substantial improvements in air quality have been made in Texas. Over the period from 2000 to 2013, average design values of ozone concentrations* at regulatory monitors decreased by 24% in Texas, double the national average rate (Figure 1.1.1; TCEQ, 2015a). The Houston metropolitan area went from, in 1999, having the highest number of days exceeding the NAAQS for ozone of any U.S. city and one of the highest ozone design values, to, in 2014, having no monitors that had a fourth highest maximum daily 8-hour average ozone concentration greater than 85 ppb (the 1997 level of the NAAQS). Similar ozone reductions have occurred in other Texas cities, as shown in Figure 1.1.2).

*An ozone design value is the fourth highest daily maximum, 8-hr averaged concentration over the course of a year, averaged over three years. The design value is used to compare measurements at regulatory monitors to the NAAQS.

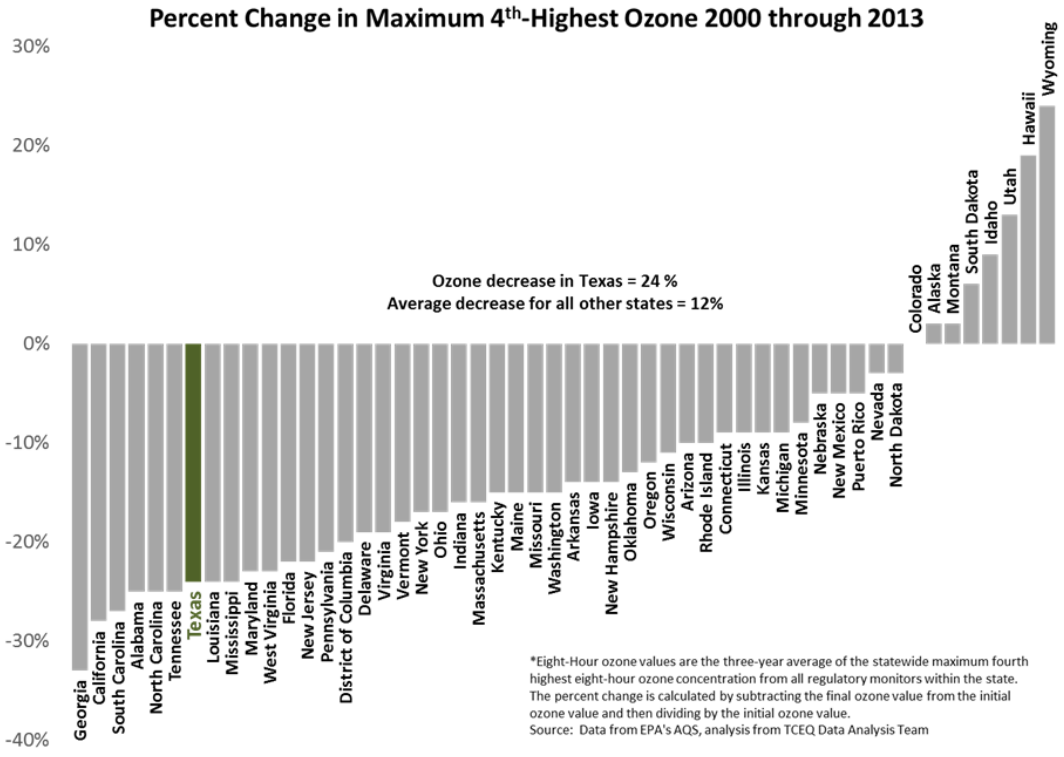

Figure 1.1.1 Comparison of ozone reductions in Texas to other States, 2000-2013.
Source: TCEQ (http://www.tceq.texas.gov/airquality/airsuccess/air-success-criteria)

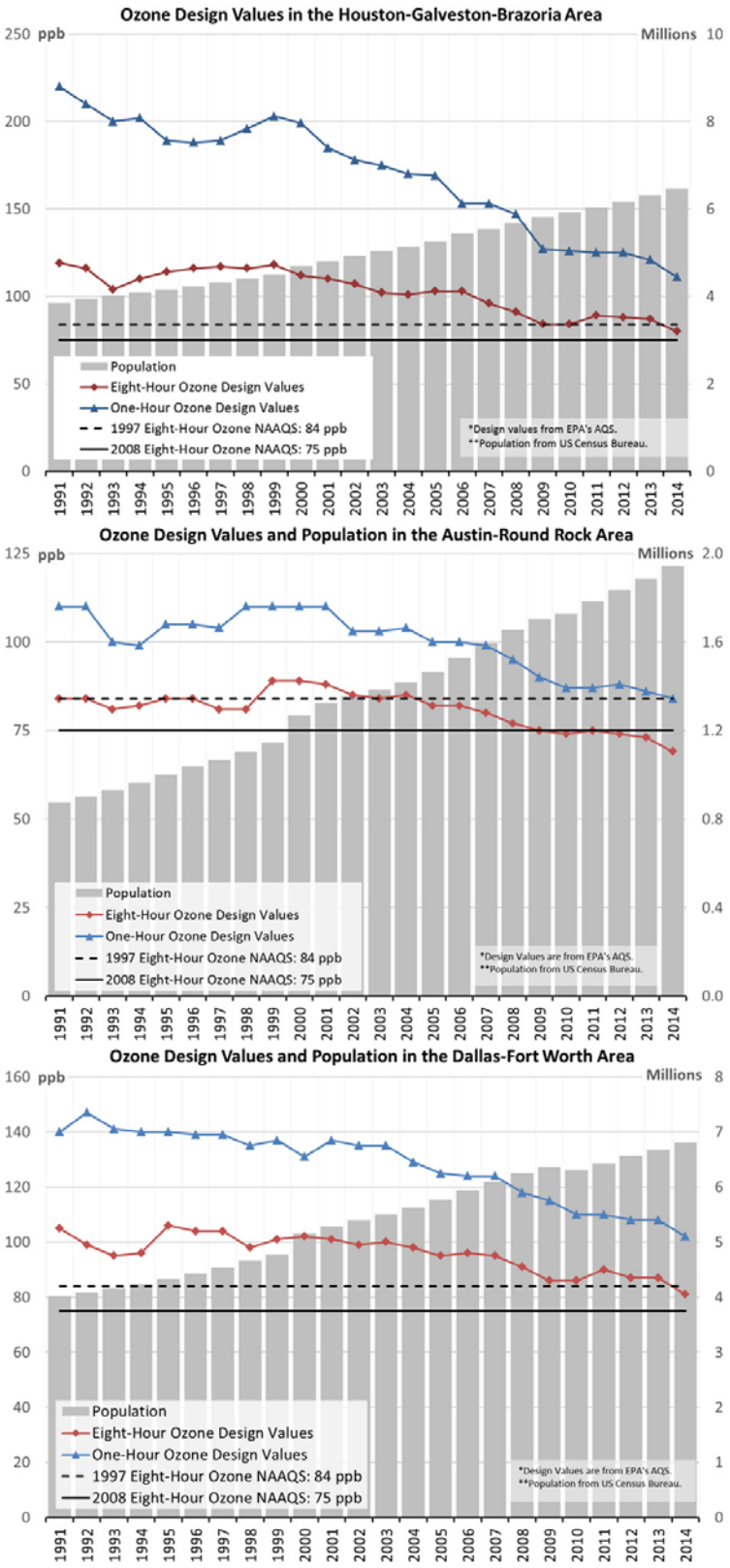

Figure 1.1.2. Trends in population and ozone design values in Texas cities over the past 25 years (TCEQ, 2015b); in all Texas cities, ozone design values have either decreased or remained constant, despite increases in population; two ozone design values are shown: design values based on eight hour averages of ozone concentrations, which are the design values used in the most recent NAAQS, and design values based on one hour averages of ozone concentrations, which were the design values used in standards prior to 1997; in 1997, EPA revoked the 1-hour ozone standard (0.12 ppm, not to be exceeded more than once per year) in all areas, although some areas have continued obligations under that standard.

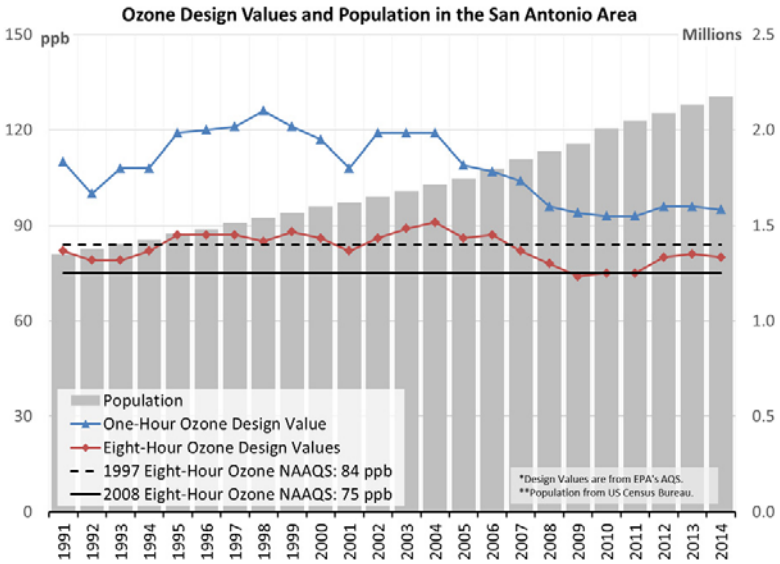

Figure 1.1.2 (continued). Trends in population and ozone design values in Texas cities over the past 25 years (TCEQ, 2015b); in all Texas cities, ozone design values have either decreased or remained constant, despite increases in population; two ozone design values are shown: design values based on eight hour averages of ozone concentrations, which are the design values used in the most recent NAAQS, and design values based on one hour averages of ozone concentrations, which were the design values used in standards prior to 1997; in 1997, EPA revoked the 1-hour ozone standard (0.12 ppm, not to be exceeded more than once per year) in all areas, although some areas have continued obligations under that standard.

Identifying the most effective and efficient approaches to improving air quality in Texas requires a sound understanding of the emissions and atmospheric processes that lead to air pollution. One reason for the success that the State of Texas has had in reducing ozone concentrations is its investments in air quality research. These investments have helped to identify focused strategies for emission reductions, designed to be most effective for conditions in Texas.

While progress in air quality over the past decade has been impressive, challenges remain. The Dallas-Fort Worth, Houston-Galveston-Brazoria area and the San Antonio region still do not meet the NAAQS for ozone, established in 2008. In addition, the U.S. Environmental Protection Agency (EPA) has recently (October 2015) lowered the NAAQS for ozone, potentially changing the attainment status for multiple regions in Texas. Continuing to make improvements in air quality will require new strategies, which in turn will require continuing improvements in scientific understanding. For example, it is becoming increasingly recognized that regional, continental and even global factors now have a significant influence on air quality in many parts of Texas (McDonald-Buller et al., 2011; Berlin, et al., 2013). Identifying the most effective and efficient balance between local, regional and national air quality improvement actions will require a new body of scientific information. In addition, driven by advances in drilling technology, oil and gas production activities in Texas have seen a substantial resurgence. These activities have the potential to impact air quality in complex ways. Direct emissions associated with the production activities include ozone precursors and some air toxics. Indirectly, the availability of relatively inexpensive natural gas and natural gas liquids has changed emissions associated with electricity generation and chemical manufacturing. Again, identifying effective and efficient approaches to reducing emissions, as energy development continues, will require new scientific information.

These are just a few of the examples of the types of challenges Texas will face in continuing to improve air quality. This document summarizes the current state of scientific understanding of air quality in Texas. It draws on and builds on previous State of the Science assessments (Allen et al., 2004; Allen et al., 2012). Findings from recent work, particularly work funded by the Texas Air Quality Research Program (AQRP), are summarized.

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Texas Commission on Environmental Quality (TCEQ, 2015b), Air Quality Successes, available at: http://www.tceq.state.tx.us/airquality/airsuccess/airSuccessMetro

1.2 Field measurement campaigns

Air pollutant formation and accumulation depends on emissions, meteorology, atmospheric chemistry and other inter-dependent phenomena. Because of the complexity and interdependence of atmospheric processes, experimental studies often involve simultaneous measurements of many chemical and physical features of the atmosphere. These coordinated measurement efforts are referred to as field measurement campaigns.

Box 1.2.1. Field Measurement Campaigns

- Texas Air Quality Study (TexAQS 2000)
- Texas Air Quality Study II (TexAQS 2005-2006)
- Study of Houston Atmospheric Radical Precursors (SHARP, 2009)
- Formaldehyde and Olefin from Large Industrial Sources (FLAIR) measurements (Houston and Texas City, 2009)
- 2010 Flare Study (Controlled, full scale flare tests)
- 2010-date Shale oil and gas production region field measurements
- DISCOVER-AQ 2013

Since 2000, multiple field measurement campaigns have been conducted in Texas (Box 1.2.1), and these measurement campaigns have generally been a focal point for both measurements and modeling done to improve the scientific understanding of air quality in Texas. The campaigns have ranged greatly in size and scope, with the smallest programs involving approximately a dozen investigators, and the largest involving several hundred. One of the largest campaigns was conducted in southeastern Texas in the summer of 2000 and focused on air pollutant formation, accumulation, and transport. Known as the Texas Air Quality Study, or TexAQS, this field campaign involved approximately 300 researchers drawn from around the world. TexAQS led to the identification of the role of Highly Reactive Volatile Organic Compounds (HRVOCs: ethene, propene, butenes, and 1,3 butadiene) in ozone formation in southeast Texas. Based on the results of TexAQS, the TCEQ substantially revised the air quality management plan (State Implementation Plan, or SIP) for the Houston-Galveston-Brazoria region. A follow-up field campaign was conducted in 2005 and 2006 (TexAQS II) and involved many of the same investigators. This field campaign documented substantial reductions in HRVOC concentrations, relative to the measurements made in 2000. In addition, TexAQS II identified new mechanisms for activation of chlorine in sea salt particles and made measurements to quantify inter-city transport of ozone.

Since 2006, more focused field studies, involving smaller numbers of investigators, have been conducted. Many of these field campaigns focused on issues associated with HRVOCs initially raised during the 2000 TexAQS campaign. For example, two campaigns in 2009 (SHARP and FLAIR) sought better characterization of olefin, formaldehyde, and free radical sources in southeast Texas. A series of full-scale flare tests conducted in 2010 at an industrial research facility in Tulsa, Oklahoma examined the emissions of flares operating at low flow rates and with low heating value gases as a potential source of HRVOC emissions. All of these studies have provided insights that will be useful in developing plans for reducing ozone formation in southeast Texas.

Beginning in 2010, the focus of field campaigns shifted from the industrial regions of southeast Texas to measurements made in regions with recently expanded oil and gas production activity, particularly production involving hydraulic fracturing of shale formations. The majority of these measurements have been made in the Barnett Shale natural gas production region near Fort Worth, although recently measurements have been initiated in the Eagle Ford production region, south of San Antonio. These measurements are continuing and analysis of data from the campaigns is on-going.

In 2013, a field campaign, titled DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality), was conducted under the leadership of the National Aeronautics and Space Administration (NASA). DISCOVER-AQ used southeast Texas as a test bed for the use of satellite measurements in characterizing air quality. Sub-orbital (aircraft and ground station) measurements were conducted in concert with satellite measurements to assess the limits of current and the needs for future satellite measurement capabilities. Augmentations of the measurements, funded by TCEQ and the AQRP, leveraged the extensive investments made by NASA, and provided additional insights into the factors that control air quality in southeast Texas.

These field programs are described in more detail in Sections 1.2.1-1.2.7.

References:

Web sites describing TexAQS and its principal findings have been maintained by the University of Texas, www.utexas.edu/research/ceer/texaqs www.utexas.edu/research/ceer/texaqsarchive

Summary of TexAQS II: Parrish, D.D., D.T. Allen, T.S. Bates, M. Estes, F.C. Fehsenfeld, G. Feingold, R. Ferrare, R.M. Hardesty, J.F. Meagher, J.W. Nielsen-Gammon, R.B.Pierce, T.B. Ryerson, J.H. Seinfeld, E.J. Williams "Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS)", *Journal of Geophysical Research – Atmospheres*, 114, D00F13, doi:10.1029/2009JD011842 (2009).

Reports describing the FLAIR, SHARP, Controlled Industrial Flare, and Barnett Shale field studies are available at the AQRP web site: http://aqrp.ceer.utexas.edu/projects.cfm ; the controlled industrial flare study is also described at: Torres, V.M., Herndon, S., Kodesh, Z., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research* 51, 12559-12568, DOI: 10.1021/ie202674t (2012); Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Industrial & Engineering Chemistry Research* 51, 12569-12576, DOI: 10.1021/ie202675f (2012).

The DISCOVER-AQ program is described at the NASA web site: http://discover-aq.larc.nasa.gov/ and in a feature article in the Air and Waste Management Association's EM (Environmental Manager) magazine (September, 2014).

1.2.1 Texas Air Quality Study (TexAQS 2000)

In August and September of 2000, an international team of more than 300 researchers, drawn from nearly two dozen universities, the National Oceanic and Atmospheric Administration (NOAA), Brookhaven National Laboratory, Pacific Northwest National Laboratory, and the EPA, undertook the largest air quality study ever conducted in the State of Texas. The study was designed to improve understanding of the formation, transport and accumulation of air pollutants along the Gulf Coast of southeastern Texas. Measurements were made at approximately 20 ground stations, shown in Figure 1.2.1. Additional sampling was carried out with aircraft that flew over broad regions of eastern Texas.

Figure 1.2.1. Ground sampling sites operated during the Texas Air Quality Study during the summer of 2000.

TexAQS led to the identification of the role of HRVOCs in ozone formation in southeast Texas. Key scientific findings were summarized in an Accelerated Science Evaluation (see citation below), and based on these findings, the TCEQ substantially revised the air quality management plan or SIP for the Houston-Galveston-Brazoria region. Understanding the sources of HRVOC emissions, which were not well quantified in emission inventories, and reducing HRVOC emissions, became a priority that has continued for more than a decade.

References:

Daum, P.H., J. Meagher, D. Allen, and C. Durrenberger. 2002. Accelerated Science Evaluation of Ozone Formation in the Houston-Galveston Area. Summary. 6 pp. http://www.utexas.edu/research/ceer/texaqsarchive/accelerated.htm

Web sites describing TexAQS and its principal findings have been maintained by the University of Texas, www.utexas.edu/research/ceer/texaqs www.utexas.edu/research/ceer/texaqsarchive

1.2.2 Texas Air Quality Study II (TexAQS 2005-2006)

The first Texas Air Quality Study, conducted in the summer of 2000 (Section 1.2.1), was focused primarily on southeast Texas, and helped inform state decisions concerning how to meet then current air quality standards for southeast Texas. After 2000, however, regulations for ozone shifted in emphasis, from concentrations averaged over short periods of time (i.e., the ozone standard with ozone concentrations averaged over one-hour), to concentrations averaged over longer time periods (e.g., ozone concentrations averaged over eight hours and particulate matter concentrations averaged over a day or year). Longer averaging times mean broader geographical regions influence air pollutant concentrations. A second Texas Air Quality Study (TexAQS II) was conducted in 2005 and 2006 to characterize pollutant transport over regional (~100-1000 km) scales. The study also characterized progress that had been made in improving air quality in Houston since 2000.

Among the most significant findings emerging from TexAQS II was the magnitude of ozone transported into Texas. Background ozone concentrations in eastern Texas, which represent the minimum ozone concentration that is likely achievable through only local controls, were found to approach or exceed 75 ppbv for an 8-hour average, which was the level of the NAAQS through 2015 (see Parrish et al., 2009, cited below).

A second set of major findings were associated with concentrations of HRVOCs, identified as critical to ozone formation in Houston during TexAQS 2000. Observed concentrations of HRVOCs in southeast Texas were lower in 2006 than in 2000, however, despite improvements in inventory estimates since the TexAQS 2000 study, significant discrepancies were still observed between reported emissions and observed concentrations (see Parrish et al., 2009, cited below). This finding led to additional field programs related to potential sources of HRVOCs (FLAIR and the TCEQ 2010 Flare Study)

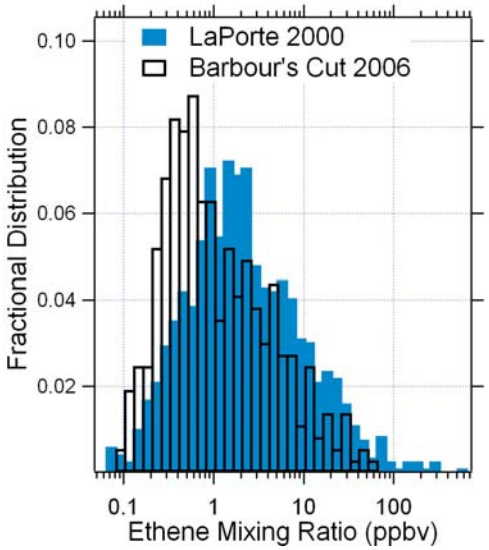

Figure 1.2.2. Comparison of ethene concentrations made at similar locations in the Houston Ship Channel region in 2000 (LaPorte) and 2006 (Barbour's Cut). A significant decrease in average and extreme ethene concentrations was observed.

Reference:

Parrish, D.D., D.T. Allen, T.S. Bates, M. Estes, F.C. Fehsenfeld, G. Feingold, R. Ferrare, R.M. Hardesty, J.F. Meagher, J.W. Nielsen-Gammon, R.B.Pierce, T.B. Ryerson, J.H. Seinfeld, E.J. Williams "Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS)", *Journal of Geophysical Research – Atmospheres*, 114, D00F13, doi:10.1029/2009JD011842 (2009).

1.2.3 Study of Houston Atmospheric Radical Precursors (SHARP)

The chemistry of atmospheric radicals, especially the hydroxyl radical (OH) and hydroperoxyl radical (HO_2), together called HOx, is deeply involved in the formation of ozone and other photochemical air pollutants. Radical precursors, such as nitrous acid (HONO) and formaldehyde (HCHO), significantly affect the HOx budget in urban environments such as Houston. The Study of Houston Atmospheric Radical Precursors (SHARP), in the spring of 2009, examined sources and sinks for free radicals and the impact of radical sources and sinks on the sensitivity of ozone formation to emissions of oxides of nitrogen (NOx) and volatile organic compounds (VOCs). Both measurements and modeling were performed and reconciling model predictions and observations was a major focus of study.

Among the HONO formation mechanisms that were considered were gas-phase photolysis of nitrophenols, heterogeneous conversion of NO_2 on fresh and aged soot particles and soil surfaces, photolysis of surface adsorbed nitric acid, and heterogeneous conversion of HNO_3 on the surface of primary organic aerosol. HO_x production during the SHARP campaign at the Moody Tower measurement site in Houston was dominated by the photolysis of HONO in the early morning and by photolysis of O_3 in the midday; at night, OH production occurred mainly via O_3 reactions with alkenes. On average, the daily HO_x production rate was 23.8 ppbv day^{-1} in the region, of which 31% was from O_3 photolysis, 23% from HONO photolysis, 12% from HCHO photolysis, and 14% from O_3 reactions with alkenes (Lefer et al., 2011).

Daytime observed HONO mixing ratios are often far larger than expected. Statistically significant vertical gradients of HONO throughout the day, with smaller mixing ratios aloft, have suggested that a likely source of daytime HONO could be photocatalytic conversion of NO_2 on the ground surfaces in Houston. Although daytime mechanisms for HONO formation have been a subject of exploration, it is evident that uncertainty remains.

References:

Ren, X., van Duin, D., Cazorla, M., Chen, S., Mao, J., Zhang, L., Brune, W.H., Flynn, J.H., Grossberg, N., Lefer, B.L., Rappenglück, B., Wong, K.M., Tsai, C., Stutz, J., Dibb, J.E., Jobson, B.T., Luke, W.T., Kelley, P., Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *JGR Atmospheres* 118, 5770-5780 doi:10.1002/jgrd.50342 (2013).

Olaguer, E.P., Kolb, C.E., Lefer, B., Rappenglück, B., Zhang, R., Pinto, J.P., Overview of the SHARP campaign: Motivation, design and major outcomes, *JGR Atmospheres*, Introduction to a Special Collection: doi:10.1002/2013JD019730 (2014).

Couzo, E., Lefer, B., Stutz, J., Yarwood, G., Karamchandani, P., Henderson, B., Vizuete, W., Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas, *Atmospheric Environment,* 112, 344-355 (2015).

Lefer, B., J. Stutz, X. Ren, W. Brune, J. Dibb, Study of Houston Atmospheric Radical Precursors (SHARP) data analysis. Air Quality Research Program, TCEQ Grant No. 582-10-94300, November 2011.

1.2.4 Formaldehyde and Olefin from Large Industrial Sources (FLAIR) measurements (Houston and Texas City, 2009)

The goal of the FLAIR program was to use a variety of remote sensing and direct field measurements to assess the strength of industrial sources of formaldehyde and olefins. Measurements were made in Texas City and the Houston Ship Channel region. The study was motivated by a variety of divergent analyses of the relative contribution of primary sources and secondary chemical production to ambient formaldehyde concentrations and fluxes in Houston.

Among the sources examined in the study were flares. Consistent with controlled flare studies done in 2010 (described in Section 1.2.5), a variety of measurement techniques used in the FLAIR study found that formaldehyde is not directly emitted by un-ignited flare stacks, but burning flares emit formaldehyde at the flare tip. Emission rates of burning flares observed during FLAIR varied between 0.3-2.5 kg/h of formaldehyde. Also consistent with results from controlled flare studies, combustion efficiencies were found to vary from 0% (unlit) to 70% (over-assisted) to 99.9% (operating as intended).

The FLAIR study also identified a large source of primary formaldehyde emissions in the Texas City refinery complex with a strength of 18 ± 5 kg/h. Analysis of the HCHO/SO_2 ratio revealed that during most of the time this source(s) co-emitted with a ratio of roughly 0.1. However, some of the formaldehyde emissions were not correlated with SO_2. Analysis of the emission inventory in Texas City, as well as triangulation and wind field analysis revealed that the most likely sources of HCHO were a Fluid Catalytic Cracking Unit (FCCU) regeneration unit and desulfurization processes (Olaguer et al., 2013).

While the measurements made during the FLAIR study in 2009 indicate that some formaldehyde is directly emitted from flares and from FCCU catalyst regeneration units, most of the formaldehyde observed in Houston (~92%) is associated with secondary formation from the oxidation of VOCs (Parrish et al., 2012). Photochemical modeling studies indicate that directly-emitted formaldehyde associated with over-assisted flares does not accentuate ozone formation as greatly as originally hypothesized.

The olefin measurements made during the FLAIR campaign continued to show discrepancies between reported emissions and observations with observations exceeding levels expected from inventories by a factor of 2 orders of magnitude or more at some sites.

References:

Parrish, D.D., T.B. Ryerson, J. Mellqvist, J. Johansson, A. Fried, D. Richter, J.G. Walega, R.A. Washenfelder, J.A. de Gouw, J. Peischl, K.C. Aikin, S.A. McKeen, G.J. Frost, F.C. Fehsenfeld, S.C. Herndon, Primary and secondary sources of formaldehyde in urban atmospheres: Houston Texas region. *Atmospheric Chemistry and Physics* 12 (2012), doi:10.5194/acp-12-3273-2012.

Olaguer, E.P., Herndon, S.C., Buzcu-Guven, B., Kolb, C.E., Brown, M.J., Cuclis, A.E., Attribution of primary formaldehyde and sulfur dioxide at Texas City during SHARP/formaldehyde and olefins from large industrial releases (FLAIR) using an adjoint chemistry transport model , *JGR Atmospheres* 118, 11,317-11,326 doi:10.1002/jgrd.50794 (2013).

Pikelnaya, O., Flynn, J.H., Tsai, C., Stutz, J., Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, *JGR Atmospheres* 118, 8716-8728 doi:10.1002/jgrd.50643 (2013).

1.2.5 TCEQ 2010 Flare Study (2010, Controlled, full scale flare tests)

One of the potential sources of HRVOCs in the Houston area is industrial flaring operations. Flares are safety devices that must be able to combust large emergency releases of hydrocarbons. These emergency events are rare, however, and most flare operations occur at flow rates much lower than the maximum flare capacity. Achieving complete combustion at low flow rates, particularly with low heating value gases, can be challenging, but little data existed on flare combustion efficiencies at these conditions. In response to this, the TCEQ contracted with the University of Texas to perform a series of full-scale flare tests at low flow conditions with low heating value gases. A 24" diameter air-assisted flare with a flow capacity of 144,000 lb/hr and a 36" steam-assisted flare with a flow capacity of 937,000 lb/hr were employed in the testing. The range of flared gas flow rates was 0.1% to 0.25% of the flare's design capacity and heating values of the flared gases were in the range of 300-600 BTU/scf.

Figure 1.2.3. Full scale flare tests

Destruction/removal efficiencies (DRE, fraction of vent gas reacted) for steam-assisted flares dropped rapidly when combustion zone heating values fell below 250 BTU/scf. Air-assisted flares showed a linear drop in DRE as a function of air flow. While DREs of 98-99% were observed in some experiments, many operating conditions produced DREs of substantially less than 99%. Since standard methods for estimating emissions would have allowed a 98-99% DRE for all the tests, some test conditions resulted in the production of flare emissions multiple times the value that would be calculated using the standard methods (from Torres et al., 2012a, cited below). Air quality modeling of theoretical scenarios associated with low flaring destruction efficiencies have shown that the majority of the ozone formation associated with low destruction efficiency flares is due to the unburned gases sent to the flare, rather than products of incomplete combustion (e.g., formaldehyde; Al-Fadhli et al., 2012).

References:

Torres, V.M., Herndon, S., Kodesh, Z., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Indus. Eng. Chem.Res.* 51, 12559-12568, DOI: 10.1021/ie202674t (2012a);

Torres, V.M., Herndon, S. and Allen, D.T. "Industrial flare performance at low flow conditions: Part 2. Air and Steam assisted flares" *Indus. Eng. Chem. Res.* 51, 12569-12576, DOI: 10.1021/ie202675f (2012b).

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research*, 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

1.2.6 Shale oil and gas production region field measurements (2010-date)

Driven by advances in drilling technology, oil and gas production activities in Texas have seen a substantial resurgence over the past decade. The use of hydraulic fracturing and other technologies has enabled significantly expanded oil and gas production in the Barnett Shale formation near Fort Worth, the Eagle Ford formation south of San Antonio, the Haynesville formation in east Texas, and in other formations throughout the state. These activities have the potential to impact air quality in complex ways. Direct emissions associated with the production activities include ozone precursors (nitrogen oxides, volatile organic compounds), and some air toxics (e.g., benzene). Indirectly, the availability of relatively inexpensive natural gas and natural gas liquids has changed emissions associated with electricity generation.

A series of field campaigns have been undertaken since 2010, primarily to characterize direct emissions of volatile organic compounds and air toxics in the shale gas and oil production regions. The majority of these measurements have been made in the Barnett Shale natural gas production region near Fort Worth, although recently measurements have been initiated in the Eagle Ford production region, south of San Antonio. With funding provided by the TCEQ and other sources, instantaneous, hourly and daily measurements of concentrations of a variety of air pollutants have been made. In addition, the Texas Air Quality Research Program funded the deployment of an augmented set of measurements in and around Eagle Mountain Lake in the summer of 2011.

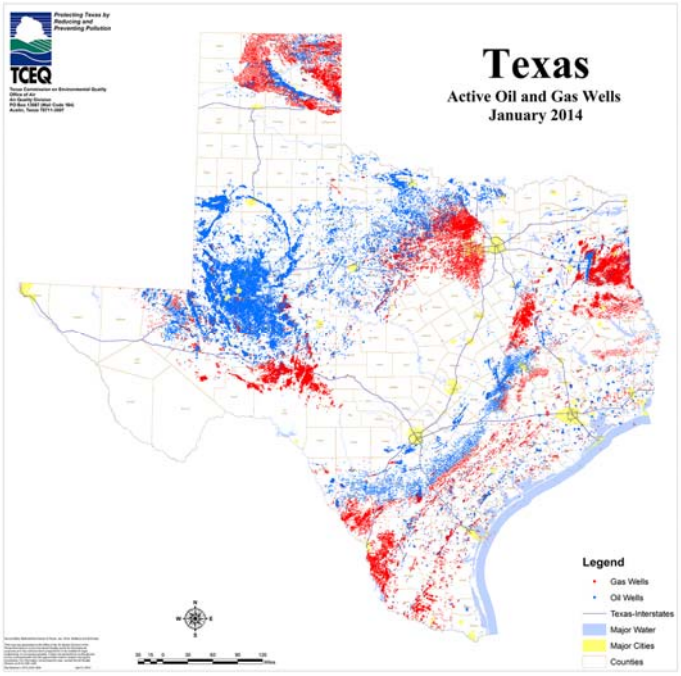

Figure 1.2.4. Locations of oil wells (blue) and gas wells (red) in Texas (2014).

http://www.tceq.state.tx.us/assets/public/implementation/barnett_shale/bs_images/txOilGasWells.png

While the results from some of these measurement studies have been summarized in the scientific literature (see references below) many analyses are on-going. Results should help to clarify the role of direct and indirect emission changes, associated with renewed oil and gas production activities, on ozone formation. For example, a series of studies (Eastern Research Group, 2011; Allen et al., 2013, 2015a,b) of emissions on and near natural gas production sites have indicated that emissions of hydrocarbons from a relatively small fraction of sites and

sources dominate total emissions. If these high emitting sources are accounted for in emission inventories, then emission estimates are generally consistent with ambient measurements (Zavala et al., 2014).

Using these emission inventories, air quality modeling has indicated that the impact of oil and gas production emissions on ozone formation is location dependent. In regions such as the Barnett Shale, changes in ozone formation in the Barnett Shale due to switching electricity generation from coal fired power plants to natural gas fired power plants is much larger than the additional ozone formation due to oil and gas production emissions in the Barnett Shale (Pacsi et al., 2013). In contrast, in regions such as the Eagle Ford Shale, NOx emissions from oil and gas operations, in concert with reactive biogenic hydrocarbon emissions, lead to increases in ozone concentrations that are 1 ppb or more in nearby urban areas on some days. While there are also regions of decreased ozone concentrations due to switching electricity generation from coal fired power plants to natural gas fired power plants, these decreases occur in different regions than the increases associated with emissions from oil and gas production in the Eagle Ford (Pacsi et al., 2015).

References:

Allen, D.T., Torres, V.M., Thomas, J., Sullivan, D., Harrison, M., Hendler, A., Herndon, S.C., Kolb, C.E., Fraser, M., Hill, A.D., Lamb, B.K., Miskimins, J., Sawyer, R.F., and Seinfeld, J.H. Measurements of Methane Emissions at Natural Gas Production Sites in the United States, *Proceedings of the National Academy of Sciences,* 110, 17768-17773, doi: 10.1073/pnas.1304880110 (2013).

Allen, D.T., Pacsi, A., Sullivan, D., Zavala-Araiza, D., Harrison, M., Keen, K., Fraser, M., Hill, A.D., Sawyer, R.F., and Seinfeld, J.H. Methane Emissions from Process Equipment at Natural Gas Production Sites in the United States: Pneumatic Controllers, *Environmental Science & Technology*, 49 (1), 633–640, doi:10.1021/es5040156 (2015a).

Allen, D.T., Sullivan, D., Zavala-Araiza, D., Pacsi, A., Harrison, M., Keen, K., Fraser, M., Hill, A.D., Lamb, B.K., Sawyer, R.F., and Seinfeld, J.H. Methane Emissions from Process Equipment at Natural Gas Production Sites in the United States: Liquid Unloadings, *Environmental Science & Technology*, 49 (1), 641–648, doi:10.1021/es504016r (2015b).

Eastern Research Group and Sage Environmental Consulting, Final Report, City of Fort Worth Natural Gas Air Quality Study, prepared for the City of Fort Worth, July 13, 2011.

Final Reports of AQRP funded projects for the Barnett Shale field campaign are available at: http://aqrp.ceer.utexas.edu/projects.cfm

Pacsi, A.P., Kimura, Y., McGaughey, G., McDonald-Buller, E.C., and Allen, D.T., Regional ozone impacts of increased natural gas use in the Texas power sector and development in the Eagle Ford shale, *Environmental Science & Technology*, 49, 3966-3973, doi: 10.1021/es5055012 (2015).

Pacsi, A.P., Alhajeri, N.S., Zavala-Araiza, D., Webster, M.D. and Allen, D.T., Regional Air Quality Impacts of Increased Natural Gas Production and Use in Texas, *Environmental Science & Technology*, 47, 3521-3527, doi: 10.1021/es3044714 (2013)

Zavala-Araiza, D., Sullivan, D.W., and Allen, D.T. Atmospheric hydrocarbon emissions and concentrations in the Barnett Shale natural gas production region, Environmental Science & Technology, 48, 5314-5321 doi: 10.1021/es405770h (2014).

1.2.7 DISCOVER-AQ 2013

"DISCOVER-AQ, a NASA Earth Venture program funded mission, stands for Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality. In recent years, progress in reaching air quality goals has begun to plateau for many locations. Furthermore, near-surface pollution is one of the most challenging problems for Earth observations from space. However, with an improved ability to monitor pollution from satellites from DISCOVER-AQ, scientists could make better air quality forecasts, more accurately determine the sources of pollutants in the air and more closely determine the fluctuations in emissions levels. In short, the more accurate data scientists have at hand, the better society is able to deal effectively with lingering pollution problems." (From NASA DISCOVER-AQ web site: http://discover-aq.larc.nasa.gov/science.php)

The DISCOVER-AQ campaign employed NASA aircraft to make a series of flights, with scientific instruments on board to measure gaseous and particulate pollution. Flights began in the Baltimore-Washington, D.C. area in 2011 and continued with flights in Houston in 2013. The State of Texas, through the TCEQ and the Air Quality Research Program, worked with NASA to develop sampling strategies for the 2013 field measurement campaign in Houston. The flight paths for DISCOVER-AQ in Houston are shown in Figure 1.2.5. The field campaign involved coordinating ground measurements and instrumented aircraft flights with satellite overpasses.

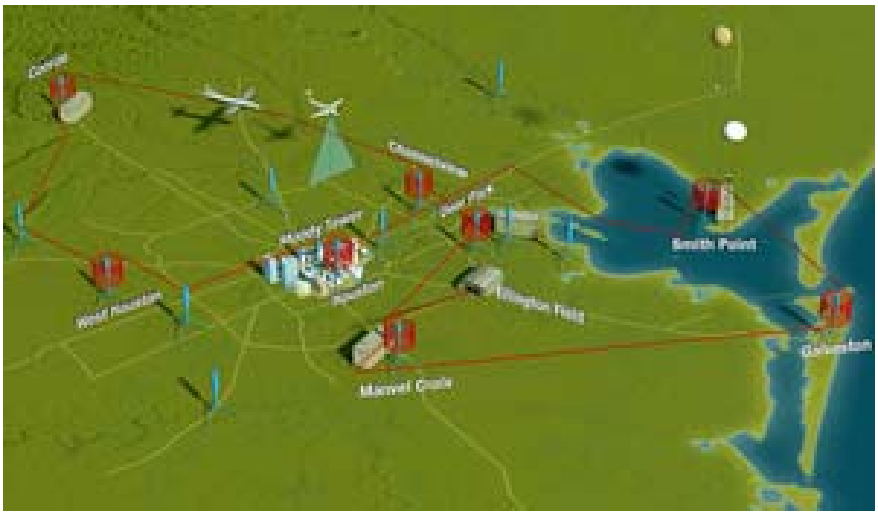

Figure 1.2.5. Flight track for NASA DISCOVER-AQ aircraft during the 2013 field campaign; the same flight track was flown on multiple days and included aircraft spirals that provided data on vertical distributions of air pollutants at eight fixed locations, shown on the map.

Reference:

The DISCOVER-AQ program is described at the NASA web site: http://discover-aq.larc.nasa.gov

2. State of the Science: Emissions, Chemistry, and Meteorology and Transport/Modeling

2.1 Overview and methods for developing state of the science findings

Scientific findings emerging from large field campaigns and data analysis programs, of the type that have occurred in Texas over the past decade, are multifaceted. Many of the scientific findings have direct and immediate policy relevance. For example, scientific findings from TexAQS were used to guide the development of the approaches used to attain the NAAQS for ozone in Houston. Other scientific findings have longer-term policy relevance. For example, scientific findings that improve understanding of emissions and chemistry associated with natural gas production may help inform the direction of air quality policies in regions such as San Antonio and the Dallas-Fort Worth area. Better understanding of how flare operating practices influence emissions can guide emission reduction strategies. The purpose of this document is to summarize the current state of scientific understanding on key issues addressed by the AQRP in Texas. Findings with both immediate and longer-term relevance are summarized.

Scientific findings have varying degrees of certainty. The findings reported in this document are not limited to those for which there is a high degree of certainty; in many cases highlighting critical areas where uncertainty exists can be important in determining the likelihood that a policy will be effective, and identifying areas where uncertainty exists is critical to continued progress in scientific understanding. However, when uncertainty or areas of disagreement concerning the implications of scientific findings exist, this document clearly identifies and, to the extent possible, characterizes the uncertainties.

Initial drafts of this report were written by AQRP staff (David Allen, Elena McDonald-Buller, and Gary McGaughey of The University of Texas at Austin). The report was then revised based on reviews by both the TCEQ and the AQRP's Independent Technical Advisory Committee.

The findings are divided into sections corresponding to the areas where the AQRP performs research: emissions, chemistry, and atmospheric transport/modeling. In each section, there is a brief statement of major findings; citations to the scientific literature provide additional details.

2.2 Ozone precursor emissions

2.2.1 Overview of emission inventories

Emission inventories are used for a variety of purposes and at a variety of spatial and temporal scales. Inventories are used at state and national spatial scales and at annual and multi-year temporal scales to establish trends in air quality. They are also used as inputs to air quality models that require kilometer-level spatial resolution and hourly temporal resolution. These variable applications of emission inventories lead to very different information needs. This assessment focuses on emission inventories that are used in air quality models that are used to evaluate air quality management plans for ozone. These models must predict atmospheric processes on days when extreme ozone concentrations have been observed, therefore emission inventories resolved at kilometer-level spatial scales and at hourly temporal scales are of greatest interest. Findings are reported for industrial flares, fires, biogenics, HRVOCs, emissions associated with oil and natural gas production, and emissions characterized by satellite measurements. Other categories of emissions (e.g., mobile sources, off-road equipment) are significant sources but have not been the focus of AQRP research activities and therefore are not summarized here, but have been described in previous scientific assessments (e.g., Allen and Durrenberger, 2003).

References:

Allen, D., Durrenberger, C. and Texas Commission on Environmental Quality, Technical Analysis Division. 2003. Accelerated Science Evaluation of Ozone Formation in the Houston-Galveston Area: Emission Inventories Version 3, February, 2003, available at http://www.utexas.edu/research/ceer/texaqsarchive/accelerated.htm

2.2.2 Emissions source characterization and inventory assessment from AQRP projects 2010-2015

Industrial flares

Studies performed during TexAQS 2000 indicated that high temporal variability in emissions from industrial sources in southeastern Texas could lead to rapid ozone formation, in particular when emissions were composed of HRVOCs (Murphy and Allen, 2005; Nam et al., 2006; Webster et al., 2007; Nam et al., 2008; Kleinman et al., 2003; Allen et al., 2004; Vizuete et al., 2008; Olaguer et al., 2009; Henderson et al., 2010). These findings motivated the collection of hourly emissions data from 141 industrial locations in the region during TexAQS II, which later were incorporated into a 2006 Special Inventory (TCEQ, 2008). Emissions from industrial flares constituted 45% of all VOC and 77% of all HRVOC emissions in the 2006 Special Inventory. The temporal patterns of emissions from industrial flaring operations were found to consist of multiple components, including nearly constant, routinely variable, or episodic (Nam et al., 2006; Webster et al., 2007; Pavlovic et al., 2009; Pavlovic et al., 2012a). Air quality modeling based on the 2006 Special Inventory suggested that the temporal variability of emissions from flaring operations could lead to additional ozone formation both locally and over large spatial scales (Pavlovic et al., 2010; Pavlovic et al., 2012b). Collectively, these studies indicated the importance of understanding and reducing emissions from flaring events in order to contribute to improvements in air quality in the region.

Industrial flares are safety devices designed to combust large emergency releases of hydrocarbons. However, emergency events are rare, and most flare operations occur at flow rates much lower than the maximum flare capacity. A key assumption had been that flares operating over the range of requirements stated in Title 40 Code of Federal Regulations (CFR) §60.18 achieve the assumed hydrocarbon destruction and removal efficiency (DRE) of 98-99 percent at varying vent gas flow rate turndown, assist ratios, and vent gas heat content. The TCEQ 2010 Flare Study (Tracking #2010-04) and AQRP Project 14-009 (Task 1; Allen and Torres, 2011) were designed to explore flare DRE performance. Field tests were conducted at the John Zink Company, LLC flare test facility in Tulsa, Oklahoma, to measure flare emissions and to collect process and operational data in a semi-controlled environment to determine the relationship between flare design, operation, vent gas lower heating value (LHV) and flow rate, destruction and removal efficiency (DRE), and combustion efficiency (CE). The tests indicated that at low flow rates, and with low heating value gases, standard emission estimation methods understated emissions if excess steam or air-assist was used. The most efficient industrial flare operation, as measured by the DRE and combustion efficiency (CE), was achieved at or near the incipient smoke point (Allen and Torres, 2011; Torres et al., 2012a; Torres et al., 2012b). Minimum levels of steam or air assist that complied with the flare manufacturer's recommendations should be used when possible. Air quality modeling of theoretical scenarios associated with low flaring destruction efficiencies showed that the majority of the ozone formation associated with low destruction efficiency flares was due to the unburned gases sent to the flare, rather than products of incomplete combustion (e.g., formaldehyde) (Al-Fadhli et al., 2011; Herndon et al., 2012). Field observations during the Formaldehyde and Olefin from Large Industrial Sources (FLAIR) campaign in Houston and Texas City in 2009 supported these findings (Parrish et al., 2012; AQRP Project 10-045, Stutz et al., 2011). The projects supported the development of remote sensing technologies, such as Passive and Active Fourier Transform Infrared (PFTIR, AFTIR)

Spectroscopy (Allen and Torres, 2011), and modeling techniques (e.g. AQRP Project 10-009 (Task 2), Rawlings et al., 2011; AQRP Project 10-022, Chen et al., 2011; Singh et al., 2012; Lou et al., 2012) that offered approaches for improving the detection, monitoring, and evaluation of flare operational conditions. Notably, the projects led to the development of a supplemental online flare operations training for plant personnel who monitor elevated, industrial-scale chemical and petrochemical flares (https://sfot.ceer.utexas.edu).

Most recently, on April 20, 2015, EPA revised AP-42 emission factors for refinery and chemical plant flaring operations as a result of a consent decree with environmental groups (http://www.epa.gov/ttn/chief/consentdecree/index_consent_decree.html). Revised emission factors for VOCs from affected flaring operations are substantially higher than previous emissions estimates.

Wildland fires and open burning

Wildland fires and open burning can be substantial sources of ozone precursors and particulate matter. The influence of fire events on air quality in Texas has been well documented by observational and modeling studies (e.g., Junquera et al., 2005; Morris et al., 2006; McMillan et al., 2010; Villanueva-Fierro et al., 2009; Kemball-Cook et al., 2014). The Fire INventory from NCAR (FINN) is a global fire emissions model that estimates daily emissions of trace gases and particles from open biomass burning. FINN is widely used in global and regional modeling studies (Wiedinmyer et al., 2011). FINN v.1 was released in 2010 and updated in 2011. FINN v.1.5 was released in 2014. AQRP Project 12-018 (McDonald-Buller et al., 2013) evaluated the sensitivity of FINN v.1 emissions estimates to the variability in input parameters and investigated the effects on modeled air quality using the Comprehensive Air Quality Model with Extensions (CAMx). Sensitivity studies used different input data sources for land cover, emission factors, fire detection, burned area, and fuel loading in FINN. The project found that variability in fire emissions is season- and region- dependent in the United States, and differences in emissions estimates due to varying input data resources could exceed a factor of two. The use of the different estimates of fire emissions had substantial impacts on predictions of ozone and fine particulate matter concentrations in Texas and other regions of the United States.

AQRP Project 14-011 (McDonald-Buller et al., 2015) conducted targeted improvements to the FINN model to benefit the global and regional air quality management and research communities, with a special focus on needs for Texas. A new algorithm for estimating area burned from satellite-derived fire detections was developed and incorporated into FINN to address a known under-prediction bias for area burned. Improvements in the area burned estimation were accompanied by better spatial resolution in the characterization of land cover, new fuel loading data with greater spatial resolution for the United States, and incorporation of new satellite-based estimates of barren land and vegetative cover. Crop-specific emission factors and fuel loadings were added to FINN as an option for users that have a land cover data resource that distinguishes major crop types typically found in the United States. These modifications have formed the basis of the next generation of the FINN model, FINN v.2. Annual emissions estimates were generated for 2012 to support TCEQ air quality modeling efforts. An approach was also developed for partitioning NO_x emissions estimates from FINN into aged NO_z forms (i.e., nitrogen dioxide [NO2], nitric acid [HNO3], peroxyacetyl nitrate [PAN], C3 and higher peroxyacyl nitrates, and organic nitrates) to account for rapid NO_x oxidation in fire plumes.

In addition, the project examined the sensitivity of FINN v.2 emissions estimates and predictions of regional air quality to land cover characterization. The MODIS Land Cover Type (LCT) product has been used as the default resource for land cover characterization in FINN, but new global, U.S. national, and Texas regional products are now available alternatives. These include the United Nations Global Land Cover (GLC-SHARE) and European Space Agency (ESA) Climate Change Initiative global data products, the U.S. Forest Service Fuel Characteristic Classification System (FCCS), the U.S. Department of Agriculture National Agricultural Statistical Service Cropland Data Layer (CDL), and a Texas (TCEQ) regional land cover product developed by Popescu et al. (2011). Differences between simulations highlighted the complex sensitivity of emissions estimates from the FINN model to various land cover inputs and associated fuel loadings and emission factors. At this time, McDonald-Buller et al. (2015) recommended use of the following combination of land cover products in FINN to support Texas air quality modeling activities: the Texas regional land cover product with the Cropland Data Layer, the U.S. Forest Service FCCS in the continental U.S., and the MODIS LCT product elsewhere. This combination provides the greatest spatial resolution and specificity in land cover and fuel loadings for the Texas regional domain and continental U.S. However, it is important to recognize the range of FINN emissions estimates that can be obtained with different land cover products and the strong need for *in situ* evaluation of fuel loadings.

Biogenic hydrocarbons

Biogenic volatile organic compounds (BVOCs), in particular isoprene (2-methyl-1, 3-butadiene, C_5H_8) and monoterpenes (a class of terpenes composed of two isoprene units), have been widely recognized for their key roles in atmospheric chemistry and climate, including contributions as precursors for tropospheric ozone (Atkinson, 2000) and secondary organic aerosol (SOA) formation (Tsigaridis and Kanakidou, 2003; Claeys et al., 2004). Globally, isoprene and monoterpenes have been estimated to comprise 70% and 11%, respectively, of total annual BVOCs emitted from vegetation (Sindelarova et al., 2014). Average Texas statewide VOC emissions reported in the EPA 2011 National Emission Inventory (Version 1) were ranked first within the continental United States at approximately 11,650 and 4,600 tons per day for biogenic and anthropogenic emissions, respectively.

Emissions of biogenic VOCs exhibit strong diurnal variability with temperature and sunlight and spatial gradients due to differences in land use and land cover. For example, observations made by Gilman et al. (2009) aboard the NOAA R/V Brown during TexAQS II/GoMACCS, indicated that BVOCs accounted for up to 20% of the VOC reactivity during the afternoon in the Houston-Galveston-Brazoria area. In sensitivity studies using a regional chemical transport model during the TexAQS 2000 time period, Li et al. (2007) found changes in ozone concentrations of ± 5 to 25 ppb over the Houston urban area and ± 5 to 10 ppb over the Houston Ship Channel in response to changes in isoprene emissions locally or from regions to the north of Houston. Characterization of land use and land cover has been an on-going priority of research in Texas since the late 1990s (e.g., Wiedinmyer et al., 2001; Feldman et al., 2010; Popescu et al., 2011). Land cover in Texas is highly diverse, varying from dense forest in East Texas to grasses and croplands towards the central regions. Huang et al. (2015a) found that misclassification between trees and grasses/crops has the potential to lead to large differences in biogenic emission estimates and maximum daily 8-hour ozone concentrations.

The TCEQ has relied on the Global Biosphere Emissions and Interactions System (GloBEIS3.1; http://www.globeis.com/) for estimating biogenic emissions for a number of years but has recently transitioned to the Model of Emissions of Gases and Aerosols from Nature (MEGAN; Guenther et al., 2012). AQRP projects have provided information about the uncertainties, sensitivities, and potential improvements to MEGAN under varying climatic conditions. These projects have evaluated current soil moisture representations using simulated and observational soil moisture datasets and explored the sensitivity of isoprene emission estimates to alternative representations of soil moisture (AQRP Project 14-008, McGaughey et al., 2015); evaluated the default drought parameterization scheme in MEGAN through comparisons with isoprene field measurements and investigated the use of different emission factors fields in MEGAN (AQRP Project 14-030, Ying et al., 2015); developed quantitative estimates of isoprene and monoterpene emissions with updated land cover and emission factor inputs using airborne measurements (AQRP Project 14-016, Yarwood et al., 2015) and generated a satellite-derived Photosynthetically Active Radiation (PAR) product, which is a requisite parameter for biogenic emissions models (AQRP Project 14-017, Pour Biazar et al., 2015).

Through the AQRP projects, essential inputs to the MEGAN model, including leaf area index, plant functional type characterization, and emission factors, have been updated based on available recent ground survey, remote sensing, and land surface model data products, and aircraft measurements during the DISCOVER-AQ campaign. MEGAN predictions of isoprene and monoterpene emissions have demonstrated a persistent high bias compared with aircraft flux data, suggesting large uncertainties still exist with the input data (e.g. Warneke et al., 2010). Predictions from air quality models such as CAMx and the Community Multi-scale Air Quality Modeling System (CMAQ) that have used MEGAN for biogenic emissions estimates in Texas have generally demonstrated a high bias in isoprene and ozone concentrations relative to aircraft and/or ground observations (Kota et al., 2015). Other studies over different global regions have evaluated MEGAN estimates of isoprene emissions using ground and aloft observations (e.g., Müller et al., 2008; Langford et al., 2010; Geng et al., 2011) aircraft measurements (e.g. Song et al., 2008; Warneke et al., 2010; Carlton et al., 2011), and satellite derived formaldehyde data (e.g. Palmer et al., 2006; Millet et al., 2008; Müller et al., 2008). MEGAN isoprene estimates have exhibited both high and low biases relative to observational data.

Biases in MEGAN estimates have been attributed to uncertainties in default emission factors (e.g. Langford et al., 2010; Ferreira et al., 2010), land cover data (e.g., Geng et al., 2011), spatial and temporal resolution of climate data (Pugh et al., 2013; Ashworth et al., 2010), and simulation of solar radiation and temperatures by the Weather Research and Forecast (WRF) model associated with the underestimation of aerosols and clouds, among other factors. AQRP projects have aimed at improving MEGAN estimates and understanding the implications on photochemical model predictions. Ying et al. (2015), for example, indicated that the use of emission factor fields from BEIS v3.61 and its input data (BELD4) could significantly improve MEGAN's capabilities in reproducing the observed isoprene concentrations at locations in Texas. Pour Biazar et al. (2015) found that use of satellite-derived PAR in MEGAN resulted in lower isoprene emissions estimates (by 15%~29%) relative to PAR fields derived from WRF over Texas climate regions during August and September of 2013. Sensitivity studies by Yarwood et al. (2015) examined the effects of altering the chemical mechanism, dry deposition

velocities for biogenic trace gases, and emission factors in the photochemical model CAMx on concentrations of a subset of species (isoprene, isoprene products, sum of monoterpenes, ozone, OH); the results indicated the need for further verification of emission factors, reconciliation of substantial differences between leaf-, tower-, aircraft-, and satellite-based emission estimates, use of assimilation approaches (satellite and/or in-situ observations) for improving solar radiation and temperature inputs to MEGAN, and application of current land cover data.

Extreme climate events such as severe drought are a recurring phenomenon in Texas and have the potential to affect regional air quality through stresses to biogenic systems. Despite previous leaf- and ecosystem-level studies, the impact of drought on biogenic emissions (primarily isoprene) remains somewhat controversial. Limited ecosystem-level studies have shown stimulated isoprene emissions under drought conditions (Pressely et al., 2006) as well as short-term increases followed by long-term decreases (Potosnak et al., 2014). MEGAN estimates of biogenic emissions are influenced by competing effects of model input parameters (i.e. reductions in leaf area index and soil moisture may lead to negative impacts on isoprene emissions while elevated temperatures may enhance emissions during drought; Huang et al., 2015b) and also uncertainties in input data. The parameterization of water stress on plants during drought in MEGAN is based on soil moisture and wilting point; predicted isoprene emissions have been shown to be highly sensitive to the specific soil moisture database employed (AQRP Project 14-008, McGaughey et al., 2015). Observations of soil moisture in much of eastern Texas are sparse, although NASA's Soil Moisture Active Passive (SMAP) satellite mission and the Texas Soil Observation Network (TxSON) should result in new data resources in the future.

Emissions of Highly Reactive Volatile Organic Compounds (HRVOCs)

Observational evidence has indicated substantial reductions in emissions of ozone precursors in the Houston area during the time period between the TexAQS 2000 and TexAQS II field campaigns. Washenfelder et al. (2010) measured reductions of 29% ± 20% in NO_x emissions between August 2000 and September 2006 in the Houston industrial area that were consistent with reductions in NO_x emissions at larger point sources throughout the southeastern United States that have implemented controls. Temporal trends in the ratios of the HRVOCs, ethene and propene, respectively, to oxides of nitrogen (i.e., C_2H_4/NO_x and C_3H_6/NO_x) over the same time period indicated decreases of 30% ± 30%; median ambient concentrations of ethene and propene within the Houston urban area decreased by 52% and 48%, respectively. However, even with declines in emissions and ambient concentrations, measurements during TexAQS 2000 and TexAQS II indicate that the best emission inventories significantly underestimate industrial VOC emissions in Houston (e.g., Ryerson et al., 2003; De Gouw et al., 2009; Parrish et al., 2009; Mellqvist et al., 2010; Washenfelder et al., 2010; Kim et al., 2011). For example, Washenfelder et al. (2010) had found that measured ratios of C_2H_4/NO_x and C_3H_6/NOx exceeded emission inventory values by factors of 1.4-20 and 1-24, respectively.

During 2009 (SHARP, Lefer, 2009), 2011 (AQRP Project 10-006, Johansson et al., 2013) and 2013 (DISCOVER-AQ, AQRP Project 13-005, Johansson et al., 2013; AQRP Project 14-007, Johansson et al., 2015), atmospheric VOC gas columns downwind of specific local source regions in the Houston area have been repeatedly investigated using a combination of mobile Differential Optical Absorption Spectroscopy (DOAS) and Solar Occultation Flux (SOF). Johansson et al. (2014) reported that although alkane emissions between 2006 and 2011 were

generally stable, emissions of ethene and propene have declined. For example, measurements downwind of the Houston Ship Channel indicated ethene and propene emissions during 2006 of 1511 kg h^{-1} and 878 kg h^{-1}, respectively, compared to approximately 600 kg h^{-1} for both species during both 2009 and 2011. In the most recent analysis of limited mobile DOAS sampling performed in Houston during DISCOVER-AQ (2013), Johansson et al. (2015) found additional decreases in alkene concentrations; for example, Houston Ship Channel emissions for ethene and propene were estimated at 475 kg h^{-1} and 394 kg h^{-1}, respectively. However, the authors noted that measured VOC emissions were 5-15 times higher than those based on year-specific emission inventories, while for SO_2 and NO_2 the ratios were typically 0.5–2 (Johansson et al., 2014). The results of Johansson et al. (2014) were generally consistent with those from previous studies for Houston that have suggested an under representation of alkenes within emissions inventories of up to an order of magnitude (e.g., the findings of Mellqvist et al. (2010), which were based only on SOF measurements collected during 2006, as well as Air Quality Project 10-045 (Stutz et al., 2011) which estimated ethene and propene emissions using inverse modeling and in-situ observations collected during 2009).

Barnett Shale 2011 field campaign

The Barnett Shale is an oil and gas production region located largely to the west of the Dallas area that saw rapid expansion and economic growth between 2005 and 2010. An AQRP-sponsored field campaign conducted in 2011 sought to better understand the effects of Barnett Shale activity on air quality in the region. Aircraft measurements collected by AQRP Project 10-044 (Alvarez et al., 2011) over portions of the Barnett Shale did not find enhancements in ozone concentrations clearly associated with oil and gas emissions, but persistent southerly winds (~10 mph) may not have favored mixing of urban Dallas-Fort Worth and Barnett Shale emissions that would alter the VOC/NO_x ratio towards a regime favoring ozone production. On some occasions, elevated concentrations of reactive alkenes (up to 10 ppbv) and formaldehyde (4-6 ppbv compared to background concentrations of 2-3 ppbv) were measured, such as immediately downwind of a large compressor station in the Eagle Mountain Lake area.

Fourier Transform InfraRed Spectroscopy (FTIR) and canister sampling analysis performed by AQRP Project 10-006 (Johansson et al., 2011) estimated significant rates of ethene emissions from large compressor stations (0.4 kg/hr) and from flash venting from a single condensate tank (2 kg/hr); however, high ethene concentrations have not been observed in other contemporary studies (e.g., Sullivan, 2010; TITAN, 2010; Zielinska et al., 2011). The largest oil and gas sources of methane and other hydrocarbon emissions near Fort Worth were gas treatment facilities combined with large compressor stations. Flashing emissions on one occasion from a condensate tank were estimated at 140 kg/h for methane and 10 kg/h for ethane (among other species).

Deployment of the Measurement of Ozone Production Sensor (MOPS) during August – October 2011 at the Meacham site near Dallas-Fort Worth by AQRP Project 10-034 (Lefer and Brune, 2011) showed that ozone production on sunny days peaked at 40-60 ppbv/h during mid-morning, suggesting that Meacham may be an ozone source region. Ozone production rates at Eagle Mountain Lake were generally lower, with peak ozone productivities of 40 ppbv/h in the late mornings on only a few days. Findings from AQRP Project 10-024 (Griffin et al., 2011) suggested that the air masses transported to Eagle Mountain Lake were aged and originated over

the Dallas-Fort Worth metropolitan area; the impact of local sources were detected only intermittently. Aircraft measurements collected by Alvarez et al., (2011) within the photochemically aged plume downwind of Dallas-Fort Worth showed modest concentrations of NO, NO_2, and reactive alkenes and indicated enhancements in maximum ozone concentrations by factors ranging from 1.5-2.5 relative to upwind concentrations.

Satellite observations of NO_2 column densities

Nitrogen oxides are precursors to both ozone and fine particulate matter. Over the past decade, anthropogenic NO_x emissions have declined substantially due, largely, to reductions from mobile and stationary point sources (e.g., http://www.epa.gov/ttnchie1/trends/); between 2005 and 2014, NO_x emissions reported to EPA's National Emission Inventory (NEI) indicated that U.S. anthropogenic emissions have declined by approximately 39%. Emissions from point sources, such as electric generating units, are commonly measured directly using continuous emission monitors (CEMs); however, other spatially distributed NO_x sources and the sparseness of ground-level monitoring present challenges in tracking the spatial and temporal variations in emissions.

Satellite NO_2 column observations provide an effective proxy to infer NO_x emissions from surface-based sources (e.g., Boersma et al., 2008a; Lamsal et al., 2011, 2015; Streets et al., 2013; Tang et al., 2013; Vinken et al., 2014, among many others) and are widely used to estimate trends (e.g., Boersma et al., 2008b; Russell et al., 2012; Zhou et al., 2012; Schneider et al., 2015, among many others). In a study focused on eastern Texas, McDonald-Buller et al. (2012) found that NO_2 column densities were highest over urban areas and highway corridors and had decreases between 2005 and 2010 in reasonable agreement with changes in ground-based observations. A comparison of trends between satellite observations and results from photochemical modeling indicated largest differences in rural regions suggesting possible under-estimation of emissions associated with oil and gas activities. More recent studies have also demonstrated declines in NO_2 column densities during the past decade within various eastern Texas metropolitan areas (e.g., Choi and Souri, 2015; Lamsal et al., 2015; Tong et al., 2015). Lamsal et al. (2015) estimated that atmospheric NO_2 concentrations over Dallas and Houston decreased by 35-40% between 2005 and 2013 and noted the importance of accounting for seasonal and interannual variability in the vertical concentration profiles required by standard satellite retrieval algorithms,. Further analyses using a high-resolution chemical transport model suggested that emissions reductions were greater during 2005-2010 compared to 2010-2013.

Although uncertainties remain (e.g., refer to review by Streets et al., 2013), NO_2 column retrievals are widely used to constrain emissions inventories for global and regional modeling (e.g., Boersma et al., 2008a; Kim et al., 2009; Lin et al., 2010; Tang et al., 2013; 2015; Vinken et al., 2014). In studies for Texas, Tang et al. (2013, 2015) found that a regionally-based inversion approach to adjust NO_x emissions deteriorated model performance (as evaluated by comparison to ground-based measurements) while an emission sector-based methodology showed some improvement. AQRP Project 13-TN2 (Kim et al., 2013) developed techniques and software that can be used to more efficiently process and integrate geo-spatial datasets with air quality modeling predictions; for example, urban emission features can be refined by downscaling and re-gridding relatively coarse resolution GOME-2 column NO_2 observations using fine-scale photochemical model (CMAQ) predictions. AQRP Project 14-014 (Choi and Li, 2015) used a

sector-based inversion methodology and NO_2 columns derived from Ozone Monitoring Instrument (OMI) observations to downwardly adjust an NEI inventory with a known high bias. Additional treatment of the OMI dataset included adjustments for cloud fraction, solar angle, and, importantly, removal of the a priori "first-guess" influences in the vertical concentration profiles. The adjustments to the inventory, which reduced emissions from anthropogenic sectors and increased emissions associated with biogenic activity, showed improved agreement with available surface and aircraft observations. However, a recent study by Kemball-Cook et al. (2015) noted large differences in top-down emissions using two different operational products derived from the same satellite dataset suggesting high sensitivity to the specific dataset employed.

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2.3 Tropospheric chemistry

2.3.1 Overview

Atmospheric chemistry in Texas has a number of unique features. The combinations of industrial and urban emissions, and forested and coastal environments, cause certain chemical pathways to become more significant in Texas than in other regions. Specific findings arising from the AQRP program that address tropospheric chemistry under Texas conditions are summarized in this Section.

2.3.2 Tropospheric chemistry assessment from AQRP projects 2010-2015

NO_x sink and recycling reactions and gas-particle partitioning of organic nitrates

Reaction products arising from the oxidation of anthropogenic or biogenic volatile organic compounds can act to reduce the availability of NO_x for ozone formation by forming NO_x sink compounds, including organic nitrates and nitric acid. NO_x sink species may eventually react to return NO_x back to the atmosphere in a process known as NO_x recycling. Organic nitrates and their role as NO_x sink species, their participation in NO_x recycling reactions, and their gas-particle partitioning have been the subject of several coordinated studies involving experimental chamber measurements and photochemical modeling and have received increasing attention recently because of the implications for ozone and organic aerosol formation on local, regional, and global scales.

The chemistry of organic nitrates in the atmosphere has been reviewed in detail by Perring et al. (2013), AQRP Project 12-012 (Hildebrandt Ruiz and Yarwood, 2013), and elsewhere, and is summarized only briefly here. Organic nitrates ($RONO_2$) are primarily formed as products of the reaction of organic peroxy radical (RO_2) and nitric oxide (NO). RO_2 radicals arise from the oxidation of anthropogenic or biogenic volatile organic compounds (VOCs) by hydroxyl radical (OH), ozone (O_3), nitrate (NO_3) or photolysis. Although information for many compounds is not complete, the organic nitrate functionality and formation yields (α) depend upon the size and structure of the organic backbone (R) of the peroxy radical. For example, alkanes have higher reported yields than alkenes at an equivalent number of carbon atoms; yields generally increase with an increasing number of carbon atoms (Perring et al., 2013). Precursors to organic nitrates vary by location with anthropogenic and biogenic emission source regions (Perring et al., 2013). Larger $RONO_2$ molecules are semi-volatile and are expected to partition between the gas and particle phases. Gas-particle partitioning and hydrolysis of organic nitrates in the condensed phase influence their role as sources and sinks of NO_x. Once formed, organic nitrates can be transported, chemically processed, removed by deposition to vegetation and other surfaces, or partition into the aerosol phase, depending on their structure. Organic nitrates have sufficiently long atmospheric chemical lifetimes (hours to days) to be affected by regional or longer-range transport, such that they have the potential to influence NO_x budgets and air quality over extended spatial scales. For example, organic nitrates extend the range of downwind transport of NO_x and the potential for ozone formation on regional scales.

Recent advances have been made in understanding $RONO_2$ chemistry and gas-particle partitioning in ambient and laboratory studies (e.g., Rollins et al., 2010; Liu et al., 2012; Rollins et al., 2013; Rindelaub et al., 2015; Bean and Hildebrandt Ruiz, 2015; Lee et al., 2015) and early modifications to the chemical mechanisms have begun to represent these processes in CAMx and

other photochemical grid models. Environmental chamber experiments conducted as part of AQRP Project 10-042 (Yarwood et al., 2012) provided experimental evidence for NO_x production when organic nitrates degraded by OH reaction and photolysis and provided an initial foundation for modifications to the Carbon Bond mechanism in CAMx (CB6r1 mechanism). The CB6r2 mechanism was developed during AQRP Project 12-012 (Hildebrandt Ruiz and Yarwood, 2013) to improve the level of detail regarding the formation and fate of organic nitrates.

Influence of nitryl chloride chemistry on tropospheric oxidation capacity and ozone formation

Dinitrogen pentoxide (N_2O_5) is a nocturnal reservoir of NO_x, formed from the reaction of nitrate radical (NO_3^-) and NO_2. Heterogeneous reaction of N_2O_5 can proceed via two pathways: (1) hydrolysis to form soluble nitrate, the rate of which depends on the availability of aerosol surface area and on the heterogeneous uptake coefficient of N_2O_5 to aerosol (Brown et al., 2009; Parrish et al., 2009), or (2) reaction with chloride to form nitryl chloride ($ClNO_2$) and nitrate, which depends on, among other factors, particulate chloride (PCl) availability (Finlayson-Pitts et al., 1989; Behnke et al., 1997; Kercher et al., 2009; Osthoff et al., 2008; Thornton et al., 2010; Roberts et al., 2008). At sunrise, $ClNO_2$ photolysis can affect the cycling of oxidants by providing a source of chlorine atoms that enhance VOC oxidation (Osthoff et al., 2008; Knipping and Dabdub, 2003; Tanaka et al., 2003). Simpson et al. (2015) provide a comprehensive overview of the current understanding of the chemistry of nitryl halides in polluted regions. The presence of nitryl chloride has been characterized in the coastal environments of Houston during the 2006 TexAQS/Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS) (Osthoff et al., 2008) and the Los Angeles area during the 2010 CalNex campaign by Riedel et al. (2012) and Mielke et al (2013), as well as for the inland regions of Boulder, Colorado (Thornton et al., 2010), Calgary, Alberta, Canada, (Mielke et al., 2011), southwestern Germany (Phillips et al., 2012), and the Uintah Basin of Utah (Edwards et al., 2013).

The influences of nitryl chloride production and chemistry on regional air quality and implications for air quality management have been examined using chemical transport models (e.g., Simon et al., 2009; Sarwar et al., 2012; Sarwar et al., 2014). Results of these studies have suggested increases in ozone due to $ClNO_2$ production are generally within 1-6 nmol/mol in the Northern Hemisphere with seasonal and spatial variations. AQRP Project 10-015 (Koo et al., 2012) developed an initial parameterized mechanism for $ClNO_2$ chemistry in CAMx, which has typically been used for regulatory air quality modeling in Texas. CAMx version 6.20 (v.6.20; http://www.camx.com/files/camxusersguide_v6-20.pdf) incorporates an extension of CB6r2 chemistry (CB6r2h) to address reactions involving ocean-borne halogen compounds. The CB6r2h includes updates to the chlorine (Cl) reaction mechanism of Koo et al. (2012) as well as reaction mechanisms for bromine and iodine (Yarwood et al., 2014).

Contribution of intermediate Volatile Organic Compounds (IVOCs) to secondary organic aerosol formation

Understanding the composition and sources of fine particulate matter ($PM_{2.5}$) in Houston is important to air quality planning as the region experiences concentrations close to the level of the NAAQS. Over half of fine particulate matter in the Houston region is composed of organic material including primary organic aerosol (POA), which is comprised of compounds that are emitted as particles and have not reacted in the atmosphere, and secondary organic aerosol (SOA), which is formed when gas-phase compounds undergo one or more chemical

transformations in the gas-phase, forming less volatile compounds that then partition between the gas- and particle-phases. These gas-phase precursors of SOA are classified (in decreasing order of vapor pressure/volatility) as volatile organic compounds (VOC), intermediate volatility organic compounds (IVOC) or semivolatile organic compounds (SVOC). Sources of organic aerosol (OA) in Houston include POA and SOA from urban anthropogenic activity, the petrochemical industry, and fires, as well as SOA from biogenic VOCs. The importance of organics in controlling fine PM mass in the Houston region has been recognized through ambient air quality data collection during field campaigns such as TexAQS 2000 and DISCOVER-AQ.

Recent studies have suggested the importance of intermediate volatile organic compounds as precursors of SOA (e.g., Ait-Helal, 2014; Yuan et al., 2013; Robinson et al., 2007). In a review of emissions inventories from the point source sector in Harris County, AQRP Project 14-024 (Hildebrandt Ruiz et al., 2015) identified butyl CARBITOL™ and methyl naphthalene as potential IVOCs, as well as compound mixtures associated with petrochemicals processing that could contain IVOCs. Hildebrandt Ruiz et al. (2015) found that of six IVOCs (n-pentadecane, 2,6,10-trimethyldodecane, 2-methylnapthalene, butyl CARBITOL™, Texanol™, and mineral spirits) examined in laboratory chamber experiments, all but Texanol™ formed SOA.

A state of the science approach for modeling gas-aerosol partitioning and chemical aging of primary and secondary atmospheric organic aerosols based on the Volatility Basis Set (Donahue et al., 2006) has recently been added as an option in CAMx but has yet to be widely applied for air quality planning efforts in Texas. AQRP Project 14-024 used CAMx with the 1.5 dimensional volatility basis set (1.5-D VBS) to simulate organic aerosol formation in the Houston region during the 2013 DISCOVER-AQ campaign. The 1.5-D VBS scheme accounts for systematic variations in both volatility and oxidation state (O:C ratio) to model the magnitude and chemical aging of OA. Emissions of IVOCs from major combustion sources were added using IVOC fractions of total non-methane organic gas (NMOG) emissions estimated from environmental chamber studies. Analysis of ambient air quality data analysis during DISCOVER-AQ was used to guide model improvements; biases of modeled versus observed organic carbon and chemically aged oxygenated OA (OOA: anthropogenic and biogenic) were generally within 30% at Houston area sites.

Chemical pathways for secondary organic aerosol from isoprene

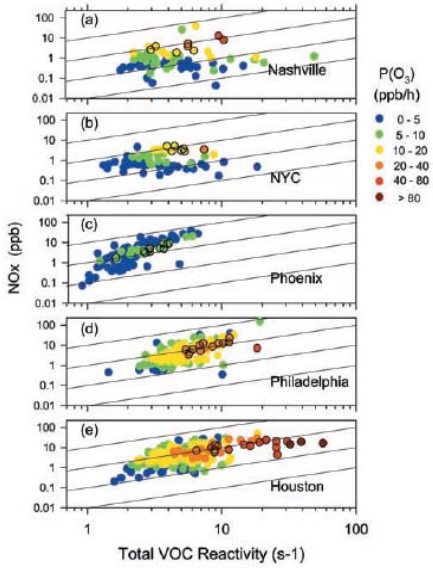
Within the last decade, it has been recognized that photochemical oxidation of isoprene leads to significant yields of gas-phase intermediates that contribute to SOA formation. The production of isoprene-derived SOA is enhanced by anthropogenic emissions, including NO_x and SO_2 typical of urban areas (Budisulistiorini et al., 2015; Surratt et al., 2006, Kroll et al., 2006). Recent studies have identified important reactive intermediates formed under low and high NO_x conditions (Surratt et al., 2006; Kroll et al., 2006) and the influence of varying aerosol acidity (Surratt et al., 2006; Surratt et al., 2010) and relative humidity (Carlton et al., 2009). Predictions of isoprene-derived SOA formation have required fundamental improvements in the gas and aerosol-phase chemical mechanisms in regional and global scale models and identified the need for evaluation of revised mechanisms against controlled chamber experiments (Chen et al., 2015; AQRP Project 14-003, Vizuete and Surratt, 2015); evaluation of model revisions against ambient measurements has indicated overall better performance in representing seasonal and spatial

patterns of biogenic SOA (Carlton et al., 2009; Karl et al., 2009; Baek et al., 2011; Ying et al., 2015; Li et al., 2015; Lin et al., 2013), although uncertainties remain.

Ozone production rates and efficiencies in the Houston Area

The proximity of NO_x and reactive VOC-rich plumes in Houston's extensive petrochemical complex lead to conditions that favor rapid ozone formation (e.g., Kleinman et al., 2002, 2005; Ryerson et al., 2003; Mao et al., 2010). During TexAQS 2000, ozone production rates and ozone production efficiencies (OPE) in plumes originating from the Houston Ship Channel industrial complex were found to be greater than those for the Houston urban core and others areas of the United States (Ryerson et al., 2003; Daum et al., 2003; Berkowitz et al., 2004; Kleinman et al., 2005). For example, comparisons of ozone production rates for five U.S. cities by Kleinman et al. (2005), shown in Figure 2.3.1, indicates that the top 10% of the distribution of ozone production rates for Houston are substantially higher than those in Philadelphia, Phoenix, New York City, and Nashville.

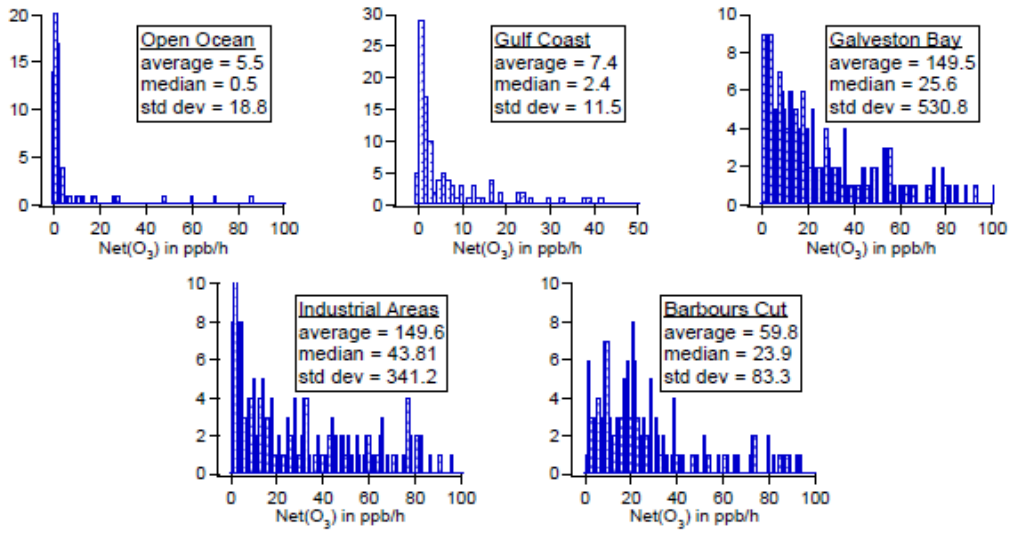
Figure 2.3.1. Ozone production rates for five U.S. cities in the style of an ozone isopleths diagram from Kleinman et al. (2005). Samples comprising the top 10% of the distribution in each city are outlined in bold.



During TexAQS 2000, strong spatial gradients in the rates of ozone formation were found across the Houston area (Berkowitz et al., 2005) with levels between 3 and 18 ppb h^{-1} over downtown Houston and 3 and 80 ppb h^{-1} in the eastern industrial plume (Daum et al., 2003). Net ozone production rates by Sommariva et al. (2011), shown in Figure 2.3.2, during TexAQS II varied spatially throughout the Houston/Galveston region and Gulf Coast. More recently, AQRP Project 13-024 (Ren et al., 2013) found OPEs of approximately 16 based on observations during the summer of 2013 at a Galveston monitoring location. Zhou et al. (2014) indicated that large OPEs (8–15) occurred in diluted industrial plumes transported over the isoprene-rich northern rural areas, while lower OPEs (5-7) are generally found in urban and industrial plumes transported southward. Using measurements collected aboard the NOAA P-3 during DISCOVER-AQ, AQRP Project 14-020 (Ren, 2015) calculated an average OPE of approximately 8, which is greater than the value of 5.9 +/- 1.2 ppbv calculated for the TexAQS II (2006) period (Neuman et

al., 2009). Overall, these findings suggest that highly reactive air masses continue to be important in ozone formation in Houston, that the high reactivity is due to both anthropogenic and biogenic emissions, and that the locations of high ozone concentrations resulting from highly reactive emissions are variable, due to Houston's complex meteorology.

Figure 2.3.2. Frequency distributions of Net(O_3) at locations during the NOAA R/V Brown cruise in the summer of 2006 as part of TexAQS II from Sommariva et al. (2011). The bin size is 0.1 ppb h-1 for the open ocean and 1 ppb/h for all other locations. Values on the y-axis are the number of data points in each bin.



AQRP Project 10-032 (Lefer et al., 2011) investigated ozone production sensitivity during three campaigns: TexAQS 2000 (late summer), TexAQS II Radical and Aerosol Measurement Program (TRAMP, fall 2006), and SHARP 2009 (spring), and found similar behavior across the campaigns, during which the early morning and late afternoon periods were most sensitive to VOC and NO_x, respectively. Lefer et al. (2011) noted that afternoon ozone sensitivity had a longer NO_x-sensitive period during SHARP 2009 compared to the results for 2000 and 2006 (e.g., Mao et al., 2010). Using measurements collected aboard the NOAA P-3 during DISCOVER-AQ and at eight surface sites where the P-3 conducted vertical spiral profiles, AQRP Project 14-020 (Ren, 2015) employed an observation-constrained box model based on the Carbon Bond mechanism, Version 5 (CB05), to investigate ozone production sensitivities. Across the surface sites, ozone formation ranged from VOC sensitive for the entire day at Deer Park to mostly NO_x sensitive at Smith Point and Conroe; Moody Tower and Channelview were either VOC sensitive or in the transition regime. Throughout the Houston area, overall ozone production tended to be VOC sensitive in the mornings with average rates of 20-30 ppbv hr^{-1} and maximum rates of 30-50 ppbv h^{-1}; these relatively high rates suggested that VOC controls may be an effective way to control ozone in Houston. In the afternoon, average ozone production rates were 5-10- ppbv hr^{-1} under mostly NO_x sensitive conditions but spatial variability existed.

Zhou et al. (2014) also noted that periods with the most rapid ozone formation were VOC-sensitive while slow ozone formation was NO_x-limited. Zhou et al. (2014) indicated that despite reductions in both NO_x and HRVOCs between 2000 and 2006 (e.g., Cowling et al., 2007;

Gilman et al., 2009; Washenfelder et al., 2010) that have reduced ozone production by 40-50% in Houston, OPEs were similar between the two periods consistent with results from previous studies (e.g., Cowling et al., 2007; Neuman et al., 2009). In an investigation of the impact of structural and parametric uncertainties on predicted ozone and precursor concentrations, AQRP Project 10-008 (Cohan et al., 2011) identified the importance of emission rates, reaction rate constants, and boundary conditions on predicted Dallas-Fort Worth area ozone concentrations during June 2006 under predominantly NO_x-limited conditions. Collectively, these results and those from other studies (e.g., Kleinman et al., 2005; Xiao et al., 2010; Sommariva et al., 2011) have indicated the importance of both HRVOC and NO_x controls to further reduce ozone concentrations in Texas.

β-Hydroxynitrates as unique markers for ozone enhancements in Houston industrial plumes

Quantifying the relative contributions of individual HRVOCs to ozone formation has remained challenging despite their long-recognized role in ozone formation in the Houston Ship Channel. β-hydroxynitrates (βHNs) are formed when HRVOCs react in the atmosphere in the presence of nitrogen oxides (NO_x). Using a combination of data analysis and reactive plume modeling, AQRP Project 14-026 (Yarwood et al., 2015) leveraged recent aircraft measurements of C_2-C_5 hydroxynitrates, made during the National Aeronautics and Space Administration (NASA) Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC^{4}RS) campaign in the fall of 2013, as a novel initial approach to link observed enhancements of ozone and formaldehyde to reactions of specific HRVOCs and isoprene in Houston Ship Channel plumes.

Ozone enhancements in plume intercepts ranged from 4 to 54 ppb. The fraction of these enhancements directly attributable to HRVOC and isoprene emissions (as indicated by the O_3/βHN ratios) ranged from 6% to 24%. Isoprene contributed, on average, 35% (range of 9% to 56%) of the directly attributable ozone enhancement. Direct contributions of individual HRVOCs to the anthropogenic ozone enhancement were ranked on average as ethene (49%), propene (32%), butenes (13%), and butadiene (6%). Variability in these relative contributions reflected in part, differences in HRVOC reaction rates as plumes were photochemically processed downwind of release.

The modeled direct contributions of HRVOCs determined for one flight day using the SCICHEM Lagrangian puff model were generally consistent with the observational data. Direct formation of ozone from the HRVOC emissions in the Houston Ship Channel explained 12-25% of the plume ozone increments; the remaining ozone was formed indirectly by the interaction of Houston Ship Channel emissions with emissions of other species such as isoprene. The project found that representing Houston Ship Channel emissions by multiple, narrower source plumes accelerated plume chemistry and improved model performance. Plume chemistry was found to be sensitive to whether HRVOCs and NO_x were released together or segregated in separate plumes that interact as they disperse and overlap each other.

Mechanisms for HONO formation

Nitrous acid (HONO) is a precursor to the formation of hydroxyl radical (OH). Collectively known as HO_x, OH, and hydroperoxyl radical (HO_2) have important roles in the formation of ozone and fine particulate matter. Field campaigns, such as the TexAQS II, TRAMP, SHARP,

and FLAIR, have sought to improve the characterization of HONO and understanding of its influence on radical budgets, primarily in the Houston-Galveston-Brazoria airshed. Findings during these studies have been used to guide improvements in the formation pathways for HONO in CAMx (Couzo et al., 2014; Karamchandani et al., 2014).

Measurements during the SHARP campaign indicated that photolysis of HONO in the early morning is an important radical production source in Houston (AQRP Project 12-028, Lefer et al., 2014; Karamchandani et al., 2014). Sources of HONO include production by homogeneous gas-phase reactions, direct emissions from combustion sources, or production by heterogeneous reactions on ground or aerosol surfaces (Karamchandani et al., 2014). Recent measurements have indicated though that daytime observed HONO mixing ratios are often far larger than the expected photostationary state with OH and NO in urban and rural locations throughout the world (e.g., Wong et al., 2012; Acker et al., 2006a; Acker et al., 2006b, Zhou et al., 2007; Carter and Seinfeld, 2012; Spartaro et al., 2013), including the Houston area (Olaguer et al., 2009; Wong et al., 2012). Moreover, the dominant HONO formation pathway in both the Carbon Bond and SAPRC chemical mechanisms commonly used in air quality models was the homogeneous gas-phase reaction of OH with NO, which was insufficient to replicate observed nocturnal and daytime HONO formation. Direct emissions of HONO could also not account for observed concentrations. Additional work is necessary to reconcile HONO measurements with observations.

Daytime formation mechanisms that account for enhanced HONO formation have been a focal point of studies over the past several years. Both gas-phase and heterogeneous mechanisms on aerosol surfaces have been investigated, including gas-phase photolysis of ortho-nitrophenols (Bejan et al., 2006), daytime reaction of photo-excited NO_2 with water vapor (Li et al., 2008), heterogeneous conversion of NO_2 on fresh and aged soot particles (Zhang et al., 2009; Lefer et al., 2010), humic acids and soil surfaces (Stemmler et al., 2006), photolysis of surface adsorbed nitric acid (Zhou et al., 2011), and heterogeneous conversion of HNO_3 on the surface of primary organic aerosol (Ziemba et al., 2010). In the Houston area during SHARP, Wong et al. (2012) and AQRP Project 10-032 (Lefer et al., 2011) found statistically significant vertical gradients of HONO throughout the day, with smaller mixing ratios aloft, and suggested that a likely source of daytime HONO could be photocatalytic conversion of gas-phase NO_2 on the ground. Karamchandani et al. (2014) have developed and implemented a surface model to CAMx that allows heterogeneous production of HONO through a representation of the surface as a reservoir of deposited species that can sorb or penetrate into soils and vegetation and undergo chemical processing and re-emission to ambient air. Couzo et al. (2014) found that heterogeneous HONO formation through this parameterization reduced the normalized mean error by 30% - 45% for modeled daytime and nighttime concentrations relative to SHARP measurements and had more significant effects than increases in direct HONO emissions.

Sources and concentrations of ambient formaldehyde

As described in detail by Seinfeld and Pandis (1998) and others (e.g., Parrish et al., 2012; Olaguer et al., 2014), formaldehyde originates from primary emissions sources (e.g., flares, industrial processes such as catalytic cracking, motor vehicles) as well as from secondary chemical production through the oxidation of biogenic and anthropogenic VOCs, including alkenes, alkanes, and aromatic compounds. Secondary production of formaldehyde occurs via

photochemical oxidation of precursor VOCs initiated by OH during the day; while at night, oxidation of precursor VOCs occurs via ozone and nitrate radical.

Measured formaldehyde concentrations in the Houston Ship Channel exceeded 50 ppb during TexAQS II (Eom et al., 2008) and 20 ppb during DISCOVER-AQ (AQRP Project 14-002, Fried and Loughner, 2015). During 2009 (SHARP; Lefer, 2009) and 2011 (AQRP Project 10-006, Johansson et al., 2013; AQRP Project 13-005, Johansson et al., 2015), atmospheric columns of HCHO associated with specific local source regions were repeatedly investigated using mobile Differential Optical Absorption Spectroscopy (DOAS) and Solar Occultation Flux (SOF). Emissions from two Texas City and two Mont Belvieu sources were estimated to range from 6 to 15 kg h^{-1}, compared to emissions of approximately 40 and 22 kg h^{-1} from a Ship Channel source during 2009/2011 and 2013, respectively. AQRP Project 14-045 (Stutz et al., 2011) used comparable measurement technology during FLAIR to infer an emissions flux from a collection of Texas City industrial facilities on the order of 20 kg h^{-1}. Stutz et al., 2011 noted direct HCHO emissions from burning flares at rates that ranged from 0.3 to 2.5 kg h^{-1} similar to results from other flare measurement studies (e.g., Pikelnaya et al., 2013).

The relative contribution of primary sources and secondary chemical production to ambient formaldehyde concentrations and fluxes in Houston has been a topic of focus and divergent analysis during the past several years (Rappengluck et al., 2010; Buzcu et al., 2011; Parrish et al., 2012; Olaguer, 2013; Olaguer et al., 2013; Zhang et al., 2013; Johansson et al., 2014). For example, using CO and SO_2 as primary markers for mobile and industrial source emissions, respectively, Rappenglück et al. (2010) calculated formaldehyde source contributions during TexAQS II at Moody Tower of 38.5% from primary vehicular emissions, 24.1% from secondary photochemistry, and 8.9% from industrial emissions. Analyzing the Moody Tower dataset but using Positive Matrix Factorization (PMF), Buzcu et al. (2011) attributed 23% of HCHO to primary emissions from motor vehicles, 24% from the oxidation of biogenic or industrial isoprene, 17% from other industrial emissions, and the remainder from OH driven secondary photochemistry. Using a plume chemistry model to investigate 13 individual HCHO events sampled in the Houston-Galveston-Brazoria area during 2009 and 2011, Johansson et al. (2014) found that primary emissions contributed 90%, on average, to measured concentrations and that only three cases had modeled contributions greater than 10% attributed to photochemical production.

Parrish et al. (2012) undertook a reanalysis of the quantification of primary and secondary sources of formaldehyde in the Houston area using archived data from airborne, mobile, and elevated surface (i.e., Moody Tower) studies collected during 2000-2009 and a measurement constrained inventory based upon the 2005 National Emissions Inventory (NEI). In contrast to earlier studies, they concluded that secondary production of formaldehyde from alkenes emitted by petrochemical facilities and on-road vehicles is the major source of formaldehyde in the Houston-Galveston-Brazoria area (92 ± 4%), with only 4 ± 2% directly emitted from these facilities. The authors noted there are cases where targeted reductions of primary formaldehyde emissions may be warranted, for example, Fried et al. (2015) indicated the importance of episodic spikes in emissions. Using a source apportionment technique within CMAQ, Zheng et al., (2013) attributed 20 to 30% of regional HCHO concentrations to primary emissions (biogenic, natural gas combustion, and vehicles) and 30 to 50% associated with secondary

formation (biogenic, industrial, and vehicles) with the remainder from upwind sources (30 to 50%).

Olaguer et al. (2014) indicated that discrepancies between primary and secondary attributions may be due, in part, to differences in the assumed relationship between tracer combustion species (e.g., CO) and primary emissions as well as in the spatial and temporal representation of the corresponding measurements. For example, Johansson et al. (2014) noted that the highest HCHO emission rate included in their study was approximately 120 kg h^{-1}; on a regional scale, these emissions are small compared to HCHO formed from secondary production, which may be an order of magnitude higher. Nonetheless, there is recognition by air quality stakeholders that understanding formaldehyde sources is critical to defining effective ozone control strategies in the Houston area.

Representation of alkene chemistry in an atmospheric chemical mechanism

Using reliable atmospheric chemical mechanisms in regulatory air quality modeling is necessary to formulate effective and efficient emission control strategies for achieving ozone reductions. Seven alkenes (ethene, propene, 1,3-butadiene, 1-butene, isobutene, trans-2-butene, and cis-2-butene) associated with industrial emissions have been classified as HRVOCs (Texas Administrative Code, Title 30, Part 1, Chapter 115; TCEQ, 2012) and have been a focus of novel emissions reduction strategies in southeastern Texas due to their recognized impacts on ozone production. Condensed chemical mechanisms commonly used for air quality modeling in the U.S., including versions of the CB (Yarwood et al., 2005; Whitten et al., 2010; Yarwood et al., 2010) and Statewide Air Pollution Research Center (SAPRC) (Carter, 2000; Carter, 2010) mechanisms, have historically been designed to model ozone formation from typical urban ambient VOC mixtures, not under atmospheric conditions significantly influenced by highly variable HRVOC emissions. AQRP Project 12-006 (Heo and Carter, 2014) designed and conducted environmental chamber experiments to evaluate the representation of alkene chemistry for HRVOCs and non-HRVOCs in the SAPRC, and to a more limited extent the CB, chemical mechanisms. SAPRC mechanisms with varying levels of VOC lumping were implemented in CMAQ (Byun and Schere, 2006) to simulate a summer ozone episode during the TexAQS II.

Statistical analysis of peak and hourly ozone concentrations by Heo and Carter (2014) indicated that SAPRC-11D, the most detailed SAPRC mechanism ever applied in regional air quality simulations that used approximately 300 explicit VOC species, exhibited the best performance overall in southeastern Texas. However, its performance was not drastically better than SAPRC-11L, a condensed and fixed-parameter version of SAPRC-11D, suggesting that an intermediate explicit representation could yield benefits in performance as well as computational feasibility for routine air quality modeling applications. The project provided insights on the need for reliable emissions data as well as lumping methods for alkenes that could guide future chemical mechanism developments indicating, for example, that unbranched C_{3+} terminal alkenes shared similar ozone formation mechanisms but also have non-negligible differences, that unbranched internal alkenes share similar ozone formation chemistries, and that lumping branched terminal alkenes and branched internal alkenes with unbranched internal alkenes introduces significant inaccuracies. Explicitly modeling propene and 1,3-butadiene is potentially useful to improve the

accuracy of ozone predictions based on the spatial variability of their emissions in southeastern Texas.

Effects of emissions reductions on nighttime power plant plume chemistry and transport

Plumes from coal-fired power plants, which are frequently located in relatively rural areas, are subject to nocturnal transport and chemical processing that may affect air quality downwind. Coal-fired electric power plants have historically produced a large fraction of total U.S. NO_x emissions, but emissions from this sector have been declining during the last decade driven by federal regulations. AQRP Project 10-020 (Yarwood et al., 2012) and Brown et al. (2012) analyzed nighttime aircraft intercepts of plumes from two different Texas power plants (Oklaunion near Wichita Falls and W. A. Parish near Houston) with different control technologies to demonstrate the effect of NO_x emissions reductions on nighttime NO_x oxidation rates. In 2006, the Oklaunion plant had low NO_x burner technology, but not selective catalytic reduction (SCR). In contrast, the W. A. Parish plant coal-fired units had both technologies. The spatial extents of nighttime-emitted plumes was found to be limited, and mixing of highly concentrated plume NO_x with ambient ozone was a determining factor for its nighttime oxidation. The plume from Oklaunion had full titration of ozone through 74 km/2.4 hours of downwind transport that suppressed nighttime oxidation of NO_2 to higher oxides of nitrogen across the majority of the plume. The plume from W.A. Parrish did not have sufficient NO_x to titrate background ozone, which led to rapid nighttime oxidation of NO_2 during downwind transport. Plume modeling showed that NO_x controls not only reduced emissions directly but also led to an additional overnight NO_x loss of 36% to 44% on average. The maximum reduction for 12 h of transport in darkness was 73%. The results implied that power plant NO_x emissions controls may produce a larger than linear reduction in next-day, downwind ozone production following nighttime transport. The findings have been used to guide improvements in the Plume-in-Grid (PiG) formulation in CAMx.

Nighttime nitrate radical chemistry in the Houston urban boundary layer

Aircraft measurements during the second Texas air quality study provided unique insights on the nighttime chemistry and structure of the Houston urban boundary layer. AQRP Project 10-020 (Yarwood et al., 2012) found that nocturnal boundary layer depths vary between 100 – 400 m with overlying residual layer depths of 0.8 – 1.5 km. Nitrate radical had a strong influence on hydrocarbon oxidation (Stutz et al., 2009). Production rates for NO_3 ranged from 1-2 ppbv h^{-1} (Brown et al., 2009; Brown et al., 2011; Brown and Stutz, 2012) with maximum values of 2.7 ppbv h^{-1} (Yarwood et al., 2012) within NO_x plumes of industrial origin, but were generally smaller in rural plumes and plumes that originated from urban Houston and were transported downwind.

Nitrate radical was the dominant nighttime oxidant, with net oxidation rates 3 - 5 times faster than those due to ozone (Brown et al., 2011; Brown and Stutz, 2012). Net VOC oxidation rates due to NO_3 and O_3 varied between 0.1 - 1 ppbv hr^{-1}, (Yarwood et al., 2012) primarily associated with highly reactive alkenes, including isoprene, isobutene (2-methyl-1-propene) and 1,3-butadiene (Stutz et al., 2009; Brown et al., 2009; Brown et al., 2011; Brown and Stutz, 2012). Biogenic emissions were frequently observed at modest levels within the nocturnal boundary layer and underwent rapid oxidation (0.2 - 1 ppbv hr^{-1}), mainly by NO_3 (Yarwood et al., 2012; Brown et al., 2011). These NO_3-VOC reactions were more significant as a NO_3 loss pathway

than heterogeneous reactions of either NO_3 or N_2O_5 in the Houston urban boundary layer in contrast to other urban locations (Stutz et al., 2009).

Rate of sulfur dioxide to sulfate transformation in the Houston Ship Channel

In June of 2010, the EPA promulgated a more stringent primary NAAQS for sulfur dioxide (SO_2), requiring that the 99th percentile of 1-hour daily maximum concentrations averaged over 3 years not exceed 75 ppb. Fossil-fueled power plants and industrial facilities are the main sources of SO_2 emissions within the United States. The EPA recommends the use of the AERMOD steady-state Gaussian plume model (EPA, 2010) for near-source 1-hour SO_2 modeling assuming no chemical transformation of SO_2. Photochemical oxidants convert SO_2 to sulfate thereby reducing SO_2 concentrations. AERMOD does not treat photochemical oxidants and represents SO_2 transformation as a simple exponential decay process. This approach may not be appropriate for the reactive atmosphere of the Houston Ship Channel that may have more rapid SO_2 to sulfate conversion rates. Using NOAA P-3 aircraft measurements collected during the 2006 Texas Air Quality Study in the Houston Ship Channel area, AQRP Project 12-013 (Koo and Morris, 2013) determined a representative SO_2 transformation rate of 0.04 hr^{-1} (half-life of 17 hours). This rate can be used with the AERMOD model to simulate 1-hour SO_2 concentrations and is higher than that reported for power plant plumes. Investigations to determine sulfur dioxide to sulfate conversion rates within the Houston Ship Channel region that can be used with AERMOD under a range of meteorological conditions should continue to be examined.

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2.4 Atmospheric physical processes and long-range transport of pollutants

2.4.1 Overview

Models of atmospheric physical processes, emissions, and atmospheric chemistry are all incorporated into photochemical air quality models. The photochemical air quality models mathematically and numerically process the information to yield predictions of air pollutant concentrations. The models are used to quantitatively assess the potential effectiveness of air quality management strategies. Because of their importance in air quality management, AQRP projects have focused on improving model performance by improving the description of emissions and atmospheric chemistry (described in previous sections), as well as by improving models of physical pollutant loss mechanisms, cloud characterizations, cloud processes, and wind fields. This Section describes those model improvements, as well as analyses performed to understand the long-range transport of pollutants.

2.4.2 Atmospheric physical processes and long-range transport of pollutants: Assessment from AQRP projects 2010-2015

Regionally high ozone episodes and synoptic-scale weather patterns

Continental-scale weather patterns establish the frequency of local meteorological conditions favorable for high ozone concentrations, such as high temperatures, low wind speeds, clear skies, and stagnation (e.g., Jacob and Winner, 2009; Ngan et al., 2011; Zhu et al., 2013). The synoptic weather conditions during high ozone episodes in eastern Texas often exhibit a ridge of high pressure in the lower atmosphere that extends south or southwest into the region (McGaughey et al., 2013). This large-scale circulation pattern often occurs in a post-frontal environment that is associated with the long-range (multi-day) transport of continental air, which is characterized by elevated concentrations of ozone and/or its precursor compounds, into Texas from geographic areas located to the north and/or east of the state (Rappenglück et al., 2008; Ngan et al., 2011; 2012; AQRP Project 13-016, Morris and Lefer, 2013; AQPR Project 14-006, Alrick and Morris, 2015; McGaughey et al., 2015). These background ozone concentrations entering Texas have been shown to vary by transport direction and season (Nielsen-Gammon et al., 2005; Berlin et al., 2013; Morris et al., 2013), and are correlated, in part, to the predominant continental-scale weather patterns. For example, the Bermuda High, a quasi-permanent high-pressure system centered over the North Atlantic Ocean in summer, has a significant influence on surface ozone concentrations in the eastern U.S. (Hogrefe et al., 2004; Hegarty et al., 2007; Li et al., 2012; Zhu et al., 2013; Shen et al., 2015). In a large-scale meteorological analysis specific to Texas during 1998-2013, AQRP Project 14-010 (Wang, 2015) developed a linear regression model that captured 58% - 72% of the interannual summer variance of monthly mean Houston-Galveston-Brazoria maximum daily average 8-hour (MDA8) ozone concentrations; variations in the westernmost extent of the Bermuda High was the most important predictor of monthly ozone concentrations in this region.

Improved representation of vertical mixing and land surface processes for meteorological modeling

Because large-scale meteorological influences are often weak during conditions of poor air quality, the potential impacts from local-scale circulations (such as terrain flows, sea/land breezes, nocturnal jets) become especially important (Olaguer et al., 2009). Numerous studies have evaluated treatments of vertical diffusion and convective mixing in support of Texas air

quality modeling applications in recent years (e.g., Emery et al., 2009; ENVIRON, 2011; Tang et al., 2011; Li and Rappengluck, 2014; Haman et al., 2014) as well as sensitivity of near-surface meteorological predictions to the choice of planetary boundary layer scheme (e.g., Hu et al., 2010, 2013; Yerramilli et al., 2010; Kolling et al., 2013; Cuichiara et al., 2014; Wilmot et al., 2014) and sensitivity to land surface modeling (Cheng et al., 2008; Misenis and Zhang, 2010). Using a single-layer urban canopy model (UCM), Lee et al. (2011) found that more realistic prediction of sensible and latent heat fluxes was associated with improved replication of diurnal profiles of temperature and planetary boundary layer height over the Houston area. In a similarly-focused study, AQRP Project 12-TN1 (Tong et al., 2013) analyzed the impact of different combinations of surface and planetary boundary layer schemes on the over-prediction of nighttime near-surface wind speeds in the Houston-Galveston-Brazoria area; although the simulation of physically-relevant parameters such as friction velocity were improved, the overall model biases were aggravated suggesting that optimization of WRF physics schemes might be needed.

Meteorological models used in support of air quality modeling applications typically incorporate data assimilation (i.e., "nudging") to observations or other analyses to reduce uncertainties in near-surface meteorological predictions (e.g., Ngan et al., 2012, Li and Rappengluck, 2014; TCEQ, 2015; AQRP Project 14-014, Choi and Li, 2015). One of the most successful efforts to reduce uncertainties in the simulation of daytime lower-tropospheric winds and planetary boundary layer heights has been the assimilation of radar wind profiler data (e.g., Nielsen-Gammon et al., 2007; Zhang et al., 2007; Stuart et al., 2007; TCEQ, 2015). AQRP Project 14-004 (Loughner and Follette-Cook, 2015) used an iterative observational and data assimilation technique newly developed by EPA (Appel et al., 2014) to improve WRF's simulation of the sea/bay breezes that proved critical to capturing the magnitude and spatial distribution of ozone concentrations in Houston during 2013. AQRP Project 14-022 (McNider et al., 2015) investigated a technique that utilized the difference between satellite-observed and land surface model-simulated skin temperatures to nudge soil moisture and thermal resistance. Root mean square error (RMSE) and bias was calculated for a control WRF run and for the nudging case using skin temperatures (evaluated by the satellite dataset) as the performance metric. The results for the model grid domain that included the continental U.S. and surrounding regions showed improvements in bias across much of the region; however, increased bias in limited areas caused a slight overall increase in the absolute bias. RMSE was improved by approximately 20% with even larger improvements in Texas. An evaluation of WRF wind speed and wind direction performance compared to NWS observations demonstrated slight decreases in both bias and RMSE. Because skin temperatures are physically related to relevant land surface characteristics, the results suggested that simple land surface models constrained by observations using similar data assimilation techniques can improve the specification of land surface parameters leading to improved meteorological predictions.

Simulation of clouds and precipitation

Photochemistry is strongly influenced by clouds, which can both attenuate and enhance the actinic flux of ultraviolet (UV) radiation (e.g., Emery et al., 2010). Accurate simulation of cloud cover is necessary to simulate photolysis rates, and ozone predictions are very sensitive to photolysis rates (Byun et al., 2007; TCEQ, 2011). In addition, clouds impact the rate and depth of vertical mixing in the lower troposphere (e.g., Langford et al., 2010) as well as the chemical

composition of the atmosphere (e.g., Flynn et al., 2010). The vertical depth and spatial/temporal distribution of clouds are some of the most difficult meteorological phenomena to accurately simulate (Pour-Biazar et al., 2007; Emery et al., 2010). Spurious thunderstorms and clouds are also common in air quality modeling (Olaguer et al., 2009), suggesting the need for flexibility in the selection of modeling parameterizations (TCEQ, 2011).

In support of Texas applications, Pour-Biazar et al. (2007) used GOES satellite data to correct the photolysis rates in CMAQ for a TexAQS episode. The results demonstrated that clouds increased the lifetime of ozone precursors leading to increased ozone production and improvements in model performance. A study by ENVIRON (2010) found that surface ozone predictions in CAMx were more responsive to the placement of sub-grid clouds than to how photolysis rates were applied (TCEQ, 2011). Efforts by Pour-Biazar et al. (2011) to develop a GOES cloud assimilation technique in WRF relied on adjustments to the modeled vertical velocities to force better agreement between predicted and satellite-observed cloudiness. Although the study showed improvements of 7-10% in cloud prediction, additional work is needed. To capture the effects of sub-grid clouds (i.e., clouds that are not fully resolved by air quality grid models), AQRP Project 14-025 (Emery et al., 2015) developed a "Cloud-in-Grid" treatment that simulates the impact of vertical convective transport for both in-cloud and ambient fractions of the grid column. A comparison to limited observational aircraft data demonstrated improvement in the simulation of boundary layer concentrations of ozone and nitrogen oxides.

Project 14-022 (McNider et al., 2015) found that large differences between WRF and satellite insolation at the surface was largely due to the placement of clouds. A set of simulations was performed that employed the NASA Short-term Prediction Research and Transition Center (SPoRT) Geostationary Operational Environmental Satellite (GOES)-derived insolation product that had better performance statistics against pyranometer data compared to a control WRF simulation. Using National Weather Service (NWS) 2-meter temperature as the performance metric, replacement of satellite insolation into the WRF control run reduced model bias and error within Texas; however, the overall performance across the entire continental U.S. and surrounding regions was slightly degraded. McNider et al. (2015) indicated that the differences in results between the satellite and WRF insolation cases appeared to be related to surface albedo and that using satellite-derived albedo in place of WRF defaults might improve performance; however, further investigation is needed.

Contributions of North American Background (NAB) ozone to Texas air quality

Over the past decade, hemispheric transport of ozone and pollutants with longer atmospheric lifetimes to and from the United States has received increasing recognition as potential influences on local and regional air quality management. The definition of "background ozone" can vary widely, and its estimation can depend on global-scale models and/or ambient observations. Within the United States, North American Background (NAB) ozone, formerly known as Policy Relevant Background (PRB) ozone, is a specific construct that has been instrumental to the establishment of the NAAQS for ozone. The EPA (2013) defines NAB ozone as concentrations that would occur in the absence of anthropogenic emissions in continental North America. Contributors to NAB include emissions that react to form ozone from anthropogenic sources outside North America and natural sources globally (e.g., wildfires,

lightning, biogenic except agricultural activities) and stratospheric-tropospheric exchange of ozone.

Establishing NAB ozone concentrations throughout the United States currently requires the application of global-scale chemical transport models (CTMs) alone or in combination with regional CTMs. Recent modeling studies have estimated NAB ozone concentrations to vary between 25 ppb and 50 ppb across the United States (e.g., Zhang et al., 2011; Emery et al., 2012; Fiore et al., 2014), with maximum values (>60 ppb) in western intermountain regions attributed, in part, to stratospheric-tropospheric exchange processes (e.g., Lin et al., 2012; AQRP Project 12-011, Emery et al., 2013; Lefohn et al., 2014), wildfires (e.g., Mueller and Mallard, 2011; Jaffe et al., 2012; Zhang et al., 2014), and intercontinental pollution (e.g., Brown-Steiner and Hess, 2011; Verstraeten et al., 2015).

Regional and global modeling studies have specifically examined the contributions of long-range transport on Texas air quality. Using a regional CAMx episode for June 2006 with boundary conditions from GEOS-Chem, McDonald-Buller et al. (2014) found median NAB ozone concentrations were 18 - 22 ppb in eastern Texas urban areas and 20 - 29 ppb in El Paso, consistent with other studies that have found higher concentrations at intermountain west sites (e.g., Emery et al., 2012; Zhang et al., 2014). NAB ozone concentrations increased with altitude over Texas, with less pronounced gradients at higher elevation sites in west Texas. Tai et al. (2013) investigated the effects of removing anthropogenic emissions from geographic regions outside of North America (zROW – i.e., zero out the rest of the world) on predicted ozone concentrations in Texas using GEOS-Chem for selected years during 2006 through 2012. Monthly MDA8 ozone concentrations were relatively lower in El Paso than the Dallas-Fort Worth and Houston urban areas but were subject to higher contributions by sources outside of North America (exceeding 10 ppb in the winter). Anthropogenic emissions were projected to increase in Asia and the Middle East but decline in member countries of the Organization for Economic Cooperation and Development (OECD90) between 2012 and 2018; emissions reductions in Western Europe during this time period were projected to provide at least some benefit to the Eastern U.S., particularly in the Gulf Coast States (Tai et al., 2013).

Boundary conditions for regional chemical transport models

The use of regional-scale photochemical models allows for refined grid resolution, geographic topography, emissions inventories, and meteorological data that may not be achievable with global-scale models because of their computational intensity or that present challenges to their performance. However, regional chemical transport models, such as CMAQ (Foley et al., 2010) and CAMx (ENVIRON, 2014) require lateral and top boundary conditions that are now routinely obtained from global-scale models (Giordano et al., 2015). Common global models employed for North American studies have included the Goddard Earth Observing System – Chemistry model (GEOS-Chem; Bey et al., 2001), The Model for OZone and Related chemical Tracers (MOZART-4; Emmons et al., 2010) and AM3 (Donner et al., 2011). Because the outer boundaries of regional modeling domains are often located over remote maritime areas, evaluation and validation of model predictions is challenging; recent studies have employed satellite datasets (Tang et al., 2009; Pfister et al., 2011; Henderson et al., 2014; McGaughey et al., 2014), comparisons with observations collected at ground-based monitoring stations in remote U.S. regions (e.g., refer to review by McDonald-Buller et al., 2011), ozonesondes (Pfister

et al., 2011; Li and Rappenglück, 2014), and/or aircraft measurements (Tang et al., 2009; Pfister et al., 2011).

AQRP Project 12-011 (Emery et al., 2013) developed boundary condition inputs for CAMx utilizing output from three global models (GEOS-Chem, MOZART, and AM3) and conducted an evaluation of surface ozone predictions focused on the southwest, south central, and southeast regions of the U.S. surrounding Texas and the Gulf of Mexico. In general, performance of the models tracked each other throughout the 2008 simulation, with differences associated with the representation of lightning NO_x and stratospheric intrusions. AM3 performance was superior in the southwest where the influence of higher ozone concentrations in the upper troposphere and lower stratosphere played a substantial role in the springtime regional surface ozone pattern. These findings and those of other studies (e.g. McDonald-Buller et al., 2011) suggest the utility of continuing to evaluate and further the evolution of multiple global models as resources for regional modeling simulations.

Dry deposition

Dry deposition is broadly defined as the transport of gaseous and particulate species from the atmosphere by turbulent transfer to surfaces in the absence of precipitation (Seinfeld and Pandis, 2012). Dry deposition is estimated to account for 20-25% of total ozone removal from the troposphere globally (Lelieveld and Dentener, 2000; Wild, 2007). On a regional level in Texas, dry deposition represents the most important physical removal mechanism for ozone during the warm spring through early fall seasons (McDonald-Buller et al., 2001); therefore, accurate estimates of dry deposition of ozone and its precursors are required for air quality modeling and management.

In regional air quality models such as CAMx or CMAQ, dry deposition is often treated as a first-order removal mechanism, where a characteristic dry deposition velocity V_d (ratio of deposition flux and concentration) is used to describe the process. Dry deposition of a gas is modeled as the product of its dry deposition velocity and concentration. Dry deposition models, such as those of Wesely (1989) and more recently of Zhang et al. (2003) that are included as options in CAMx, typically employ a resistance approach analogous to Ohm's law in electrical circuits. Three resistances to transport and surface uptake are included: an aerodynamic resistance, quasi-laminar sub-layer resistance, and surface resistance.

Validation of dry deposition models against observations, as well as intercomparisons between models have been conducted (Zhang et al., 2002; Michou et al., 2005; Schwede et al., 2011; Park et al., 2014; Val Martin et al., 2014; Wu et al., 2011), yet significant uncertainties remain (Pleim and Ran, 2011). Dry deposition velocities remain uncharacterized for many compounds or require reconciliation between predictions from algorithms in global and regional chemical transport models and observations (e.g. Nguyen et al., 2015). Observations of ozone dry deposition velocities are extremely limited in Texas, making it difficult to evaluate model estimates. Huang et al. (2015) identified a study, by Kawa (1986), that reported ozone V_d in the range of 1.1 to 1.2 cm/s using an eddy covariance technique over the Big Thicket National Preserve (forest) located in East Texas in June of 1982.

Similar to models used to estimate biogenic emissions, dry deposition algorithms require characterization of land use and land cover, as well as meteorological parameters for evaluating component resistances. Characterizing land cover, in particular in forested and heavily vegetated areas, has been a primary consideration for determining surface resistances; the heterogeneity of the urban environment has typically not been represented in the dry deposition algorithms used in regional-scale transport models. AQRP Project 10-021 (Corsi et al., 2011) conducted laboratory experiments to determine the surface resistance of fresh and weathered built environment surface materials, developed a refined characterization of the urban built environment of Austin, Texas using extensive geospatial data, and examined the effects on the dry deposition of ozone. Changes in predicted daily maximum 8-hour average ozone concentrations were primarily attributed to deposition to urban vegetation and highlighted the importance of characterizing Texas urban landscapes undergoing rapid development.

Responses of vegetation to changes in climate have the potential to alter dry deposition velocities. Recently Huang et al. (2015) modeled seasonal and interannual changes in estimated ozone dry deposition velocities and component resistances over eastern Texas during representative drought years (2006 and 2011). Predicted ozone dry deposition velocities increased during the spring but decreased during the summer and fall seasons reflecting complex and competing responses of deposition pathways (i.e., stomatal and non-stomatal) in vegetated areas. Forests exhibited the most significant reductions in simulated dry deposition velocities. Results from this study emphasized the need for field measurements and the importance of understanding the spatial distribution of impacts on dry deposition over eastern Texas and other regions of the world subject to recurring drought.

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2.5 Particulate matter

2.5.1 Overview

Most of the research of the AQRP program has focused on improving the understanding of emissions, chemistry and atmospheric physical processes that lead to ozone formation and accumulation. This is because ozone is the air pollutant for which the State has the greatest number of regions that do not meet the NAAQS. With the recent tightening of the NAAQS for fine particulate matter, however, some regions in Texas are approaching non-attainment for fine particulate matter as well; a number of AQRP projects have been funded to specifically address particulate matter. These projects are summarized in this Section.

2.5.2 Particulate matter sources and composition in Southeastern Texas: Assessment from AQRP projects 2010-2015

Over the past 15 years, measurements during field campaigns have been made to better characterize particulate matter size, composition and concentrations in southeastern Texas. TexAQS 2000 coincided with Gulf Coast Aerosol Research and Characterization Program (GC-ARCH) or the Houston Supersite, which had the aim of improving the understanding of the concentrations, spatial and temporal variability, composition, and sources of fine particulate matter (i.e., particles with diameters less than or equal to 2.5 micrometers) in southeastern Texas (Russell et al., 2004). Measurements conducted during the SHARP, TexAQS/GoMACCS 2006, and more recently DISCOVER-AQ campaigns have sought to continue to improve the spatial and temporal characterization of fine particulate matter composition and sources and to develop new measurement approaches for characterizing aerosol concentration, size distribution, and optical properties (AQRP Project 14-005, Brooks and Yang, 2015). In 2012, the EPA promulgated a more stringent primary annual NAAQS for fine particulate matter of 12 $\mu g\ m^{-3}$, a decrease from the level of the 1997 standard of 15 $\mu g\ m^{-3}$. Although the Houston area has experienced declines in fine particulate mass matter concentrations over the past decade at regulatory monitoring sites, it remains close to the level of nonattainment with the 2012 federal standard. As of January 15, 2015, the Houston area was designated by the EPA as "unclassifiable/attainment" (HGAC, 2015).

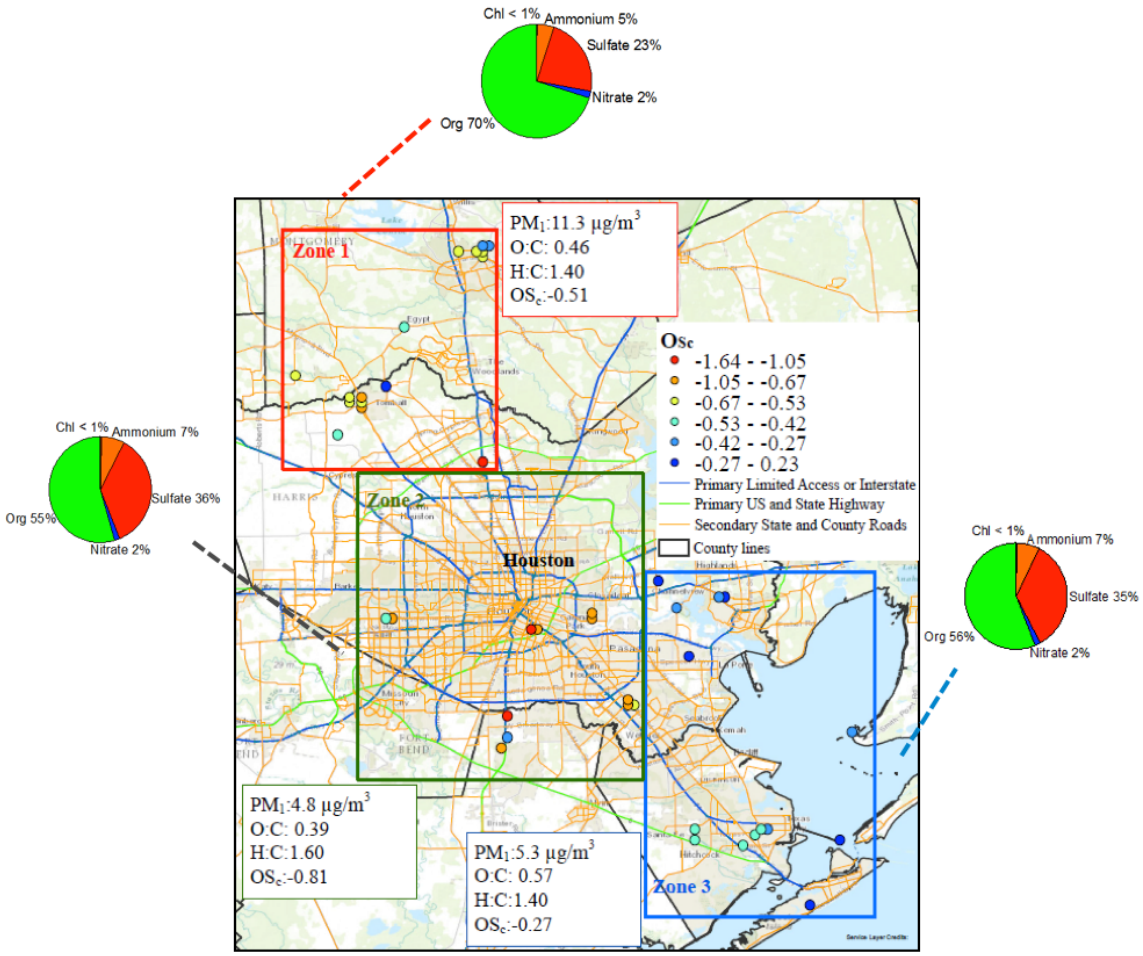
Zhang et al. (2015) have a recent critical review of urban fine particular matter with an overview of Houston and other metropolitan areas (Beijing, Los Angeles, and Mexico City) that have had intensive atmospheric field measurement campaigns. AQRP Projects 13-022 (Griffin et al., 2014) and 14-009 (Griffin and Lefer, 2015) provided a recent characterization of the spatial variation of submicron particulate matter composition across Houston during the DISCOVER-AQ campaign. Figure 2.5.1, which is drawn from this work, indicates the relative importance of organic aerosol and sulfate as particulate matter species (Griffin and Lefer, 2015). Positive Matrix Factorization (PMF) analysis was applied for zonal-based identification of organic aerosol components, including hydrocarbon-like organic aerosol (HOA), which is a proxy for POA, and various forms of oxygenated organic aerosol (OOA-I representing less aged fresh SOA and OOA-II representing aged and oxidized regional SOA). Secondary organic aerosol represented more than 90% of organic aerosol in Zones 1 (northwest Houston) and 3 (east and southeast Houston); the OOA-I factor was more important than the OOA-II factor, suggesting overall the influences of regional transport and anthropogenic and biogenic VOC emission sources. Sources likely differed between zones. For example, higher levels of isoprene and

monoterpenes were predicted in northwest Houston than the other zones. Monoterpene concentrations exhibit statistically significant moderate correlation with levels of SOA and OOA-I in this zone; Principal Component Analysis (PCA) suggested that monoterpenes may impact SOA formation through oxidation by nitrate radical. Although the composition of OA in Zone 2 (central Houston) also indicated the dominant contribution of SOA (67%), it had a more primary character than the other zones suggesting greater impacts by sources of primary aerosol such as motor vehicles.

Radiocarbon measurements made during DISCOVER-AQ for AQRP Projects 12-032 (Sheesley and Usenko, 2013) and 14-029 (Sheesley and Usenko, 2015) distinguished fossil (i.e., primary fossil fuel combustion and SOA produced in the atmosphere from fossil-derived volatile organic carbon) and contemporary sources (i.e., primary biogenic emissions, biomass combustion and SOA produced in the atmosphere from biogenic- and biomass combustion-derived volatile organic carbon) at selected sites in Houston. Moody Tower, a site indicative of urban Houston, had a consistent primary motor vehicle exhaust contribution of 18-27%, a fossil SOA contribution that varied from 5% to 33% depending on atmospheric conditions, and biogenic SOA contribution ranging from 40% to 75%. Conroe, a site indicative of aged urban aerosol combined with biogenics located north of Houston, had a lower contribution of motor vehicle exhaust (5% to 10%), a similarly variable fraction of fossil SOA (4% to 25%), and a biogenics contribution of 60% to 79%.

These findings were broadly consistent with those of earlier studies that have been conducted during field campaigns in southeastern Texas over the past 15 years. Measurements made during TexAQS 2000 and GC-ARCH (Allen, 2005) indicated that fine particulate matter composition in southeast Texas was dominated by sulfate primarily from regional sources and organic carbon of regional and local origin. Fires can be an important event-based contribution to fine particulate matter mass. Secondary organic aerosol formation was associated with reactions of biogenic and anthropogenic precursors. Particle size distributions were not spatially homogeneous; industrial sites had higher concentrations of ultrafine particles than more residential sites. Yu and Cowin (2009) found that the averages and ranges of organic, elemental, and total during the SHARP campaign were comparable to observations in the early 2000s (Allen, 2004, 2005). The average OC to EC ratio was 6.9, indicating that secondary organic aerosols were a component in the carbonaceous aerosols observed in Houston. Bahreini et al. (2009) found greater organic aerosol mass downwind of the Houston industrial center relative to the urban area during TexAQS 2006. Observed ratios of the enhancement above background in OA, ΔOA, to the enhancement above background in carbon monoxide (CO), ΔCO, downwind of the Houston urban center were within a factor of two of the same values in plumes from urban areas in the northeastern United States (de Gouw, 2008) indicating similar concentrations of precursors and chemical processes. However, ΔOA/ΔCO in plumes originating from the Houston Ship Channel exceeded that in the urban area by factors ranging from 1.5 to 7.

Figure 2.5.1. From Griffin and Lefer (2015; ref. Table 12): Average contribution of particulate matter constituents, concentrations, and oxidation metrics in three analysis zones defined by average carbon oxidation state (OSc) and geography. Zone 1- northwest Houston; Zone 2 - greater central Houston; Zone 3 - east and southeast Houston. Average concentrations (µg m^{-3}) and associated standard deviations (in parentheses) of PM species in the defined analysis zones are shown in the accompanying table.



Zone	OA	Sulfate	Nitrate	Ammonium	Chloride
1	8.16 (±3.54)	2.4 (±0.60)	0.23 (±0.15)	0.53 (±0.15)	0.019 (±0.007)
2	2.68 (±1.73)	1.68 (±1.01)	0.08 (±0.09)	0.37 (±0.26)	0.013 (±0.008)
3	3.03 (±1.9)	1.58 (±0.63)	0.08 (±0.047)	0.33 (±0.16)	0.0076 (±0.004)

2.5.3 References

AQRP Projects:

AQRP Project 12-032: Sheesley, R., and S. Usenko, (2013), Collect, analyze, and archive filters at two DISCOVER-AQ Houston focus areas: Initial characterization of PM formation and emission, Prepared for the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/

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AQRP Project 14-005: Brooks, S. and P. Yang, (2015), Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation, Prepared for the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/

AQRP Project 14-009: Griffin, R. and B. Lefer, (2015), Analysis of surface particulate matter and trace gas data generated during the Houston operations of DISCOVER-AQ, Prepared for the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/

AQRP Project 14-029: Sheesley, R., and S. Usenko, (2015), Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ, Prepared for the Texas Air Quality Research Program, http://aqrp.ceer.utexas.edu/

Other:

Allen D., (2005), Gulf Coast Aerosol Research and Characterization Program (Houston Supersite). Center for Energy and Environmental Resources, The University of Texas at Austin, Cooperative Agreement Number R-82806201 between the Environmental Protection Agency and The University of Texas at Austin, April 2005.

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Russell, M., D. Allen, D. Collins, and M. Fraser, (2004), Daily, seasonal, and spatial trends in PM2.5 mass and composition in Southeast Texas, Aerosol Science and Technology 38 (S1), 14-26.

Yu, X-Y., J. Cowin, N. Laulainen, M. Iedema, B. Lefer, D. Anderson, D. Pernia, and J. Flynn, (2009), Radical initiated secondary aerosol formation (RISAF) - Particle measurements during SHARP, Houston Advanced Research Consortium (HARC), Project H-105.

Zhang, R., G. Wang, S. Guo, M.L. Zamora, Q. Ying, Y. Ling, W. Wang, M. Hu, and Y. Wang, (2015), Formation of urban fine particulate matter, Chemical Reviews, 115(10), 3803-55, doi: 10.1021/acs.chemrev.5b00067.

3. Summary of Projects and Publications from the Air Quality Research Program (AQRP, 2010-2015)

Fifty research projects and two science synthesis projects were funded by the AQRP between 2010 and 2015. The projects are listed, by category, in Table 3-1. Full project reports are available at the AQRP web site (http://aqrp.ceer.utexas.edu/reports.cfm).

Table 3-1. AQRP Research Projects 2010-2012

Project Number	Title
Dallas-Fort Worth Area Studies	
10-DFW, 11-DFW	Logistical Support for Dallas-Fort Worth (Barnett Shale) Measurement Study
10-024	Surface Measurements and One-Dimensional Modeling Related to Ozone Formation in the Suburban Dallas-Fort Worth Area
10-034	Dallas Measurements of Ozone Production
10-044	Airborne Measurements to Investigate Ozone Production and Transport in the Dallas/Fort Worth (DFW) Area During the 2011 Ozone Season
Houston Area Studies	
10-032	SHARP Data Analysis: Radical Budget and Ozone Production
10-045	Quantification of Hydrocarbon, NOx and SO_2 Emissions from Petrochemical Facilities in Houston: Interpretation of the 2009 FLAIR Dataset
12-013	Development of Transformation Rate of SO_2 to Sulfate for the Houston Ship Channel using the TexAQS 2006 Field Study Data
14-010	Impact of large-scale circulation patterns on surface ozone concentrations in HGB
DISCOVER-AQ (Houston) Studies	
12-004	Logistical Support for DICOVER-AQ Measurement Study
13-005	Quantification of industrial emissions of VOCs, NO_2 and SO_2 by SOF and mobile DOAS during DISCOVER-AQ
13-016	Ozonesonde launches from the University of Houston and Smith Point, Texas in Support of DISCOVER-AQ
13-022	Surface Measurements of PM, VOCs, and Photochemically Relevant Gases in Support of DISCOVER-AQ
13-024	Surface Measurement of Trace Gases in Support of DISCOVER-AQ in Houston in Summer 2013
12-032	Collect, Analyze, and Archive Filters at two DISCOVER-AQ Houston Focus Areas
14-002	Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC4RS Campaigns
14-004	Emission Source region contributions to a high surface ozone episode during DISCOVER-AQ
14-005	Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation
14-006	Characterization of Boundary-Layer Meteorology during DISCOVER-AQ Using Radar Wind Profiler and Balloon Sounding Measurements

14-007	Improved Analysis of VOC, NO_2, SO_2 and HCHO data from SOF, mobile DOAS and MW-DOAS during DISCOVER-AQ
14-009	Analysis of Surface Particulate Matter and Trace Gas Data Generated during the Houston Operations of DISCOVER-AQ
14-014	Constraining NO_X Emissions Using Satellite NO_2 and HCHO Column Measurements over Southeast Texas
14-020	Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC4RS
14-024	Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ Data, Modeling and Experiments
14-026	Quantifying ozone production from light alkenes using novel measurements of hydroxynitrate reaction products in Houston during the NASA SEAC4RS project
14-029	Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ
Flares and Emission Inventories	
10-006	Quantification of Industrial Emissions of VOCs, NO_2 and SO_2 by SOF and Mobile DOAS
10-009	Additional Flare Test Days for TCEQ Comprehensive Flare Study
10-022	Development of Speciated Industrial Flare Emission Inventories for Air Quality Modeling in Texas
12-011	Investigation of Global Modeling and Lightning NOx Emissions as Sources of Regional Background Ozone in Texas
12-018	The Effects of Uncertainties in Fire Emissions Estimates on Predictions of Texas Air Quality
14-011	Targeted Improvements in the Fire Inventory from NCAR (FINN) Model for Texas Air Quality Planning
14-023	Assessment of Two Remote Sensing Technologies to Control Flare Performance
Emissions and Chemistry of Biogenic Volatile Organic Compounds	
14-003	Update and evaluation of model algorithms needed to predict Particulate Matter from Isoprene
14-008	Investigation of Input Parameters for Biogenic Emissions Modeling in Texas during Drought Years
14-016	Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations
14-017	Incorporating Space-borne Observations to Improve Biogenic Emission Estimates in Texas
14-030	Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation
Modeling and Atmospheric Chemistry	
10-008	Factors Influencing Ozone-Precursor Response in Texas Attainment Modeling
10-015	An Assessment of Nitryl Chloride Formation Chemistry and its Importance in Ozone Non-Attainment Areas in Texas
10-020	NOx Reactions and Transport in Nighttime Plumes and Impact on Next-Day Ozone
10-021	Dry Deposition of Ozone to Built Environment Surfaces
10-029	Wind Modeling Improvements with the Ensemble Kalman Filter

10-042	Environmental Chamber Experiments to Evaluate NOx Sinks and Recycling in Atmospheric Chemical Mechanisms
12-006	Environmental chamber experiments and CMAQ modeling to improve mechanisms to model ozone formation from HRVOCs
12-012	Interactions Between Organic Aerosol and NOy: Influence on Oxidant Production
12-028	Implementation and evaluation of new HONO mechanisms in a 3-D Chemical Transport Model for Spring 2009 in Houston
12-TN1	Investigation of surface layer parameterization of the WRF model and its impact on the observed nocturnal wind speed bias
12-TN2	Development of IDL-based geospatial data processing framework for meteorology and air quality modeling
14-022	Use of satellite data to improve specifications of land surface parameters
14-025	Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model
State of the Science Evaluations	
10-SSA	State of the Science Synthesis, 2012
	State of the Science Synthesis, 2015

PUBLICATIONS

FY10-11

10-006

Johansson, J., Johan Mellqvist, Jerker Samuelsson, Brian Offerle, Jana Moldanova, Bernhard Rappenglück, Barry Lefer, and James Flynn (2014) , Formaldehyde Quantitative Measurements and Modeling of Industrial Formaldehyde Emissions in the Greater Houston Area during Campaigns in 2009 and 2011, Journal of Geophysical Research: Atmospheres, 119, DOI: 10.1002/2013JD020159

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10-009

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Pavlovic, R.T., Al-Fadhli, Kimura, Y., Allen, D.T., and McDonald-Buller, E.C. Impacts of Emission Variability and Flare Combustion Efficiency on Ozone Formation in the Houston-Galveston-Brazoria Area, *Industrial & Engineering Chemistry Research,* 51, 12593-12599, DOI: 10.1021/ie203052w (2012).

Knighton, W.B., Herndon, S.C., Franklin, J.F., Wood, E.C., Wormhoudt, J., Brooks, W., Fortner, E.C., and Allen, D.T. Direct measurement of volatile organic compound emissions from industrial flares using real-time on-line techniques: Proton Transfer Reaction Mass Spectrometry and Tunable Infrared Laser Differential Absorption Spectroscopy, *Industrial & Engineering Chemistry Research,* 51, 12674-12684, DOI: 10.1021/ie202695v (2012)

Torres, V.M., Herndon, S., Kodesh, Z., Nettles, R., and Allen, D.T. "Industrial flare performance at low flow conditions: Part 1. Study Overview" *Industrial & Engineering Chemistry Research,* 51, 12559-12568, DOI: 10.1021/ie202674t (2012).

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Herndon, S.C., Nelson, D.D., Wood, E.C., Knighton, W.B., Kolb, C.E., Kodesh, Z., Torres, V.M., and Allen, D.T., Application of the carbon balance method to flare emissions characteristics, *Industrial & Engineering Chemistry Research,* 51, 12577-12585, DOI: 10.1021/ie202676b (2012)

Al-Fadhli, F.M., Kimura, Y., McDonald-Buller, E.C., and Allen, D.T. Impact of flare destruction efficiency and products of incomplete combustion on ozone formation in Houston, Texas, *Industrial & Engineering Chemistry Research,* 51, 12663-12673, DOI: 10.1021/ie201400z (2012).

The following presentations were given at the Air& Waste Management Association June 2012 Conference, and papers were published in the Conference Proceedings:

Torres, V.M., Allen, D.T., Herndon, S. and Kodesh, Z., Overview of the Texas Commission on Environmental Quality 2010 Flare Study, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-437-AWMA, San Antonio, June, 2012.

Torres, V.M., Al-Fadhli, F.M., Allen, D.T., Herndon, S., and Wood, E., NOx Emissions from Industrial Flaring, Air and Waste Association Annual Meeting, Extended Abstract 2012-A-315-AWMA, San Antonio, June, 2012.

10-015
The following papers are currently under development:

Measurements of Nitryl Chloride in Several Metropolitan Areas and Comparison with Regional Models
J.M. Roberts, H. Osthoff, E.J. Williams, B. Lerner, J.A. Neuman, J.B. Nowak, S.B. Brown, W.P. Dube, N.L. Wagner, T.B. Ryerson, I.B. Pollack, J.S. Holloway, A. Middlebrook, R. Bahreini, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

Hydrochloric acid at the Pasadena ground site during CalNex 2010 and its role as a source of aerosol chloride
J.M. Roberts, P.R. Veres, A.K. Cochran, C. Warneke, J. de Gouw, R. Weber, R. Ellis, T. Vandenboer, J. Murphy, B. Koo, G. Yarwood
In preparation for Journal of Geophysical Research

10-020
Brown, S. S. et al. (2012), Effects of NO_xcontrol and plume mixing on nighttime chemical processing of plumes from coal-fired power plants, J. Geophys. Res., 117, D07304, doi:10.1029/2011JD016954.

Brown, S. S., Dubé, W. P., Bahreini, R., Middlebrook, A. M., Brock, C. A., Warneke, C., de Gouw, J. A., Washenfelder, R. A., Atlas, E., Peischl, J., Ryerson, T. B., Holloway, J. S., Schwarz, J. P., Spackman, R., Trainer, M., Parrish, D. D., Fehshenfeld, F. C., and Ravishankara, A. R.: Biogenic VOC oxidation and organic aerosol formation in an urban nocturnal boundary layer: aircraft vertical profiles in Houston, TX, Atmos. Chem. Phys., 13, 11317-11337, doi:10.5194/acp-13-11317-2013, 2013.

In preparation for Atmosphere:
Reactive Plume Modeling to Investigate NOx Reactions and Transport at Night
Prakash Karamchandani, Shu-Yun Chen, Greg Yarwood, Steven S. Brown, David Parrish

In preparation for Atmosphere:
Modeling Overnight Power Plant Plume Impacts on Next-Day Ozone Using a Plume-in-Grid Technique
Greg Yarwood, Chris Emery, Steven S. Brown, David Parrish

10-021
The Project Investigators presented findings from this project at the Air & Waste Management Association June 2012 Conference. The title of the submitted abstract was *Dry Deposition of Ozone to Built Environment Surfaces* and the authors are Yosuke Kimura, Dustin Poppendeck, Erin Darling, Elena McDonald-Buller, and Richard Corsi

10-022
Kanwar Devesh Singh, Tanaji Dabade, Hitesh Vaid, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, Kuyen Li, and Christopher B. Martin "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Model,"*Industrial & Engineering Chemistry Research* **2012** *51* (39), 12611-12620

Kanwar Devesh Singh, Preeti Gangadharan, Daniel Chen, Helen H. Lou, Xianchang Li, P. Richmond, " Parametric Study of Ethylene Flare Operations and Validation of a Reduced Combustion Mechanism," Engineering Applications of Computational Fluid Mechanics, Vol. 8, No. 2, pp. 211–228 (2014).

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K. Singh, T. Dabade, H. Vaid, P. Gangadharan, D. Chen, H. Lou, X. Li, K. Li, C. Martin, "Computational Fluid Dynamics Modeling of Industrial Flares Operated in Stand-By Mode," Industrial Flares special issue, Ind. & Eng. Chem. Research, 51 (39), 12611-12620, October, 2012.

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10-024

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B. Karakurt Cevik, A.P. Rutter, L. Gong, R.J. Griffin, J.H. Flynn, B.L. Lefer, and S. Kim (2016), Estimates of airmass aging using particle and other measurements near Fort Worth, *Atmos. Environ.*, *126*, 45-54.

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L. Gong, R. Lewicki, R.J. Griffin, A. Rutter, F.K. Tittel, B.L. Lefer, J.H. Flynn, J.E. Dibb, and E. Scheuer (2012), Gas-particle partitioning of ammonia in the Fort Worth, TX area, *American Association for Aerosol Research Annual Conference*, Minneapolis, MN, October 2012. (poster)

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A. P. Rutter, B. Karakurt Cevik, K.M. Shakya, L. Gong, C. Gutierrez, M. Calzada, S. Kim, R.J. Griffin, J.H. Flynn, and B.L. Lefer, Source apportionment of organic aerosols and VOCs near Fort Worth, TX (2012), *American Association for Aerosol Research Annual Conference*, Minneapolis, MN.

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10-032
Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhan, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappengluck, K. W. Wong. C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke and P. Kelley (2013), Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, *Journal of Geophysical Research-Atmospheres,118*,5770-5780,doi:10.1002/jgrd.50342.

10-042
Heo, G., McDonald-Buller, E.C., Carter, W.P.L., Yarwood, G., Whitten, G.Z. and Allen, D.T. "Modeling Ozone Formation from Alkene Reactions using the Carbon Bond Chemical Mechanism, *Atmospheric Environment*, 59, 141-150, DOI: 10.1016/j.atmosenv.2012.05.042 (2012).

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In preparation for Atmospheric Environment: *Environmental chamber experiments to evaluate NOx removal and recycling represented in atmospheric mechanisms for air quality modeling*
Gookyoung Heo, William Carter, Greg Yarwood, Gary Z. Whitten, David T. Allen

In preparation for Atmospheric Environment: *Evaluation of mechanisms for modeling ozone formation from isoprene in SAPRC-07 and CB6 using environmental chamber data with low initial NOx*
Gookyoung Heo, William Carter, Greg Yarwood

10-045
Olga Pikelnaya, James H. Flynn, Catalina Tsai, and Jochen Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, Journal of Geophysical Reserch, Volume 118, Issue 15, pages 8716–8728, 16 August 2013, DOI: 10.1002/jgrd.50643

The following papers were published in Industrial & Engineering Chemistry Research Special Issue on Industrial Flaring. The paper edition of this special edition came out in Fall 2012.

W. Berk Knighton, Scott C. Herndon, Ezra C. Wood, Edward C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Detecting Fugitive Emissions of 1,3-Butadiene and Styrene from a Petrochemical Facility: An Application of a Mobile Laboratory and a Modified Proton Transfer Reaction Mass Spectrometer," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12706-12711

Ezra C. Wood, Scott C. Herndon, Ed C. Fortner, Timothy B. Onasch, Joda Wormhoudt, Charles E. Kolb, W. Berk Knighton, Ben H. Lee, Miguel Zavala, Luisa Molina, and Marvin Jones. "Combustion and Destruction/Removal Efficiencies of In-Use Chemical Flares in the Greater Houston Area," *Industrial & Engineering Chemistry Research* 2012 *51* (39), 12685-12696

Pikelnaya, O., J. H. Flynn, C. Tsai, and J. Stutz (2013), Imaging DOAS detection of primary formaldehyde and sulfur dioxide emissions from petrochemical flares, J. Geophys. Res. Atmos., 118,8716–8728, doi:10.1002/jgrd.50643.

This project has also resulted in the following publications:
Olga Pikelnaya, Jochen Stutz, Scott Herndon, Ezra Wood, Oluwayemisi Oluwole, George Mount, Elena Spinei, William Vizuete, Evan Couzo, "*Formaldehyde and Olefin from Large Industrial Sources (FLAIR) in Houston, TX – Campaign Overview",* in preparation for Journal of Geophysical Research

Olga Pikelnaya, Scott Herndon, Ezra Wood, and Jochen Stutz, "*Observations of emissions from ships in the Houston Ship Channel during 2009 FLAIR campaign,"* under development.

FY12-13

12-006
Journal Papers:
Gookyoung Heo, Peng Wang, Qi Ying, Ron Thomas, William P.L. Carter. Using chemically detailed emissions data to test assumptions used in developing chemical mechanisms: a case study for southeast Texas, USA. [To be submitted to Atmospheric Environment in Summer 2014]

Peng Wang, Gookyoung Heo, William P.L. Carter, Qi Ying. Comparison of a detailed and a lumped version of SAPRC-11 photochemical mechanism during a summer ozone episode. [To be submitted to Atmospheric Environment in Summer 2014]

Gookyoung Heo, Chia-Li Chen, Ping Tang, William P.L. Carter. Evaluation of mechanisms for major terminal and internal alkenes with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2014]

Gookyoung Heo, Shunsuke Nakao, William P.L. Carter. Evaluation of mechanisms for 1,3-butadiene with environmental chamber data. [To be submitted to Atmospheric Environment in Summer 2014]

Conference Paper:
Heo, G., Carter, W.P.L., Wang, P., Ying, Q., Thomas, R. (2013). Evaluating and improving atmospheric chemical mechanisms used for modeling ozone formation from alkenes. Presented at the 12th Annual CMAS Conference, Chapel Hill, NC, October 28-30, 2013.

12-012

Conference presentations:

C. Faxon, J. Bean, L. Hildebrandt Ruiz. Evidence of atmospheric chlorine chemistry in Conroe, TX: Regional implications. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

J. Bean, C. Faxon, L. Hildebrandt Ruiz. Atmospheric processing of pollutants in the Houston Region: First insights from DISCOVER-AQ. American Chemical Society Southwest Regional Meeting, November 2013, Waco, TX.

L. Hildebrandt Ruiz, J. Bean, G. Yarwood, B. Koo, U. Nopmongcol. Formation and Gas-Particle Partitioning of Organic Nitrates: Influence on Ozone Production. American Association for Aerosol Research Annual Meeting, October 2013, Portland, OR.

Planned publications:

C. Faxon, J. Bean and L. Hildebrandt Ruiz. Preliminary title "Significant Inland Concentrations of ClNO2 Detected in Conroe TX during DISCOVER-AQ 2013". Submission planned for August 2014.

J. Bean, C. Faxon and L. Hildebrandt Ruiz. Manuscript summarizing particle-phase measurements from DISCOVER-AQ. Submission planned for late 2014.

13-016

Gary Morris presented a poster entitled "Tropospheric Ozone Pollution Project (TOPP) Overview: A Context for DISCOVER-AQ Houston 2013" at the DISCOVER-AQ Science Team Meeting on February 27, 2014.

13-022

A. Bui, Y.J. Leong, N. Sanchez, H.W. Wallace, and R. Griffin, Distribution, influential factors, and sources of aerosol liquid water during the DISCOVER-AQ 2013 campaign in Houston, TX, *American Association for Aerosol Research Annual Meeting*, Minneapolis, MN, October 2015. (poster)

Y.J. Leong, N. Sanchez, H.W. Wallace, B. Karakurt Cevik, J. Flynn, Y. Han, P. Massoli, C. Floerchinger, E. Fortner, S. Herndon, B. Lefer, and R. Griffin, Overview of surface measurements of submicron particulate matter in the greater Houston area during the DISCOVER-AQ 2013 field campaign, *American Association for Aerosol Research Annual Meeting*, Minneapolis, MN, October 2015.

B. Lefer, J. Flynn, L. Judd, X. Ren, M. Estes, and R. Griffin, The spatial and temporal variability of ozone in the Houston metropolitan area during DISCOVER-AQ and its relation to meteorological conditions, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014.

R. Sheesley, T. Barrett, S. Yoon, A. Clark, L. Hildebrandt-Ruiz, R. Griffin, B. Karakurt Cevik, R. Long, R. Duvall, and S. Usenko, Spatial trends in surface-based carbonaceous aerosol,

including organic, water-soluble, and elemental carbon, during DISCOVER-AQ in Houston, TX, *American Geophysical Union Winter Meeting*, San Francisco, CA, December 2014. (poster)

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

R. Ferrare, J. Crawford, R. Griffin, C.Hostetler, B. Anderson, B. Holben, R. Hoff, A. Beyersdorf, and L. Ziemba, DISCOVER-AQ investigation of aerosol impacts on air quality over Houston, *American Association for Aerosol Research Annual Meeting*, Orlando, FL, October 2014.

H.W. Wallace, Y.J. Leong, B.K. Cevik, M.G. Camp, J.H. Flynn, B.L. Lefer, and R.J. Griffin, Characterization of nocturnal aerosol formation in Houston during DISCOVER-AQ, *International Global Atmospheric Chemistry Quadrennial Meeting*, Natal, Brazil, September 2014. (poster)

H.W. Wallace, Y.J. Leong, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, and R.J. Griffin, Characterization of aerosol organic nitrate in the outflow from Houston, TX, during the DISCOVER-AQ campaign, *American Chemical Society Annual Meeting*, San Francisco, CA, August 2014.

Y.J. Leong, H.W. Wallace, B. Lefer, B.K. Cevik, J.H. Flynn, R.W. Talbot, P.L. Laine, B.C. Sive, X. Lan, D. Anderson, Y. Zhou, M. Camp, R.J. Griffin, Chemical characterization of submicron aerosol emissions in the greater Houston area using an aerosol mass spectrometer on a mobile platform, *American Geophysical Union Winter Meeting,* San Francisco, CA, December 2013. (poster)

13-024

NASA AQAST meeting at Rice University in Houston, TX (Jan. 14-16, 2014), where Xinrong Ren gave a talk titled: "Measurements of trace gases at the Manvel Croix and Galveston sites during DISCOVER-AQ."

NASA DISCOVER-AQ science meeting at NASA Langley in Hampton, VA, where Winston Luke gave a talk titled: "NOAA/Air Resources Laboratory Surface Observations at Galveston and Manvel-Croix: Summary and Comparison with Aircraft Data."

A paper is in preparation with the intent to submit to Atmospheric Chemistry and Physics within about 3 months.

12-028

Implementation and Refinement of a Surface Model for HONO formation in a 3-D Chemical Transport Model. Prakash Karamchandani[1], Chris Emery[1], Greg Yarwood[1], Barry Lefer[2], Jochen Stutz[3], Evan Couzo[4], and William Vizuete[5]. ([1]ENVIRON, [2]University of Houston, [3]University of California-Los Angeles, [4]Massachusetts Institute of Technology, and [5]University of North Carolina.)

Impacts of heterogeneous HONO formation on radical sources and ozone chemistry in Houston, Texas. Evan Couzo[1], Barry Lefer[2], Jochen Stutz[3], Greg Yarwood[4], Prakash Karamchandani[4], Barron Henderson[5], and William Vizuete[1]. ([1]University of North Carolina (now at MIT), [2]University of Houston, [3]University of California-Los Angeles, [4]ENVIRON, [5]University of Florida.)

12-032
Poster at the American Geophysical Union national meeting (Dec 2013) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Poster at the DISCOVER-AQ Science Working Group meeting (Feb 2014) *Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX* Rebecca J. Sheesley, Tate E. Barrett, Subin Yoon, Adelaide Clark and Sascha Usenko

Manuscript in preparation. Submission planned to Atmospheric Environment in summer 2014. Draft title: "*Initial characterization of surface-based carbonaceous aerosol during DISCOVER-AQ in Houston, TX*."

12-TN1
Presentation:
"A regional chemical reanalysis prototype" Pius Lee , Greg Carmichael, Tianfeng Chai, Rick Saylor, Li Pan, Hyuncheol Kim, Daniel Tong, and Ariel Stein

Poster:
"Preliminary analyses of flight measurements and CMAQ simulation during Southeast Nexus (SENEX) field experiment" Li Pan, Pius Lee , Hyun Cheol Kim, Daniel Tong ,Rick Saylor and Tianfeng Chai

Publication:
Pius Lee, Fantine Ngan, Hang Lei, Barry Baker, Bright Dornblaser, Gary McGauhey,and Daniel Tong. An Application for Improving Air Quality: a Houston Case Study, Earthzine 2014 [available at: http://www.earthzine.org/2014/03/29/an-application-for-improving-air-quality-a-houston-case-study/?shareadraft=baba698217_53330c8eab882]

12-TN2
The project team presented at the Community Modeling and Analysis System (CMAS) Conference in October 2013.

Presentations:
"HCHO and NO2 column comparisons between OMI, GOME-2 and CMAQ during 2013 SENEX campaign (21 slides)" Hyun Cheol Kim, Li Pan, Pius Lee, Rick Saylor, and Daniel Tong

Posters:
Fine-scale comparison of GOME-2, OMI and CMAQ NO2 columns over Southern California in 2008" Hyun Cheol Kim, Sang-Mi Lee, Fong Ngan, and Pius Lee