AIR QUALITY RESEARCH PROGRAM

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

Quarterly Report

December 1, 2010 through February 28, 2011

Submitted to

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Texas Air Quality Research Program

Quarterly Progress Report

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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 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 were initiated. The subcontracting involves two phases. First, a sub-agreement is established with each institution specifying terms and conditions. Second, once a sub-agreement is in place and a project Work Plan is approved, a Task Order is issued authorizing work to commence. At the end of the current quarter, all but one of the sub-agreements were in place and Task Orders or Letter Agreements for 6 of 14 projects were activated. An additional 9 Task Orders for 5 different projects were issued and are currently pending signature. The work underway on the 6 projects with active Task Orders is described in this progress 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.
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> (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 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 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. 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 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.

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. 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 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. 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.

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; 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.

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-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.

RESEARCH PROJECTS

During the third quarter of operation, Program Administration focused on issuing Task Orders for projects with approved Work Plans. Project Managers continued to work with the Principal Investigators (PIs) to finalize project Work Plans, which include the Statement of Work, a detailed budget, and a Quality Assurance Project Plan (QAPP). As of the end of this quarter Agreements were fully executed with all participating institutions, with the exception of one. That institution has issued a verbal approval and signatures are in process. Six projects are Active. A total of 9 Task Orders representing 5 projects are pending, meaning they have been issued to the participating organizations and are awaiting signature. It should be noted that each Task Order specifies the project start date as the day following TCEQ authorization of the Work Plan; however, this is not official until the Task Orders have been signed by both parties.

Two projects that had approved Work Plans are currently being modified due to contractual issues. These are mainly related to changes in project leadership roles. It is anticipated that the modified Work Plans will be submitted and approved in March, as there are no substantive changes to the scope of the project.

During the previous quarter two institutions (both from outside of the State of Texas) were unable to agree to the terms of the AQRP sub-agreement and one PI withdrew from the program leaving additional research project funds available to be awarded. During this quarter, those funds were awarded to 2 projects that were named as alternates by the Advisory Council. One of those projects has Task Orders Pending and the other project is the last project without a finalized Work Plan. This project's Work Plan is expected to be submitted for approval during the week of March 7, 2011.

A detailed summary of each of the projects approved for funding and their status follows:

Project 10-006 **STATUS: Task Order Pending**

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

Funded Amount: $484,662
($262,179 Chalmers, $222,483 UH)

Executive Summary:
In a collaboration between the University of Houston and the Chalmers University of Technology in Gothenburg/Sweden, a measurement study will be conducted which will help to locate and quantify industrial emissions of VOCs (alkanes, alkenes and other species), NO_2 and SO_2 utilizing the Solar Occultation Flux (SOF) and the mobile Differential Optical Absorption Spectroscopy (DOAS) methods. During part of the campaign, a mobile extractive Fourier Transform Infrared Spectroscopy (meFTIR) will also be used. These methods allow estimates of pollutant concentrations in a column of air from a point on the ground. This study will follow up previous measurements in 2006 and 2009 to obtain a trend analysis for selected sites, but also will be extended to new areas and improve the understanding of short and long term pollutant variability. Thus, the study objectives are relevant for the AQRP priority research area about emissions, emphasizing the need to improve the uncertainty of industrial gas emissions (VOC, NO_x) that lead to the formation of tropospheric ozone. The measurements will be conducted from a van with a specially equipped sunroof to be able to conduct SOF measurements. The availability of such a platform will be valuable for future SOF studies. During the project, complementary wind measurements will be conducted using GPS radiosondes and from a 10 meter portable mast that will be acquired within the project. To complement the path measurements taken by the SOF, DOAS, and meFTIR, canister samples will be taken downwind the sites and analyzed afterwards using gas chromatography. In this way fugitive emissions for VOCs will be derived. The study areas will include locations in Houston (Houston Ship Channel, Mont Belvieu, Texas City, Chocolate Bayou, Freeport and Sweeny), Dallas - Fort Worth (DFW), Longview, Beaumont and Port Arthur. The priorities for the measurement areas outside Houston will be discussed with TCEQ and the AQRP project manager prior to the measurements.

The measurement campaign will take place largely in April and May 2011. The measurements in the DFW area will be carried out to augment other measurements taken by AQRP projects that are part of the DFW Field Campaign. The SOF measurements will be conducted 1 month earlier than the other DFW projects in order to get more sunshine hours and have better chances of cooler temperatures which will optimize SOF measurements, and for other logistical reasons.

The overall measurements in this project will be carried out in the same manner as in previous studies in the Houston area during 2006 and 2009, but a few qualitative studies will be conducted in addition, measuring CO and formaldehyde (HCHO) in parallel with VOCs. We also plan to perform thermal emission measurements with FTIR, targeting flares as a source of emissions.

Project Update:
In collaboration with UT and TCEQ, work has focused on finalizing the Work Plan and the Quality Assurance Project Plan (QAPP) for this project. These were approved on February 15, 2011, and a Task Order has been issued to each institution for signature. Once the signed Task Orders are returned, this project will be active.

This is one of four AQRP projects conducting air sampling activities in the DFW area. In order to enhance collaboration and take advantage of economies of scale, the DFW Field Study Committee was formed. More information about the committee can be found in this report following the research project descriptions.

Project 10-008 **STATUS: Active – Oct. 21, 2010**

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

Funded Amount: $178,796
($128,851 Rice, $49,945 ENVIRON)

Executive Summary:
This project aims to characterize how various model inputs and formulations influence predictions of ozone-precursor response in Texas ozone attainment modeling episodes. Bayesian inference is being used to consider model performance for alternate structural and parametric scenarios to develop probabilistic representations of ozone response to emissions. The expected outcomes of this research are to improve understanding of how various factors (anthropogenic and biogenic emission rates, chemical mechanisms, photolysis rates, boundary conditions, and dry deposition schemes) influence ozone response predictions; to help prioritize future improvements to Texas SIP modeling; and to demonstrate how probabilistic analyses via an ensemble approach can supplement deterministic estimates of ozone response.

Project Update:
Development of alternate model structural inputs

With the original TCEQ model inputs for the 2006 Houston-Galveston-Brazoria (HGB) and Dallas-Fort Worth (DFW) ozone modeling episodes (HGB8H2 and DFW8H2) as the base case setting, ENVIRON has developed alternate model formulations and input parameter settings to be used for the structural uncertainty cases:

- Updated photochemical model and chemical mechanism: ENVIRON has implemented the CB-6 chemistry mechanism into the latest version of CAMx (Version 5.32). The new photolysis rate inputs for the CB6 mechanism were also prepared.
- Alternate boundary conditions: Boundary conditions (BCs) for both episodes on the 36-km master modeling grid were extracted from the 2006 annual GEOS-CHEM global model simulation outputs. These and the original TCEQ BC inputs were also adjusted for use in CB-6, in which acetone and propane have been subtracted from the species PAR, and added explicitly in the BCs.
- Alternate biogenic emissions: Alternate biogenic emissions inputs were prepared for each modeling grid using the Model of Emissions of Gases and Aerosols from Nature (MEGAN) biogenic emission model (Version 2.03a) which employs updated land cover data with 1-km of spatial resolution based on satellite and ground observations.
- Land use inputs for the Zhang dry deposition scheme: CAMx Version 5.3 offers two dry deposition options: the original approach based on the work of Wesely (1989) and Slinn and Slinn (1980); and an updated approach based on the work of Zhang et al. (2001; 2003), which are formulated for 11 and 26 land use categories, respectively. A new land

use input file format is introduced that supports both land use categorizations as well as an optional leaf area index data field. ENVIRON prepared the new land use inputs for the Zhang scheme for each modeling grid.

Preliminary analysis of model performance

- Set up of the new base case for the project by using CAMx Version 5.32: Rice has run the new CAMx Version 5.32 with CB-05 Chemistry for the June 2006 episode by using the base inputs provided by TCEQ. The new base case run focuses on 2 grids (the 36-km and 12-km domains). Therefore the original Albedo_Haze_Ozone files have been modified for matching the 2 grids. Rice also compared the base case simulation results to those generated from the earlier version (Version 5.20 with CB-05) of CAMx by TCEQ and found the differences to be small.
- Validation of the accuracy of High-order Decoupled Direct Method (HDDM) in the new CAMx code: Ozone sensitivities simulated by CAMx-HDDM have been tested against the sensitivities computed by brute force with good consistency. The sensitivity parameters that have been tested are (36-km) domain-wide NO_x emissions, initial conditions of all species, boundary conditions of all species, and the reaction rate of $NO+O_3$.
- Simulations of structural scenarios: Rice has performed simulations for alternate structural cases by using the CB-6 mechanism (with the new photolysis rate inputs), the Zhang dry deposition scheme (with the new land use inputs), GEOS-CHEM-generated BCs for the 36-km master grid, and MEGAN-generated biogenic emissions, with each structural factor changed one at a time from the base case.
- Model performance evaluation: Rice has evaluated the model performance against TCEQ and EPA ozone measurements for the structural scenarios listed above. Simulated ozone concentrations for the above structural scenarios have been evaluated against TCEQ and EPA observations. Linear regression equations and correlation coefficients (R^2) have been derived. Weighted root-mean-squared error and relative likelihood function for each case have been computed.

Issues as related to the projects during the reporting period

Categorized emission files for the Aug/Sept 2006 HGB Ozone Modeling Episode from TCEQ are needed to separately consider uncertainties in and sensitivities to biogenic and anthropogenic emissions categories. This is also necessary in order to substitute the alternate (MEGAN) biogenic emissions. Project personnel have been in communication with Jim MacKay and Weining Zhao of TCEQ and categorized emissions files for this episode are expected, as they have provided for June 2006.

Detailed testing of CAMx-HDDM against brute force became necessary because we are using an updated version of CAMx (Version 5.32) with new features (e.g., Zhang deposition, CB-6 chemistry) for which HDDM performance had not been tested. Initial attempts showed major discrepancies, because CAMx-HDDM has not been extended to the ACM2 vertical diffusion scheme. The discrepancies have been resolved by limiting work to the older vertical diffusion scheme, and HDDM is now validated to provide results consistent with brute force.

Project 10-009 **STATUS: Active – Sept. 8, 2010**

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

Funded Amount: $591,332

Executive Summary:
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 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 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 with nitrogen 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.

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 will be compared to the extractive measurement results.

The data from this study have been and continue to be quality assured and are being analyzed. An external review committee selected by the TCEQ will review the draft project final report.

Project Update:
This project is on schedule. The final report will be delayed slightly to accommodate some additional review activities and presentations requested by the TCEQ. This new schedule is being developed with the TCEQ and will be updated during the next quarter.

One of the remote-sensing contractors, Telops, has delayed significantly in providing their data. This delay in reporting their data was reported to the TCEQ Project liaison during the last quarter. They recently submitted their data. This delay will impact production of the section of the final report that compares the Telops remote sensing measurements to the primary extractive measurements but should only slightly delay production of the final report.

Due to favorable weather and test conditions, twice as many steam-assisted test points and 25% more air-assisted test points were conducted than originally planned. Data analyses for the project final report are being performed.

It is anticipated that the project as initially defined would be completed slightly under budget. This information was reported to the TCEQ during this quarter along with a request to expend these funds to leverage the original scope of work for this project by adding a new task. The additional task proposed will build on computational fluid dynamics (CFD) modeling work performed at The University of Texas at Austin using two –dimensional modeling of flame and wind tunnel data available in the literature. The proposed task will build on this expertise by applying the model to full sized flares to assess the relative impact on flare combustion efficiency by altering operating variables such as gas flow, waste gas heating value, amount of steam assist, flame temperature, and presence of certain HRVOCs (ethylene, propylene). Parametric sensitivity of the model will be evaluated. Data from the 2010 pilot scale flare tests at John Zink in Tulsa, OK, will be used to evaluate the performance of the model. The work on this Task will be completed by August 31, 2011.

The information for the new Task was submitted to the TCEQ Liaison for review. Since this was an addition to the previously approved scope of work, the request was forwarded to the Project Review Panel with input solicited from the ITAC and Advisory Council. The request to add the Task was approved by the Project Review Panel on February 22, 2011. The PI has submitted a fully revised Work Plan to the TCEQ Project Liaison for review and final authorization.

Project 10-015 **STATUS: Work Plan under Modification**

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 – Jim Neece

Funding Requested: $201,280

Executive Summary:
Generally urban air pollution occurs during hot, sunlit, stagnant weather when ozone and aerosols (very fine particles suspended in the air) are produced in copious amounts from the interaction of sunlight with emissions from natural sources, vehicles and industry. However, a very different chemistry proceeds in the atmosphere in the absence of sunlight. Indeed, at night an entirely different family of chemical species, which cannot persist in sunlight, actively modifies the composition of the urban atmosphere. In some cases, this modified composition sets the stage to jumpstart the next day's sunlight driven chemistry, and thereby increases the amount of ozone and aerosol that are formed. In other cases, the nighttime chemistry removes ozone and aerosol precursors and thereby reduces the next day's ozone and aerosol formation.

Work conducted by the National Oceanic and Atmospheric Administration (NOAA) during the TexAQS 2006 study has shown that heterogeneous uptake and reaction of the important nighttime chemical species dinitrogen pentoxide (N_2O_5) can form the active halogen species, nitryl chloride ($ClNO_2$), potentially in high enough abundance to impact the next day's photochemistry. Nitryl chloride is produced when sufficient chloride-containing aerosol co-exists with high nighttime nitrogen oxides and ozone. This process is likely particularly important in Houston due to high levels of chloride-containing aerosol from airborne sea salt, high NOx emissions, and high ozone concentrations. This project aims to characterize nitryl chloride formation in urban areas of Texas as inferred from existing data sets from the TexAQS I, II and SHARP field campaigns in the region, and the CalNex 2010 data set conducted in another polluted coastal urban area (Los Angeles). This project will also include both box modeling of the N_2O_5- $ClNO_2$-aerosol system to test and refine chemistry algorithms, and photochemical grid modeling with the CAMx model as used by TCEQ for SIP development.

The expected outcomes of this research are improvement in our understanding of nighttime atmospheric chemistry, particularly with regard to active chlorine chemistry, and its influence on the production of ozone and aerosols in urban areas. This improved understanding will be directly incorporated into the photochemical grid models so that more reliable SIP planning can be conducted.

Project Update:
On November 9, 2010, the TCEQ Liaison recommended that Project 10-015 should commence. A Task Order was issued to NOAA on November 22, 2010, and it was sent to their central office for signature. In February, 2011, the PI notified AQPR Project Management that NOAA was unable to sign the contract documents due to a conflict with the indemnity clause. It was determined that ENVIRON could take the lead on the project, enabling the work to move forward. Currently, the Work Plan is being modified to reflect ENVIRON's leadership role. It will be resubmitted to the TCEQ Liaison in March 2011.

Project 10-020 **STATUS: Work Plan under Modification**

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 Requested: $202,498

Executive Summary:
During the second Texas Air Quality Study in 2006 the National Oceanic and Atmospheric Administration (NOAA) P-3 aircraft measured a wide suite of atmospheric species including important a critical nighttime chemical species: the nitrate radical (NO_3), a strong oxidant for highly reactive VOC. Reactions between NO_3 and highly reactive VOC can remove them from the atmosphere and prevent their participation in ozone and aerosol formation. This project aims to characterize how the nighttime chemistry affected the NOx and VOC concentrations in the atmosphere over Houston, with particular focus on the petrochemical industrial and power plant emissions. This project will also evaluate the success of plume modeling in reproducing the observations, and improve the algorithms presently incorporated into the photochemical grid models that are used in SIP development.

The expected outcomes of this research are improvement in our understanding of nighttime atmospheric chemistry, particularly with regard to the NO_3-VOC chemistry, and its influence on the production of ozone and aerosols in urban areas. This improved understanding will be directly incorporated into the photochemical grid models so that more reliable SIP planning can be conducted.

Project Update:
On November 8, 2010, the TCEQ Liaison recommended that Project 10-020 should commence. A Task Order was issued to NOAA on November 22, 2010, and it was sent to their central office for signature. In February 2011, the PI notified AQPR Project Management that NOAA was unable to sign the contract documents due to a conflict with the indemnity clause. It was determined that ENVIRON could take the lead on the project, enabling the work to move forward. Currently, the Work Plan is being modified to reflect ENVIRON's leadership role. It will be resubmitted to the TCEQ Liaison in March 2011.

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

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

Executive Summary:
In January of 2010 the USEPA proposed to strengthen the 8-hour primary National Ambient Air Quality Standards (NAAQS) for ozone to between 0.060 and 0.070 ppm and established a new seasonal secondary standard. The increased stringency of the primary and secondary NAAQS is expected to result in nonattainment designations for many more counties throughout the United States, including Texas. 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 the most 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. 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 such as roofing, building façades, and roadways.

The overall objective of this project is to improve existing knowledge of the effects of the urban built environment on dry deposition of ozone and predicted ozone concentrations. This project uses Austin, Texas, as the case study area but the experimental data and air quality modeling approach will be applicable to other ozone nonattainment and near nonattainment areas in eastern Texas. The project has the following objectives:

1. To conduct laboratory and field experiments to better characterize ozone removal by large-area outdoor built environment surfaces.
2. To characterize built environment surfaces in the Austin, Texas urban landscape using geospatial data.
3. To modify the dry deposition algorithms in CAMx, the air quality model used in regulatory applications for Texas, to include information from (1) and (2).
4. To conduct CAMx simulations to investigate the impacts of improvements in the characterization of dry deposition to built environment surfaces and of potential increases in built environment surfaces due to future urbanization on predicted ozone concentrations in Austin, Texas.

The deliverables to TCEQ will include revised deposition information, obtained from laboratory experiments, for a minimum of sixteen materials representing a range of urban built environment surfaces. Modified CAMx code to recognize these new urban land use categories will be

provided, as well as an updated land use database for Austin, Texas, based upon the latest available geospatial information. Collectively, these deliverables should allow the TCEQ to readily adapt this work to photochemical modeling of other urban areas in Texas with similar built environment surfaces to that of Austin.

Project Update:

Phase 1

During Phase 1, ozone surface reaction resistances for a wide range of building materials will be quantified in laboratory experiments. These measured reaction resistances will then be used in Phase 2 of the project to modify the CAMx air quality model to provide a better representation of ozone dry deposition to the urban built environment. Phase 1 includes two major tasks: (P1-1) determination of surface resistances and (P1-2) estimation of quasi-laminar sub-layer resistance at field sites.

Task P1-1: Determination of bulk surface resistances.

P1-1.1. Selection of materials. A minimum of sixteen materials representing a range of urban built environment surfaces have been selected for laboratory experiments to quantify ozone surface reactions. The materials are listed in Table 1 along with an indication of the testing status.

Table 1. Building materials included in Phase 1 experiments to quantify ozone surface resistances.

Type	Material	Description	Test Status
Road	Asphalt	5% Binder	Completed
Road	Asphalt	6% Binder	Completed
Road	Asphalt		
Road	Concrete	Roads/buildings (0.42 porosity with fly ash)	Completed
Road	Concrete	Roads/buildings (0.42 porosity without fly ash)	Completed
Road	Concrete	Buildings/bridges (0.32 porosity without fly ash)	Completed
Wall	Concrete	Driveways (0.7 porosity without fly ash)	Completed
Wall	Brick	Clay unpainted	Completed
Wall	Stone	Limestone	
Wall	Wood	Painted	
Wall	Wood	Fence, unpainted	
Wall	Fiber cement		
Roof	Asphalt shingle	Three tab (flat)	
Roof	Asphalt shingle	Dimensional (raised)	
Roof	Membrane 1		
Roof	Built up asphalt		

P1-1.2. Modification and performance testing of experimental system. Construction of the experimental system, shown in Figure 1, was completed on November 31, 2010. Preliminary testing, including quality assurance tests and corrective actions, was completed on January 17, 2011.

Figure 1. Experimental system for the ozone deposition experiments.

Acquisition of a six-port sampling valve was required for the system, which slowed the initial experimental system construction and testing. In addition, initial investigations showed 10-20% ozone loss in control (empty) chambers. The ozone removal could have been due to heterogeneous ozone reactions with the walls, adsorption to walls, or possibly absorption to layers of water molecules that accumulate on wall surfaces (even without visible condensation) due to the elevated water vapor concentrations used during experiments. In order to minimize ozone loss, the chamber walls are now being cleaned with distilled water and methanol, and are heat treated after each experiment. For experiments that include test materials, results are being corrected for ozone removal to walls of the control chamber.

P1-1.3. Determination of initial surface resistances and diurnal variations/regeneration. This task began in January 2011. As of February 18th, the initial surface resistance experiments have been completed for 7 of the 16 materials shown in Table 1. Revisions to

the experimental schedule have allowed for the quantification of the initial surface resistance for three materials every two weeks, which should allow this task to be completed as planned in April 2011.

P1-1.4. Determination of longer-term in-field variations in material reactivity. Two samples of each material that is listed in Table 1 were placed on the roof of the Center for Energy and Environmental Resources (CEER) at the University of Texas at Austin after the conclusion of the regeneration phase. These samples will be retested every two months after aging in the field. It is expected that some materials will be analyzed for up to six months while others will be analyzed for approximately four months in the field.

Task P1-2: Estimation of quasi-laminar sub-layer resistance at field sites. These experiments aim to estimate the transport resistance, i.e., the sum of the aerodynamic and boundary layer resistances, near buildings and to compare these with the existing diffusion resistances used in the CAMx model.

P1-2.1. Selection of the test compound. This task has been completed. Naphthalene was selected as the test compound for the preliminary investigations.

P1-2.2. Fabrication of mass transfer plates. This task has been completed. Stainless steel paint can lids were selected for use as the mass transfer (coated) plates.

P1-2.3. Preliminary testing. This task has been completed. Twelve preliminary tests were completed to show the viability of using naphthalene volatilization from plates to estimate transport resistance at field sites.

P1-2.4. Field studies. Fifteen experiments have been completed to calculate the transport resistance of naphthalene and, by theoretical corrections, for ozone to horizontal built environment surfaces. Plates have been tested on the roof of the Center for Energy and Environmental Resources (CEER) and the roof of the UTest House at the J.J. Pickle Research Campus of the University of Texas at Austin. Three vertical surfaces (a total of nine more experiments) remain to be completed in order to finish this task. This task is two months ahead of schedule; it was not scheduled to be started until March 2011.

Phase 2

The second phase of the project focuses on modifications to the dry deposition algorithm used in CAMx based on new experimental data related to material surface resistances and spatially resolved characterization of built environment surfaces in the urban landscape. This phase of the project is divided into three major tasks: (P2-1) characterization of built environment surfaces in the Austin urban landscape, (P2-2) pre-processing of the new land use/land cover data into the appropriate format for CAMx and modification of the dry deposition algorithms in CAMx, (P3-3) and air quality modeling and analysis of the impacts on ozone concentrations .

Task P2-1: Characterization of built environment surfaces in the Austin urban landscape. Data collection efforts have focused on three types of built environment surfaces in Travis County: (1) paved surfaces in the transportation network and parking lots, (2) residential properties, and (3) commercial properties. The primary objectives are to identify datasets with

information on the location, surface area, elevations, and types of built environment surface materials, to create a set of new urban land use categories that describe built environment surface types and their compositions, and to develop a new dry deposition land use and land cover file for use in CAMx that provides the spatial extent of the new urban land use categories to replace the existing single categorization of "urban". These data have also been used to guide the selection of materials for the experimental phase of the project.

For the Travis County transportation network, the team has continued to analyze the Texas Department of Transportation (TxDOT) Pavement Management Information System (PMIS) database for 2010 and to combine it with information from the City of Austin's 2003 Transportation ArcGIS shape file. The PMIS database includes the length, width, and pavement types for seven roadway classes and ten pavement types. The product of the length and width was used to determine the paved surface for the road segment. Of the roadway classes included in the PMIS database, the dominant surface material was medium thickness asphaltic concrete (2.5-5.5") and to lesser extents continuously reinforced concrete and surface treatment pavement.

The TxDOT PMIS database does not include residential streets, parking lots, or driveways. The City of Austin's 2003 transportation ArcGIS shape file included the following roadway classes within the City of Austin and Travis County: paved/unpaved streets, paved/unpaved alleys, paved/unpaved driveways greater than 150 ft, parking areas, open storage areas, medians greater than 10 feet, and bridges. It did not provide information regarding paved surface materials, nor was it as recent as the TxDOT PMIS database. However, it provided spatial data for other transportation-related classes not included in the TxDOT PMIS database. The City of Austin's transportation shape file was intersected with the TCAD parcels. It was found that most parking lots and open storage areas could be attributed to commercial improved and multi-family (i.e. apartment) parcels. Overall, 81% of parcels identified as multi-family residences, 74% identified as commercial improved parcels, and 85% of industrial improved parcels intersected with polygons for parking and/or open space areas. Thus, it appears that for these land use types, the City of Austin's transportation shape file captured most parking lot and open space areas. In contrast, paved areas for single family residences are not well represented. A field survey for single family residences in conjunction with assessments in Google Earth is planned to address this gap.

The Travis County Appraisal District (TCAD) offered the most comprehensive and current data regarding real and business personal property in Travis County. TCAD provided their 2010 dataset for the project with a waiver of their usual fees. These data included information on property square footage, improvement details, land area, and location, and in particular for residential properties, material construction types and roofing class. TCAD has three basic strategies to establish the value of properties: market, cost and income. Valuation by market reflects trading between similar properties. Valuation by cost reflects the cost of building a similar property. Valuation by income reflects the expected income from the property. Residential properties are evaluated based on cost, whereas commercial properties are often evaluated by income. Because of these differences, residential properties have a stronger link to building materials in the TCAD database than commercial buildings.

Residential floor area (72%) is substantially larger than commercial floor area (28%) in Travis County. Single family residences followed by apartments (100+ units) represent the most significant residential types. Office buildings (+35,000 sq. ft), bulk warehouses (over 20,000 sq. ft), warehouse (less than 20,000 sq. ft.), office buildings (+6 floors), and discount stores represent the most significant commercial types. With respect to residential structures, the floor areas of single family residences and large apartment complexes have increased over time in Travis County. In contrast, the floor areas of duplexes and small apartments peaked during the 1960s through 1980s and have decreased since. Collectively, the data for single family residences indicate changes in practices that have occurred over time. Prior to the 1990s, residential construction was primarily wood framing with wood siding; after this period, wood framing with veneer brick or stone became more prevalent. Overall, large apartment complexes have a higher proportion of wood framing with plaster or stucco than single family residences.

A survey of single family residential homes in the urban and suburban areas of Travis County was designed by the project team. The objective of the survey effort was to compare actual exterior construction material types to those reported in the TCAD database and to address missing information in the TCAD data such as the type and length of fencing and the percentage and type of accenting on the façade of residential homes. Seven age groups were identified for the survey: pre-1950, 1950s, 1960s, 1970s, 1980s, 1990s, and 2000+. Within each age group, five or six streets were randomly selected within Travis County, for a total of 36 streets. Approximately 20 homes were surveyed on each street. The survey was conducted on January 25, 2011 by two groups of project team members. The completed residential survey dataset is currently under analysis. The team anticipates conducting similar surveys for apartment complexes and commercial properties in Travis County.

Task P2-2: Preparation for CAMx modeling.

P2-2.1. Land cover/land use data processing for CAMx.
No work on this task was conducted during the reporting period.

P2-2.2. Modification of the CAMx Dry Deposition Algorithms.
No work on this task was conducted during the reporting period.

Task P2-3: CAMx Modeling and Sensitivity Studies. No work on this task was conducted during the reporting period.

Funding
All funds allocated to this project are expected to be used by the project end date of 8/31/2011.

Project 10-022 **STATUS: Task Order Pending**

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 Limited to: $150,000

Executive Summary:
Current methodologies for calculating VOC emissions from flaring activities generally apply a simple mass reduction to the VOC species sent to the flare. While it is assumed that a flare operating under its designed conditions and in compliance with 40 CFR 60.18 may achieve 98% destruction/removal efficiency (DRE), a flare operating outside of these parameters may have a DRE much lower than 98%. Basic combustion chemistry demonstrates that many intermediate VOC species may be formed by the combustion process.

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) and AQRP Project 10-009 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-assist and steam-assist flares under open-air conditions. This project will (1) primarily use CFD modeling as a predicting tool for the Tulsa flare performance tests (2) further compare the CFD modeling with the flare performance data and speciated volatile organic compound (VOC) concentrations if the data are available by May 31, 2011. 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 mechanism is reduced from the combined GRI and USC mechanisms with the goal of allowing NOx formation and handling light hydrocarbon combustion. This Lamar mechanism has been validated against methane, ethylene, and propylene experimental data. More photochemically important NOx species will also be added to the existing mechanism and an evaluation with lab data will be carried out for this new mechanism.

Lamar University (LU) will acquire the operating, design, and meteorological data of the flare test campaign from the University of Texas (UT) and conduct CFD modeling and prediction. The test data, if acquired by May 31, 2011, will be compared with the model results. The test data include Combustion Efficiency (CE), Destruction & Removal Efficiencies (DRE) and monitored CO/CO2, NO, NO2, methane, acetylene, ethylene, propylene, formaldehyde, acetaldehyde, and acetone concentrations. Cases will be modeled for the effect of varying steam

flow and heating value for the steam-assist flare and the effect of varying air flow and heating value for the air-assist flare.

Project Update:
A fully executed contract is in place with Lamar University. The project Work Plan was approved on February 15, 2011, and a Task Order was submitted to Lamar University on February 25, 2011. Once the Task Order is returned with signature, the project will be Active.

Project 10-024 **STATUS: Task Order Pending**

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

Executive Summary:
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 (NAAQS) 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) will investigate this hypothesis by performing an air quality sampling campaign that is described below.

The Rice, UH, and UNH team will install 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 15 to June 15, 2011. Eagle Mountain Lake is located approximately 30 kilometers to the northwest of downtown Forth Worth. This location was chosen for several reasons. First, there is a wealth of natural gas activity in this region. Second, wind in the DFW area often blows toward the northwest, indicating that the site will be subject to the emissions from Forth Worth. Lastly, other monitoring 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 will include 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 will conduct computational modeling that will be 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.

Project Update:
Fully executed contracts are in place with Rice University, the University of Michigan and the University of Houston. UT has received a verbal approval of the contract from the University of New Hampshire, and signatures are pending. The project Work Plan was approved on February 15, 2011, and Task Orders were issued on February 25, 2011. Once all Task Orders are returned with signature, the project will be Active.

This is one of four AQRP projects conducting air sampling activities in the DFW area. In order to enhance collaboration and take advantage of economies of scale, the DFW Field Study Committee was formed. More information about the committee can be found in this report following the research project descriptions.

Project 10-029 **STATUS: Active – Dec. 1, 2010**

Wind Modeling Improvements with the Ensemble Kalman Filter

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

Funding Awarded: $80,108

Executive Summary:
Meteorological models provide essential inputs to photochemical models that are used to simulate and study the formation and transport of air pollutants such as ozone. The appropriate treatment of vertical mixing in the lower atmosphere is a crucial component of meteorological and air quality models. Models use various schemes to simulate the vertical changes in heat, momentum, and other constituents within the lower portion of the atmosphere. Errors and uncertainties associated with these schemes remain one of the primary sources of inaccuracies in model predictions.

The purpose of this project is to improve meteorological analyses and forecasts, particularly of low-level winds and vertical diffusion, using a technique known as the Ensemble Kalman Filter (EnKF) data assimilation system. EnKF provides a methodology, using a combination of independent sources of observed and model-predicted information, to reduce errors in the model state resulting in an improved meteorological simulation. Previous work with a single case study demonstrated improvements in both analyses and forecasts using an initial version of EnKF. This project will obtain firmer conclusions regarding improved model performance by testing the procedure on other ozone episodes, increasing the number of considered model variables, and expanding the study to include a larger variety of meteorological conditions.

This meteorological research is directed toward the modeling priority area of the AQRP Strategic Plan. It specifically addresses the need for better use of data assimilation for more accurate modeling of individual ozone episodes and improvements in the physical representation of processes within the models. It also indirectly addresses all other modeling aspects of the AQRP Strategic Plan, because improved representation of winds and transport will allow more accurate conclusions to be drawn in all modeling studies involving meteorology, including but not limited to TCEQ attainment demonstrations.

This project utilizes the WRF (Weather Research and Forecast) mesoscale meteorological model and the Asymmetrical Convection Model, version 2 (ACM2) vertical mixing scheme. The final results will include software modifications for use in WRF along with the appropriate documentation. TCEQ can use the results of this project to potentially improve the meteorological model performance in their own models, and to continue to refine or improve the EnKF technique. Any improvements in meteorological model performance may lead to improved photochemical model performance and improved development of ozone control strategies and forecasts.

Project Update:
A fully executed contract is in place with Texas A&M University (TAMU). The project Work Plan was submitted to TCEQ on November 26, 2010 for final review. On November 29, 2010, the TCEQ Liaison recommended that Project 10-029 should commence. A Task Order was issued on Dec. 2, 2010, but was not returned with signature by TAMU until mid-February. This project is now Active.

Despite the delay in executing the Task Order, low-level activities have been initiated on Task 1. First, a graduate student has been learning about the fundamentals of data assimilation and the details of the Ensemble Kalman Filter (EnKF) as it relates to other assimilation techniques. He is close to complete on this activity.

Second, have been provided the following deliverables: (1) the software and scripts necessary to run the WRF meteorological model with the EnKF data assimilation system, including parameter estimation for certain parameters used by the ACM2 vertical mixing scheme; (2) a descriptive overview of the primary scripts, including their organization, functionality, and user-specified options; and (3) an annotated bibliography of the key papers regarding EnKF parameter estimation.

An "annotated bibliography" is a list of pertinent papers and resources, including brief summaries of why each of the papers and resources are pertinent. It describes the progression of technological development of the particular version of the EnKF that we use for parameter estimation. This particular annotated bibliography includes and describes seventeen papers, theses, and dissertations. Links are provided through which each of the papers, theses, and dissertations may be downloaded.

Project 10-032 **STATUS: Task Order Pending**

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

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

Executive Summary:

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:
A fully executed sub-agreement is in place with the University of Houston and UCLA. UT has received a verbal approval of the contract from the University of New Hampshire, and signatures are pending. The project Work Plan was approved on Feb. 8, 2011 and Task Orders were issued on February 15, 2011, to UH and UCLA. The Task Order to UNH will be issued once the contract is fully executed. Once all Task Orders are returned with signature, the project will be Active. At that time, the University of Houston will issue Purchase Orders to the University of Miami and Pennsylvania State University for their portions of the project activities.

Project 10-034 **STATUS: Task Order Pending**

Dallas Measurements of Ozone Production

University of Houston – Barry Lefer

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

Requested Funding: $195,054

Executive Summary:
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 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:

A fully executed sub-agreement is in place with the University of Houston. The project Work Plan was approved on Feb. 1, 2011 and a Task Order was issued on February 14, 2011. Once the Task Order is returned with signature, the project will be Active with a start date of February 2, 2011. At that time, the University of Houston will issue a Purchase Order to Pennsylvania State University for their portion of the project activities.

The progress towards the goals put forth in the scope of work have been limited to planning and making revisions to the QAPP, Work Plan, and Budget for this project.

This is one of four AQRP projects conducting air sampling activities in the DFW area. In order to enhance collaboration and take advantage of economies of scale, the DFW Field Study Committee was formed. More information about the committee can be found in this report following the research project descriptions.

On February 8th, UH project personnel and the DFW Site Committee Project Manager performed a preliminary site visit to the Eagle Mountain Lake monitoring site (CAMS 75) to survey the area and determine the feasibility of installing the MOPS. Sufficient power and space were found at the site, and it was determined that a 2m scaffold platform will be constructed for the MOPS to minimize the impacts of local structures (i.e. lab trailers, towers, and fencing) on the measurements.

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

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 – Jim Neece

Funded Amount: $237,481

Executive Summary:
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 chemical compounds, called NOx sinks. 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 will carry out new environmental chamber experiments to characterize NOx sinks for VOCs that are poorly understood (e.g., toluene, isoprene). At the same time, a literature search will be performed for chamber experiments performed in Europe that have not been utilized in the US for developing chemical mechanisms. The data obtained will be 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.

Project Update:

1. Progress
1.1. Data Obtained from Environmental Chamber Experiments at EUPHORE

The chemical mechanisms used in the TCEQ's SIP modeling were developed using environmental chamber data from the Universities of California and North Carolina. The European Commission has funded an environmental chamber in Spain (called EUPHORE) where experiments have been performed that are relevant to the characterization of NOx-sinks in the chemistry of aromatic hydrocarbons. Scientists at EUPHORE have been contacted, and data from selected experiments have been obtained and prepared for use in chemical mechanism evaluation. Preliminary modeling confirms that the data are useful but also revealed uncertainties in the data. The project team is currently working with EUPHORE scientists to improve the characterization of sunlight for each experiment. The data obtained from EUPHORE will be used in this project to improve chemical mechanisms for aromatic hydrocarbons.

1.2. Design of New Chamber Experiments

This project will perform environmental chamber experiments of a new type designed to quantify the strength of NOx-sinks introduced by different VOCs. Experiments will be performed at the University of California at Riverside (UCR). A base mixture of propene and NOx will be loaded into the chamber and irradiated until the initial NOx is consumed and the final concentration of ozone is limited by the initial NOx. Then, the experiment will be repeated with addition of a target compound (e.g., toluene) and the final ozone concentrations will altered by the NOx sinks introduced by the target compound. Propene is chosen for the base mixture because it has strong ozone forming tendency and weak NOx sinks. Computer simulations were performed to design the chamber experiments, specifically to determine initial concentrations of NOx, propene and several target compounds that will provide useful results for mechanism development. Figure 1 shows chamber simulation results for the base propene/NOx mixture and additions of toluene and cresol. The final ozone is reduced by both toluene and cresol because their reaction mechanisms include strong NOx sinks (stronger for cresol than toluene) and the concentrations of NOx products (NO_2 and HNO_3) also change. Chamber experiments also were designed to test whether NOx sink compounds (e.g., organic nitrates) can themselves react under atmospheric conditions to release NOx and thereby prolong ozone formation, a process called NOx recycling.

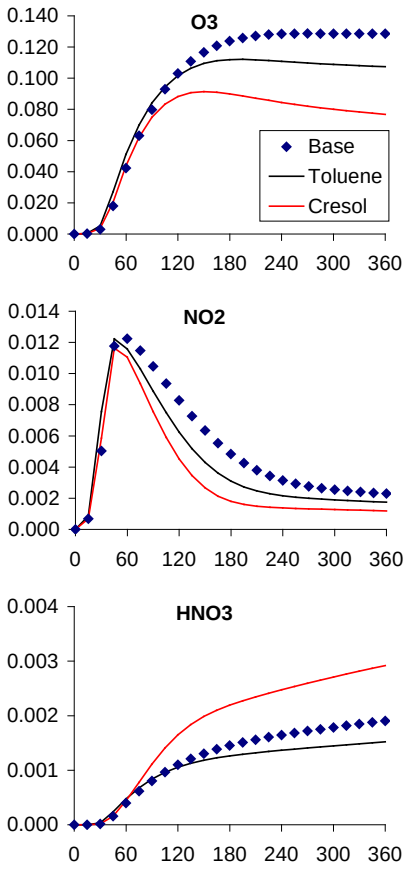

Figure 1. Simulated pollutant concentrations (ppm) to design chamber experiments that test NOx sinks in the reaction mechanisms for toluene and cresol.

1.3. Improvements to the UCR Chamber Experiments

Progress was made on readying the UCR environmental chamber for use in this project. A new cavity ring-down instrumentation (funded by a separate project) to be used for measuring NO_2, total PANs, organic nitrates and glyoxal was made operational in the UCR environmental chamber laboratory. Work is still needed in interfacing the instrument to the data collection system for modeling and some modifications need to be made to obtain environmental health and safety approval of the lasers, but this is not expected to delay the program.

2. Issues as related to the projects during the reporting period

The environmental chamber at UCR is housed in a temperature controlled building for which the cooling compressor failed preventing any experiments until the compressor is replaced. A replacement compressor has been ordered and should be installed in February, 2011.

The UCR environmental chamber has two alternate sources of UV radiation for conducting experiments, an arc light and black lights. The arc light approximates the spectrum of solar radiation whereas the black lights are designed to produce UV light and so have a different

spectrum than natural sunlight. The arc light source has experienced problems recently and is still not operational. Despite many attempts at repair, UCR is unable to get the light to operate without shutting down because of leaking cooling water around the arc. UCR sought advice from the manufacturer, who examined some parts involved and found no problems. Their current recommendation is that the leaks may be caused by a misalignment, and UCR is obtaining a low power laser to check the alignment. If this solves the problem experiments for this project may start before the end of February. If the arc light system cannot be repaired, a project conference call will be held to discuss the option of using the black lights for this project.

Additional Information:
Environ has issued purchase orders (POs) to Smog Reyes and the University of California – Riverside for services related to mechanism development, and specialized technical assistance and use of the chamber, respectively.

Project 10-044 **STATUS: Work Plan under Development**

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 Requested: $380,261

Executive Summary:
The University of Houston (UH) aircraft-based Air Quality Monitoring Team will conduct an airborne measurements investigation in the Dallas Fort Worth (DFW) area during the 2011 ozone season. The proposed measurement campaign includes 45 flight hours to be conducted during mid-May to mid-July using the twin-engine Piper Aztec aircraft. The constituents and mechanics of ozone formation and transport of ozone and ozone precursor compounds are the primary measurements of interest for this effort. The aircraft airborne sampling data will be used as a complement to ground based monitoring to better understand the atmospheric chemistry, meteorology, and transport of pollutants of interest in and around the DFW area.

Information obtained using an instrumented aircraft enables investigators to better understand the mechanisms associated with the transport of precursors and their contribution to ozone formation under various meteorological conditions. This and other similar aircraft have been used in previous projects in Texas to obtain this type of information. The aircraft has a full complement of instrumentation and is extensively modified for the purpose of air quality characterization.

UH will collect airborne monitoring samples on a minimum of five flights in and around DFW. The UH team will develop detailed flight plans in coordination with AQRP. Flights will have specific sampling goals; potential flights might be designed to:

(1) map pollutant concentrations throughout DFW on high ozone days in DFW.

(2) measure pollutant concentrations downwind of power plants.

(3) measure pollutant concentrations in the vicinity of active gas wells and/or compressor stations located on the Barnett Shale.

(4) investigate the impact in DFW of biomass burning episodes that might occur during the period of the study.

The University of Houston Aztec aircraft will provide observations of ozone, nitrogen oxides, sulfur dioxide, formaldehyde, reactive alkenes, volatile organic compounds, and meteorological parameters.

Project Update:
Dr. Shauck was notified in January 2011 that this project would be partially funded at a level of $279,715. The PI and the AQRP Project Manager are working to finalize the Work Plan for submission to TCEQ.

This is one of four AQRP projects conducting air sampling activities in the DFW area. In order to enhance collaboration and take advantage of economies of scale, the DFW Field Study Committee was formed. More information about the committee can be found in this report following the research project descriptions.

Project 10-045 **STATUS: Active - Jan. 22, 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)

Executive Summary:
In Spring 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 volatile organic compounds (VOCs), oxides of nitrogen (NO_x) and formaldehyde (HCHO), which all contribute to ozone formation. At the same time an Imaging Differential Optical Absorption Spectrometer (I-DOAS) operated by the University of California Los Angeles (UCLA) sampled flares and other individual sources for emissions of HCHO 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 in order to determine facility-wide emissions of HCHO and NO_2. As a result of all above mentioned efforts, a unique observational dataset of VOCs, HCHO, and NO_x observations was created.

The current project is a collaborative effort between the University of California Los Angeles (UCLA), Aerodyne Research Inc. (ARI), Washington State University (WSU) and University of North Carolina Chapel Hill (UNC), to interpret the observational dataset collected during 2009 FLAIR campaign. The observational data acquired by the different groups will be used to estimate emission rates of ozone precursors, such as VOCs, HCHO and NO_x, for the specific times and locations of the observation. These emission rates then will be compared to the hourly special inventories (SI) to provide an illustrative comparison for emission sources that are potentially critical for ozone formation.

Specific goals of this project are:

1. Characterize source-and date-specific emissions and atmospheric chemistry using the ARI mobile laboratory FLAIR dataset. Identify where the pollutant sources are, how much is emitted, and what happens to these pollutants in the atmosphere.
2. Determine of facility averaged fluxes of NO_2, HCHO, and SO_2 using dual MAX-DOAS data acquired during FLAIR 2009.

3. Characterize source-and date-specific fluxes of HCHO, NO_2 and SO_2 from point sources in Houston based on I-DOAS observations during FLAIR.
4. Estimate source-specific emission rates through interpretation and consolidation of the combined observations of all platforms during FLAIR. Qualitatively compare observations with hourly special inventories for 2006 and determine the uncertainty of the observations.

Project Update:
A fully executed contract is in place with UCLA, Aerodyne, UNC-Chapel Hill, and Washington State University. The Work Plan was approved on Jan. 21, 2011 and Task Orders have been fully executed with all parties. Work has now begun on this project and the initial Monthly Technical Report will be due on March 8, 2011.

Because of the limited dollar amount budgeted and the scope of the work to be done, Aerodyne has issued purchase orders (POs) to Montana State University and the University of Massachusetts, Amherst for $20,000 each for work related to this project.

DFW Field Study Committee

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).

Several conference calls have been held to coordinate the overall study plan and to coordinate monitoring site logistics. Eagle Mountain Lake was selected as the primary ground site for the study by the Committee. Site access agreement negotiations with the landholder are underway, led by AQRP staff. A site plan, including power requirements has been developed, again by AQRP staff, and preliminary contacts have been made with contractors to construct a pad, erect fencing, and install electrical utilities to the site.

Vincent Torres is acting as the lead AQRP Project Manager for the Committee, handling the site logistics and site access agreement negotiation.

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 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 eight 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. Ms. Maria Stanzione, AQRP Grant Manager, with assistance from Rachael Bushn, Melanie Allbritton, and Susan McCoy assisted with program organization and financial management. This included assisting with the contracting process, issuing Task Orders, and invoicing functions. Mr. Denzil Smith is responsible for the AQRP Web Page development and for data management.

Table 1: AQRP Administration Budget

Administration Budget (includes Council Expenses)

Budget Category		FY10	FY11	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$173,100	$148,755	$321,855	$187,557.80	$16,711.00	$117,586.20
Fringe Benefits		$38,082	$32,726	$70,808	$31,864.36		$38,943.64
Travel		$8,500	$7,500	$16,000	$346.85		$15,653.15
Supplies		$34,215	$2,744	$36,959	$6,520.99	$2,565.00	$27,873.01
Equipment		$6,000	$0	$6,000			$6,000.00
Other			$4,007	$4,007			$4,007.00
Total Direct Costs		$259,897	$195,732	$455,629	$226,290.00	$19,276.00	$210,063.00
Authorized Indirect Costs		$17,310	$14,876	$32,186	$17,418.40		$14,767.60
10% of Salaries and Wages							
Total Costs		**$277,207**	**$210,608**	**$487,815**	**$243,708.40**	**$19,276.00**	**$224,830.60**
Fringe Rate		22%	22%				

Dr. Mariana Dionisio, a post-doctoral associate is 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.

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 is an estimate, and actual fringe benefit expenses will be 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. For example, the amount of fringe benefits will be 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 for the months of December and January are included in the spreadsheet above. February fringe benefit expenses have not posted as of the writing of this report.

Supplies and materials expenditures included monthly telecom charges, postage, and office supplies. In addition, a computer was purchased to serve as a web server for the AQRP web site and backup storage was added to prepare for the submission of project data.

Indirect costs for the months of December and January are included in Table 1. February indirect costs have not posted as of the writing of this report.

At the initiation of the AQRP, funds were budgeted and expenses were projected based on assumptions made with the information known at that time. As the AQRP has progressed, spending decisions and staffing allocations have been made to most efficiently meet the needs of the program. Since the program started later than anticipated, the contracting and other program start-up activities have been pushed into FY 11 and concentrated into a shorter period of time. Thus the amount of time (FTE) spent on the program in FY 10 was reduced and the amount of time (FTE) those individuals working within the Administrative roles are spending on necessary program start-up functions has increased in FY 11. Their original percent time was estimated and divided between FY 10 and FY 11. As stated above, these tasks still need to be completed within FY 11 and thus the increase of FTE within FY 11

As these start-up activities are essential, 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.

ITAC

There were no ITAC expenses during this reporting period.

A conference call was held with the ITAC on December 2, 2010 to provide an update on the status of the AQRP, discuss the disposition of remaining Research/Contractual funds (if any projects were not able to proceed), discuss the DFW Field Program, and begin the Strategic Plan for the next biennium.

Table 2: ITAC Budget

ITAC Budget

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$16,500	$16,600	$33,100	$8,990.45		$24,109.55
Supplies		$2,364	$2,800	$5,164	$249.38		$4,914.62
Equipment							
Other							
Contractual							
Total Direct Costs		$18,864	$19,400	$38,264	$9,239.83	$0.00	$29,024.17
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$18,864**	**$19,400**	**$38,264**	**$9,239.83**	**$0.00**	**$29,024.17**

Project Management

Project Managers (PMs) have been assigned to each of the research projects. During the period from December 1, 2010 through February 28, 2011, PMs have worked with PIs to complete project Work Plans. A significant amount of time has been focused on the development and review of Quality Assurance Project Plans (QAPPs). For those projects that are now active, the role of the PM has evolved to helping the PIs accomplish project goals and ensuring that all reporting requirements are met.

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.

Table 3: Project Management Budget

Project Management Budget

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$139,653	$101,011	$240,664	$92,988.41	$10,280.00	$137,395.59
Fringe Benefits		$30,725	$22,223	$52,948	$16,981.50		$35,966.50
Travel		$4,000	$5,200	$9,200			$9,200.00
Supplies		$1,657	$1,465	$3,122	$16.93		$3,105.07
Equipment							
Other							
Contractual							
Total Direct Costs		$176,035	$129,899	$305,934	$109,986.84	$10,280.00	$185,667.16
Authorized Indirect Costs		$13,965	$10,101	$24,066	$8,564.40		$15,501.60
10% of Salaries and Wages							
Total Costs		**$190,000**	**$140,000**	**$330,000**	**$118,551.24**	**$10,280.00**	**$201,168.76**

Research Projects

As of February 28, 2011, a total of 6 projects are active. Table 4 on the following 2 pages illustrates the funding awarded to each project and the total expenses reported on each project as of February 28, 2011.

The projects that have the Cumulative Expenditures and Remaining Balance shadowed are not yet active, meaning their Task Orders have not been signed. Project 10-044 is the only project whose Work Plan has not been approved, so they have not yet been issued a Task Order. Task Orders has also not been issued to the University of New Hampshire for Projects 10-024 and 10-032. They will be issued upon full execution of the master contract. This is expected to occur in the first week of March 2011.

At this time, it is anticipated that all funding for research projects will be allocated to the projects listed above. It is still early in the Program, but it is anticipated that all Program funds will also be used.

Table 4: 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	$27,083	$101,768
10-008	Environ International	$49,945	$31,587	$18,358
10-009	UT-Austin	$591,332	$450,458	$140,874
10-021	UT-Austin	$248,786	$88,090	$160,696
10-022	Lamar University	$150,000		
10-032	University of Houston	$176,314		
10-032	University of New Hampshire	$23,054		
10-032	UCLA	$49,284		
10-034	University of Houston	$195,054		
10-042	Environ International	$237,481	$69,154	$168,327
10-045	UCLA	$149,773	$0	$149,773
10-045	UNC - Chapel Hill	$33,281	$0	$33,281
10-045	Aerodyne Research Inc.	$164,988	$0	$164,988
10-045	Washington State University	$50,000	$0	$50,000
FY 10 Total Contractual Funding Awarded		$2,248,143		
FY 10 Contractual Funding Remaining to be Awarded		$37,857		
FY 10 Contractual Funds Expended to Date*			$666,371	
FY 10 Contractual Funds Remaining to be Spent				$1,619,629

FY 11 Contractual Funding		**$1,736,063**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
10-006	Chalmers University of Tech	$262,179		
10-006	University of Houston	$222,483		
10-015	Environ International	$201,280		
10-020	Environ International	$202,498		
10-024	Rice University	$225,662		
10-024	University of New Hampshire	$70,747		
10-024	University of Houston	$64,414		
10-024	University of Michigan	$98,134		
10-029	Texas A&M University	$80,108		
10-044	University of Houston	$279,715		
FY 11 Total Contractual Funding Awarded		$1,707,220		
FY 11 Contractual Funding Remaining to be Awarded		$28,843		
FY 11 Contractual Funds Expended to Date*			$0	
FY 11 Contractual Funds Remaining to be Spent				$ 1,736,063
Total Contractual Funding		$4,022,063		
Total Contractual Funding Awarded		$3,955,363		
Total Contractual Funding Remaining to be Awarded		$66,700		
Total Contractual Funds Expended to Date*			$666,371	
Total Contractual Funds Remaining to be Spent				$3,355,692

*(Expenditures Reported as of February 28, 2011.)

Appendix

Financial Reports by Fiscal Year

(Expenditures reported as of February 28, 2011. Does not include all expenditures for the month of February 2011.)

Administration Budget (includes Council Expenses)

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$173,100	$159,682.24	$12,441.00	$976.76
Fringe Benefits		$38,082	$28,998.03		$9,083.97
Travel		$8,500	$346.85		$8,153.15
Supplies		$34,215	$6,520.99	$2,565.00	$25,129.01
Equipment		$6,000			$6,000.00
Other					
Total Direct Costs		$259,897	$195,548.11	$15,006.00	$49,342.89
Authorized Indirect Costs		$17,310	$15,794.43		$1,515.57
10% of Salaries and Wages					
Total Costs		**$277,207**	**$211,342.54**	**$15,006.00**	**$50,858.46**

Administration Budget (includes Council Expenses)

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$148,755	$27,875.56	$4,270.00	$116,609.44
Fringe Benefits		$32,726	$2,866.33		$29,859.67
Travel		$7,500			$7,500.00
Supplies		$2,744			$2,744.00
Equipment					
Other		$4,007			$4,007.00
Total Direct Costs		$195,732	$30,741.89	$4,270.00	$160,720.11
Authorized Indirect Costs		$14,876	$1,623.97		$13,252.03
10% of Salaries and Wages					
Total Costs		**$210,608**	**$32,365.86**	**$4,270.00**	**$173,972.14**

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**

Project Management Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$139,653	$92,988.41	$10,280.00	$36,384.59
Fringe Benefits		$30,725	$16,981.50		$13,743.50
Travel		$4,000			$4,000.00
Supplies		$1,657	$16.93		$1,640.07
Equipment					
Other					
Total Direct Costs		$176,035	$109,986.84	$10,280.00	$55,768.16
Authorized Indirect Costs		$13,965	$8,564.40		$5,400.90
10% of Salaries and Wages					
Total Costs		**$190,000**	**$118,551.24**	**$10,280.00**	**$61,169.06**

Project Management Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$101,011			$101,011.00
Fringe Benefits		$22,222			$22,222.00
Travel		$5,200			$5,200.00
Supplies		$1,465			$1,465.00
Equipment					
Other					
Total Direct Costs		$129,898			$129,898.00
Authorized Indirect Costs		$10,102			$10,102.00
10% of Salaries and Wages					
Total Costs		**$140,000**	**$0**	**$0**	**$140,000**

AQRP Budget

FY 2010

Budget Category		FY10 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$173,100	$159,682.24	$12,441.00	$976.76
Fringe Benefits		$38,082	$28,998.03	$0.00	$9,083.97
Travel		$8,500	$346.85	$0.00	$8,153.15
Supplies		$34,215	$6,520.99	$2,565.00	$25,129.01
Equipment		$6,000	$0.00	$0.00	$6,000.00
Other		$0	$0.00	$0.00	$0.00
Contractual		$2,286,000	$666,371.00	$0.00	$1,619,629.00
ITAC		$18,864	$9,239.83	$0.00	$9,624.17
Project Management		$190,000	$118,551.24	$10,280.00	$61,169.06
Total Direct Costs		$2,754,761	$989,710.18	$25,286.00	$1,739,765.12
Authorized Indirect Costs		$17,310	$15,794.43	$0.00	$1,515.57
10% of Salaries and Wages					
Total Costs		**$2,772,071**	**$1,005,504.61**	**$25,286.00**	**$1,741,280.69**

AQRP Budget

FY 2011

Budget Category		FY11 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$148,755	$27,875.56	$4,270.00	$116,609.44
Fringe Benefits		$32,726	$2,866.33	$0.00	$29,859.67
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		$1,736,063	$0.00	$0.00	$1,736,063.00
ITAC		$19,400	$0.00	$0.00	$19,400.00
Project Management		$140,000	$0.00	$0.00	$140,000.00
Total Direct Costs		$2,091,195	$30,741.89	$4,270.00	$2,056,183.11
Authorized Indirect Costs		$14,876	$1,623.97	$0.00	$13,252.03
10% of Salaries and Wages					
Total Costs		**$2,106,071**	**$32,365.86**	**$4,270.00**	**$2,069,435.14**