AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-15-50047
Awarded to The University of Texas at Austin

Quarterly Report

March 1, 2017 through May 31, 2017

Submitted to

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Texas Air Quality Research Program

Quarterly Report

March 1, 2017 – May 31, 2017

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.

PROGRAM ACTIVITIES FOR THE QUARTER

Between March 1, 2017 and May 31, 2017, the AQRP Program Administrative staff worked with each research project's lead institution to ensure that all project investigators were informed of, and meeting, all reporting requirements, both technical and financial, and that project invoices were complete and all expenses were allowable. Project Managers worked with the Investigators to ensure that all project activities were moving forward and all technical reporting requirements were being met. These activities will continue throughout the term of the projects.

In March 2017, the TCEQ contacted the AQRP Administration requesting additional oversight on projects taking place in the San Antonio area in May 2017. A logistics project was proposed and then approved by the ITAC and the Advisory Council. Funding was allocated from funds remaining (unallocated) in the research project category. This project, led by David Sullivan at UT Austin, worked with the PIs to find acceptable sites to take measurements, gain permission from those site owners to utilize those locations, and prepare the sites, including providing fencing and electrical hook-ups. The primary site was at the University of Texas at San Antonio. The field study took place in May 2017. More information on the field study activities can be found in the individual project summaries below.

The redesign of the AQRP website is in the final stages of review and will be launched during the next quarter.

The AQRP Workshop will be held at the UT Austin Pickle Research Campus in August 2017.

BACKGROUND

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

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

The University of Texas at Austin was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and the University of Texas at Austin on July 29, 2015 for the 2016-2017 biennium. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

RESEARCH PROJECT CYCLE

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

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

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

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

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

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

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

7.) Funded projects are assigned an AQRP Project Manager at UT-Austin and a Project Liaison at TCEQ. The AQRP Project Manager 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 AQRP Project Manager has responsibility for documenting progress toward project measures of success for each project. The AQRP Project Manager works with the researchers, and the TCEQ, to create an approved work plan for the project.

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

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

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

Steps 7 and 8 are in progress for the quarter being reported.

RESEARCH PROJECTS

FY 2016 – 2017 Projects

Project 16-008 **STATUS: Active – Sept. 22, 2016**

High Background Ozone Events in the Houston-Galveston-Brazoria Area: Causes, Effects, and Case Studies of Central American Fires

University of Houston – Yuxuan Wang

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Doug Boyer

Funded Amount: $191,366

Abstract
A significant fraction of surface ozone in Texas comes from regional background originating from outside the state. Background ozone is particularly variable over the Houston-Galveston-Brazoria (HGB) region due to its unique geographical location and meteorology. Prior analyses of the HGB background ozone have focused predominantly upon averages, not high concentration days or exceptional events. To bridge this gap, the objectives of this project are to identify high background ozone events across the HGB area over the past 16 years (2000-2015), characterize meteorological conditions and anomalous emissions that cause these events, and understand their effects on ozone exceedances. With regard to emission anomalies, the focus will be on fire events from Mexico and Central America, a large fire region globally of unique importance to Texas air quality in springtime and summer whose impact on Texas background ozone has not been quantified.

Integrated analyses of observations and modeling will be conducted to achieve the project objectives. Daily HGB background ozone estimated by researchers at the Texas Commission on Environmental Quality (TCEQ) will be used as the data source to identify high background ozone days. Different types of meteorological events which may be potentially associated with high background ozone (e.g., cold fronts and thunderstorms) or high local photochemical production (e.g., heat waves and stagnation) will be identified based on the analysis of meteorology data. The relationship between high background ozone days and the meteorological 'event days' will be characterized, e.g., in terms of their overlapping (or the lack of it), and background ozone difference between meteorological 'event days' and 'non-event days' will be evaluated. Anomalies in fire emissions leading to high background ozone will be mapped through spatiotemporal sampling of the Fire INventory from NCAR (FINN) along background trajectories of air masses affecting the HGB area prior to and during the selected high background ozone days. The GEOS-Chem global chemistry transport model, with the FINN inventory implemented, will be used to simulate a number of case studies of large Central American fires and estimate the perturbations caused by ozone precursor emissions from those fires on background ozone concentrations in Texas and the HGB area. Finally, we will develop a quantitative estimate of the effects of background ozone versus local production on ozone exceedance cases in the HGB area and the dependence of such effects on meteorology and Central America fire emissions.

Project Update

The following progress has been made towards project goals:

In addition to stagnation, two more metrological events, cold front and thunderstorm, were identified and their effects on HGB ozone were investigated. Figure 1 shows the probability distribution of MDA8 and background ozone mixing ratio during each type of events respectively. The ozone distribution during top 15% MDA8 ozone days and top 15% background ozone days is also shown for comparison. Because it includes some "high" ozone days in low ozone years and months (e.g., July 2014, 2015): 15% MDA8 and background O_3 have distributions that extend to very low ozone values. Each type of event shows similar effects on MDA8 and background ozone. Stagnation increases MDA8 and background ozone in terms of both the mode and right tail of their respective distributions, while thunderstorm has the opposite effect. Cold front does not show a clear effect on MDA8 and background ozone. It might be because cold front is a regional event and ozone response to cold front may differ from pre-front to post-front but the front statistics compiled so far do not label distinct stages of the front.

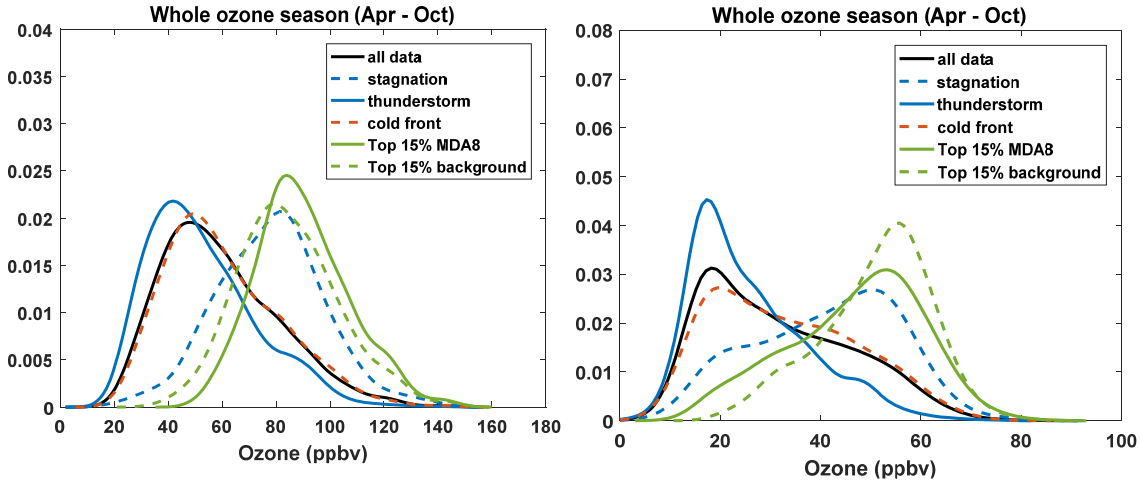

***Figure 1**. Probability density curves of MDA8 (left) and background (right) ozone mixing ratio.*

To investigate cold front effects on ozone in different stages of the front life cycle, the seasonality and distributions of the cyclone data were reexamined. Figure 2 shows the tracks of cyclone centers and cyclone counts in each month of the ozone season during 2000-2015. Cyclone distributions show large variations in each month. The number of cyclones is largest in spring (e.g. April) and fall (e.g. October), and smallest in July and August. In addition, the cyclone centers become far away from Texas during the summer (e.g. July). Considering the large variability of cyclone center distributions by month and by year, it is not practical to trace the identified cyclones one by one and examine their effects on HGB ozone individually. The challenge is to define a method that could automatically screen the cycle data to select those whose cold front had passed through the eastern half of Texas and influenced HGB ozone. This issue will be the focus of our ongoing work.

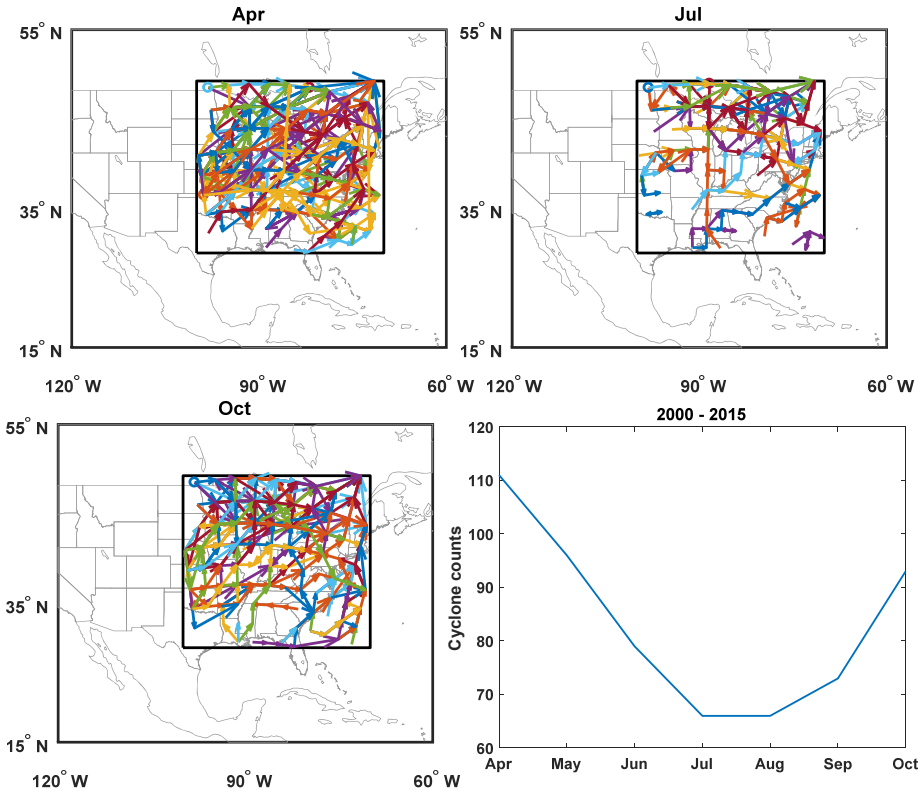

Figure 2. *Cyclone center tracks in (a) April, (b) July, (c) October and (d) Cyclone counts April to October during 2000-2015.*

Passive tracer simulation was conducted using the GEOS-Chem model with a horizontal resolution of 2°x 2.5° to track air mass origins influencing HGB air quality for the two case months (April 2011 and May 2008). Six synthetic passive tracers were added in the model with a fixed lifetime of 30 days and were emitted at a constant rate from the following six source regions of importance to HGB air quality: Houston, Texas (excluding Houston), US (excluding TX), Gulf of Mexico (referred to as the Gulf tracer), Mexico, and the Rest of Central America (RCA).

A composite indicator (CI) metric was developed to determine the days when HGB is predominantly influenced by northerly or southerly flows. CI is calculated according to Equation (1), which is the sum of the northern tracers (including Texas and the US tracer described above) minus the sum of the southern tracers (including the Gulf, Mexico and RCA tracer described above). All the tracer concentrations included in the calculation are normalized. Figure 3 shows how the CI value can catch the influence of different sources on HGB background ozone. In most cases, positive CI values overlap with background ozone peaks, which suggests those background ozone peaks were caused by transport of air pollutant from the north. However, there are few background ozone peaks coinciding with negative CI values, which is likely caused by the transport of pollutants from Central America fires.

$$Composite\ indicator\ (CI) = (US + TX) - (Mexico + Gulf + RCA) \quad (1)$$

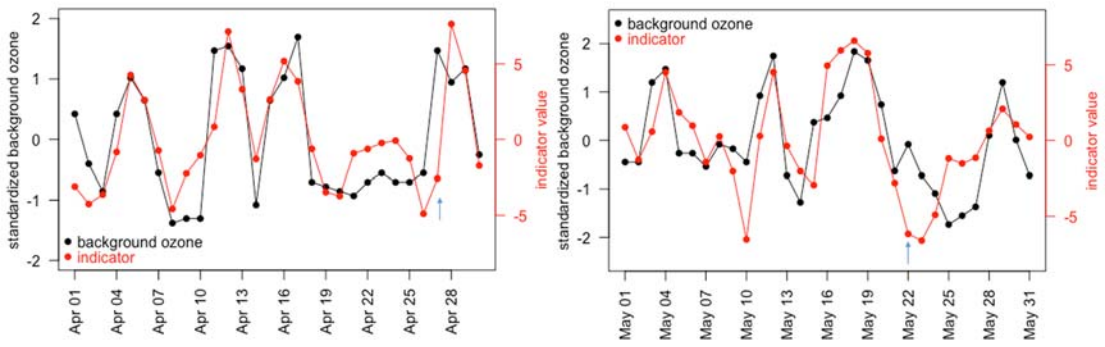

Figure 3*. Time series of standardized background ozone and composite indicator over HGB region of April 2011 (left) and May 2008 (right).*

The days were classified into three predominant source groups based on CI values: northern impact, southern fires impact, and the clean Gulf impact. Here the southern fires refer to fires from Central America. A clean-Gulf day is defined when the standardized Gulf tracer is positive and all other tracers are negative, indicating the dominant influences from clean marine air from the Gulf of Mexico. Figure 4 shows the boxplot of simulated and observed HGB MDA8 ozone in each category for April 2011 and May 2008. The model tends to overestimate MDA8 ozone in the clean Gulf and the southern fires impact group in both months. The southern fires group has a mean ozone enhancement above the clean Gulf group of 4 ppbv and 6 ppbv at HGB during April 2011 and May 2008, respectively. The corresponding enhancement from fires above the clean Gulf group from the GEOS-Chem model is 3.8 ppbv and 10.6 ppbv, respectively.

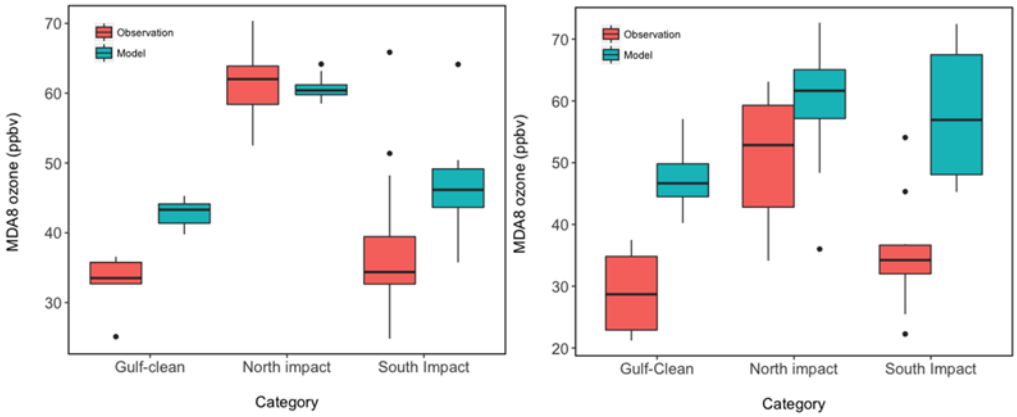

Figure 4*. Boxplot of model and observed HGB MDA8 ozone in each category based on CI values for April 2011 (left) and May 2008 (right).*

There were no delays or issues related to the project during this reporting time period. The project team intends to use all funds allocated to the project by 8/31/2017 to complete the planned work tasks.

Project 16-010 **STATUS: Active – Oct. 20, 2016**

MOVES-Based NOx Analyses for Urban Case Studies in Texas

Sonoma Technology, Inc. – Stephen Reid

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Chris Kite

Funded Amount: $69,075

Abstract
Emissions inventories are an important component of air quality planning and a key input to photochemical grid models that support air quality assessments. Findings from recent studies suggest that nitrogen oxides (NOx) emissions may be overestimated in the U.S. Environmental Protection Agency's (EPA) National Emissions Inventory (NEI), perhaps by as much as a factor of two. This overestimate has generally been attributed to the mobile source sector (e.g., on-road motor vehicles), for which emission estimates are prepared using EPA's MOVES model. A number of potential issues have been identified with MOVES, including reliance on the model's default input data rather than more representative local inputs.

The overall goals of this project are to examine MOVES emission estimates at the local scale and identify which input parameters have the greatest influence on NOx emission estimates. Specifically, we will use a well-established emissions reconciliation technique to quantitatively compare MOVES emission results with ambient near-road monitoring data. These analyses will be performed for case studies in three Texas metropolitan areas: Dallas-Fort Worth, Houston, and El Paso. In addition, we will perform sensitivity analyses comparing MOVES emission results using default vs. local data to identify key parameters that have substantial influence on NOx emissions. The results of this work will support emissions inventory development and air quality management efforts in Texas by providing information on the accuracy of current MOVES emission estimates and MOVES input parameters, for which local data are critical.

Project Update
Over this quarter (March to May, 2017), the project team followed the project plan and continued work on Task 1 Emissions Reconciliation Analyses and Task 2 MOVES Sensitivity Analyses. Using the pollutant concentration data collected from three near-road monitoring sites in Houston, Fort Worth, and El Paso, as well as MOVES modeling data obtained from TCEQ (Texas Commission on Environmental Quality), NCTCOG (North Central Texas Council of Government), and HGAC (Houston-Galveston Area Council), the team continued work to develop and compare ambient and emission-based CO/NO_x ratios (e.g., in data tables and plots). The team also identified four key input parameters (fleet mix, vehicle speed, vehicle age, and meteorology) and designed a range of MOVES sensitivity testing scenarios for each of the three analysis areas.

Over the next quarter, work will focus on conducting MOVES scenario runs, summarizing MOVES modeling results, and comparing ambient-based and emission-based pollutant ratios for all three analysis areas. The project team will also work on the draft project report, final project report, and presentation of findings in the next quarter.

There were no delays or issues related to the project during this reporting time period. The project team intends to use all funds allocated to the project by 8/31/2017 to complete the planned work tasks.

Project 16-011 **STATUS: Active – Oct. 6, 2016**

A Next Generation Modeling System for Estimating Texas Biogenic VOC Emissions

Ramboll Environ US Corporation – Gregory Yarwood

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Doug Boyer

Funded Amount: $158,134

Abstract
The exchange of gases and aerosols between the Earth's surface and the atmosphere is an important factor in determining atmospheric composition and regional air quality. Emissions of reactive gases from the earth's surface drive the production of ozone and aerosol and other atmospheric constituents relevant for regional air quality. Emissions of some compounds, including biogenic volatile organic compounds (BVOCs), are highly variable and can vary more than an order of magnitude over spatial scales of a few kilometers and time scales of less than a day. This makes estimation of these emissions especially challenging and yet accurate quantification and simulation of these fluxes is a necessary step towards developing air pollution control strategies and for attributing observed atmospheric composition changes to their causes.

The overall goal of this project is to improve numerical model predictions of regional ozone and aerosol distributions in Texas by reducing uncertainties associated with quantitative estimates of BVOC emissions from Texas and the surrounding region. Although there have been significant advancements in the procedures used to simulate BVOC emissions, there are still major uncertainties that affect the reliability of Texas air quality simulations. This includes significant gaps in our understanding of BVOC emissions and their implementation in numerical models including 1) isoprene emission factors, 2) missing compounds, and 3) and unrepresented processes including canopy heterogeneity and stress induced emissions. In this project, we will develop new emission factors and incorporate missing BVOC compounds and unrepresented BVOC emission processes into the Model of Emissions of Gases and Aerosols from Nature (MEGAN) framework. To accomplish this, we will develop a transparent and comprehensive approach to assigning isoprene and monoterpene emission factors and will update MEGAN to include additional BVOC and processes including stress induced emissions and canopy heterogeneity. We will evaluate MEGAN BVOC emission inventories for Texas and surrounding regions using surface and aircraft observations and a photochemical model.

The overall benefit of this project will be more accurate VOC emission estimates for the Texas air quality simulations that are critical for scientific understanding and the development of regulatory control strategies that will enhance efforts to improve and maintain clean air.

Project Update
The project consists of five tasks: (1) develop and apply a transparent approach for estimating BVOC emission factor distributions, (2) synthesize, reconcile and calculate isoprene and monoterpene (terpenoid) emission factors for Texas and the surrounding region, (3) develop the MEGAN3 model, (4) perform a MEGAN3 evaluation and sensitivity study and (5) project

management and reporting. The project began on October 6, 2016. Progress to date is described below. We anticipate that all funds allocated for the project will be utilized by August 31, 2017.

During the March 2017- May 2017 quarter, work was carried out on Tasks 1- 5.

Task 1: Development and Application of a Transparent Approach for Estimating BVOC Emission Factor Distributions

During March, Dr. Guenther completed review and testing of the draft BVOC emission factor (EF) database system (Figure 1) and provided guidance to Ramboll Environ for additional tasks. The additional tasks included development of preprocessors to create two new land cover input files (growth form and ecotype) for the EF processor and calculation of the Light Dependent Fraction (LDF) for all emission categories. Following completion of these tasks, Dr. Guenther reviewed the BVOC emission factor (EF) database system and code. During May, a user specified J-rating threshold was applied to EF and LDF measurements. The J-rating (expert judgment) assigns a rating to the measurements in the EF database based on the underlying information, including but not limited to, data collection methods and documentation.

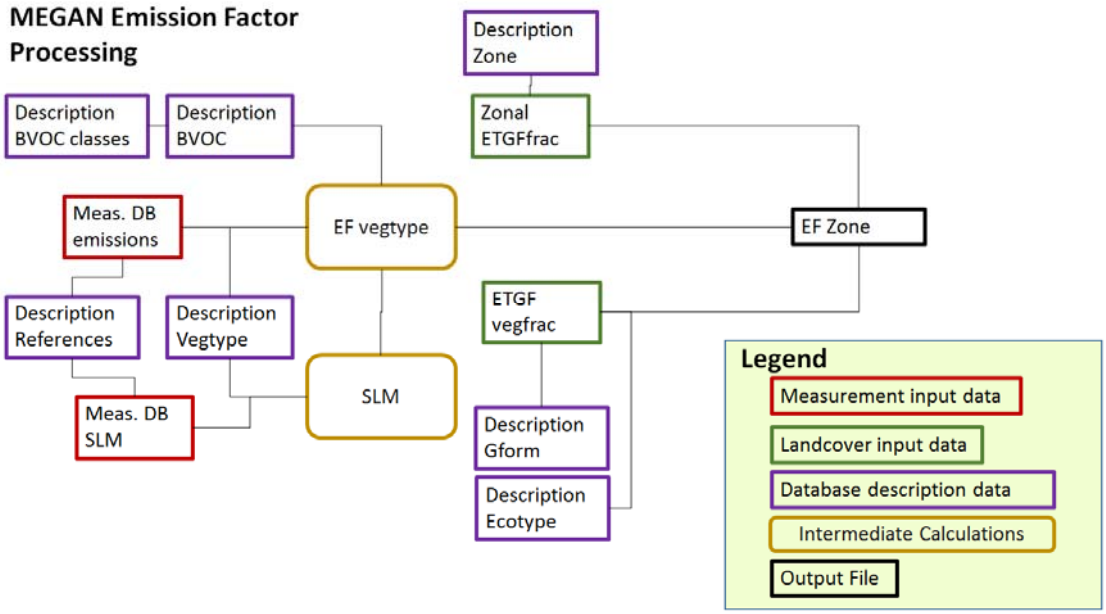

Figure 5*. Schematic of MEGAN emission factor processing.*

Task 2: Emission Factor Development

During March, Dr. Guenther continued compilation and integration of emissions data from studies in the literature into the emission measurement database. In April, Dr. Guenther developed an approach for setting default data including zero values, and flagged suspect emissions data. Dr. Guenther then integrated additional emissions data from studies reported in the literature into the emission measurement database.

Task 3: Development of MEGAN3

Throughout March and April, Dr. Guenther and Ramboll Environ collaborated on the MEGAN3 programming and overall structure. Ramboll Environ worked closely with Dr. Guenther to implement required updates to the initial draft of MEGAN3 source code and added new code as needed. For example, Ramboll Environ generated an input file estimating long-term ozone exposure from air quality modeling output. The purpose of this input file is to determine whether plants are undergoing stress due to air pollution.

In April, Ramboll Environ provided the updated package of MEGAN3 source code to Dr. Guenther for his review. Dr. Guenther recommended final modifications to complete the code. By the end of April, Dr. Guenther had evaluated and assessed the MEGAN code and began writing documentation for code and inputs.

Task 4: MEGAN Evaluation and Sensitivity Study

Task 4 was initiated in May. MEGAN3 emissions were evaluated against aircraft flux data from the 2013 Southeast Atmosphere Study (SAS) and compared with two other MEGAN emission inventories: (1) MEGAN v2.1 using the default landcover database and emission factors, and (2) MEGAN v2.1 updated high-resolution landcover database and emission factors from AQRP Project 14-016. Emissions sensitivity tests were carried out with MEGAN3 to evaluate changes in emissions due to use of different J-rating criteria. We began base case photochemical modeling of the June 1-July 15, 2013 period that encompassed all of the SAS C-130 and P-3 aircraft flights using MEGAN v2.1 biogenic emissions and using the most recent versions of the CAMx model and CB6r4 chemical mechanism.

Task 5: Project Management and Reporting

This task is ongoing. Dr. Guenther continued compiling information for the final report.

Project 16-019 **STATUS: Active – Sept. 30, 2016**

The Influence of Alkyl Nitrates from Anthropogenic and Biogenic Precursors on Regional Air Quality in Eastern Texas

University of Texas at Austin – Elena McDonald-Buller
Ramboll Environ US Corporation – Gregory Yarwood

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Jim Smith

Funded Amount: $180,641
($118,019 UT Austin, $62,622 Ramboll Environ)

Abstract
Mono and multifunctional alkyl nitrates (ANs) are formed from the oxidation of biogenic or anthropogenic volatile organic compound (VOC) precursors and serve as a reservoir or sink of nitrogen oxides (NO_x). Alkyl nitrates have sufficiently long atmospheric chemical lifetimes (hours to days), such that they can influence tropospheric ozone and secondary organic aerosol (SOA) formation over regional to global spatial scales. Their functionalities, yields, and fates are known to depend upon the size and structure of the VOC. Depending on their structure, ANs can be transported, chemically processed, removed by deposition to vegetation and other surfaces, or undergo partitioning to and from the aerosol phase where hydrolysis is thought to be a loss mechanism. Although knowledge gaps still exist, recent laboratory and field studies have provided new insights on these processes for ANs formed from biogenic and anthropogenic hydrocarbon precursors. An ongoing need will be to incorporate these findings into the chemical mechanisms of photochemical models used to assess regional air quality. The objectives of this work are to apply the findings of ongoing experimental studies examining alkyl nitrates formed from the OH-initiated oxidation of C8-C11 alkanes at the University of Texas at Austin in addition to those of new publications that have focused on other hydrocarbon precursor classes relevant to Texas emissions inventories to improve how ANs are represented in the version 6 of the Carbon Bond mechanism (CB6). Revision 4 of CB6 (CB6r4) will soon be available in version 6.32 of the Comprehensive Air quality Model with extensions (CAMx v6.32). Sensitivity tests with CAMx will evaluate the formation and fate of ANs in central and southeastern Texas, the influence of ANs on regional ozone by recycling NO_x, and dependencies on organic aerosol concentrations.

Project Update
The project consists of three tasks: (1) develop modifications to the CB6r4 mechanism in CAMx, (2) evaluate the CB6r4 updates in CAMx modeling during the time period of the DISCOVER-AQ campaign through sensitivity studies that evaluate the formation and fate of ANs and effects on regional ozone and organic aerosol concentrations in central and southeastern Texas, and (3) disseminate results through reporting, publications, and presentations. The project began on October 6, 2016. Progress to date is described below. We anticipate that all funds allocated for the project will be utilized by August 31, 2017.

Task 1: Refinements to the CB6r4 Mechanism in CAMx

CAMx 6.40, the most recent released version, includes two algorithms for organic gas-aerosol partitioning and oxidation: the hybrid 1.5-dimension (1.5-D) Volatility basis Set (VBS) or Secondary Organic Aerosol Partitioning (SOAP) schemes. SOAP was recently updated with the latest information on SOA yields, saturation concentrations, and water solubility; the most recent version, SOAP2, is available in CAMx 6.40. The SOAP2 scheme has been the focus of this study as it is expected it to be more widely used than the 1.5-D VBS scheme.

Initial CAMx v.6.40 base case simulations were completed at the Texas Advanced Computing Center (TACC) at the University of Texas at Austin using the 1.5-D VBS or SOAP2 schemes. We evaluated model performance using surface and aircraft observations for the DISCOVER-AQ time period in southeastern Texas. Both simulations exhibited a high bias in hourly average $PM_{2.5}$, organic aerosol, and organic carbon concentrations relative to surface observations, in particular with the SOAP2 scheme. Sodium and nitrate indicative of sea salt emissions also exhibited a high bias. Predictions of contemporary carbon contributions were biased low relative to radiocarbon source apportionment analysis at Conroe. The Particulate Source Apportionment Technology (PSAT) tool in CAMx was enabled in runs with SOAP2 for diagnostic purposes. The results were used to guide a refinement in the CAMx simulations with SOAP2 with the aim of improving model performance. SOAP2 did not include SOA loss by photolysis, which can be competitive with other aging mechanisms of atmospheric SOA. To account for this removal process in the particle phase, the photolytic loss of SOA, as a first-order decay reaction with a photolysis rate derived by scaling the NO_2 photolysis rate, was implemented in a new version of SOAP identified as SOAP2r3.

The performance of CAMx v.6.40 with the SOAP2r3 scheme was evaluated against observations at CAMS sites throughout eastern Texas and surface and aircraft measurements in southeastern Texas collected during the DISCOVER-AQ campaign. Predictions from CAMx v6.40 with SOAP2r3 were generally comparable to those based on the 1.5-D VBS scheme. This configuration is serving as the base case for sensitivity simulations that are evaluating updates to the CB6r4 mechanism. We are currently drafting the final report, including the results of the CAMx performance evaluation with SOAP2r3 and comparisons with SOAP2 and the 1.5-D VBS schemes.

Updates to the CB6r4 mechanism are on-going. Terpenes have been differentiated into two classes, α-pinene represented by the new model species APIN and other terpenes represented by the existing model species TERP. Reactions of APIN and TERP with oxidants OH, O_3 and NO_3 were developed by updating the reactions for TERP in CB6r4 using published laboratory studies and analyses of ambient data. In particular, yields of alkyl nitrate from APIN and TERP reactions have been defined that are consistent both with laboratory studies and ambient data.

The CB species, NTR2, represents organic nitrates that can partition significantly to organic aerosol. NTR2 is assumed to undergo reaction with OH or hydrolysis within aerosols. The gas-particle partitioning of NTR2 and subsequent hydrolysis of NTR2 in the particle phase are implemented as a pseudo gas-phase reaction in CAMx v.6.40 with a hydrolysis lifetime of 6-hours. Recent laboratory experiments as well as findings from field studies in the southeastern U.S. have indicated much shorter atmospheric lifetimes are appropriate for acidic aerosols. We reduced the particle-phase NTR2 hydrolysis lifetime in the CB6 mechanism to 1-hour.

Collectively the changes to the terpene chemistry and the NTR2 hydrolysis lifetime were implemented in a new version of the CB mechanism identified as CB6r6T.

Task 2. Evaluating CB6r4 Updates in CAMx Modeling for DISCOVER-AQ

The CAMx emission inventory was updated to split TERP into APIN and TERP. A CAMx simulation that replaced the CB6r4 mechanism with CB6r6T but was otherwise identical to the base case (i.e., with the SOAP2r3 scheme) has been completed. Analysis of the results of this simulation relative to the base case is on-going.

Task 3. Project Reporting and Presentation

On-going per requirements.

Project 16-031 **STATUS: Active – Oct. 18, 2016**

Condensed Chemical Mechanisms for Ozone and Particulate Matter Incorporating the Latest in Isoprene Chemistry

University of North Carolina – Chapel Hill – William Vizuete

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

Funded Amount: $225,000

Abstract
Isoprene, the most emitted non-methane hydrocarbon on the planet, is known to influence ozone (O_3) formation in Houston, Texas. Eastern Texas and northern Louisiana feature some of the largest biogenic emission sources of isoprene in the United States. It is also now known that the photochemical oxidation of isoprene, when mixed with anthropogenic emissions from urban areas like those found in Houston, can produce significant yields of fine particulate matter ($PM_{2.5}$) through acid-catalyzed multiphase chemistry of isoprene epoxydiols (IEPOX) that leads to secondary organic aerosol (SOA) formation. Next-generation regulatory models in Houston will attempt to capture this recent discovery even though there exists great uncertainty in both gas-phase isoprene oxidation and SOA formation chemistry. This work will produce a fully updated condensed gas-phase mechanism based on SAPRC-07 and PM formation parameters suitable for use in a regulatory air quality model. The updated parameters will be evaluated against an archive of UNC smog chamber experiments, including new isoprene SOA experiments that investigate the effect of organic coatings/mixtures on the acid-catalyzed multiphase chemistry of IEPOX.

Our previously funded Air Quality Research Program (AQRP) work has directly derived the multiphase kinetics of IEPOX only on pure inorganic aerosols. In the atmosphere, however, IEPOX will more likely encounter mixed particles containing both pre-existing organics and acidic sulfate. As a result, there is a need to constrain the impact of pre-existing organics within acidic sulfate aerosol on the kinetics of IEPOX multiphase chemistry. We will also produce a regulatory air quality modeling episode focused on Houston to test these new updates in a simulated urban environment. This work directly addresses the stated priority area of improving the understanding of O_3 and PM formation and the interaction with PM precursors. Further, the regulatory air quality modeling system developed by this work can begin to address the stated priority of quantifying the impacts of uncertainty due to the treatment of atmospheric chemical processes by condensed models.

Project Update
The following progress has been made towards project goals:

Task 1 - Updated SAPRC-07 and Aerosol Module for Isoprene Oxidation

Preliminary Analysis

N/A

Data Collected

We have completed the development of the input files needed to evaluate the updates in the SAPRC-07 mechanism.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

This past quarter has been focused on finishing the experimental data while certain equipment was available to us. As a result, we had to move all resources to complete task 2 and postponed progress on Task 1 until next quarter.

Goals and Anticipated Issues for the Succeeding Reporting Period

We will also begin simulating our chamber experiments using the SAPRC-16 chemical mechanism.

Detailed Analysis of the Progress of the Task Order to Date

The progress on the task is on schedule.

Task 2 - Chamber Experiments: Interplay of Particle-Phase Composition, Phase, and Viscosity on IEPOX Multiphase Chemistry

Preliminary Analysis

The overall experimental setup is shown in Figure 1. At this point, we have conducted kinetic measurements using Flow Tube Reactor to derive IEPOX uptake coefficient onto aerosols coated with organic matter produced by oxidation of α-pinene, toluene, and naphthalene under various relative humidity. Ammonium bisulfate seed aerosols are generated by atomizing a solution mix of ammonium sulfate and sulfuric acid. Upon generation, seed aerosols pass through a diffusion dryer before entering the Potential Aerosol Mass (PAM) Oxidation Flow Reactor (Aerodyne Research, Inc) [3,4]. The injection rate of pure precursor VOCs is controlled by a syringe pump. Depending on the precursors, ozonolysis and/or photo-oxidation of the VOCs takes place in the PAM to form organic coatings on existing seed aerosols by condensational growth. A carbon strip denuder is introduced downstream to the PAM to remove excess gas phase species to prevent secondary reactions inside the flow tube as well as suppression of IEPOX detected by High Resolution Time-Of-Flight Chemical Ionization Mass Spectrometer (ToF-CIMS, Aerodyne Research, Inc.). Aerosol size and bulk composition are measured in real time by scanning mobility particle sizer (SMPS, TSI Inc.) and aerosol chemical speciation monitor (ACSM, Aerodyne Research, Inc.). Filters (Teflo 47mm, 1 μm poresize, PALL Corp.) and Multi-Plate Sampler samples are collected for offline analyses to gain detailed chemical and morphological information of aerosols.

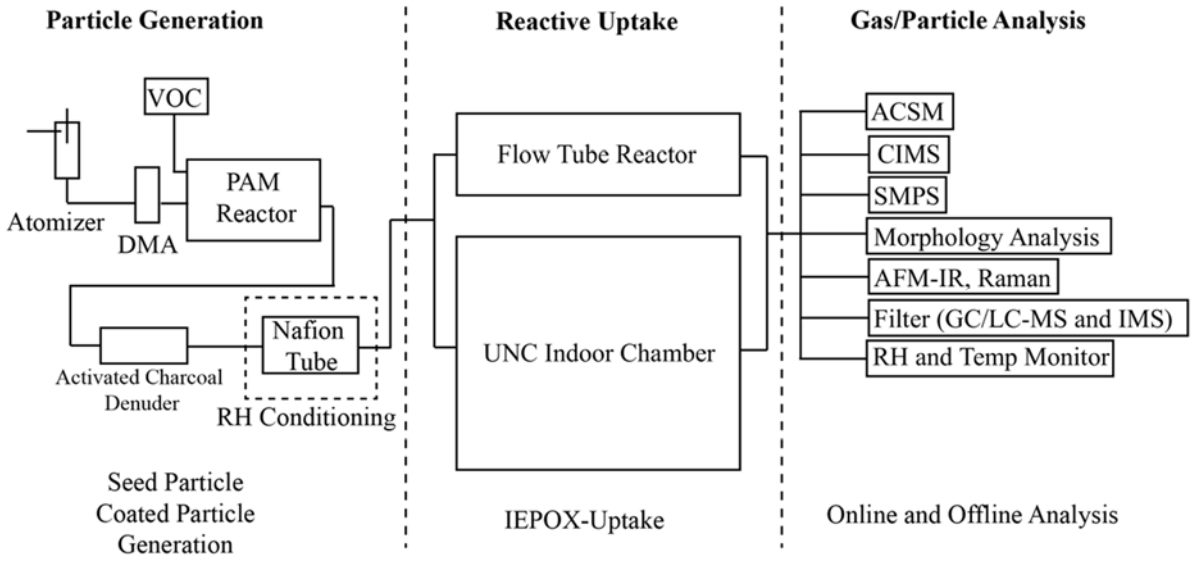

Figure 1. *IEPOX Reactive Uptake Experiment Setup*

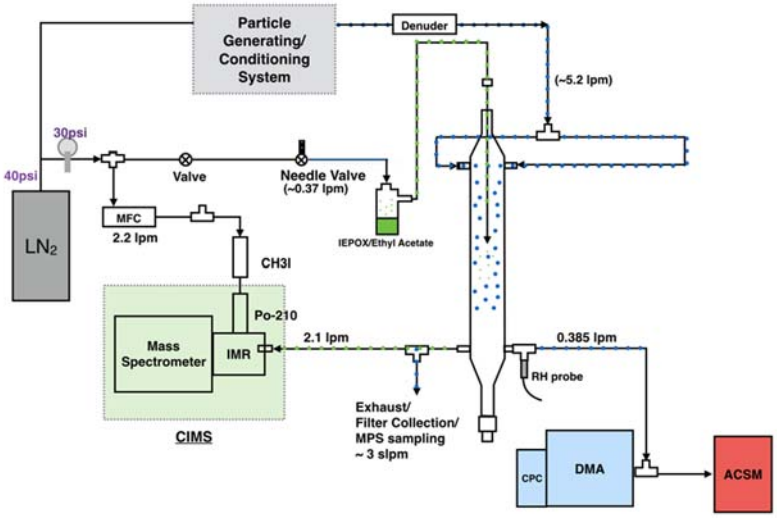

Figure 2. *Flow tube setup*

Figure 2 shows the detailed schematic for the flow tube experiments. The setup has been modified and improved in various aspects to better cater to the purpose of this project and to reduce uncertainties in measurements compared to previous practices in the literature [3,4]. IEPOX is introduced into the flow tube through axially moveable injector in the center. Aerosol flow output from PAM is evenly split into two streams, connected to two top nozzles on the reactor. By varying the axial position of the injector along the flow tube reactor, IEPOX is allowed to

interact with aerosols for different period of time, and hence the heterogeneous reaction rate, k_{het}, of IEPOX with aerosols can be calculated by subtracting IEPOX loss rate to the wall, k_{wall}, from the total loss rate, k_{total}, i.e.,

$$k_{het} = k_{total} - k_{wall} \qquad (1)$$

After correcting k_{het} for non-plug flow condition, the uptake coefficient, γ, is calculated by

$$\gamma = \frac{4k_{het}}{S_a \omega} \qquad (2)$$

where Sa is the total surface area of the sulfate aerosols and ω is the mean molecular speed of gaseous IEPOX molecule in the air.

Data Collected

SOA Precursor	Concentration (ppb)	Reactant(s)	Coating Thickness (nm)	Relative Humidity
α-pinene	200-650 ppb	O_3		
Toluene	420-1200 ppb	O_3/OH	0/5/10/15	15%/30%/50%
Naphthalene	100-500 ppb	O_3/OH		

Table 1. *Flow Tube Experimental Conditions*

Experiments conducted to date are summarized in Table 1. Raw data from abovementioned online measuring techniques have been collected and partly analyzed. Filters samples collected are stored in a freezer at -20 ℃ for future analysis.

Figure 3 gives an example of the data we are obtaining and processing. On the left, the IEPOX signal normalized by reagent ion signal is plotted against the time during which IEPOX injector was gradually moved from top to bottom and back to top. Reaction time at each injector position can be calculated at given flow rate. The slopes obtained by linearly fitting natural logarithm of IEPOX signal and reaction time are the IEPOX loss rates (right figure), pseudo-first order reaction assumed. Appling equation 1 and 2 to reaction rates yields reactive uptake coefficient γ. The reaction uptake coefficient γ's from α-pinene experiments are summarized in Figure 4. Diffusion limitations are increasingly noticeable for experiments at 15% and 30% RH as coating thickness increases in spite of the outlier with no coating at 30% RH. At 50% RH, a reversed trend is observed, which needs further investigation. One possible explanation is that the original seed acidity is diluted by elevated aerosol-phase liquid water content but extra acidity from α-pinene ozonolysis products under wet condition breaks the status quo and promotes IEPOX acid catalyzed reaction in the aerosol phase. Difference of phase state from dryer conditions is also possible. Repeated experiments and phase state investigation are warranted.

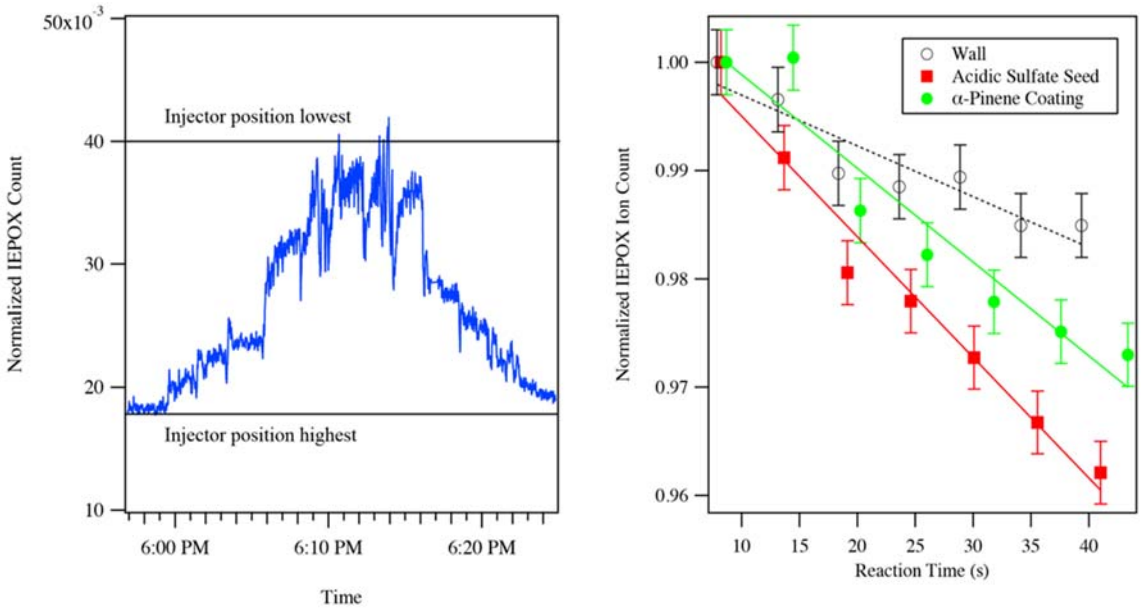

Figure 3. *Sample experimental results from flow tube measurements: Left – CIMS measured IEPOX signal in two full decays; Right – IEPOX loss rate without aerosols, with acidic sulfate seed and seed coated by α-pinene ozonolysis products. Initial values normalized to 1 for ease of comparison.*

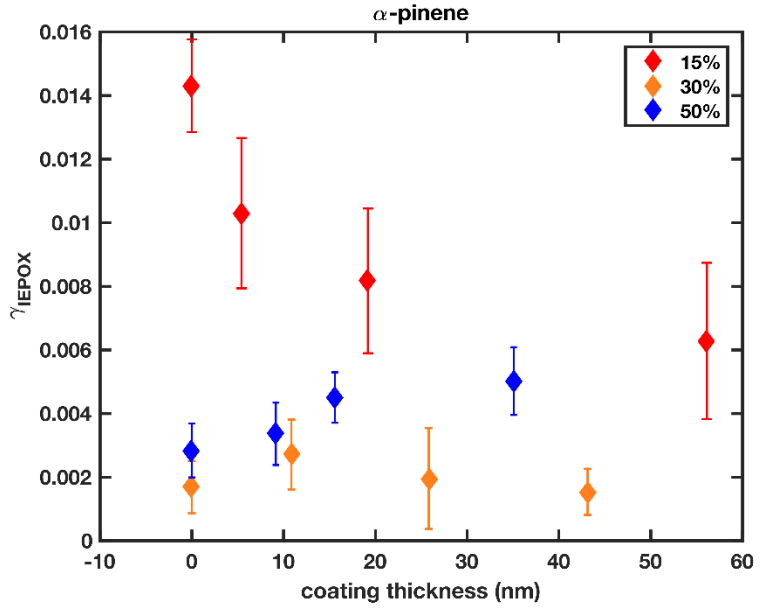

Figure 4. *γ_{IEPOX} obtained at various coating thicknesses under 15%, 30% and 50% relative humidity*

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Identified problems:

Reproduction of flow configuration previously described in the literature didn't yield interpretable CIMS measurements. Gas-phase products from oxidation of VOCs in the PAM in addition to increased water vapor in wet experiments posed a problem to IEPOX sensitivity on the CIMS due to ion suppression.

Adjustment:

The flow configuration has been modified and improved in various aspects to better cater to the purpose of this project and to reduce uncertainties in measurements compared to previous practices in the literature. In wet experiments where ion suppression is more severe, two carbon strip denuders are used in tandem to remove gas-phase compounds coming from PAM.

Goals and Anticipated Issues for the Succeeding Reporting Period

Goals:

1) Finishing up processing data from online measurements and obtaining γ_{IEPOX} for toluene and naphthalene coating experiments.

2) Nucleation, though a minor path to form organic aerosols in our case, cannot be neglected if they do take up IEPOX and favor nucleophilic reaction with IEPOX to form low volatility products. We have already conducted nucleation experiments with the three precursor VOCs. Experimental procedures are the same except acidic sulfate seed aerosols was not injected. We will follow the method described above to calculate and compare IEPOX loss rate to bulk nucleated aerosols with that to the wall. We want to see whether there is a statistically significant difference between the two.

References

1. Lambe *et al.* Characterization of aerosol photooxidation flow reactors: heterogeneous oxidation, secondary organic aerosol formation and cloud condensation nuclei activity measurements. *Atmospheric Measurement Techniques* 445–461 (2011). doi:10.5194/amt-4-445-2011

2. Kang, Root, Toohey & Brune. Introducing the concept of Potential Aerosol Mass (PAM). *Atmospheric Chemistry and Physics* 5727–5744 (2007). doi:10.5194/acp-7-5727-2007

3. Gaston, C. J. *et al.* Reactive Uptake of an Isoprene-Derived Epoxydiol to Submicron Aerosol Particles. *Environmental Science and Technology* **48,** 11178–11186 (2014).

4. Riedel, T. P. *et al.* Heterogeneous Reactions of Isoprene-Derived Epoxides: Reaction Probabilities and Molar Secondary Organic Aerosol Yield Estimates. *Environ. Sci. Technol. Lett.* **2,** 38–42 (2015).

Detailed Analysis of the Progress of the Task Order to Date

The progress on the task is on schedule.

Task 3 Implementation in a regulatory air quality model

Preliminary Analysis

During this quarter, we have begun analyzing results from our CMAQ-BOX model simulations where we have completed a series of sensitivity analysis on IEPOX-SOA reactive uptake equation with updated aerosol phase diffusivity and henry's law constant that is influenced by organic coating of the aerosol.

Data Collected

We have collected the Look Rock Site observational data from the SOAS campaign and using it to compare our simulations generated by the CMAQ-BOX model.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

During this month we had issues configuring the CMAQ-BOX model and constraining unknown parameters in our modified reactive uptake equation. We have successfully addressed installation issues and have quality assured our installation.

Goals and Anticipated Issues for the Succeeding Reporting Period

Sensitivity runs generated from CMAQ-BOX model will be compared against Look Rock site data.

Detailed Analysis of the Progress of the Task Order to Date

The progress on the task is on schedule.

Project 17-007 **STATUS: Active – Nov. 3, 2016**

Evaluating Methods for Determining the Vapor Pressure of Heavy Refinery Liquids

University of Texas at Austin – Vincent Torres

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Russell Nettles

Funded Amount: $205,500

Abstract
During the last five years, crude oil and natural gas production and petroleum refinery operations have seen an increased focus on their emissions of volatile organic compounds (VOCs), hazardous air pollutants (HAPS) and greenhouse gases (GHGs), especially those from storage tanks. These actions have been taken by the United States Environmental Protection Agency (US EPA) "because EPA and state investigations have identified Clean Air Act compliance concerns regarding significant emissions from storage vessels, such as tanks or containers at onshore oil and natural gas production facilities" and to "collect information on processing characteristics, crude slate, emission inventories, and limited source testing to fill information gaps". State and federal laws require certain facilities to design, install, operate and maintain effective pollution control measures to minimize the emissions of VOCs and HAPs. For example, the federal New Source Performance Standards for Crude Oil and Natural Gas Production "requires that new, reconstructed or modified storage vessels with the potential for VOC emissions of equal to or greater than six tons per year reduce VOC emissions by at least 95%." The Texas Commission on Environmental Quality (TCEQ) funded two projects recently to better understand the composition and properties of heavy refinery liquids and the most appropriate method of determining their true vapor pressure (TVP).

The purpose of this research is to improve the estimates of VOC emissions from storage tanks holding heavy refinery liquids. These tanks are found at storage terminals and refineries and are frequently heated in order to reduce the viscosity of their contents and make them pumpable. Evidence is mounting that the emissions from these tanks are underreported and may explain some of the VOC inventory gap in parts of Texas.

During the course of this project, the most accurate, reliable, convenient, and reasonably priced means of measuring the TVP of heavy refinery liquids stored in tanks will be identified. Identifying an appropriate means of measuring the TVP of these heavy refinery liquids is important because direct measurement of VOC emissions from storage tanks is inherently inexact and expensive, so equations are used to estimate emissions from storage tanks. The value used for the TVP in these equations has a profound impact on the results. The results of this research will facilitate efforts being made by the US EPA, TCEQ, and agencies in other states to better understand, more accurately estimate, and manage emissions from tanks holding heavy refinery liquids.

Project Update
The project team (PT) has obtained samples for three No. 6 oil, two asphalts and one residual material, in addition to a hydraulic fluid sample and the three pure chemicals that will be used to produce the "known" material. A dispensing system for transferring material samples from bulk

containers to small vials of various sizes (from 10 to 200 ml as required by the commercial labs) to send samples to the labs was designed and assembled. The PT also developed and prepared a standard operating procedure for dispensing samples from the bulk shipping containers and the handling of samples until their vapor pressure has been measured. At the end of this quarter or early in the next, the samples will be sent to the labs for vapor pressure (VP) measurements. During the next quarter, the commercial labs will perform their measurements and UT Austin will make measurements using the two mini-method instruments.

There is no gold standard, i.e., a readily available reference method for measuring the vapor pressure of complex mixtures like heavy refinery liquids. So the PT had to identify a reference standard to use for the project. It will do so using two independent approaches. One approach will be to rely on the use of detailed vapor pressure information provided by the manufacturer of the material and the second approach will rely on estimation of the vapor pressure of a mixture prepared from pure substances, whose vapor pressure and molecular weight would be similar to typical heavy liquids. For the latter, referred to as the "known", because its vapor pressure can be estimated computationally, the PT has used a NIST-modified UNIFAC model to identify the recipe for and estimate the vapor pressure of the "known" material. Work was performed to calibrate this model.

The impact of water on the vapor pressure of the sample must also be accounted for when presenting vapor pressure measurements as emissions models depend on the use of vapor pressures without the water contribution**.** Work was performed to develop a method to estimate the contribution of the water in mixture when the water content is known. The water vapor pressure contribution will be subtracted from any vapor pressure measurements made at UT Austin that have not excluded its effect.

The PT has secured two mini-method instruments to use during the study for measurement of the vapor pressure of the heavy liquids by the PT. One instrument (Grabner VP Vision) has arrived and the project's chemist has been familiarizing himself with its operation. The second instrument (Eralytics ERAVAP) will arrive late this quarter. The greatest challenge in making the VP measurements will be keeping the viscosity of the liquid samples low enough to ensure it flows easily through the instrument and does not thicken to the point where it could harm the operation of the instrument. The heavy liquid samples will be kept at a temperature that is elevated slightly above ambient temperature to reduce their viscosity and keep it low enough to prevent harm to the instrument. A standard operating procedure for making vapor pressure measurements using these instruments will be developed early in the next quarter.

A project extension from August 31, 2017 to November 30, 2017 was requested by the PI on March 23, 2017 and approved by AQRP on March 31, 2017. The reason for this is that our project received final approval in November 2016. It was proposed as a 13 month project. Although the project is making good progress, at this point, it does not appear that we can complete the work in less than 13 months.

The project team intends to use all funds allocated to the project by 11/30/2017 to complete the planned work tasks.

Project 17-024 **STATUS: Active – Oct. 17, 2016**

Improving the Modeling of Wildfire Impacts on Ozone and Particulate Matter for Texas Air Quality Planning

Atmospheric and Environmental Research, Inc. – Matthew Alvarado

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Erik Gribbin

Funded Amount: $170,039

Abstract
Fires can have a large impact on ozone and particulate matter concentrations, and thus air quality, in Texas. Current air quality models (also called chemical transport models) take estimates of the primary emissions from biomass burning (such as forest and grass fires) and unphysically dilute them, which can lead to incorrect estimates of the impact of biomass burning on air quality. Smaller scale models like AER's Aerosol Simulation Program allow us to examine the chemical and physical transformations of trace gases and aerosols within biomass burning plumes and to develop new methods for accurately including this aging process in standard air quality models. In this project, we will improve our understanding of the impacts of local and out-of-state fires on air quality in Texas by implementing an improved approach for modeling the near-source chemistry of biomass burning plumes into the CAMx (Comprehensive Air Quality Model with Extensions) model used in Texas air quality planning. This improved approach will allow CAMx to better represent the impact of forest and grass fires on air pollutants such as ozone and fine particulate matter ($PM_{2.5}$). We will also investigate the impact that long-range transport of wildfire smoke has on air quality in Texas. This project thus addresses two strategic topics of the Texas Air Quality Research Program: "Improving the understanding of ozone and particulate matter (PM) formation [and] the interactions of ozone and PM precursors" and "Investigating global, international, and regional transport of pollutants using data and modeling analyses."

Project Update
The overarching goal of this project is to use an advanced smoke plume chemistry model (AER's Aerosol Simulation Program, or ASP) to improve understanding of the formation of O_3 and $PM_{2.5}$ in biomass burning (BB) plumes, and improve estimates of the impacts of in-state and out-of-state biomass burning on Texas air quality. The project is split into the following two tasks:

- To develop and evaluate an improved sub-grid scale parameterization of biomass burning for CAMx based on ASP coupled with the large eddy simulation model SAM (SAM-ASP) and an analysis of O_3 and SOA production in fire plumes observed during BBOP.
- To explore the impact of BB plumes on the boundary conditions used for CAMx and the resulting impact on Texas air quality with ASP coupled with the Lagrangian particle dispersion model STILT (STILT-ASP).

The progress to date and challenges encountered for each task are discussed below. We currently estimate that we will use all of the funds allocated to this project by 08/31/2017.

Task 1: Develop improved parameterization and assess the impact on Texas air quality

In this reporting period we were able to successfully complete the simulations needed to fill a determined latin-hypercube sampling of SAM-ASP model runs. The variables that we decided to investigate included biomass burning fuel type, overhead O_3 column (reported in Dobson Units, DU), temperature, latitude, start day and start time. We also were able to run the Gaussian Emulator Machine (GEM) on the sampled model output files, as well as successfully compile and run fortran code that uses the emulator prediction inputs from the GEM to evaluate the emulator at a desired point in order to predict the mean and standard deviation for trace gas enhancement ratios. This second step is critical to make the developed parameterizations interface with the CAMx model.

Figure 1 shows the initial results from the emulator evaluation of ozone for the full range of temperatures and starting days, while overhead O_3 (300 DU), latitude (45° N), and start hour (12:00 local solar time) are held fixed. These initial results had some odd features, such as a shift in maximun O_3 to the spring that we traced to a bug in the SAM-ASP model that was giving the incorrect seasonal dependence of the solar zenith angle and thus the photolysis rates. We also determined that including all four fuel types in the same GEM fit gave odd results due to the fact that when running the Gaussian Emulator Machine we treated the fuel type as a numeric value, so the fuel types may be influencing each other's results unintentionally. To address this we re-ran the latin-hypercube sampling using 100 simulations of each fuel type separately, and repeated the GEM development and evaluation. These changes resulted in a more reasonable dependence of the modeled $\Delta O_3/\Delta CO$ on the day of the year (Figure 2), although the revised parameterization still appears to be producing a relatively low amount of O_3 for the conditions matching the Williams fire (Alvarado et al., 2015) and suggests a slight fall-off in O_3 production at high temperatures.

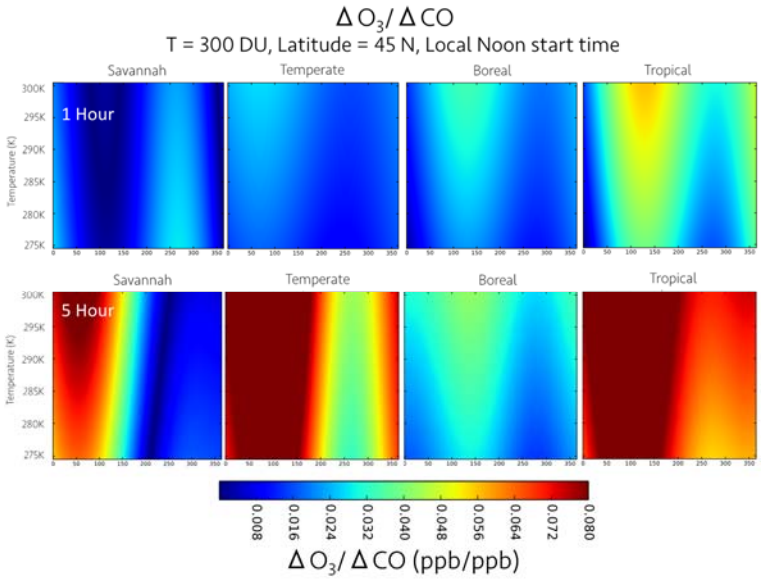

Figure 1. *Evaluation of the GEM ozone enhancement ratio outputs for a range of temperatures (y-axis) and start days (x-axis. From left to right the fuel types include Savannah, Temperate Forests, Boreal Forests and Tropical Forests. The top row shows model output 1 hour downwind, and the bottom row shows model output 5 hours downwind.*

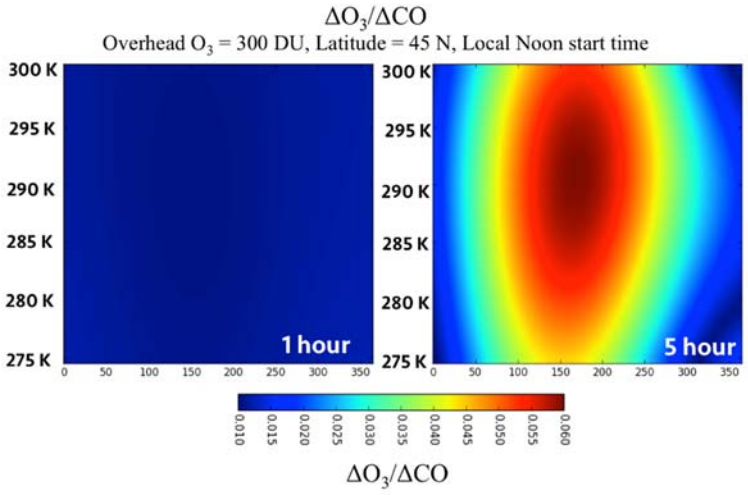

Figure 2*. Evaluation of the GEM ozone enhancement ratio outputs for Savannah/Grassland fires for a range of temperatures (y-axis) and start days (x-axis), at fixed latitude, overhead ozone and model start hour. The left panel shows model output 1 hour downwind, and the right panel shows model output 5 hours downwind.*

Task 2: Investigate the impact of long-range transport of BB pollution on Texas air quality

In this reporting period we analyzed our STILT-ASP simulations for the impacts of fire CO on the boundaries of the TCEQ modeling domain. Figure 3a shows that STILT-ASP and GEOS-Chem both predict significant CO emissions over Eastern/Southeastern CONUS for May 11, 2012, but STILT-ASP predicts a higher CO concentration relative to GEOS-Chem at the Eastern receptor. In addition, both models show elevated CO along the southern border on this day. STILT-ASP predicts larger concentrations than GEOS-Chem, although both models are within ~30 ppbv CO of each other at both locations. In contrast, Figure 3b shows that for June 1, 2012, STILT-ASP predicts mean CO of approximately 120 ppbv at the northern SK boundary receptor, but GEOS-Chem shows CO levels in excess of 10^3 ppbv. We are still investigating whether this discrepancy is due to different fire emissions (FINN in STILT-ASP versus GFED in GEOS-Chem), differences in transport, or other causes. Along the southern border, both models capture the influence of wildfires over Central America and predict similar levels of CO along the southern border of the grid.

In the next reporting period we will expand the number of receptors we run to look at issues related to potential numerical diffusion of biomass burning plumes in the GEOS-Chem boundary conditions.

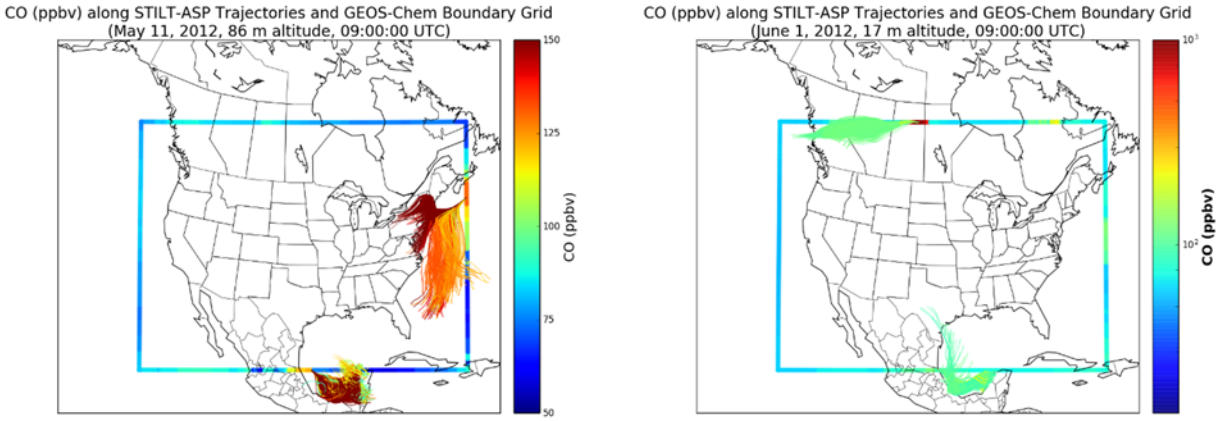

Figure 3. *(a) CO along two STILT-ASP back-trajectory calculations (500 Lagrangian parcels each) overplotted on the GEOS-Chem boundary conditions for May 11, 2012 at 09:00 UTC. (b) same for June 1, 2012 at 09:00 UTC. Note the change in scale from Figure 3a.*

Alvarado, M. J., C. R. Lonsdale, R. J. Yokelson, S. K. Akagi, H. Coe, J. S. Craven, E. V. Fischer, G. R. McMeeking, J. H. Seinfeld, T. Soni, J. W. Taylor, D. R. Weise, and C. E. Wold (2015), Investigating the Links Between Ozone and Organic Aerosol Chemistry in a Biomass Burning Plume from a Prescribed Fire in California Chaparral, *Atmos. Chem. Phys.*, 15, 6667–6688, doi:10.5194/acp-15-6667-2015.

Project 17-032 **STATUS: Active – Dec. 6, 2016**

Spatial Mapping of Ozone Formation near San Antonio

Drexel University – Ezra Wood

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Mark Estes

Funded Amount: $59,000

Abstract
Ozone (O_3) is the main component of smog and causes adverse effects on human health, especially to sensitive groups such as children and the elderly. Unlike "primary" pollutants which are emitted directly from vehicles and industrial processes, ozone is formed in the atmosphere from photochemical reactions involving volatile organic compounds (VOCs) and nitrogen oxides ("NO_x"). In order for San Antonio to comply with the new National Ambient Air Quality Standard for ozone of 70 ppb, regulators will need to make science-based decisions on effective mitigation strategies, including emission reduction programs. Such decisions will require knowledge of the amount of ozone that is transported into the city from upwind regions (usually located southeast of San Antonio), the absolute rates of ozone formation in and around San Antonio, the relative importance and interaction of emissions from various sources (e.g., upwind oil and gas activity and urban emissions from the city itself), and when and where ozone formation occurs under "NO_x-limited" or "VOC-limited" conditions. In contrast to Houston and Dallas, little is known about ozone formation in San Antonio. This research project will address this major shortcoming and elucidate the mechanisms and rates of ozone formation that affect air quality in San Antonio using novel measurements of peroxy radicals aboard a mobile supersite during a 3-week field project during late spring of 2017. Instantaneous ozone production rates $P(O_3)$ will be quantified aboard the Aerodyne Mobile Laboratory using new but tested measurements of total peroxy radicals. These measurements will be used to "map" the rate of ozone formation upwind, downwind, and inside of the urban core of San Antonio. Measurements of organic nitrates will also be used to investigate the role of alkanes and organic nitrate formation as a terminator of ozone chemistry.

The main goals of the project are to quantify how much ozone is produced inside the city compared to upwind, and to quantify the role of alkanes in ozone formation.

Project Update
Major activities for the March – May quarter are listed below:

1. The thermal dissociation – cavity attenuated phase shift spectrometer (TD-CAPS) instrument for measuring organic nitrates was re-assembled, the quartz thermal dissociation tubes were assembled and housed, the temperature controllers were adapted for dual zone control, and temperature scans of n-propyl nitrate were recorded. These temperature scans, in which the temperature of the heated quartz tube inlet is scanned from ambient temperature up to 400 °C, agreed with prior results showing full dissociation of n-propyl nitrate at 300 °C for a flow rate of 2 LPM.

2. Jessica Pavelec, a Drexel co-op undergraduate student, started work in the lab on April 2 and executed much of the day to day tasks for the TD-CAPS instrument above.

3. The ECHAMP radical sensor was calibrated with two calibration sources by postdoc Daniel Anderson. Various parts of this instrument were reconstructed following the PI's move from U. of Massachusetts to Drexel University, including replacement of six of the eight mass flow controllers.

4. The two instruments and supporting equipment were shipped to Aerodyne Research, Inc. (MA). Daniel Anderson and Ezra Wood traveled to Aerodyne in mid-April to integrate the instruments into the Aerodyne Mobile laboratory (AML). Upon integration in the laboratory, both CAPS units suffered from a sporadic noise source, and rather than travel to San Antonio on the AML were instead shipped separately to San Antonio following an additional two days of diagnostics.

5. The field deployment in San Antonio commenced. Set-up for measurements of total peroxy radicals ($RO_2 + HO_2$) and organic nitrates commenced on May 8 and will continue through May 31. The mobile lab has been stationed at the University of Texas – San Antonio (May 8 – 15), Floresville (May 16 – 21), Mathis (May 22 – 26), and UTSA (May 27 – 31). The noise source in the ECHAMP CAPS sensors has been resolved and was likely due to intermittent electrical connections in both CAPS, and none of the three CAPS systems (two for ECHAMP, one for TD-CAPS) have suffered from this noise during the field measurements.

Figure 1 shows time series data for O_3, $RO_2 + HO_2$, NO, NO_2 photolysis rates (jNO_2), and calculated ozone production rates $P(O_3)$ for the first deployment at UTSA.

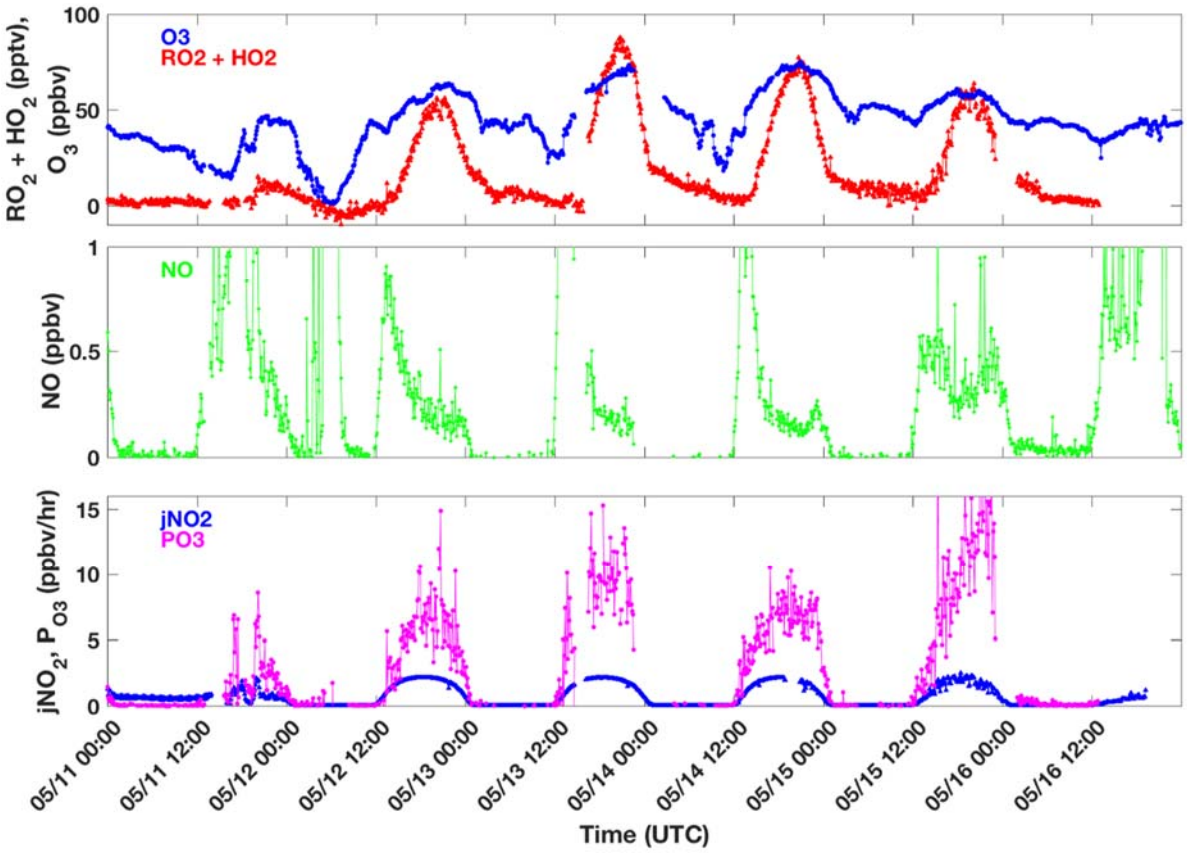

Figure 1. *Preliminary measurements and calculated quantities ($P(O_3)$) from the UTSA measurements.*

$P(O_3)$ is calculated using equation 1:

$$P(O_3)\ (ppb/hr) = k_{HO2+NO}([HO_2]+[RO_2][NO] \qquad \text{Eq 1.}$$

where k_{HO2+NO} is the bimolecular rate constant for the reaction between HO_2 and NO, which forms NO_2 (and O_3 following photolysis). The sum of $[RO_2]$ and $[HO_2]$ is measured by ECHAMP and NO is measured by a Thermo model 42i-TL chemiluminescence sensor. The preliminary calculations show modest values for $P(O_3)$ peaking at 15 ppb/hr. In comparison, values exceeding 50 ppb/hr have been observed in Houston, Mexico City, and other major metropolitan areas. Daytime NO values in at all sites visited have been lower than the typical transition concentration between "NOx-limited" and "VOC-limited" chemistry, suggesting that ozone formation chemistry is "NOx-limited", though more in-depth analysis is required. Figure 2 shows one type of analysis procedure that will be used to assess the nature of ozone production – plotting the calculated ozone production rate as a function of NO. This curve is expected to increase at low NO values and decrease later at higher NO values. Higher $P(O_3)$ values are expected at higher HOx radical production rates (i.e., faster O_3 formation is expected under sunny conditions with high concentrations of radical precursors including formaldehyde, water vapor, and ozone itself). The graph in figure 2 is colored by the formaldehyde concentration as a proxy for HOx production rates, and indeed the highest

$P(O_3)$ values are observed at the highest formaldehyde concentrations. Future analysis will incorporate more data, and use the radical production rates calculated from the measurements of photolysis rates, formaldehyde, ozone, water vapor, hydrogen peroxide, acetaldehyde and other oxygenated VOCs, and alkenes (from ozonolysis).

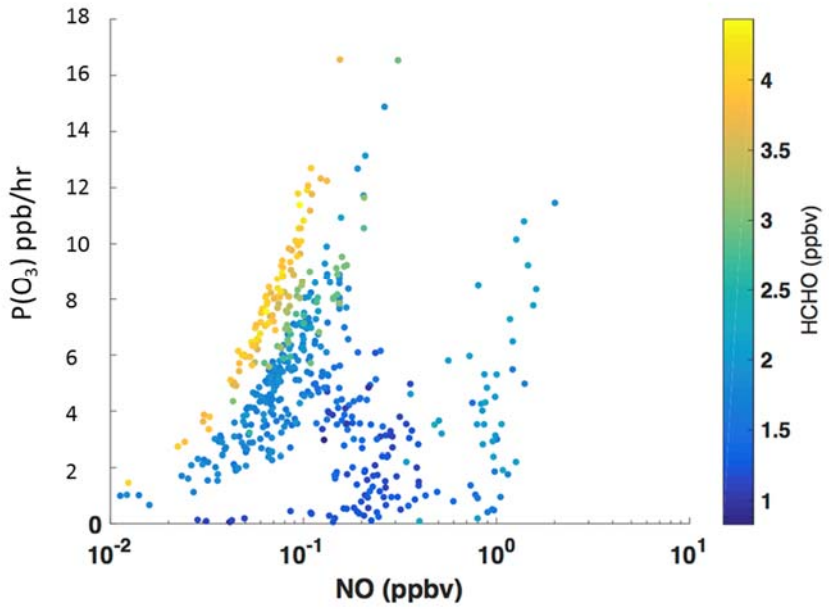

Figure 2. *$P(O_3)$ as a function of NO, colored by formaldehyde concentration, suggesting most ozone formation observed at UTSA was "NOx-limited".*

The TD-CAPS system has been challenged by low mixing ratios of alkyl nitrates and the difficulty of measuring these compounds on top of a time varying NO_2 concentration, which forms the background signal for the measurement. For the last few days of the field measurements this instrument switched to measuring the sum of peroxyacyl nitrates and alkyl nitrates, i.e. total organic nitrates, rather than just alkyl nitrates, in order to attain higher signal-to-noise ratios. Initial results are successful, with mixing ratios of 0.5 to 1 ppb of organic nitrates.

All funds are anticipated to be spent by 8/31/2017.

Project 17-039 **STATUS: Active – Nov. 16, 2016**

Use of Satellite Data to Improve Specifications of Land Surface Parameters

University of Alabama - Huntsville – Richard McNider

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Bright Dornblaser

Funded Amount: $149,227

Abstract
It is the purpose of this project to continue a process to evaluate and improve the performance of the land surface models used in WRF by the use of satellite skin temperatures to better specify physical parameters associated with land use classes. Improved temperature performance impacts biogenic emissions, thermal decomposition (chemical chain lengths and slopes of ozone/NOy curves) and thermally driven winds. Also, land surface parameters control surface deposition which impacts the efficacy of long-range transport. Physical parameters such as heat capacity, thermal resistance, roughness, surface moisture availability, albedo etc. associated with a land use class are actually used in the land surface model. Many of the land use class associated parameters such as surface moisture availability are dynamic and ill-observed depending on antecedent precipitation and evaporation, soil transport, the phenological state of the vegetation, irrigation applications etc. Other parameters such as heat capacity, thermal resistance or deep soil temperature are not only difficult to observe they are often unknowable *a priori*. Despite the difficulty in specifying these parameters they are incredibly important to model predictions of turbulence, temperature, boundary layer heights and winds.

This project is directed toward the Meteorology and Air Quality Modeling and Biogenic Emissions Priority. Biogenic emissions are highly sensitive to temperature. Improvement in temperature predictions in conjunction with improved radiation inputs into biogenic emission model (MEGAN or BEIS) should increase the quality of biogenic emissions. The project is responsive to three areas in the Meteorology and Air Quality Modeling Priority- (1) boundary layer performance can impact local circulations driven by thermal gradients and the strength of low level jets is controlled by nighttime surface cooling rates; (2) boundary layers can impact clouds both boundary layer topped cumulus and clouds in sea breeze convergence zones; (3) dry deposition of ozone and nitrogen species is often controlled by stomatal uptake which depends on soil moisture.

The project will continue and expand activities under a 2015 funded AQRP project using satellite observed skin temperatures. That project was a late selected reduced scope project. Despite some initial issues with a NOAA skin temperature data set, the project ended up showing improvement in model performance for skin temperatures and in wind performance. However, the improvements were not as large as in previous uses of skin temperature data. Part of this may be due to following the Pleim-Xiu air temperature approach in the project, in which absolute differences between model and observed skin temperatures were used rather than skin temperature tendencies. Differences between the model and satellite skin temperatures not related to the boundary layer parameters such as emissivity or atmospheric correction in the satellite product might be an issue. Under this activity skin temperature tendencies will be tested

instead which avoids such problems. The DISCOVER AQ period of 2013 was an unusually cloudy and windy period over most of the Eastern U.S. and not characteristic of the conditions usually associated with ozone episodes in Texas. While significant effort went into QA for the skin temperature data set, cloud contamination in the skin temperatures may still be an issue. Under the current activity alternative skin temperature products such as MODIS data will used in conjunction with the tendency method that may reduce cloud contamination issues. Also, in consultation with TCEQ additional periods such as TEXAQS 2006 or the 2012 SIP period will be examined. Finally, the work on the previous project included emphasis on the large 12-km domain. Under this activity a greater emphasis will be given to fine scale model performance around Houston and Dallas. Particular attention will be given to wind changes due to changes in boundary layer parameters including changes in sea breezes and low level jets.

Project Update

The progress to date and challenges encountered are discussed below.

Reruns of 2013 Discover AQ Period: As follow-up to last year's project the period September 1-30, 2013 period is being re-run and model performance re-evaluated. Since making these runs that were reported last year, new nudging strategies both for the large scale analysis and satellite data have been developed. As an example, wind nudging in the boundary layer was used in the prior runs. It is felt that for the present study that boundary layer physics should be allowed to develop both at the surface and in the residual layer. The control experiment has been run (i.e. with no satellite assimilation). An analysis of its performance compared to the previous control run is being made. The satellite assimilation run will be run in June. For the assimilation run an aggressive scheme for not carrying out moisture assimilation when either clouds are present in the satellite data or clouds are present in the model. While this will reduce the amount of data to be assimilated it may improve performance.

Additional Model Evaluation Period: As noted in the proposal for this project, the Discover AQ period was not a particularly representative period for air quality concerns. Many active fronts and pervasive cloudiness dominated the period. Thus, as part of this year's effort an additional modeling period was to be chosen in conjunction with TCEQ. After discussion with TCEQ it was decided that the period July 1, 2012 – August 31, 2012 would be the new period. The drier 2012 year is a contrast to the 2013 Discover AQ period. This period may coincide with potential SIP work in in Texas.

Skin temperatures from GOES and MODIS have been processed for this period. Additional QA/QC procedures have been developed to remove clouds especially near cloud edges. Initial Model set up has been completed. Some differences in nudging protocols have been changed as described above. It is expected that the first control simulation for this new period will be carried out in June.

MODIS Greenness Values: Previous simulations for the 2013 Discover AQ period indicated that the seasonal adjustment in the Pleim-Xiu scheme produced erroneously high vegetation values especially in the arid West. In consulting with Jon Pleim at EPA they had also found that the seasonal adjustment was over-specifying vegetation fractions. They had made tests using MODIS Greenness Products and were in the process of converting to MODIS to specify seasonal vegetation. Under this activity we proposed to use a new MODIS Greenness product produced by the NASA SPorT Center. This product has a shorter averaging period than the standard

MODIS product so that short term vegetative changes are better captured. This product has already been incorporated in WRF by NASA. We are using the file structure set up by NASA in our WRF simulations for the 2013 simulations. However, this product was not available until 2013 so we will employ the standard MODIS greenness product for the 2012 simulation period.

Sea Surface Temperatures: As part of a small EPRI and NASA project looking at WRF and air quality over the Great Lakes it was found that the standard surface water temperatures were too warm. This led to an unstable layer at night over the water. A procedure was established to use MODIS skin temperatures in WRF. This uses a running ten day average to ensure continuous spatial data. This may be employed in the Texas runs since it may improve performance in coastal areas. Previous studies by Rice University has also pointed to use of satellite sea surface temperatures improving winds in Houston air quality

Funds: Charges and time devoted the project during the first 4 months were below targets in part due to some competing projects and set up of accounts. However, charges have accelerated so that charges will meet project targets.

Project 17-053 **STATUS: Active – Jan. 10, 2017**

Identifying and Apportioning Ozone Producing VOCs in Central American Fires

Aerodyne Research, Inc. – Scott Herndon

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Mark Estes

Funding Amount: $185,193

Abstract
Aerodyne Research, Inc. will conduct measurements using a mobile laboratory as a portable photochemistry super site to study ozone production and the emission sources that ultimately impact air quality in central Texas. Work will be done at locations upwind, downwind and lateral to San Antonio. The suite of instrumentation has been selected to quantify key oxygenated volatile organic carbon species (OVOC) and nitrogen containing species (e.g. alkyl nitrates) to pinpoint and apportion ozone within broad categories of VOC emission sectors. The instrument payload will also directly quantify the instantaneous production rate of ozone to determine whether the chemical regime is NOx limited or VOC limited. An additional component of this research project will be to characterize emission sources associated with oil and natural gas production in the Eagle Ford Shale play, including active medium to large processing flares, as well as oil and condensate tanks at wellpads.

The project will provide scientific insight into the VOCs that are contributing to the ozone in central Texas. The effectiveness of mitigation strategies will be informed by these results. This work will isolate ozone production due to VOC oxidation from biogenic sources, refinery emissions, emissions from oil producing well pads and emissions from natural gas production. The dataset will inherently contain regional transport of emissions and processed air. The project will quantify local ozone production rates and evaluate the ozone sensitivity regime.

Project Update
This report discusses the progress from March 1st to May 31st, 2017. It includes a summary of the actual measurement site locations, instrument performance, and initial observations. Each topic will be discussed and summarized below.

During May 2017, Aerodyne Research, Inc. conducted measurements using a portable photochemistry super-site. The study involved quantification of ozone production and the emission sources that ultimately impact air quality in central Texas. The deployment locations were upwind and downwind of San Antonio. The suite of instrumentation was selected to quantify key oxygenated volatile organic carbon species (OVOC) and nitrogen-containing species (e.g. alkyl nitrates). Ultimately, with additional analysis, this suite of measurements will be used to apportion ozone within broad categories of VOC emission sectors. The instrument payload has quantified the instantaneous gross production rate of odd-oxygen (effectively the sum of ozone and nitrogen dioxide). Initial analysis suggests the chemical regime is NOx-limited. We have performed measurements in areas upwind of San Antonio and collected data on various VOC emission profiles (e.g. biogenic vs oil and gas).

Measurement Sites

To meet the science objectives of the project, we conducted measurements at three different sites. The timing of the moves was done in coordination with the TCEQ weather forecasting resources. A map, depicting the locations of this monitoring is below.

Figure 1. *Measurement locations for Project 17-053*

The red diamond symbols in Figure 1 indicate the locations where the mobile labs were stationed. The white line indicates the route of the two mobile labs where a limited set of tandem *mobile* data was collected.

The University of Texas at San Antonio was selected as a core measurement site. It was also the location of the Baylor measurements and the vertical wind profiling project. Additionally, during the last few days of the project, the Aerodyne and University of Houston mobile labs sampled contemporaneously, and performed extensive cross-calibrations.

The Floresville station was selected because it is an approved TCEQ location for conducting measurements and has a lengthy time series of monitoring data in the vicinity of the Eagle Ford oil and gas production region. The site was secure and power was installed at relatively low cost to the project.

The Corpus Christi State Park served two purposes: the first was to sample gulf air before it was exposed to inland biogenic and oil and gas emissions. Under the right circumstances, it would also be a vantage from which to sample industrial emissions and initial photochemistry from the refineries in Corpus Christi.

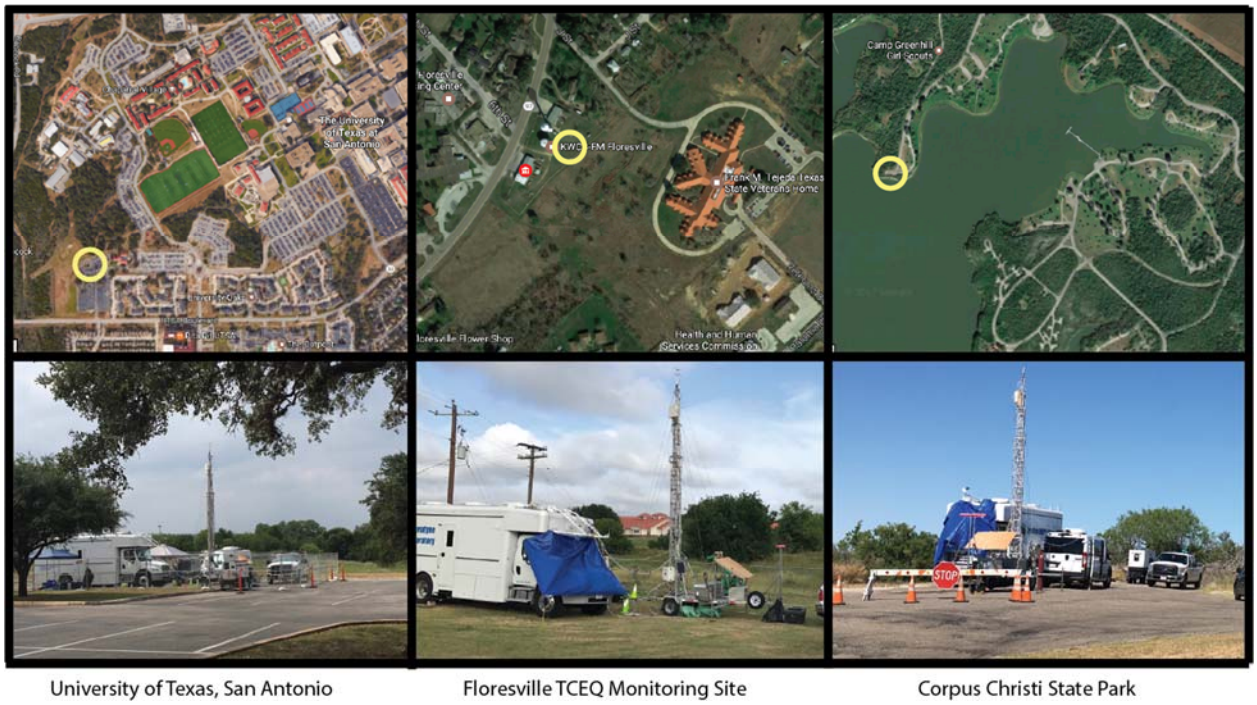

Figure 2. *Site Details for the Three Measurement Locations for Project* 16-053.

Instrumentation Performance

Trace Gases. A number of the instruments that were deployed are Aerodyne Research, Inc. brand laser spectrometers (referred to as TILDAS instruments hereafter), and can be configured to measure different gases depending on the application.

TILDAS	*Species*	*Wavelength* (cm^{-1})	*Performance*
Dual 157 m (a)	HCHO, HCOOH, H_2O	1765	HCHO excellent[a]
Dual 157 m (b)	N_2O, H_2O_2, H_2O	1278	H_2O_2 will require refit
Mini 83 m C-1	N_2O, CO, H_2O	2199	CO, N_2O, H_2O excellent
Mini 76 m C-4	HCN, C_2H_2	3287	HCN excellent C_2H_2 good
Dual 76 m (a)	CH_4, C_2H_6	2990	CH_4 good C_2H_6 excellent[b]
Dual 76 m (b)	C_2H_6, C_3H_8	2967	C_3H_8 will require selected refitting
deployed in the UH lab			
Mini 76 m C-3	CH_4, C_2H_6	2996	excellent

[a]A malfunction of the cooling airflow caused slight data loss during the initial UTSA deployment

[b]The instrument has performed well, but the ECHAMP instrument emitted ethane on-site which occasionally contaminated the sample. This will require additional quality assurance through manual examination of the data.

Table 1. *Trace Gases*

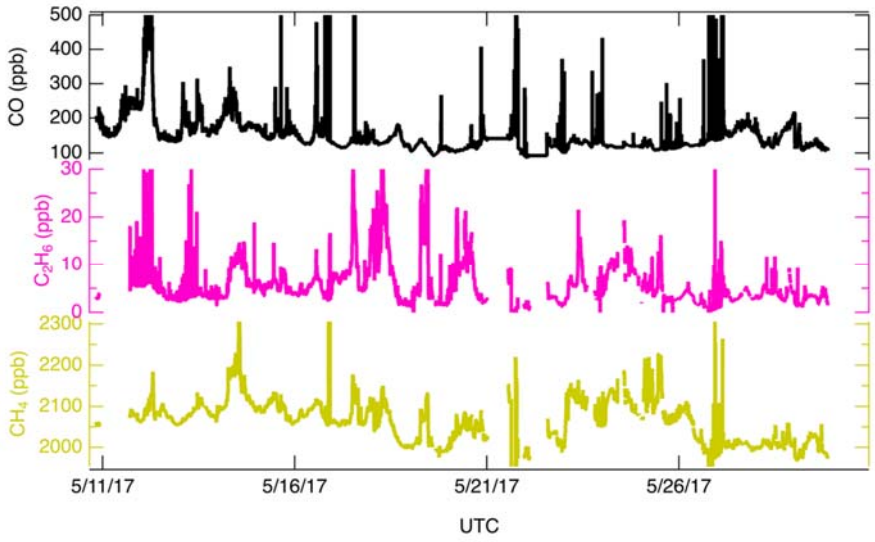

Figure 3. *An overview of the preliminary uncalibrated campaign data for selected TILDAS species. The performance and time on-line of the three species above is representative of the trace gas instrument suite.*

Speciated Particulates. The Aerosol Mass Spectrometer (AMS) measured speciated particulates including sulfates (SO4), organics (Org), nitrates (NO3) and black carbon (BC). The Soot Particle High Resolution Time of Flight Aerosol Mass Spectrometer (SP-HR-ToF-AMS) has sampled in 1 minute mode at the UTSA, Floresville and Lake Corpus Christi sites. It has also sampled in 1 second mode during mobile operations as the AML transported from Lake Corpus Christi to UTSA with traverses both in the immediate downwind vicinity of Corpus Christi refineries and in the Eagle Ford natural gas play zone. This instrument provides a measurement of Organic, NO_3, SO_4, NH_4, Chl and black carbon in ug/m^3. Preliminary analysis has revealed elevated SO_4 levels occasionally at both the UTSA and the Floresville site. These SO_4 levels have also been observed by the University of Houston mobile laboratory utilizing Rice Universities HR-ToF-AMS. The intercomparison of the data from both instruments indicates promising agreement. Investigation of the air mass associated with the elevated SO_4 signal should reveal the SO_4 source and will be a focus of further data analysis.

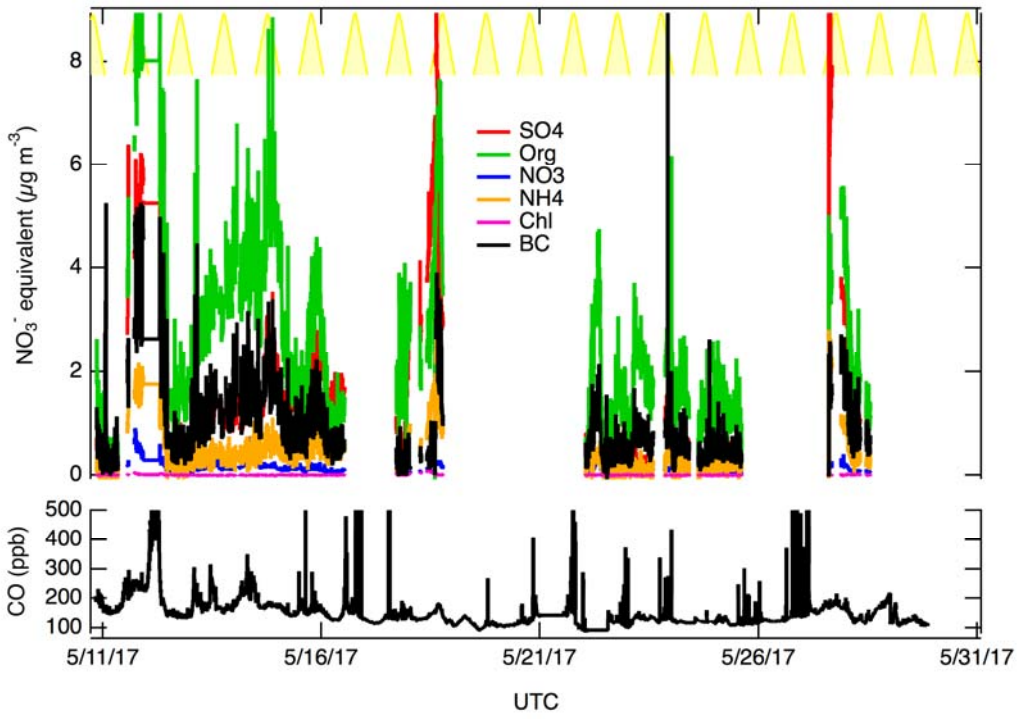

Figure 4. *Time series of analyzed AMS data, so far. The AMS data is a mixture of high-resolution and unit mass resolution analysis.*

VOCs via GC-TOF. The gas chromatograph coupled to a time of flight detector (GC-TOF) was operated with sample loop injection system. A multicomponent adsorbent (Graphsphere 1016 and Carboxen 1000) sample pre-concentration method has been selected. The instrument has had some challenges in the heat and humidity. *A leak developed during the transit from Corpus Christi (5/27/17) and the unit was deemed to be unrepairable in the field.*

HOx and ROx radicals via ECHAMP.

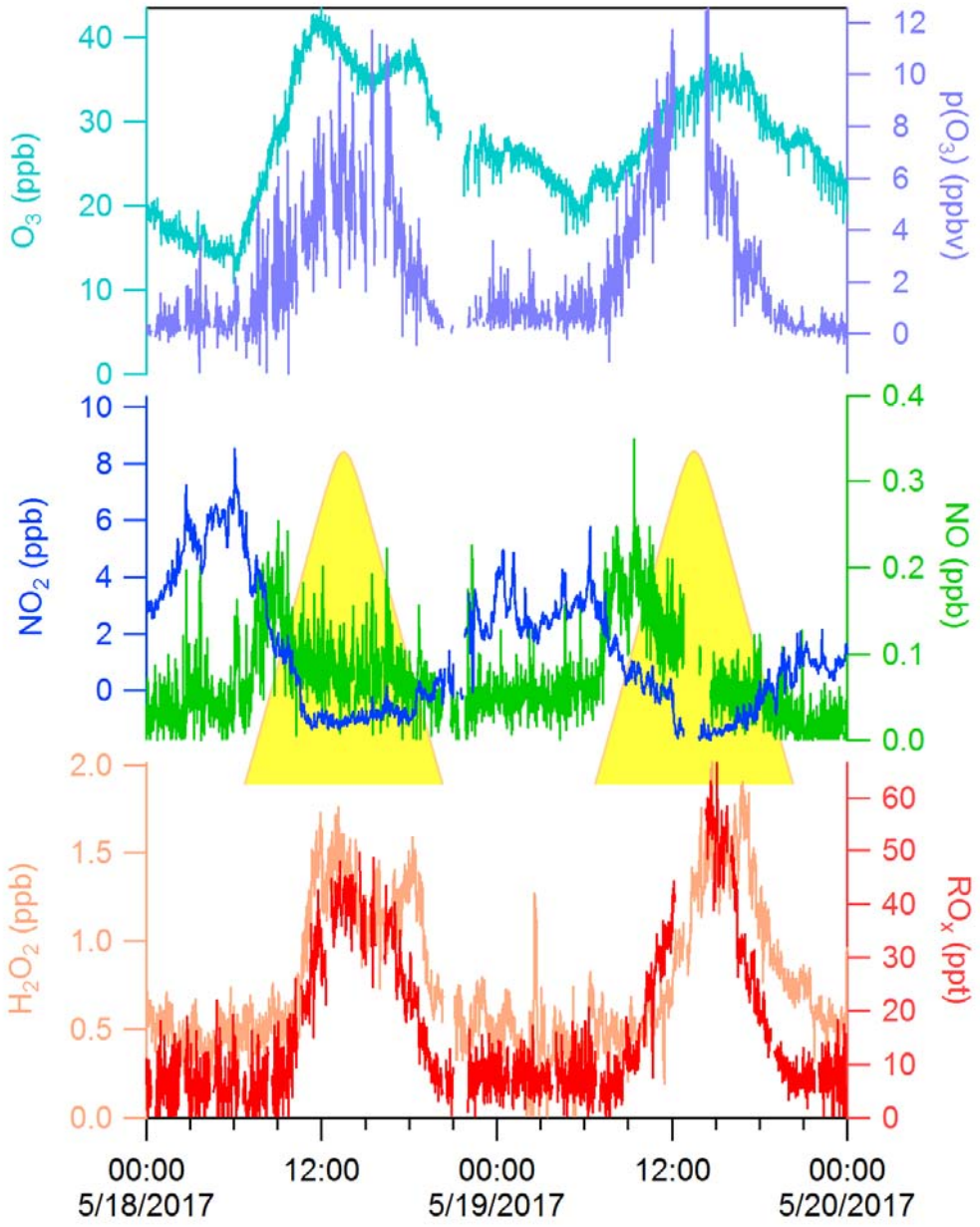

Figure 5. *HOx and ROx radicals via ECHAMP.*

Figure 5 above depicts an exemplary event at Floresville. The Drexel ECHAMP quantification of HOx/ROx is featured in the calculation of $p(O_3)$. When the sun rises, there is a photochemically-induced drop in NO_2, concomitant with a rise in HOx/ROx and O_3. We also observe a rise in H_2O_2; a sink for HO_2 radicals in low-NOx environments. While H_2O_2 rises with HOx/ROx, we observe a delayed decay relative to HOx/ROx.

Mid-volatility species via I^- CIMS and VOCs via PTR-MS. The chemical ionization mass spectrometer using the iodide-reagent ion (I^- CIMS) was integrated into the Aerodyne Mobile Laboratory (AML) in April 2017. The proton transfer reaction mass spectrometer (PTR-MS) was integrated into the minAML at the same time.

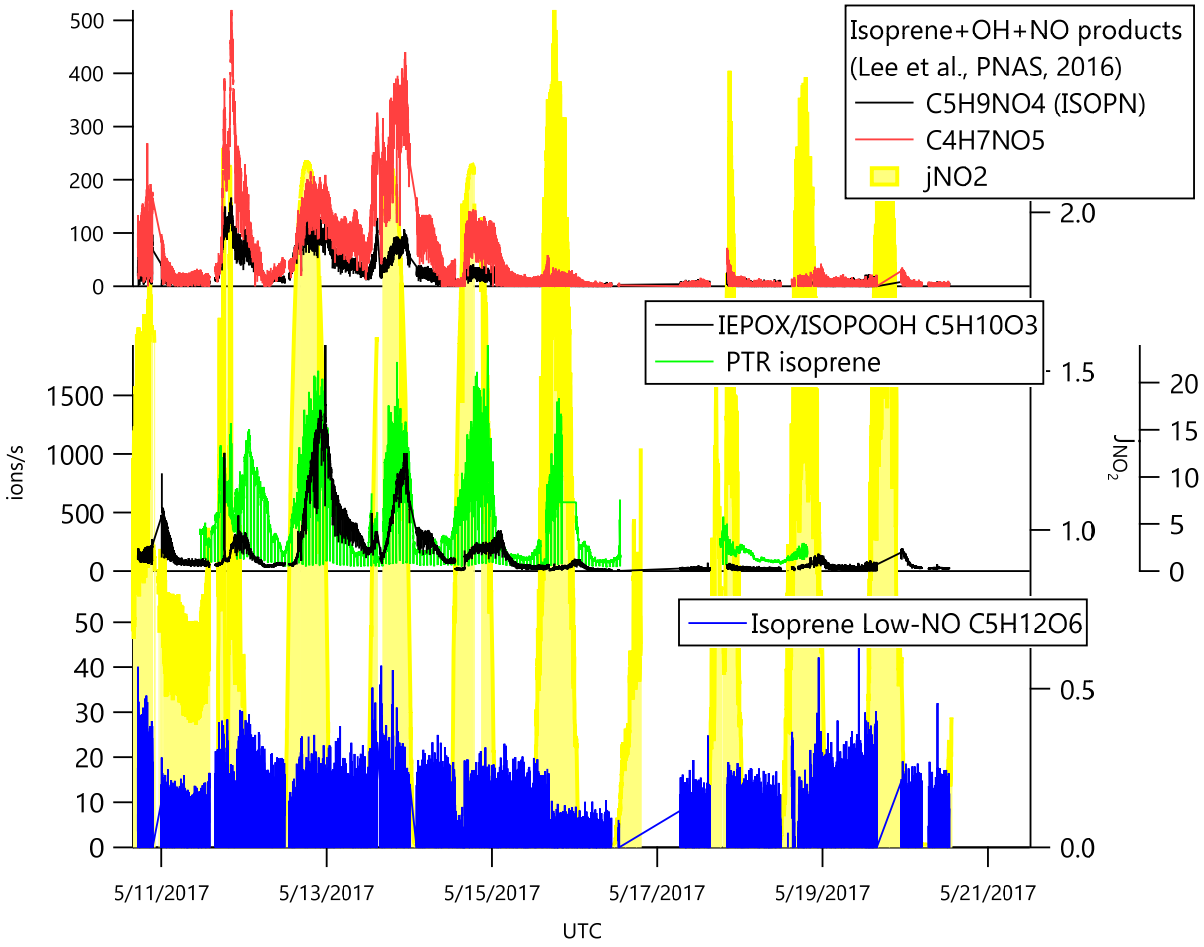

Figure 6. *Mid-volatility species via I^- CIMS and VOCs via PTR-MS.*

The I-CIMS and PTR-MS data require additional time for analysis. At this initial stage through some observations can be made. We see abundant isoprene products at UTSA site that are dominated by organic nitrates (high-NO OH-oxidation products) and we see much lower isoprene (PTR) and products at Floresville site. This is somewhat of a mystery to us and we are working to make sure there isn't an interference in the urban UTSA data at the isoprene mass to charge ratio.

Project 17-SAFS **STATUS: Active – April 13, 2017**

San Antonio Field Study Logistics

University of Texas at Austin – David Sullivan

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Mark Estes

Funding Amount: $46,000

Abstract
In May 2017, AQRP and TCEQ will conduct a field campaign in and around San Antonio to study the causes of ozone formation in the San Antonio area. The San Antonio Field Study 2017 (SAFS 2017) will deploy mobile measurement vans, wind profilers, and ozone sondes. Air quality measurements will be made by researchers from collaborating organizations, including research scientists and engineers funded wholly or in part by the AQRP and the TCEQ. This AQRP project will support the SAFS 2017 by overseeing logistical aspects of the field campaign. Specifically, it will facilitate the performance of electrical work to ensure proper access to power to operate the instrumentation, and minor site improvements to ensure access to the site locations and to prevent damage to the sites that could be caused by driving large vehicles across unpaved areas. It will also ensure other project infrastructure is in place, such as wireless access, lighting, temporary fencing, and other logistical support. In all, this project will centralize and coordinate the site infrastructure preparation for measurement sites selected for the San Antonio Field Study 2017 (SAFS 2017). The scope of work included in the project includes all aspects of site preparation and decommissioning of the measurement sites.

Project Update
This project has six (6) tasks. The current status of each task is described below.

Task 1. Sites selected for all research teams participating in SAFS 2017.

All sites were finalized in early May 2017. Infrastructure upgrades were made at the TCEQ's Floresville Hospital Blvd. CAMS 1038 site and at the primary site for several projects on the University of Texas at San Antonio (UTSA) campus by the Child Development Center.

Task 2. Obtain the necessary site access/use agreements from UTSA for the site on the campus.

This task was completed prior to the start of measurements in early May 2017.

Task 3. Site pad preparations.

This task was completed prior to the start of measurements in early May 2017.

Task 4. Provide limited support of researchers should problems arise with the site accommodations, which would be provided as needed.

Some historic information from another project were provided to the Aerodyne research team.

Task 5. Site Decommissioning.

At the end of the May operations of SAFS, some fencing may be removed at UTSA if the TCEQ decides to not use of the UTSA site later in the summer. The power install will remain in place for the balance of the summer for the upper air measurement instruments set on the grass by the parking area.

Task 6. Prepare Project Reports and Presentations.

Reports have been filed in a timely manner.

FINANCIAL STATUS REPORT

Initial funding for fiscal years 2016 and 2017 was established at $1,000,000 each, for a total award of $2,000,000 for the FY 2016/2017 biennium. The funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

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

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

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

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

Program Administration

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

During the reporting period several staff members were involved, at various levels of effort, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. Maria Stanzione, AQRP Program Manager, with Terri Mulvey, Melanie Allbritton, and Susan McCoy each provided assistance with program organization and financial management. Denzil Smith is responsible for the AQRP Web Page development and for data management. Gina Palacios is providing assistance with the website redesign.

Fringe benefits for the administration of the AQRP were initially budgeted to be 24% of salaries and wages across the term of the project. It should be noted that this was an estimate, and actual fringe benefit expenses are reported for each month. The fringe benefit amount and percentage fluctuate each month depending on the individuals being paid from the account, their salary, their FTE percentage, the selected benefit package, and other variables. For example, the amount of fringe benefits is greater for a person with family medical insurance versus a person with individual medical insurance. Actual fringe benefit expenses to date are included in the spreadsheets below.

Table 1: Administration Budget

Administration Budget (includes Council Expenses)
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$73,895.00	$70,040.00	$143,935.00	$108,105.09	$35,829.91
Fringe Benefits		$17,731.00	$16,806.00	$34,537.00	$26,416.22	$8,120.78
Travel		$34.00	$150.00	$184.00	$34.00	$150.00
Supplies		$950.00	$6,000.00	$6,950.00	$291.84	$6,658.16
Equipment						
Total Direct Costs		$92,610.00	$92,996.00	$185,606.00	$134,847.15	$50,758.85
Authorized Indirect Costs		$7,390.00	$7,004.00	$14,394.00	$10,810.51	$3,583.49
10% of Salaries and Wages						
Total Costs		**$100,000.00**	**$100,000.00**	**$200,000.00**	**$145,657.66**	**$54,342.34**

ITAC

All ITAC expenses for FY 2016 were accounted for by the end of September 2016. No changes were made to the ITAC budget and no expenditures occurred during the reporting period.

Table 2: ITAC Budget

ITAC Budget
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary						
Fringe Benefits						
Travel		$4,900.00	$10,000.00	$14,900.00	$4,076.57	$10,823.43
Supplies		$1,100.00	$5,000.00	$6,100.00	$1,079.20	$5,020.80
Total Direct Costs		$6,000.00	$15,000.00	$21,000.00	$5,155.77	$15,844.23
Authorized Indirect Costs						
10% of Salaries and Wages						
Total Costs		**$6,000.00**	**$15,000.00**	**$21,000.00**	**$5,155.77**	**$15,844.23**

Project Management

No changes were made to the Project Management budget during this quarter. Project Management funds are budgeted at 8.22% of Contractual/Research Project funds, below the 8.5% threshold.

Table 3: Project Management Budget

Project Management Budget
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$50,182.00	$44,000.00	$94,182.00	$70,142.31	$24,039.69
Fringe Benefits		$12,083.00	$10,600.00	$22,683.00	$15,347.52	$7,335.48
Travel		$0.00	$500.00	$500.00	$0.00	$500.00
Supplies		$500.00	$5,500.00	$6,000.00	$0.00	$6,000.00
Other		$2,000.00	$5,000.00	$7,000.00	$0.00	$7,000.00
Total Direct Costs		$64,765.00	$65,600.00	$130,365.00	$85,489.83	$44,875.17
Authorized Indirect Costs		$5,019.00	$4,400.00	$9,419.00	$7,014.23	$2,404.77
10% of Salaries and Wages						
Total Costs		**$69,784.00**	**$70,000.00**	**$139,784.00**	**$92,504.06**	**$47,279.94**

Research Projects

A total of $1,630,000 was originally budgeted for research projects. In previous quarters those funds were increased by $9,216, due to the reduction in funds allocated to Other and ITAC. A total of ten (10) projects were selected for funding out of fifty four (54) proposals submitted to the AQRP RFP for the 2016-2017 biennium. An additional project to oversee the logistics of the San Antonio Field Study was added in April 2017. With the addition of this project $1,639,916 has been allocated across the eleven 2016-2017 research projects. Table 4 on the following page shows the distribution of the projects across the fiscal years and the cumulative expenditures to date.

Table 4: Contractual/Research Project Budget

Contractual Expenses				
FY 16 Contractual Funding		**$815,000**		
FY 16 Contractual Funding Transfers		**$9,216**		
FY 16 Total Contractual Funding		**$824,216**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
16-008	University of Houston	$191,366	$41,722.25	$149,643.75
16-010	Sonoma Technology, Inc.	$69,075	$33,936.25	$35,138.75
16-011	Ramboll Environ	$158,134	$96,231.58	$61,902.42
16-019	Univ. of Texas - Austin	$118,019	$75,059.52	$42,959.48
16-019	Ramboll Environ	$62,622	$26,553.27	$36,068.73
16-031	UNC - Chapel Hill	$225,000	$0.00	$225,000.00
FY 16 Total Contractual Funding Awarded		$824,216		
FY 16 Contractual Funds Expended (Init. Projects)			$273,502.87	
FY 16 Contractual Funds Remaining to be Spent				$550,713.13
FY 17 Contractual Funding		**$815,000**		
FY 17 Contractual Funding Transfers		**$0**		
FY 17 Total Contractual Funding		**$815,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
17-007	Univ. of Texas - Austin	$205,500	$81,942.87	$123,557.13
17-024	Atmospheric and Environmental Research, Inc.	$170,039	$121,660.62	$48,378.38
17-032	Drexel University	$59,000	$6,908.77	$52,091.23
17-039	Univ. of Alabama - Huntsville	$149,227	$16,392.12	$132,834.88
17-053	Aerodyne Research, Inc.	$185,193	$21,668.75	$163,524.25
17-SAFS	Univ. of Texas - Austin	$46,000	$0.00	$46,000.00
FY 17 Total Contractual Funding Awarded		$814,959		
FY 17 Contractual Funding Expended (Init. Projects)			$248,573.13	
FY 17 Contractual Funds Remaining to be Spent				$566,426.87
Total Contractual Funding		$1,639,216		
Total Contractual Funding Awarded		$1,639,175		
Total Contractual Funding Remaining to be Awarded		$41		
Total Contractual Funds Expended to Date			$522,076.00	
Total Contractual Funds Remaining to be Spent				$1,117,140