AIR QUALITY RESEARCH PROGRAM

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

Quarterly Report

December 1, 2017 through February 28, 2018

Submitted to

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March 12, 2018

Texas Air Quality Research Program

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OVERVIEW

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

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

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

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

PROGRAM ACTIVITIES FOR THE QUARTER

Program activities during this reporting period were focused on the completion of the research projects, completion of the State of the Science Assessment, and the development of the Strategic Research Plan for a new Request for Proposals.

The final research project ended on January 15, 2018. By the end of February, all final reports were completed and accepted, all final invoices were paid, and all project data was received. Complete project information is now posted on the AQRP website. The Research Project section of this report provides the Executive Summary and details the funds utilized in the performance of each of the projects.

The draft State of the Science Assessment, providing a comprehensive overview of the research performed under the AQRP, was completed in December and sent to the Independent Technical Advisory Committee for review and comment. Comments received in January were addressed and a revision of the report was sent to the TCEQ and the Advisory Council for additional review and comment. Advisory Council comments were addressed in February and a new revision was sent to TCEQ for comment.

Utilizing State of the Science Assessment's evaluation of the program successes, challenges, and areas that should be considered a priority for future research activities, and in consultation with the TCEQ and the Advisory Council, a draft Strategic Research Plan was developed. A meeting will be held next quarter to finalize this document. Once the Strategic Research Plan is finalized, a new Request for Proposals will be developed and released.

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).

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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.
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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).

On September 4, 2017, the AQRP contract was renewed for the 2018 – 2019 biennium and additional funding of $750,000 per year was awarded.

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.

The final research project for FY 2016-17 ended on January 15, 2018, and all final reports were posted to the AQRP website. The strategic research priorities for the FY 2018-19 program cycle have been developed and are being reviewed by TCEQ and the ITAC.

RESEARCH PROJECTS

FY 2016 – 2017 Projects

Project 16-008	**STATUS: Active – September 22, 2016** **Completed – October 31, 2017**

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   **Expended Amount:** $189,684.87

Amount Returned to AQRP: $1,681.13

Executive Summary

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 two main factors: meteorology and out-of-state emissions. This project first estimated and quantitatively separated the effects of a number of meteorological events on peak ozone and background ozone in HGB. With regard to out-of-state emissions, the second part of the project focused on fire emissions from Central America, a large fire region globally of unique importance to Texas air quality whose impact on Texas background ozone has not been quantified previously.

Long-term meteorological and ozone data were analyzed to identify the days of five meteorological events (heat wave, stagnation, thunderstorm, cold front, and post front) and three high ozone events (exceedance, top 15% peak ozone, and top 15% background ozone) in the HGB region during the ozone season (April - October) of 2000 – 2015. Changes in peak ozone and background ozone distributions were compared for each event, except for heat wave because of its extremely uneven distribution. The effects of meteorological events on peak and background ozone were ranked by changes in median ozone during the event days as compared to the non-event days. These analyses led to the following major findings:

1. High background ozone days often have high peak ozone; for example, the top 15% background ozone days have 30 ppbv higher peak ozone than the other 85% of days and coincide with 55.5% of ozone exceedances.
2. Background ozone plays a more important role than local ozone in relative contribution to ozone exceedance at HGB. About 62% of exceedance days would have been avoided during the study period if background ozone had been reduced by 30%. The same fractional reduction of local ozone would have avoided only 40% of exceedance days.
3. The ranking of meteorological events according to their effects on HGB peak ozone is: stagnation > post front > cold front > thunderstorm, and the ranking based on background ozone effects is: post front > cold front > stagnation > thunderstorm. Only thunderstorm shows a decreasing effect on peak and background ozone; other meteorological events are all associated with higher levels of peak and background ozone.

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4. Stagnation has the largest effect on both peak ozone and background ozone at HGB, causing an increase in the median of peak ozone by 26 ppbv and background ozone by 16 ppbv. The associated effects are largest in spring, with 50% co-occurrence with exceedance, followed by 40% during fall.
5. Post front increases ozone in all seasons, with the median enhancement of 11 ppbv for peak ozone and 12 ppbv for background ozone. Cold front has a comparatively smaller effect. Both events are interconnected and co-occur with 15% of high ozone days.

The second part identified the days when Central American fires were transported to HGB and quantified those fire impacts on HGB background ozone during April and May of 2000 to 2015 using back trajectory analysis and GEOS-Chem model simulations. Observational and modeling analyses of Central American fire impacts led to the following major findings:

6. Strong evidence is found consistently from ground measurements, satellite observations, and modeling that Central American fires cause significant ozone enhancements at HGB on episodic bases during springtime.
7. The average number of days when HGB experience significant influences from long-range transport of Central American fire plumes is estimated of 2.1 days per month during April and May, with large temporal variability.
8. Two independent methods give qualitatively consistent estimates of ozone enhancements at HGB due to Central American fires in springtime: 5.67 ± 1.00 ppbv from the back trajectory method and 8.8 ± 1.6 ppbv from the GEOS-Chem passive tracer simulation.
9. Both MOPITT and MODIS satellite instruments detect significant enhancements of CO column densities and AOD, respectively, along the transport route from Central America fire regions to HGB during the GEOS-Chem identified fire-impact days, leading support to the modeling methodology.

Project Update

Project 16-008 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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   **Expended Amount:** $69,075

Amount Returned to AQRP: $0.00

Executive Summary
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 emissions of nitrogen oxides (NO_x) may be overestimated in the EPA's National Emissions Inventory (NEI), perhaps by as much as a factor of two. This overestimate has generally been attributed to the mobile source sector, for which emission estimates are prepared using EPA's MOVES model (Fujita et al., 2012; Anderson et al., 2014; Canty et al., 2015). 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 (Koupal et al., 2014; Warila et al., 2017).

Starting in 2014, the EPA mandated air quality monitoring next to selected major roadways throughout the United States; near-road air quality data for various pollutants, including CO and NO_x, have been collected by monitoring agencies (DeWinter et al., 2015). These routinely collected near-road pollutant concentrations and assessments provide an important resource to support evaluation of mobile source emissions inventories and air quality impacts. This study used near-road monitored concentration data to examine MOVES emissions estimates for NO_x at the local scale and identified which input parameters have the greatest influence on MOVES-based NO_x emissions estimates. Using emissions reconciliation and sensitivity analyses for three case studies in Texas, the results of this work support emissions inventory development and air quality management efforts in Texas by providing information on (1) the accuracy of current MOVES emissions estimates for NO_x, and (2) the MOVES input parameters for which local data collection is most important.

Methods
A CO and NO_x emissions reconciliation analysis was performed at three urban near-road sites in Texas: El Paso, Houston, and Fort Worth. The emissions reconciliation method has been used for more than two decades to identify omissions or inaccuracies in an emissions inventory by comparing emissions data and ambient concentration data (Fujita et al., 1992; Wallace et al., 2012). This method includes selective, quantitative comparisons of emissions-derived (e.g., using MOVES emissions output) and ambient-derived (based on monitored concentrations) metrics, such as carbon monoxide (CO)-to-NO_x (CO/NO_x) molar pollutant ratios (e.g., Chinkin et al., 2005). In this reconciliation analysis, a regression approach was used to derive ambient CO/NO_x ratios, with the data selection process targeting morning commute hours when the monitoring sites were downwind of the adjacent roadway. The MOVES model (MOVES2014a), using national default and county-level local inputs, was used to develop on-road mobile source

CO and NO$_x$ emissions and the corresponding emissions-based CO/NO$_x$ ratios on an annual and seasonal basis. The ambient- and emissions-based CO/NO$_x$ ratios were compared.

For each of the three case study sites, a base scenario and 18 MOVES sensitivity testing scenarios were developed to represent various levels of selected input data. Changes in NO$_x$ emissions and CO/NO$_x$ ratios were quantified with respect to fleet mix (truck percentage), vehicle speed (VMT by speed distribution), vehicle age (VMT by age distribution), and meteorology (ambient temperature and relative humidity).

Results
The ambient-based annual CO/NO$_x$ ratios near roadways during morning hours were calculated as 7.76 ± 0.10 at El Paso, 8.56 ± 0.17 at Houston, and 7.04 ± 0.19 at Fort Worth; these ratios are generally within the range of historic values calculated in previous studies. For all cases, CO/NO$_x$ ratios based on MOVES default estimates were much lower than ambient-based ratios, ranging from 2.7 (Houston winter weekday) to 4.7 (Fort Worth summer weekday). Overall, using default inputs in MOVES consistently resulted in underestimation of observed ambient CO/NO$_x$ ratios; this implies that, based on MOVES default input data, emissions estimates for CO or NO$_x$, or both pollutants, are not modeled correctly and do not reasonably represent on-road mobile sources in the emissions inventory.

When best available local (BAL) data inputs are used in MOVES, the resulting CO/NO$_x$ ratios are in much better agreement with ambient-based ratios, though these ratios differed from the ambient ratios depending on the period and location. The ambient-based ratios are comparable to the MOVES emissions-based ratios for the annual and winter weekdays when local data inputs were used (within the acceptable 25-50% range of agreement): at the El Paso site, on average, the difference between ambient-based and MOVES-based ratios was within 24%; similar mean results were shown at Houston (within 19%) and Fort Worth (within 30%). In general, the comparison indicates the importance of using BAL MOVES inputs to generate more accurate emissions estimates. Both ambient- and emissions-based CO/NO$_x$ ratios were higher in summer than in winter; this is expected given that near-road measurements indicate a larger increase in NO$_x$ than in CO mixing ratios from summer to winter. However, CO/NO$_x$ ratios modeled in MOVES exhibit a larger seasonal variation than ambient-based ratios.

The El Paso, Houston, and Fort Worth case studies in the emissions sensitivity analysis demonstrated the importance of replacing and improving MOVES default inputs with local data to allow a more robust assessment of on-road vehicle emissions. Among the MOVES input parameters tested in the sensitivity study, fleet mix and vehicle age distribution have larger effects than vehicle speed distribution and meteorological data on NO$_x$ emissions estimates. Therefore, these input parameters should be of highest priority for data collection. The results from this study suggest that, when appropriate local data are used, MOVES can reasonably reflect mobile source emissions in the inventory; MOVES emissions-based ratios are comparable to the ratios derived from ambient measurements in reconciliation analyses. However, relying on MOVES default inputs can generate biased ratios and lead to incorrect emissions assessments and conclusions. The evaluation of the mobile source NO$_x$ emissions inventory (e.g., the assessment of NEI in recent studies) should consider how MOVES default inputs are used and what their effect is on emissions estimates.

Recommendations

Further analysis will be useful, based on the existing emissions reconciliation and sensitivity analyses, to improve MOVES-based NOx emissions estimates. Recommended studies include:

- Revisiting how MOVES emissions were developed and what key assumptions were made (especially related to MOVES default) in recent studies that concluded over-estimation of mobile source NOx emissions in the NEI. An important practical issue to address is building the connection between EPA's NEI development and local emissions inventory development. Carefully designed assessment is needed to understand how default data were used in MOVES modeling for the NEI, and how the NEI can be improved by ensuring consistency with MOVES emissions inventories developed by state or regional air quality agencies using local data.

- Assessing more temporally and spatially refined MOVES emissions modeling results (e.g., by season, month, weekday vs. weekend, and facility type) to better understand the larger seasonal variation in MOVES emissions-based ratios.

Identifying challenges related to preparation of local MOVES input data, developing potential methods to fill local data gaps, and implementing the methods to improve local data use for the NEI and MOVES-based mobile source emissions inventories.

Project Update

Project 16-010 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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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   **Expended Amount:** $158,127.36

Amount Returned to AQRP: $6.64

Executive Summary
Emissions of reactive gases and particles from terrestrial ecosystems (biogenic emissions) drive atmospheric distributions of several constituents relevant for air quality and climate. Biogenic emissions tend to be 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 strategies for mitigating air pollution and climate change. Biogenic VOC emission estimation activities date back more than 50 years when Dr. Fritz Went made a first attempt to quantify biogenic VOC emissions into the atmosphere. A series of models was developed in the in the US, specifically BEIS, BEIS2, BEIS3, MEGAN and MEGAN2, using a similar framework and base data and yet the results often differed by more than a factor of two (Warneke et al. 2010). The BEIS models were intended to be used for regulatory air quality modeling with fixed landcover and parameters. MEGAN was designed to be more flexible and for use by both regulatory air quality modeling and scientific research. Comparison of these models has been complicated by emission factors, response functions and environmental conditions calculations that were difficult to extract from the models and to determine their origin. A transparent approach for determining emission factors and other variables and a modular approach for evaluating each model component would facilitate efforts to assess and improve biogenic emission models.

The goal of AQRP Project 16-011 was to improve numerical model predictions of regional ozone and aerosol distributions in Texas by reducing uncertainties associated with quantitative estimates of biogenic volatile organic compound (BVOC) emissions from Texas and the surrounding region. We aimed to reduce emission uncertainties associated with the absolute magnitude of the emissions and the response of the emissions to changes in plant stress (e.g., water and heat stress) and to improve the ability of biogenic emission estimation tools to better predict emissions of monoterpenes and responses to short- and long-term drought stress. This project incorporated biogenic emission findings from previous Texas projects into a version of a biogenic model appropriate for Texas air quality applications. Results from previous Texas AQRP projects and other studies were incorporated into a new version 3 of the Model of Emissions of Gases and Aerosols from Nature (MEGAN3).

Our specific objectives included:

1. Develop a database system that provides a transparent approach for estimating BVOC emission factors.
2. Synthesize available isoprene and monoterpenes emission and concentration observations for Texas and surrounding regions, reconcile any discrepancies, and calculate Texas isoprene and monoterpene emission factor best estimates and ranges.
3. Include in MEGAN3 missing compounds and unrepresented processes including stress induced (drought, extreme temperature and air pollution) emissions and canopy heterogeneity.
4. Investigate MEGAN3 sensitivity to data used for calculating emission factors and stress induced emission algorithms. Evaluate model emission and ambient concentration estimates using surface and aircraft observations and a photochemical model.

All four objectives were accomplished as summarized by the following:

MEGAN Emission Factor Processor:
An Emission Factor Processor for MEGAN3 (MEGAN-EFP) was developed as an open source Python code to ingest driving variables and calculate landscape scale biogenic emission factors and other model drivers. The approach is flexible so that users can use any available land cover and emissions data and can investigate the performance of various datasets. A data quality rating system was implemented so that the user can choose to omit low quality data. The framework was implemented for BVOC emissions, specific leaf area and emission light dependence fraction and can be extended to include other plant and soil traits that can vary spatially. The emission factors calculated with the MEGAN-EFP are highly transparent in that the landcover and emission data that they are based on can be traced back to specific publications.

Texas Isoprene and Monoterpene Emissions Data:
High quality enclosure measurements of isoprene emission were available for a large fraction of the tree species that comprise most of the total isoprene emission in Texas and were integrated into the MEGAN-EFP. Utilizing the MEGAN-EFP, it was determined that almost all of the Texas isoprene emitting trees are members of just three genera (oaks, sweetgum, tupelo/gum), all of which have had at least one species investigated with state-of-the-art techniques. The comparison also demonstrated that the differences between BEIS and MEGAN isoprene emission estimates are primarily due to the specific leaf area (the leaf area to leaf mass ratio) estimates and reconciled discrepancies between leaf enclosure and aircraft estimates of isoprene emission factors. The evaluation also indicated that one tree genera, the oaks, are highly diverse with many species in Texas and the surrounding region that have not been studied so the possibility exists that some of these oak species may emit isoprene at substantially different rates than those that have been studied. The assessment also revealed that there are no high quality isoprene emission data for tree species other than the high isoprene emitters in Texas and most other regions. This allows the possibility that some of the tree species thought to be non-emitters may actually have non-zero emission rates.

The available Texas monoterpene emissions data were incorporated into the MEGAN-EFP but there were no high quality enclosure measurements of monoterpene emissions for any Texas trees. Aircraft monoterpene flux measurements were incorporated into the database and currently are the best approach for constraining monoterpene emission factors.

MEGAN3 Model:
The MEGAN model code was improved by making the code more modular and easy to follow, by removing unneeded code, by adding additional compounds that may have an important role in air quality and previously unrepresented processes, and by incorporating recent results into the existing algorithms and parameters. Also, an error in the soil NOx emissions code was fixed. The resulting code, called MEGAN3, provides a modular framework that can be updated as additional knowledge and driving variables become available.

MEGAN3 Sensitivity and Evaluation:
A comparison of MEGAN2.1 and MEGAN3, with the emission factors generated by the initial runs of the MEGAN-EFP, indicated that the MEGAN3 isoprene emissions were considerably lower than MEGAN2.1 and in better agreement with aircraft flux and concentration measurements. Within Texas and across the southeastern US, there was a reduction in monoterpene emissions calculated in MEGAN3 relative to MEGAN v2.1 that degraded agreement. Concentration comparisons using the Comprehensive Air quality Model with extensions (CAMx) indicate that estimates of monoterpenes aloft and surface ozone were often considerably lower using the MEGAN3 estimates. For surface ozone, the net effect on model agreement with observations was mixed and varied by site. CAMx underestimated the aircraft monoterpene concentration measurements using MEGAN v2.1 emissions and the underestimate became more pronounced using MEGAN3. The cause of the reduction of monoterpene emissions in MEGAN3 is not known, but is under investigation. Assessment of the new stress algorithms (high temperature, low temperature, high winds, high ozone) incorporated into MEGAN3 indicated that there was relatively little impact on isoprene and monoterpenes using the initial parameterizations. These stresses are expected to have a greater impact on other biogenic VOC.

AQRP Project 16-011had the following conclusions:
MEGAN3 can be used to provide biogenic emissions estimates that are more accurate than MEGAN2.1 as demonstrated by comparison to aircraft flux measurements. MEGAN3 also facilitates assessing and improving individual model components including emission factors, canopy and soil environment conditions, and response functions which should lead to improvements over alternative models that are based on outdated emission factors and model algorithms.

The MEGAN3 framework can be used for assessing available landcover and emissions data and identifying gaps. The available landcover and emissions data that were incorporated for the initial database used for this project improved isoprene emissions for the regions investigated by the 2013 SAS aircraft study. Discrepancies between enclosure and aircraft measurements of isoprene emissions pointed out in previous studies were reconciled. Specific Leaf Area (ratio of leaf area to mass) was identified for the first time as a major reason for differences in BEIS and MEGAN isoprene emission estimates. Additional gaps were identified associated with isoprene, such as oak species emission diversity, and especially monoterpene emissions, for which there are few high quality data. Other compounds, including sesquiterpenes, oxygenated VOC, and semi-volatile compounds, may be important but are relatively unstudied.

Distributions of tree species, the major source of isoprene and monoterpene emissions in Texas, can be adequately estimated with existing landcover data in forested regions. Additional efforts are needed to improve tree species distributions in urban and savannah locations. This includes

integrating all of the existing data into the MEGAN3 landcover database and developing new landcover data such as plant species composition data for non-forested landscapes. Isoprene and other VOC emission studies have focused on closed canopy forests. The performance of models in open canopies in savannas and shrublands, including those that dominate in Central Texas and other regions, has not been well characterized and the existing landcover data, canopy environment and isoprene response functions may not be suitable for these landscapes.

Project Update
Project 16-011 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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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

Executive Summary

Alkyl nitrates have the potential to influence tropospheric ozone and secondary organic aerosol formation over regional to global spatial scales. Advances in analytical techniques and their applications in laboratory studies and major field campaigns have led to new insights on the atmospheric chemistry and fate of alkyl nitrates. The objectives of this study were to integrate these findings into the Comprehensive Air quality Model with extensions (CAMx) and investigate the effects on predicted regional ozone and fine particulate mass and composition in eastern Texas. Updates to the CB6 chemical mechanism in CAMx (from a starting point of CB6r4) focused on alkyl nitrates formed from biogenic monoterpene precursors and anthropogenic alkane precursors relevant to Texas emission inventories as well as characterization of the loss of alkyl nitrates due to hydrolysis. This new mechanism version is CB6r6d4.

The most recent release of CAMx, v.6.40, with meteorological fields from the Weather Research and Forecast (WRF) model v.3.6.1 and the CB6r4 gas-phase mechanism, was applied for the time period of August 18-September 30, 2013 that spanned the Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign in southeastern Texas. Model performance was assessed using observations from CAMs surface sites in eastern Texas and observations at the surface and aloft made during DISCOVER-AQ. Three schemes for organic gas-aerosol partitioning and oxidation in CAMx were evaluated: 1.5-D Volatility Basis Set (VBS), Secondary Organic Aerosol Partitioning (SOAP2), and a new scheme developed in this work, SOAP2r3, that included secondary organic aerosol (SOA) loss by photolysis. The SOAP2r3 and 1.5-D VBS schemes provided generally comparable model performance for trace gases and $PM_{2.5}$ total mass and component concentrations. The SOAP2r3 scheme is expected to be more easily applied for modeling efforts that support air quality planning and management and was selected for the base case.

Sensitivity studies were conducted that considered the individual and net effects of modifications to the CB6r4 gas-phase mechanism and SOA yields of the base case:

Hydrolysis of Multifunctional Organic Nitrates
Hydrolysis of multifunctional organic nitrates (i.e., the CB6 NTR2 species) was represented in the base case CB6r4 mechanism as a pseudo gas-phase reaction producing nitric acid (HNO_3) with lifetime of 6-hours. The lifetime against hydrolysis was reduced to 1-hour consistent with recent findings that very short lifetimes are appropriate for acidic aerosols. Regional ozone concentrations were insensitive to more rapid hydrolysis. Hourly total $PM_{2.5}$ mass concentrations increased by as much as 0.5 $\mu g/m^3$ on average due to an increase in particulate NO_3. Maximum increases in total $PM_{2.5}$ mass concentrations were approximately 6 $\mu g/m^3$ and occurred in areas where the sensitivity of multifunctional organic nitrates to biogenic volatile organic compound (BVOC) emissions dominated anthropogenic emissions.

Monoterpene Chemistry
Recent studies have indicated the importance of nitrate radical (NO_3)-monteprene chemistry to SOA formation, but that SOA yields are variable, with α-pinene consistently lower than for other monoterpenes. The CB6r4 mechanism was modified to split terpenes to α-pinene (APIN) and other terpenes (TERP). Revisions were made to the gas-phase reactions of TERP and APIN with hydroxyl radical (OH), ozone (O_3), and NO_3 and to SOA yields for TERP and APIN reactions with NO_3. The impacts of these modifications primarily occurred in terpene-rich areas of the modeling domain including northeastern Texas, western Louisiana, southwestern Arkansas, and southern Mississippi. Average decreases in hourly ozone concentrations were 0.5 ppb with a maximum of 1 to 2 ppb. Differences in hourly total $PM_{2.5}$ mass and organic aerosol were within ±0.5 $\mu g/m^3$ on average with maximum differences of -2 to +5 $\mu g/m^3$.

Alkane Chemistry
Long-chain alkanes are precursors to alkyl nitrates that contribute to SOA formation and serve as a potential NO_x sink via hydrolysis. Alkanes were split into PAR and PARH, which has a high AN yield, according to chain length. Revisions were made to the gas-phase reactions for PAR and PARH as well as ketones. PAR and PARH fractions were applied by emissions source sector with, for example, lower PARH fractions applied for the oil and gas sector (10%) than mobile sources (20%). Total $PM_{2.5}$ mass concentrations were relatively insensitive to the modifications in AN yields using the PARH scheme. Widespread increases in ozone were 1-2 ppb. Application of the PARH scheme decreased the total alkyl nitrate burden and increased ozone sensitivity to VOC emissions from the oil and gas sector and other anthropogenic sources.

Project Update
Project 16-019 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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   **Expended Amount:** $223,820.08

Amount Returned to AQRP: $1,179.92

Executive Summary
Isoprene is the most abundant non-methane volatile organic compound emitted into the Earth's atmosphere. Eastern Texas and northern Louisiana feature some of the largest biogenic emission sources of isoprene in the United States. Recent studies have shown that the atmospheric photo-oxidation of isoprene is a major source of fine particulate matter ($PM_{2.5}$) through the formation of secondary organic aerosol (SOA) particles. In addition, the gas phase oxidation pathways that form SOA precursors can also impact ozone (O_3) production. The goal of the work is an evaluation of the current science on estimation methods for isoprene derived SOA and the gas-phase reactions that produce their precursors. For this evaluation, a modeling system was implemented that incorporated detailed field measurement data and new experimental data was generated aimed at reducing modeling uncertainties. This work directly addresses the stated priority area of improving the understanding of O_3 and $PM_{2.5}$ formation and their interaction with precursors. The goals of the project were achieved through the completion of the following tasks:

- *Task 1:* Updated SAPRC-07 for Isoprene Oxidation Evaluation
- *Task 2:* Laboratory Experiments: The Effects of Particle-Phase Composition, Phase, and Viscosity on IEPOX-Derived SOA Formation
- *Task 3:* Implementation in an Air Quality Model

Task 1 focused on evaluating the state-of-the-science in gas-phase mechanisms in terms of its ability to produce critical SOA precursors and replicate O_3 chemistry. As part of this project the latest version of the SAPRC16 chemical mechanism was evaluated against other mechanisms and with UNC smog chamber data. The chamber data came from 40 experiments (16 characterization runs and 24 isoprene runs) completed at the UNC Dual Smog Chamber Facility (Pittsboro, NC) with isoprene runs that had a range of NO_X (NO_X = NO + NO_2) to isoprene ratios. When compared to the chamber data the SAPRC16 mechanism improves model performance with respect to predictions of peak O_3 and nitric oxide (NO)/nitrogen dioxide (NO_2) crossover times.

The goal of Tasks 2 and 3 were to assess current state of the science models for the prediction of isoprene derived SOA. Specifically, this work focused on the isoprene epoxydiols (IEPOX)-derived SOA formation chemical pathway. In summary, this chemical pathway begins with reactions with the hydroxyl radical (OH) under low NO conditions producing isoprene hydroxyl

hydroperoxide (ISOPOOH). ISOPOOH can further react with OH to form IEPOX that then partitions onto pre-existing acidic sulfate aerosol seed forming IEPOX-derived SOA. Task 2 produced new data on the impact that organic coatings could have on this uptake process. In current modeling applications the existing sulfate aerosol seed is treated as a homogeneous mixture with reactive parameters derived from empirical data. While in the real atmosphere an aerosol particle can be coated by organic layers formed by gas-phase oxidation of volatile organic compounds (VOCs) that will change the physical and chemical properties of the seed. Therefore, a more accurate IEPOX-SOA prediction should be achieved by including the effect of coatings on the heterogeneous (multiphase) reactive uptake method.

The critical findings from the experiments in Task 2 included new data showing a strong dependence on aerosol state where the reactive uptake coefficient of IEPOX was reduced by 10 times (compared to pure acidic sulfate aerosol) with only approximately 10 nm of organic coating on existing acidic sulfate aerosol particles. Furthermore, the reduction of the reactive uptake coefficient of IEPOX is non-linear with regards to the SOA coating thickness. Microscopy data was also obtained through existing collaborations that provided evidence for choosing a core-shell morphology resistor coating approach for modeling the acid-catalyzed reactive uptake of IEPOX. These results from Task 2 were also used to justify decisions in parameter values for the development of the 0-D model produced in Task 3.

The modeling in Task 3 included the implementation of a heterogeneous reactive uptake coefficient of IEPOX that included the influence of existing organic coatings on IEPOX-SOA formation. All modeling runs relied on field measurements taken during the 2013 Southern Oxidant and Aerosol Study (SOAS) in 2013 at the Look Rock (LRK), Tennessee ground site. For the model it was assumed that the SOA coated acidic sulfate particles has a core-shell morphology and a resistor coating model was adopted. In summary, the model assumes that the formation of IEPOX-derived SOA is predicted as a first order reaction with a heterogeneous reactive uptake that includes several physical and chemical parameters: aerosol acidity, relative humidity (RH), diffusion in particle phase, particle reactivity, the capability that aerosol seeds can absorb mass, and coating effects. The 0-D model was used to predict 2-methyltetrols (tetrols) and organosulfates (IEPOXOS) and found reductions in concentrations when existing coatings were included. Peak tetrol concentrations were reduced by 75% and on average by 30%. IEPOXOS had similar differences with the largest by 62% and on average by 22%. Overall, the modeling showed a 30% reduction in the reactive uptake coefficient of IEPOX across all modeling days.

Key Findings
- Experimental data show measurable reductions in the reactive uptake process of IEPOX to form SOA. The reactive uptake coefficient of IEPOX can be reduced by 10 times with only approximately 10 nm of existing SOA coating.
- The SOA coating thickness and reactive uptake coefficient of IEPOX have a negative correlation relationship. Further, the results show that the reduction of the reactive uptake coefficient is non-linear with regards to SOA coating thickness.
- The level of reduction in the reactive uptake coefficients of IEPOX depends on SOA type. α-Pinene SOA has the smallest reduction while naphthalene SOA has the largest reduction.

- Microscopy data of α-pinene SOA-coated acidic sulfate particles suggests a core-shell morphology.
- A model using a core-shell organic resistor model with consideration of existing SOA coatings improves SOA predictions when compared against field measurements.
- Evaluation of latest SAPRC16 shows improvement when compared with SAPRC-07 in simulating UNC chamber observed peak O_3 and NO/NO_2 crossover times.

Project Deliverables
- Produced modeling system, with integrated experimental data of isoprene photooxidation experiments in the presence of NO_x, for evaluation of the SAPRC16 mechanism.
- Developed and proved a methodology that allows for higher throughput of experiments and effective oxidation of aerosols for systematic understanding of how humidity, chemical composition, and existing SOA coating thickness influence the reactive uptake of gaseous IEPOX into the particle phase to yield new SOA.
- Experimental data on impact on reactive uptake coefficients of IEPOX as a function of three SOA coating types, four SOA coating thicknesses, and three relative humidity levels.
- A 0-D model fully integrated with SOAS field data for predicting heterogeneous IEPOX SOA formation that includes the influence of coatings

Project Update
Project 16-031 is complete. The final report is approved and all invoices have been paid.
Project data has been submitted to the AQRP.

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   **Expended Amount:** $202,348.21

Amount Returned to AQRP: $3,151.79

Executive Summary
This project's purpose was to identify a reliable means of measuring the vapor pressure of heavy refinery liquids. These liquids include commercial materials such as fuel oil no. 6, which is used as a marine fuel and less often for heating or power generation, and liquid asphalt, whose uses include paving and roofing. Heavy refinery liquids also include intermediate streams and blend stock, such as vacuum residual.   These materials are generally stored at elevated temperatures because they are too viscous to be pumped at ambient temperatures. For example, fuel oil no. 6 is typically stored near 120°F and liquid asphalt near 200°F.

Background
The vapor pressure of these materials is a key parameter when estimating emissions of volatile organic compounds from storage tanks (US EPA 2006), but their vapor pressures are not well understood. The properties of these materials (e.g., low vapor pressure, high viscosity, high opacity) can create challenges when measuring their vapor pressure, and measurements are rarely attempted. Vapor pressure default values are only available for vacuum residual and fuel oil no. 6 (API 2012 with addendum dated 2013; US EPA 2006), and there is no body of data that shows whether or not these default values bear any resemblance to typical vapor pressures for these materials. Results from direct measurement (US EPA 2015) and remote sensing techniques used to estimate volatile organic compound (VOC) emissions from heated storage tanks suggest that heated storage tanks might be responsible for some of the gap between estimated emissions of VOCs and observed concentrations of VOCs in some locations. If this is the case, it could be that estimated emissions are low because unrealistically low values for vapor pressure were used in the equations that are used to estimate VOC emissions from storage tanks.

Heavy refinery liquids are complex mixtures and their composition varies from source to source and from time to time at the same source. Fuel oil no. 6 and liquid asphalt are particularly complex, as they generally consist of a very heavy refinery stream that is blended with a somewhat lighter refinery stream to create the desired properties. These materials are not uniform; they vary in their physical properties and in their chemical composition.

It is the light ends in these liquids that drive vapor pressure, but accurately measuring the composition of the light ends is made difficult by the properties of the streams. Even if accurate concentrations of light ends in the streams could be obtained, the mixtures are far from ideal and an unknown amount of uncertainty would be introduced if Raoult's law were to be used to estimate the vapor pressure of these materials.

Approach
There is no gold standard for measuring the vapor pressure of a mixture, so there is no way to determine the accuracy of measured results by comparing them to a value that is known to be correct. In this project, this difficulty was addressed by applying a number of potentially appropriate methods to the study materials and by including study materials whose vapor pressure was either reasonably well understood or documented. The vapor pressure methods employed include:

At commercial laboratories:

- ASTM D2879 (2010a) (vapor pressure by isoteniscope; this is the method the US EPA (2006) refers to as defining the vapor pressure of volatile organic liquids for which vapor pressures from default values or standard reference texts are not available; it was conducted at three labs)
- ASTM E1719 (2012) (vapor pressure by ebulliometry)
- ASTM D323 Procedure A (2015) (Reid vapor pressure; in this method, the vapor pressure of an air- and water-saturated sample is taken at 100°F and its results are expected to represent an upper bound on measured vapor pressures of the study materials at 100°F)

Using two makes of automated mini method instruments (Grabner and Eralytics):

- ASTM D6378 (2010b) (triple expansion method), which can be conducted in single point mode, where a separate triple expansion is conducted for each measured temperature, and in multi point (Grabner) or curve (Eralytics) mode, where results from a triple expansion at one temperature are applied to the same sample at other temperatures
- methods based on ASTM D6378 that had instrument hardware modifications intended to make them more suitable for measuring the vapor pressure of heavy refinery liquids (Eralytics refers to this as their "low VP" method and Grabner refers to it as their "VOC" method)

The study materials were

- a "known" recipe (80 mol % n-nonadecane and 20 mol % octane) whose modeled vapor pressure can be reasonably expected to be accurate to within 10%
- a hydraulic fluid whose manufacturer provided detailed vapor pressure data
- three fuel oil no. 6 samples designated as MM, MB, and BT

Analysis of Results
Figures ES-1 through ES-5 show the results of the vapor pressure measurements for each of the five study materials in the temperature range of interest for heated storage tanks. Some of the results from commercial labs fall outside this temperature range. All of the data points can be viewed in figures in the analysis section of the main report.

In Figures ES-1 through ES-5, the y-axis is the vapor pressure in psi on a log scale and temperature is on the x-axis. The gold, yellow, and orange lines are the ASTM D2879 (vapor pressure by isoteniscope) results for three commercial labs, which are presented as measurements (large circular markers connected by a thin line) and values calculated by the labs

from a curve fit of inverse absolute temperature to base 10 logarithm of pressure for the data points obtained at higher temperatures (dotted lines). This curve fit procedure is described in ASTM (2010a). The red dotted lines represent the lab's calculated results and the red circular markers connected by thin red lines represent measured results from ASTM E1719 (vapor pressure by ebulliometry). The calculated results for ASTM E1719 are obtained from a curve fit of inverse absolute temperature to base 10 logarithm pressure, as described by ASTM (2012). The green circular markers are the low VP single point readings from the Eralytics instrument, and the blue line and blue circles are from Grabner multipoint ASTM D6378 readings and Grabner VOC single point readings, respectively. "First" Grabner refers to the first Grabner instrument used in the project and "second" Grabner is the second instrument.

The black dashed line in Figure ES-1, the "known" recipe chart, is the vapor pressure for that mixture as modeled using the Soave-Redlich-Kwong equation of state. The black dashed line in Figure ES-2 (for the hydraulic fluid) represents the manufacturer's vapor pressure values. The black dashed lines in Figures ES-3 through ES-5 (for the three fuel oil no. 6 samples) represent the API (2012 with addendum dated November 2013) default value for fuel oil no. 6.

Because there is a fair amount of confidence in the modeled expectations for the vapor pressure of the "known" recipe, it is an interesting test case for the various methods. Figure ES-1 shows that along with the Eralytics instrument's results from the low VP single point method and the ASTM D2879 results produced by Lab 3, the Grabner ASTM D6378 multipoint curve (obtained on the first instrument) and single point VOC method results (obtained on the second instrument) are in good agreement with modeled expectations above 100°F for this material. Note that lab 3, the lab whose ASTM D2879 measurements are in good agreement with the modeled vapor pressures, is the only lab that is accredited for ASTM D2879. This figure shows that in this temperature range, there were no instances where a measured vapor pressure using ASTM D2879 by any of the three commercial labs that applied this method exceeded the modeled vapor pressure. It is possible that this lower bound on vapor pressure from ASTM D2879 holds true for all of the study materials because when conducting this method the likelihood of unknowingly obtaining mistakenly high readings is low. Of the results produced by commercial laboratories (both ASTM D2879 and ASTM E1719), the best agreement with the modeled expectations for vapor pressure were the results for ASTM D2879 (vapor pressure by isoteniscope) from Lab 3 and the poorest agreement were the results for ASTM D2879 from Lab 1. The mini method instrument results show better agreement with modeled expectations for vapor pressure at the higher temperatures of the small temperature range over which they were conducted. Most of the measured values for ASTM E1719 (vapor pressure by ebulliometry), many of which were obtained over a tight temperature range above typical storage temperatures for heavy refinery liquids and do not appear in Figure ES-1, were within 10% of the modeled values.

Figure ES-2, for the hydraulic fluid, shows that the vapor pressure values from the calculated (curve-fit) results for ASTM D2879 from all the commercial labs are in very good agreement with each other and are about 1.5 to ten times higher than the manufacturer's values, with less agreement at lower temperatures. The ASTM D2879 measured results for all three labs agree at around 175°F. Labs 2 and 3 also agree at 120°F. The Grabner multipoint ASTM D6378 values and the ASTM E1719 calculated results are also in good agreement with each other, but not with the calculated ASTM D2879 results. They are also higher than the manufacturer's values, from

several hundred times higher at the lowest temperatures that can be compared to seven times higher at the highest temperature values from the Grabner instrument and 1.5 times higher for the E1719 calculated results at 300°F. For this material, the ASTM E1719 measured results were all taken at temperatures above 190°F and thus do not appear in this chart. Also, measurements taken using the Eralytics instrument are not shown in this chart because they were made using instrument methods that relied on algorithms that were later found to be in error.

Figure ES-3, for the MM fuel oil no. 6 sample, shows that the ASTM D2879 results from Labs 2 and 3 seem to be in fairly good agreement with each other but fall nearly an order of magnitude above the API default vapor pressure value. The three pairs of low VP single point readings taken on the Eralytics instrument vary across nearly an order of magnitude at 120°F and 140°F but are similar to each other at 160°F. Figure ES-3 shows that at 140°F, there are measured instrument readings, ASTM D2879 measured values for Labs 2 and 3, and the curve fit for ASTM D2879 for Labs 2 and 3, and all are on the order of a tenth of a psi. The default value (API 2012 with addendum dated November 2013) at 140°F is 0.016 psi. The lower of the two Eralytics single point readings at 140°F falls between the measured values obtained by labs 2 and 3 at this temperature. This is a wet vapor pressure measurement but this material was analyzed for water content using ASTM D95 (water by distillation) and was reported to be 0.00 vol % water.   For this material, the ASTM E1719 measured results were all taken at temperatures above 190°F and thus do not appear in this chart. Also, there are no Grabner mini method instrument results for this material because the Grabner instruments ceased operating before they could be used to test this material.

In Figure ES-4, for the MB fuel oil no. 6 sample, all of the ASTM D2879 measured results from Lab 3 fall above the default vapor pressure values, and except for the upper end of the temperature range, so do the ASTM D2879 measured results for Lab 1. Only three single point readings for the low VP method were obtained using the Eralytics instrument for this material: one at 120°F, one at 140°F, and one at 160°F. The value at 140°F falls below the values at 120°F and 160°F; in reality, the vapor pressure would increase with increasing temperature. The mini method readings, all of the ASTM D2879 measured values for Lab 3 (which begin at 176°F), and all of the measured values for Lab 1 above 140°F are 0.1 psi or higher. The default value (API 2012) reaches a value of 0.1 psi at 223°F. The lower of the two Eralytics single point readings at 140°F falls between the measured values obtained by Labs 2 and 3 at this temperature. This is a wet vapor pressure measurement but this material was analyzed for water content using ASTM D95 (water by distillation) and was reported to be 0.00 vol % water. For this material, the ASTM E1719 measured results were all taken at temperatures above 190°F and thus do not appear in this chart. Also, there are no Grabner results for this material because the Grabner instruments ceased operating before they could be used to test this material. Lab 2 did not provide ASTM D2879 results for this material because they were unable to analyze this material using ASTM D2879.

Figure ES-5, for the BT fuel oil no. 6 sample, shows that all of the ASTM D2879 measured results from Lab 3 fall well above the default vapor pressure values, sometimes two orders of magnitude higher. As with the MB fuel oil no. 6 sample, except for the upper end of the temperature range, the ASTM D2879 measured results for Lab 1 also fall above the default values. Five single point readings for the low VP method were obtained using the Eralytics instrument: two at 120°F, two at 140°F, and one at 160°F. The value at 160°F falls below the

values at 140°F and 120°F; in reality, the vapor pressure would increase with increasing temperature. Four of the five mini method readings, all of the ASTM D2879 measured values for Lab 3 (which begin at 140°F), and all of the measured values for Lab 1 above 140°F are 0.1 psi or higher. The default value (API 2012) reaches a value of 0.1 psi at 223°F. One of the two mini method instrument readings at 140°F is nearly two orders of magnitude lower than the other four instrument readings. For this material, the ASTM E1719 measured results were all taken at temperatures above 190°F and thus do not appear in this chart. Also, there are no Grabner mini method instrument results for this material because the Grabner instruments ceased operating before they could be used to test this material. Lab 2 did not provide ASTM D2879 results for this material because they were unable to analyze this material using ASTM D2879.

The ASTM D323 result for each of the five study materials was < 0.2 psi. This method measures the vapor pressure of a water- and air-saturated sample at 100°F, and the results from ASTM D323 are expected to be higher than results from the other methods at 100°F. The only method that returned a value higher than 0.2 psi at 100°F for any of the materials was the "known" recipe, where the calculated result for ASTM E1719 is higher than 0.2 psi.

Discussion and Conclusions
This project demonstrated that mini method instruments can process samples of heavy refinery liquids and that there is often order of magnitude agreement in measured vapor pressures of heavy refinery liquids using mini method instruments and the commercial lab results of this study. For both ASTM D2879 (vapor pressure by isoteniscope) and the mini method instruments, it appears that accounting for or removing dissolved air in the material being analyzed can be an important source of error in the results. For ASTM D2879, potential opportunities for overcoming this hurdle include conducting the degassing step at very low pressure at the lowest possible temperature and seeding the boil. For the mini method instruments, careful measurement of the vapor volumes and total pressures at the three expansions, along with steps to ensure that pressure measurements are made after equilibrium is established, are potential opportunities for overcoming this hurdle.

ASTM D2879 (vapor pressure by isoteniscope) results from different commercial labs disagreed by more than an order of magnitude in some cases in this project. It is likely that the conditions of the degassing step in this method are a primary cause of disagreement in results at different labs. The only lab accredited for this method produced measurements very near the modeled vapor pressure of a mixture containing a volatile compound and a nonvolatile compound (the "known" recipe), indicating that this method may be appropriate for heavy refinery liquids if the conditions of the degassing step are carefully controlled. None of the measured values of the "known" recipe that were taken using this method by any of the commercial labs were larger than the estimated vapor pressure, indicating that perhaps the measured values taken using this method represent a lower bound on vapor pressure.

The measured results for ASTM E1719 (vapor pressure by ebulliometry) were taken at temperatures higher than the temperatures of interest for estimating emissions from heated storage tanks holding fuel oil no. 6. The measured results of this method were in agreement with the estimated vapor pressure of the "known" recipe. This method generates calculated values for vapor pressure across a wide range of temperatures from measurements taken in a fairly tight

band of temperatures, and these calculated values had a flatter slope than any other method's results for all five study materials.

This project showed that the mini method instruments tested in this study show great promise as tools for measuring the vapor pressure of heavy refinery fuel oils. However, great care and understanding of the operation of the instrument and factors affecting the vapor pressure measurement of these fluids must be exercised when conducting these measurements. The results of the fuel oil no. 6 samples were very sensitive to the values for pressure and volume that were obtained at each of the expansions conducted by the instruments.

Method performance could only be assessed for the "known" recipe because there is no means of verifying the accuracy of measurements taken for any of the other study materials. A summary of method performance for the "known" recipe for temperatures ranging from 60°F to 190°F is given in Table ES-1. ASTM D2879 results from Lab 3 most closely matched the modeled expectations for this material, followed by the mini method instruments. Measured results for ASTM E1719 were in very good agreement with modeled expectations but were only made at the upper end of this temperature range and the curve-fit results for this method ranged from fair to poor. ASTM D2879 results for Lab 1 had the poorest agreement with modeled expectations, ranging from fair to poor, and ASTM D2879 results for Lab 2 ranged from fair to good.

At 100°F and above (which would include typical storage temperatures) the single point mini method results using methods intended for heavy refinery fluids were in every case near the estimated results for the "known" recipe. Except for one measurement at 140°F for the BT fuel oil no. 6 sample, the vapor pressures of the fuel oil no. 6 samples taken using the Eralytics instrument were between 0.1 and 1 psi. In addition, at least some of the Eralytics mini method results were within an order of magnitude of measured results from at least one commercial lab for each of the study's fuel oil no. 6 materials.

ASTM D95 (water by distillation) was performed on the three fuel oil no. 6 samples. The MM and MB fuel oil no. 6 samples were found to contain 0.00 volume % water, but the BT fuel oil no. 6 did contain water at 0.1 or 0.2 volume %. The contribution of water to the vapor pressure of this material was estimated by applying the results from simulation of mixtures of water and hypothetical compounds that were developed based on boiling point distribution and specific gravity of heavy fuel oils. Using this method, the estimated contribution of water at these concentrations to the vapor pressure of a fuel oil no. 6 with the density of this sample ranges from 0.01 to 0.03 psi at 100°F, from 0.02 to 0.06 psi at 120°F, and from 0.04 to 0.10 psi at 140°F. The contribution of water to the measured vapor pressures obtained during this study for this material (including all methods) were 17 to 42% at 100°F, 3 to 63% at 120°F, and 9 to >100% at 140°F.
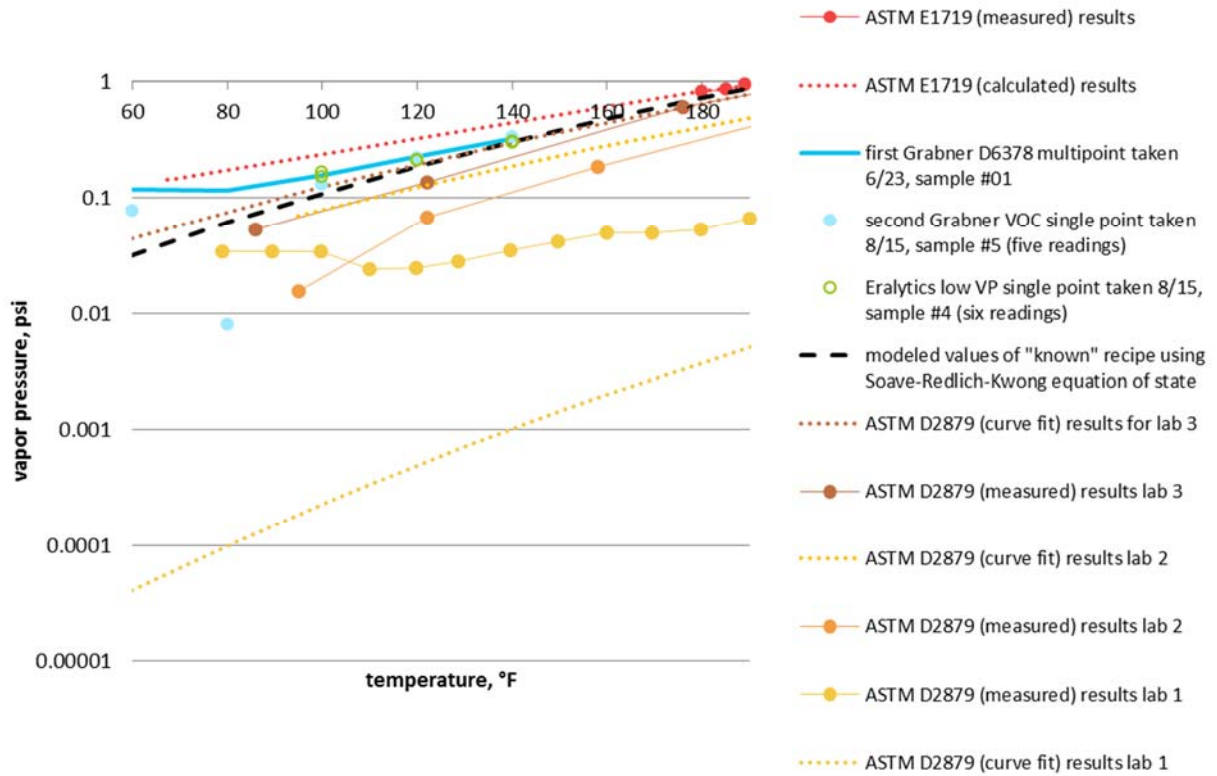
Figure ES-1. "Known" recipe vapor pressure values from 60°F to 190°F.   For the Grabner D6378 multipoint method, the values presented are the average after omitting the first injection of each syringe, per the instrument manufacturer's instructions.

Figure ES-2. Hydraulic fluid vapor pressure values from 60°F to 190°F. For the Grabner D6378 multipoint method, the values presented are the average after omitting the first injection of each syringe, per the instrument manufacturer's instructions.
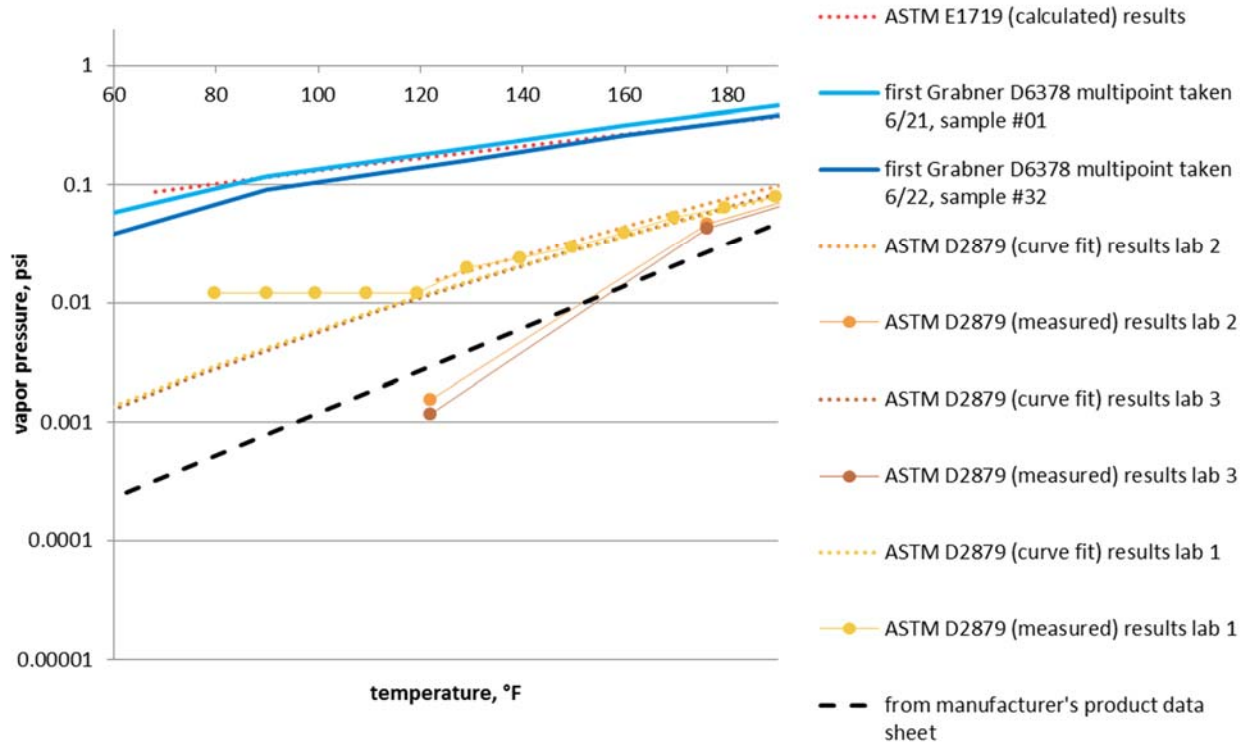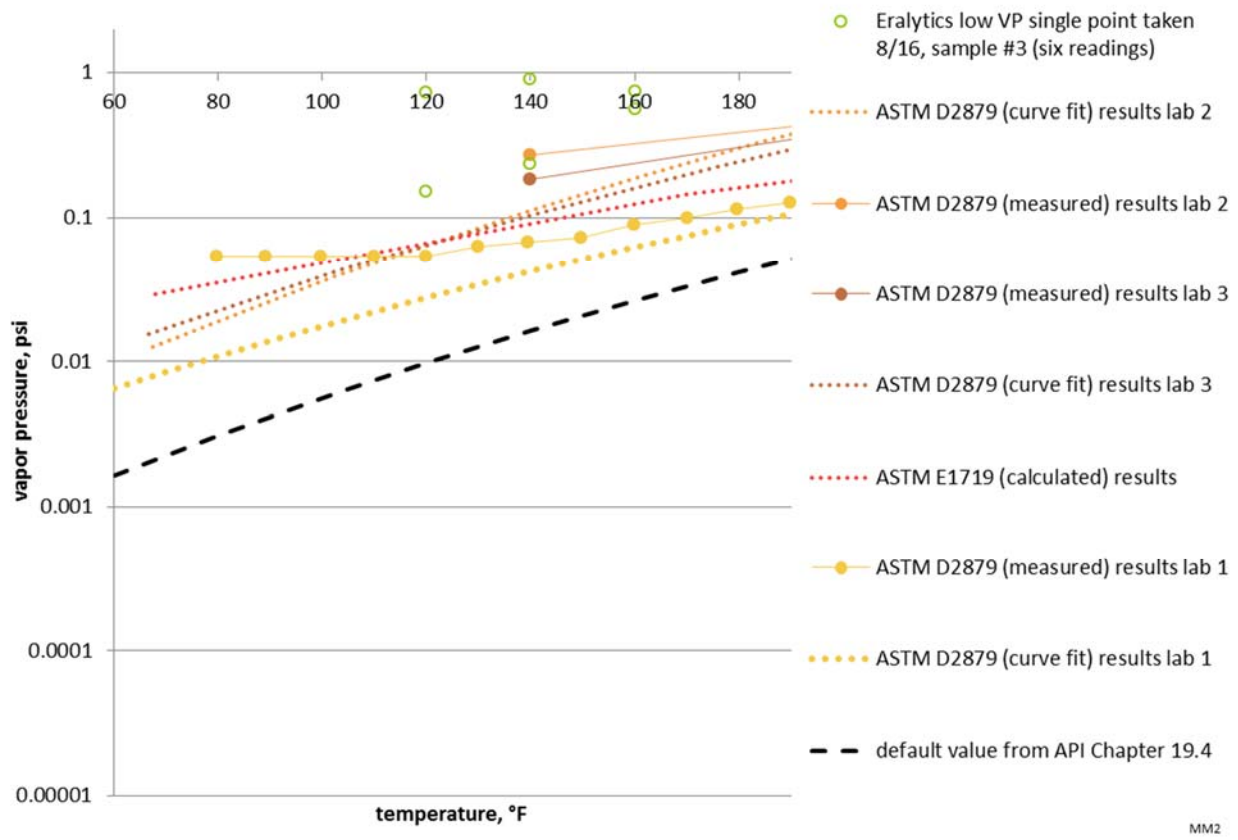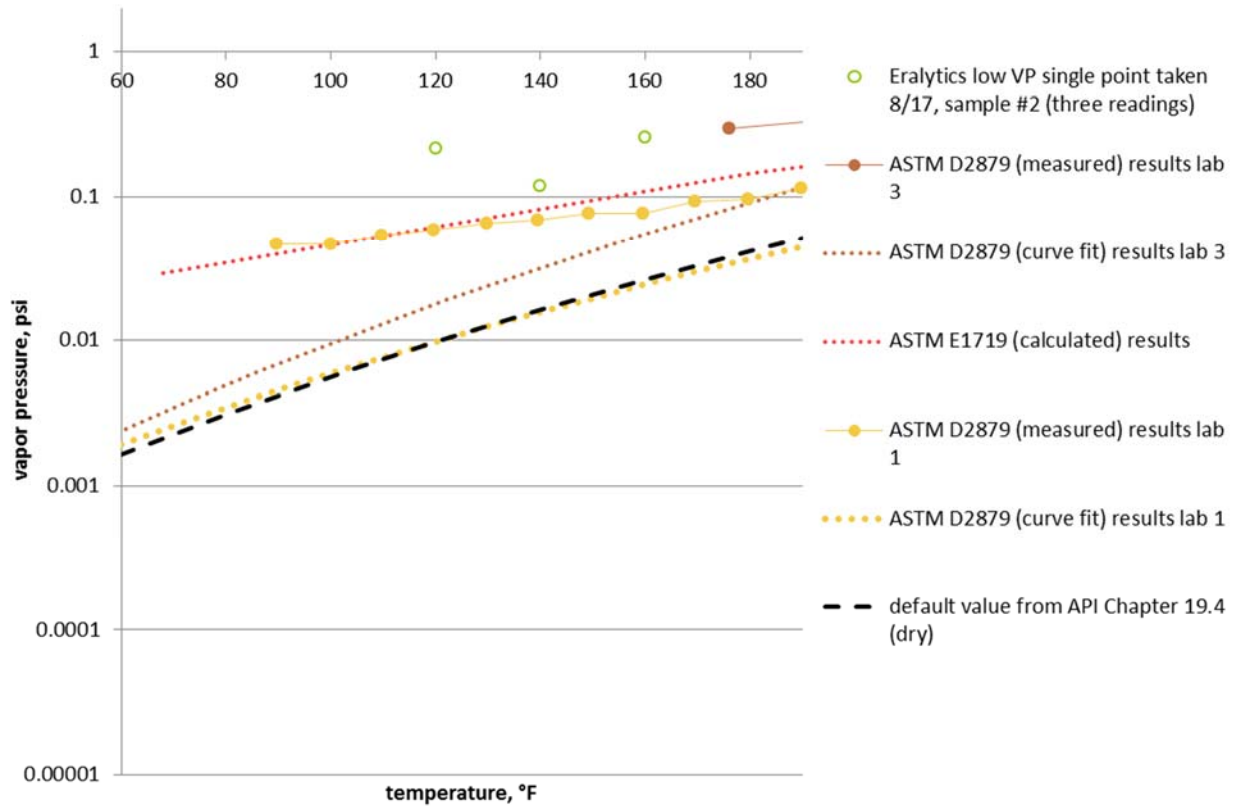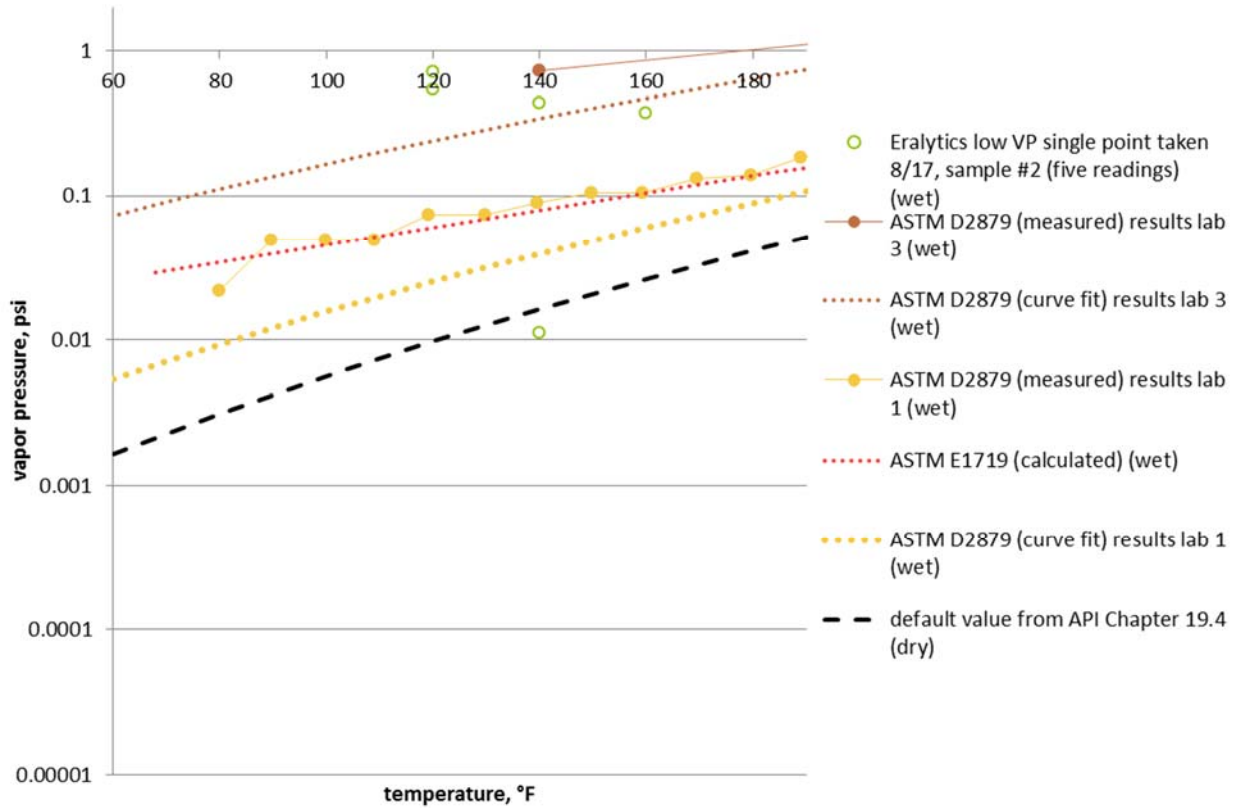
Figure ES-3. MM fuel oil no. 6 vapor pressure values from 60°F to 190°F.

Figure ES-4. MB fuel oil no. 6 vapor pressure values from 60°F to 190°F.

Figure ES-5. BT fuel oil no. 6 vapor pressure values from 60°F to 190°F.

Table ES-1. Agreement between modeled values and mini method and commercial lab vapor pressure results for the "known" recipe.

Key:

- The darkest green cells indicate very good agreement (method agrees with modeled value to within 10%)
- The medium green cells indicate good agreement (method agrees with modeled value to within 30%)
- The light green cells indicate fair agreement (method agrees with modeled value to within 90%)
- The white cells indicate poor agreement (not within 90%)
- The grey cells indicate no method value for comparison is available at this temperature

Temperature, °F	Mini method instruments			ASTM D2879 (vapor pressure by isoteniscope)						ASTM E1719 (vapor pressure by ebulliometry)	
	First Grabner ASTM D6378 multipoint taken 6/23, sample #01[a]	Second Grabner VOC single point taken 8/15, sample #5 (five readings)	Eralytics low VP single point taken 8/15, sample #4 (six readings)	Lab 1[b] measured	Lab 1 curve fit	Lab 2 measured	Lab 2 curve fit	Lab 3 measured	Lab 3 curve fit	Measured	Curve fit
60											
79											
80											
86											
95											
100											
100.04											
120											
122											
140											
158											
160											
176											
180											
185											
189											

Note: VP=vapor pressure; VOC=volatile organic compound

[a]These values are the average omitting the first injection of each syringe.

[b]Lab 1 provided vapor pressure measurements at 58 temperatures; only a sampling is provided in this table.

Project Update

Project 17-007 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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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   **Expended Amount**: $170,039

Amount Returned to AQRP: $0.00

Executive Summary
Fires can have a large impact on ozone and particulate matter concentrations, and thus air quality, in Texas. Three-dimensional Eulerian models like CAMx take estimates of the primary emissions from biomass burning and unphysically "mix" them across large-scale grid boxes, leading to inaccurate chemical modeling and incorrect estimates of the impact of biomass burning on air quality. Plume-scale process models like AER's Aerosol Simulation Program (ASP, Alvarado et al., 2015) allow us to examine the chemical and physical transformations of trace gases and aerosols within biomass burning plumes and to develop parameterizations for this aging process in coarser grid-scale models. Thus the first objective of this project was to improve our understanding of the impacts of local and out-of-state fires on air quality in Texas by implementing an improved ASP-based sub-grid scale parameterization of the formation of ozone and secondary organic aerosols in biomass burning plumes, derived from model runs of ASP coupled with the large-eddy simulation System for Atmospheric Modeling (SAM), into CAMx via the plume-in-grid (PiG) module. Our second objective was to use the Lagrangian trajectory-based modeling tool STILT-ASP to investigate the impact that long-range transport of wildfire smoke has on air quality in Texas. This project thus addressed two strategic topics of the AQRP 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."

We coupled the SAM and ASP models and made several improvements to the coupled SAM-ASP model in this project. For example, we reduced the number of model boxes that were used in the chemistry calculations in order to reduce the model run time without impacting the accuracy of the plume simulation, as this was necessary to allow us to do the 400 runs required to train the new parameterization. We also updated SAM-ASP to calculate the initial concentrations based on the mass emissions flux of the fire and emission factors for biomass burning species, rather than requiring the initial concentrations to be calculated outside of the model. This will allow SAM-ASP to better represent a wide range of fire sizes and intensities.

We evaluated the coupled SAM-ASP model by comparing the model results with measurements of the Williams Fire (Akagi et al., 2012) that was previously studied using the box model versions of ASP by Alvarado et al. (2015). Figure 1 shows the SAM-ASP calculated O_3 concentrations for the plume. The revised SAM-ASP model is able to correctly simulate the

dilution of CO in the Williams Fire smoke plume, as well as the chemical loss of NO_x, HONO, and NH_3 and formation of PAN within the plume. The formation of O_3 in the model is underestimated (model value of $\Delta O_3/\Delta CO$ of 0.05 mol/mol at 4.5 hr downwind, rather than the measured value of 0.10 mol/mol). Thus we conclude that SAM-ASP does a reasonable job of simulating CO, HONO, PAN, and NO_x within biomass burning plumes, but currently underestimates the formation of O_3.

We then ran the coupled SAM-ASP model for 100 simulations (using Latin hypercube sampling) per fire fuel type (Savannah, Tropical Forest, Temperate Forest, and Boreal Forest) and developed a Gaussian Emulator Machine (GEM) to predict the normalized mean enhancement ratio (NMER, Akagi et al., 2011) of O_3, NO_x, PAN, and other species in terms of the fuel type, temperature, latitude, day of year, and starting hour of emission. We built separate GEM parameterizations for each fuel type as our initial test of the parameterization showed that including the different fuel types in a single GEM led to unrealistic results for O_3.
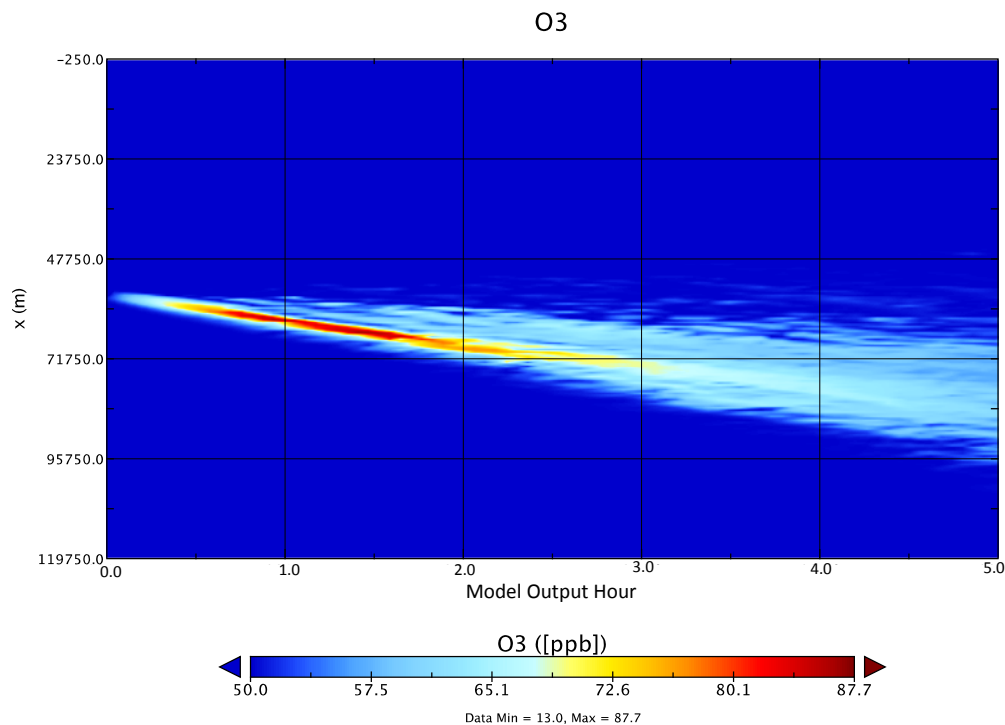
Figure 1. *SAM-ASP simulated O_3 concentrations for the Williams Fire (Akagi et al., 2012) at 1.22 km altitude. The y axis is the horizontal dimension of the SAM-ASP Lagrangian wall.*

However, our evaluation of the GEM parameterization showed that our current GEM training approach does not result in a parameterization of sufficient quality for use in regional air quality modeling. The GEM parameterization is able to represent the dependence of O_3 formation in the plume on fuel type, temperature, day of year, and latitude reasonably well, but the dependence on time of day is unrealistic, as the GEM prediction for the O_3 enhancement ratio ($\Delta O_3/\Delta CO$) is negative for plumes emitted at 14:00 local time in the summer, when these plumes should be forming O_3 up to the end of the simulation at 19:00 (7 PM) local time in the summer. Comparisons of the parameterization to the observations from the Williams Fire show that the

GEM parameterization underestimates the measured $\Delta O_3/\Delta CO$ for these conditions (GEM value of 0.04 mol/mol, as opposed to measurements of 0.10 mol/mol), similar to the results of a custom SAM-ASP simulation for these conditions (0.05 mol/mol). The GEM predictions for NO_x and other NO_y species have more serious deficiencies, with the GEM parameterization overestimating the NO_x downwind in the Williams Fire, and GEM predictions of the formation of PAN and HNO_3 being inconsistent with the GEM predictions of the loss rate of NO_x. Further work on the GEM parameterization training would be needed to identify the source of these errors and correct them.

Thus, rather than implement the GEM parameterization into CAMx, we instead implemented the parameterization of Lonsdale et al. (2015) into CAMx. This parameterization modifies the emissions of O_3, NO_y species, ethylene, and formaldehyde from fires based on a look-up-table (LUT) that is built from many runs of the ASP model within a simple Lagrangian parcel dispersion model. We added code to CAMx to read the FINN fire emission files directly and use them to initialize a biomass-burning-specific Plume-in-Grid (PiG) module. The downwind concentrations of O_3, NO_x, PAN, and other species transferred from the individual PiG puffs to the grid are determined by the parameterization based on the rate of CO transfer as well as fire and environmental conditions.

We used the modeling configuration from the 2012 CAMx modeling episode from TCEQ (May 16 – June 30, 2012) to evaluate the impact of the parameterization, as this episode and modeling configuration was used in the previous study of McDonald-Buller et al. (2015). The parameterization reduced the predicted impacts of fires on O_3 near the sources by ~30%, as expected.

For Task 2, we examined the 36-km CAMx boundary condition files (derived from the GEOS-Chem model) of the 2012 base case TCEQ modeling episode for potential episodes of biomass burning influence. Regions with CO concentration ≥ 120 ppbv along the southern boundary in May and June, which are sensitive to fires in Mexico and Central America, were simulated with STILT-ASP v2.0. The STILT-ASP v2.0 simulations show a lot of fine structure in the impacts of fires on CO along the boundaries that is not captured by the low-resolution boundary conditions from GEOS-Chem. In addition, the STILT-ASP v2.0 estimate of the $\Delta O_3/\Delta CO$ ratio during these events (mean of 0.15 mol/mol) is consistent with the review of Jaffe and Wigder (2012). However, the STILT-ASP v2.0 prediction of O_3 was high relative to GEOS-Chem (Figure 2), which appears to be due to an error in the simulation of the diurnal cycle of O_3 in STILT-ASP v2.0, especially at night. Predictions of NO_x and PAN were both much lower than the GEOS-Chem values, and this appears to be due to the chemistry of S/IVOCs used in ASP v2.1, which were derived from measurements of a biomass burning plume for the first 0-5 hours of aging (Alvarado et al., 2015). Thus the S/IVOC chemical mechanism of ASP v2.1 may need to be re-examined for the longer one to seven day runs of STILT-ASP v2.0.

We used STILT-ASP v2.0 to examine the impact of fires on CO, O_3, NO_x, and $PM_{2.5}$ during three days where the Austin/Round Rock urban area was impacted by fires from Central Mexico and the Yucatan. On the day with the highest MDA8 O_3 (May 11), the model predictions of O_3, CO, and NO_x were all consistent with the observations, with O_3 slightly overestimated (MB of +3.6 ppbv, RMSE of 5.9 ppbv) and NO_x slightly overestimated (MB of +0.3 ppbv, RMSE of 1.9 ppbv). However, due to the loss of NO_x during S/IVOC chemistry as discussed above, the impact of fire emissions on O_3 was a decrease of 0.9 ppbv of the MDA8 O_3. $PM_{2.5}$ was substantially

overestimated, likely due to an underestimation of PM$_{2.5}$ deposition. However, deposition should affect all aerosol sources relatively evenly, so the STILT-ASP v2.0 results can be used to estimate the relative fraction of PM$_{2.5}$ at the receptor that is due to fires, which for this day was 12% (0.9 μg/m^3) averaged over the MDA8 period.
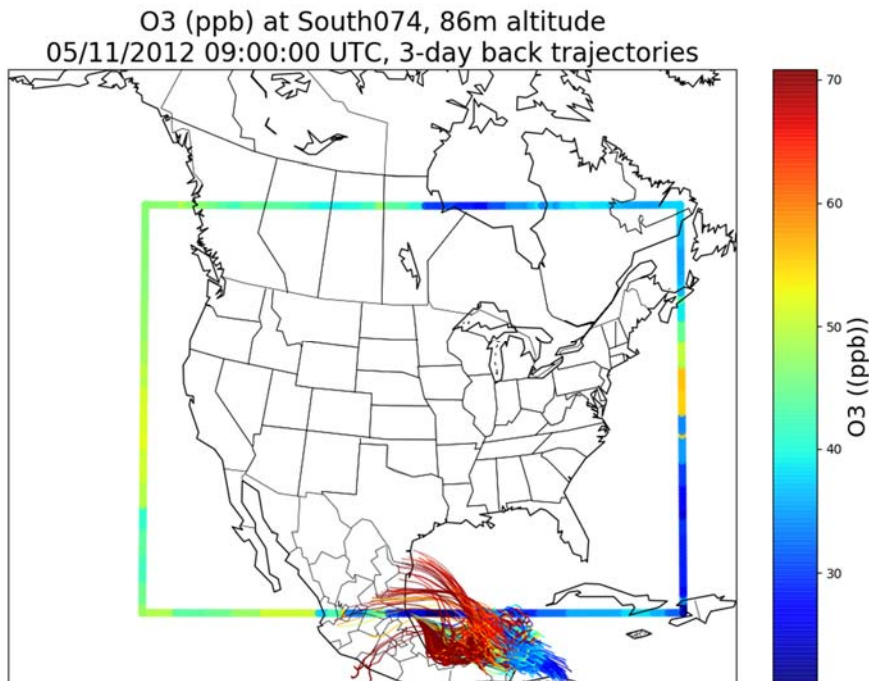

Figure 2. *O$_3$ (ppbv) from a 3-day back trajectory run of STILT-ASP v2.0 for May 11, 2012 at 09:00 UTC (03:00 CST) fire-influenced box of the southern boundary of the CAMx modeling domain. The GEOS-Chem boundary conditions are also shown.*

The results for the May 5 and May 25 Austin cases were very different, with STILT-ASP v2.0 strongly overestimating O$_3$ (MB = +40 ppbv) and underestimating NO$_x$ (MB = -2.6 ppbv) on these days, with less severe overestimates of PM$_{2.5}$. The model suggests that fires had small but positive impacts on MDA8 O$_3$ on these days (0.2 and 0.3 ppbv, respectively), but noticeable impacts on the 8-hour average PM$_{2.5}$ (2.6 and 4.0 μg/m^3, respectively).

In order to compare the STILT-ASP v2.0 predictions of the impacts of wildfires on O$_3$ and PM$_{2.5}$ with the CAMx simulations of McDonald-Buller et al. (2015), we ran STILT-ASP for the CAMS 12 site in El Paso on two dates (June 4 and June 28) that were shown to have significant fire impacts on O$_3$ in McDonald-Buller et al. (2015). However, the STILT-ASP v2.0 estimates of the impacts of fires on CO were small (2-3 ppbv), likely due to the use of the FINN v1.5 emissions rather than the FINN v2.1 emissions used by McDonald-Buller et al. (2015). Furthermore, the STILT-ASP v2.0 estimate of the impact of fires on MDA8 O$_3$ on these days is small and negative (-0.1 to -0.4 ppbv), unlike the small but positive impacts predicted by CAMx with the biomass burning parameterization (2.1 and 1.2 ppbv), but this may be due to errors in the S/IVOC chemistry as discussed above.

Project Update

Project 17-024 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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Project 17-032
            STATUS: Active – December 6, 2016
            Completed – August 31, 2017

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   **Expended Amount:** $58,964.17

Amount Returned to AQRP: $35.83

Executive Summary

Ozone formation rates and mechanisms have not been previously studied in San Antonio. Due to peak observed O_3 values that are close to the National Ambient Air Quality Standard, gaining an understanding of ozone formation rates and chemical mechanisms is important for eventually designing effective ozone abatement programs. Measurements of total peroxy radicals ($[HO_2]$ + $[RO_2]$, "$[ROx]$") were made during May 2017 in three sites upwind and downwind of San Antonio: at the University of Texas-San Antonio, which is in the Northwest of San Antonio, Floresville (Southeast of San Antonio), and Corpus Christi (Southeast of San Antonio). Combined with measurements of NO, ozone production rates were calculated for the three-week measurement project. Peroxy radicals were measured by the Ethane CHemical AMPlifier method (ECHAMP), housed in the Aerodyne Mobile Laboratory. Additionally, a thermal dissociation cavity attenuated phase shift spectrometer (TD-CAPS) was installed in the AML to measure organic nitrates. These measurements were combined with those made by collaborators at Aerodyne Research, Inc., including the radical precursors ozone, water vapor, formaldehyde, and acetaldehyde, as well as photolysis rate constants (actinic flux) to investigate the nature of ozone formation in the greater San Antonio area.

Major findings of these measurements and preliminary analysis include the following:

1. Daytime ozone production rates were typically between 5 and 10 ppb/hr and rarely exceeded 15 ppb/hr. The highest $P(O_3)$ values were observed in air masses with elevated P(HOx) and [NO] values ([NO]>0.3 ppb).
2. Primary radical production rates P(HOx) were dominated by the reaction of $O(^1D)$ with water vapor (following the photolysis of ozone) and the photolysis of formaldehyde with much smaller contributions measured or inferred from the photolysis of acetaldehyde, hydrogen peroxide, acetone, and nitrous acid. HOx radical production from alkene ozonolysis and atomic chlorine formation from photolysis of nitryl chloride ($ClNO_2$) and molecular chlorine (Cl_2) have not been quantified. Peak P(HOx) values observed were 0.6 – 0.7 ppt/s – less than half that previously observed in Houston in photochemically active air masses.
3. Analysis of estimated contributors to the HOx destruction rate L(HOx) suggests that $P(O_3)$ was almost always NOx-limited during the 3-weeks of measurements. Similarly, the dependence of $P(O_3)$ on [NO] and P(HOx) suggests that $P(O_3)$ was usually NOx-limited, and this occurs when [NO] is less than 600 ppt at the highest P(HOx) values observed (greater than 0.5 ppt/s) or less than 200 ppt at lower P(HOx) values (less than 0.25 ppt/s). During the few time periods when $P(O_3)$ was likely NOx-saturated, absolute $P(O_3)$ values were usually low – less than 5 ppb/hr.

4. During the few days that alkyl nitrates and peroxy nitrates were measured by TD-CAPS, alkyl nitrates accounted for a much smaller portion of total nitrogen oxides (NO_Y) than peroxy nitrates.

These conclusions are based on three weeks of measurements in San Antonio when there was usually southeasterly flow. Although high O_3 events are more often observed during southeasterly flow compared to other flow patterns, we cannot yet quantitatively address how representative these measurements were of other time periods.

Recommendations for Future Analysis
Based on the preliminary analysis of the field data collected for this project, there are two main topics that warrant further analysis that would greatly inform our understanding of current and future ozone pollution in San Antonio:

1. The dependence of ozone formation on NOx, VOCs, and HOx production rate should be analyzed using data collected at the upwind (Floresville, Corpus Christi), downwind (UTSA), and urban (Traveler's World) sites during the San Antonio Field Study. This will involve greatly expanding the preliminary analysis in this report. For example, the role of "non-traditional" radical sources such as alkene ozonolysis and the photolysis of nitryl chloride ($ClNO_2$) and molecular chlorine (Cl_2) has not been investigated. Similarly, the absolute $P(O_3)$ values and their dependence on NOx in the urban core have not been investigated.
2. The impact of future trends of NOx and VOC emissions on ozone concentrations and formation rates upwind of and inside San Antonio should be analyzed. This will involve analyzing emissions data, trends, and future projections for multiple emission sources (on-road, electricity generation, oil & gas activities, cement kilns, etc.), including satellite data, in concert with photochemical models.

Project Update
Project 17-032 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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   **Expended Amount:** $149,226.81

Amount Returned to AQRP: $0.19

Executive Summary
The purpose of this project was to evaluate and improve the performance of the land surface models used in the Weather Research and Forecasting model (WRF) by the use of satellite skin temperatures to better specify physical parameters associated with land use classes. This is a continuation of AQRP Project 14-022.

Improved temperature performance impacts boundary layer heights, biogenic emissions, thermal decomposition (chemical chain lengths and slopes of ozone/NO_y curves) and thermally driven winds such as sea breezes. Also, land surface parameters control surface deposition, which impacts the efficacy of long-range transport.

While considerable work has been done by the national community and especially in Texas to develop improved land use classifications, land use classes themselves are not directly used in models. Rather, physical parameters such as heat capacity, thermal resistance, roughness, surface moisture availability, albedo, etc. associated with a land use class are actually used in the land surface model. Many of the land use class associated parameters such as surface moisture availability are dynamic and ill-observed depending on antecedent precipitation and evaporation, soil moisture diffusion, 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*. In some sense they are model heuristics with different land surface models having several orders of magnitude difference in parameters such as vegetative thermal resistance. The specification of these physical parameters across grids having mixed land use types is even more problematic. Despite the difficulty in specifying these parameters they are incredibly important to model predictions of turbulence, temperature, boundary layer heights and winds.

Insolation is one of the largest components in the daytime surface energy budget. Insolation largely depends on average solar zenith angle. However, clouds can dramatically alter the solar energy received at the surface. This produces a potential source of error in air quality simulations since model clouds may be in the incorrect place or time. Thus, on certain days when clouds are present in the model but not in reality the energy difference at the surface can be large. The WRF model is run using both the default model insolation and satellite insolation.

The Pleim-Xiu (hereafter referred to as P-X) land use model in WRF has used a surface moisture and deep soil nudging technique based on differences between model 2-m air temperatures at

National Weather Service (NWS) observational sites. However, land use, vegetation coverage, and convective precipitation can all have variations on spatial scales much smaller than the spatial scale of NWS observations. The major activity under this project was to determine whether satellite observed skin temperature, which has much finer resolution (10 km) than NWS observations (~40 km), can be used to nudge soil moisture and thermal resistance and provide improved model performance.

Under the last biennium project (14-022) using skin temperatures as the performance metric, the results showed that over most of the domain that the bias was improved but there was a slight negative increase in the overall bias. This means that the few areas that had an increase in bias were larger causing a slight increase in absolute bias for the domain. An examination of time series from the nudging runs compared to the control showed that the adjustments in moisture appeared to be working as formulated. In some places part of the error may have been due to bad skin temperature data. The root-mean square statistics were also improved over the domain.

In the last biennium project comparisons with NWS observations were more mixed in regards to bias for 2-m specific humidity and 2-m temperature. Root mean square error (RMSE was unchanged for humidity and decreased slightly for 2-m temperature. For 10-m wind speed and wind direction there was a slight decrease in bias and RMSE for all regions.

Under AQRP Project 16-039, several new approaches were tested including examining small scale performance and other metrics such as wind performance, skin temperature tendencies, heat capacity assimilation, vegetative fraction, sensitivity of land surface model components, and satellite derived insolation and albedo. An additional model evaluation time period was also included that spanned the 2013 DISCOVER-AQ campaign (September 1-30, 2013). The first task was to make a model control run with which to compare successive levels of satellite assimilation. However, in making the control run several changes in model physics and nudging strategies were made that were slightly different that the last biennium runs. Additionally, the newest WRF version 3.8.1 was employed compared to version 3.6.1 used in the last biennium project. In making the control run it was found that bias and root-mean-square error statistics in the control run were significantly worse than in the last biennium control run. The source of the degradation was exhaustively investigated. While removal of the differences in model set-ups did bring the control closer to the last biennium control, it was concluded that the remaining differences were due to the new version of WRF.

Previous model set-ups had been patterned after TCEQ inputs. However, in talking to TCEQ it was found that these are fluid and have not been firmly specified for the P-X scheme. It was thus decided that the appropriate control case would be one most likely to be used within the WRF/Air Quality Community. The EPA National Exposure Research Laboratory (NERL) group was contacted to obtain their model name list and set up. Since this project was trying to show that satellite data could improve model performance in the P-X scheme, it was reasonable to use what the Pleim group at EPA would use for their control model set-up. If a different control set-up was selected and showed improvement there might be concern that a control set-up with a larger error was chosen making the use of satellite data appear better.

The satellite assimilation worked much as expected. Model comparisons to NWS observations showed improvement in most areas especially for 2-m temperatures. Texas showed even greater improvement than for the whole domain. Wind speed statistics were slightly improved.

Comparisons against profiler data showed that the assimilations improved nighttime wind speeds aloft substantially. Daytime winds aloft were either unchanged or in some cases slightly deteriorated.

Skin temperatures were also improved compared to the control case. However, examination of the spatial plots showed that a large gradient in model performance existed across the whole domain and the Texas domain. A sharp gradient in model performance east and west of a north-south longitude approximately through Amarillo was found. Model performance with the satellite assimilations was greatly improved east of this line but model performance especially for skin temperatures was degraded west of this line. The analysis suggests that the issue may be with satellite skin temperatures in the West. In the last biennium project a switch was made from the National Oceanic and Atmospheric Administration's (NOAA's) operational GSIP skin temperature product to another NOAA product, which did not seem to suffer from excessive warm temperatures in the West. However, this year's analysis suggested there may also be a problem with this product.

Model satellite assimilation was carried out for the new August 2012 period. The general performance results from the satellite assimilation were largely similar to the 2013 period. In fact, performance against NWS sites showed much better consistent agreement across the whole domain and Texas. However, it turned out that the largest impact of the assimilation for 2012 came from the satellite insolation product with skin temperature nudging producing less impact.

In summary the project shows that satellite assimilation can greatly improve model performance especially in the Eastern U.S. and East Texas.

Project Update
Project 17-039 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

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   **Expended Amount:** $185,193

Amount Returned to AQRP: $0.00

Executive Summary
A field measurement campaign was undertaken to collect data needed to identify and apportion the volatile organic compounds (VOCs) that contribute to ozone (O_3) production in Central Texas. Measurement data was collected at three primary sites from May 10th to May 31st, 2017. The sites were selected to emphasize sampling air in the San Antonio urban area, the Eagle Ford oil and gas producing shale and a site near the Gulf of Mexico in Corpus Christi State Park. The composition measurements include research and commercial grade instrumentation to quantify the following classes of compounds:

1. ozone and the oxides of nitrogen
2. light hydrocarbon photoproducts such as formaldehyde, acetone and hydrogen peroxide
3. air mass tracer species such as carbon monoxide (CO), hydrogen cyanide (HCN, from biomass burning) and sulfur dioxide (SO_2, anthropogenic tracer)
4. oil and gas light alkanes such as propane, ethane and methane
5. biogenic emissions such as isoprene, terpenes and methanol
6. anthropogenic emissions such as benzene and toluene
7. particulate matter size and composition for both primary (e.g. black carbon, hydrocarbon like organic aerosol) and secondary (e.g. oxidized organic aerosol, sulfate) particulate matter
8. minor secondary photoproducts produced with ozone from a complex mixture of VOC species.

The complete composition dataset has been quality assured and is poised to identify VOC emission categories (e.g. oil & gas; biogenic; anthropogenic) and attribute the quantified production of ozone in central Texas. This project identified ozone production under different chemical regimes. Continued analysis beyond that provided in this report could use this understanding of chemical regimes to inform ozone mitigation strategies. The goals of the State of Texas Air Quality Research Program (AQRP) are:

1. to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology and air quality modeling,
2. to integrate AQRP research with the work of other organizations, and
3. to communicate the results of AQRP research to air quality decision-makers and stakeholders.

Of the ten research priorities identified in the AQRP Strategic Research Plan FY 16-17, this project addresses two. They are 1) Improving the understanding of ozone and particulate matter formation (in central Texas), and 2) Quantifying the local ozone production that impacts the design value (DV) monitors that exceed the national ambient air quality standards (NAAQS) in central Texas. The continued analysis of the datasets collected in our project could be used to conclusively address the above research priorities.

Preliminary Findings

This project focused on collecting the measurement dataset and performing the in-depth quality assurance. The analysis using the resulting dataset is just beginning at the time of this writing. Some preliminary findings are warranted from the in-field analysis (Note that the $p(O_3)$ studies were performed in collaboration with Ezra Wood, AQRP Project 17-032):

- The quantification of low-yield nitrogen containing species involved in isoprene oxidation suggests that *biogenic VOCs play a significant role in net ozone production in San Antonio*.
- The mixing ratio enhancements of oil and gas VOCs (e.g. ethane, propane) suggest local impact in Floresville, however it is unclear that these VOCs fuel local ozone production.
- *A credible fractional attribution of the production rate of ozone ($p(O_3)$) to oil and gas VOC emissions will require additional analysis* because the nitrogen-containing oxidation products are not yet well characterized.
- When $p(O_3)$ was between $5 - 15$ ppb hr^{-1}, the chemical regime was NOx-limited.
- When $p(O_3)$, was less than 5 ppb hr^{-1} and the radical pool (e.g. HOx) was lower, either chemical regime was possible (NOx-limited or NOx-saturated).

Recommendations for Future Work

This section describes the collected research threads that follow on from the analysis of the May 2017 dataset completed as part of this project. It is divided into two sections. The first section describes the advanced analysis tasks associated with the data sets and the second describes the applied research avenues. These recommendations are meant to archive the ideas that continue the pursuit of the broad project goals as well as to describe other avenues of investigation inspired by the observed data and results.

Advanced Dataset Analysis Items
- Conduct positive matrix factorization (PMF) analysis of high-resolution proton transfer reaction mass spectrometry (PTR-MS) data. This would enable us to separate biogenic and anthropogenic emissions and first-generation oxidation products at high time resolution throughout the campaign. The resulting data would differentiate between changing masses of anthropogenic or naturally influenced air.
- PMF of the iodide chemical ionization mass spectrometry (I-CIMS) data to identify highly oxygenated products of oil and natural gas emissions. The signals isolated from this analysis could serve as tracers of aged oil and natural gas (O&NG) emissions.

- Basic laboratory experiments to oxidize simulant O&NG emissions in a flow reactor and measure the outflow with the I-CIMS. These experiments will enable us to directly identify potential O&NG tracers in the San Antonio field dataset.
- Follow on analysis of high-resolution PTR-ToF-MS data
- Propane was quantified using tunable infrared laser direct absorption spectrometry (TILDAS). This measurement principle is based upon tuning an infrared laser (near 3 μm) across the vibrational absorption of propane. The propane spectrum is broad and ill-defined. During the project, to retrieve a useful propane concentration, a simple line model was used. To improve the quantitative accuracy a computationally expensive baseline decomposition will be coupled to the full line list. This will result in an improved 1 second propane dataset.

Applied Analysis Items
- We will employ the Dynamically Simple Model for Atmospheric Chemical Complexity (DSMACC) package that uses the Master Chemical Mechanism (MCM) to calculate OH reactivity in various ways. The rich array of VOC measurements and the model running in a semi-constrained mode should be able to calculate and apportion k[OH] to defined VOC families. We will use the versions of the MCM that include detailed isoprene oxidation chemistry.
- The project was active for three weeks in May of 2017. In this task, we will evaluate the extent to which the weather, transport and associated ozone production are representative of historical data in the region. This will help inform how broadly the apportionment of ozone producing VOCs can be interpreted.
- The presence of biomass burning markers (e.g. HCN, CH_3CN) in the observational data as slowly rising enhancements above background appear to be due to transported air. A cursory examination of the preliminary back trajectory calculations (Figure 1) suggests that fire emissions from the Yucatan Peninsula represent a quantifiable portion of the air sampled at Floresville. The analysis effort described in this task will involve trying to pinpoint the source of the fire emissions and model their potential atmospheric chemistry to understand the import of O_3 to central Texas.
- Sulfur dioxide (SO_2) was observed several times at the UTSA and Traveler's World Sites. As a criteria pollutant, SO_2 emissions are part of reported inventory tabulations. This research task dovetails with the other point source inventory analysis tasks described elsewhere to investigate whether the transport and dilution model framework and inventory agree with the spatial, temporal and magnitude of reported emissions. There are multiple known SO_2 emission sources in San Antonio, however the majority of known emissions appear in the inventory as:
  - electricity generation
  - cement manufacturing
  - bulk mineral handling
- During the early morning hours of 5/11, 5/13, and 5/14, significant enhancements above background were observed for chlorine gas (Cl_2). This analysis task will examine the potential transport of industrial Cl_2 from industrial point sources in the region.
- Two distinct periods of unusually high particulate sulfate were observed. The observation was qualitatively corroborated by the Rice University AMS as well.

Preliminary results indicate that the airmass was influenced by imported sulfate aerosol from the Gulf of Mexico. This research task will be to identify the source of this sulfate.

- The Eagle Ford Shale is an oil and gas producing region that is frequently upwind of San Antonio. The mixing ratios of various oil and gas associated VOCs observed in Floresville suggests local emissions (Figure 2). In this task, we will use detailed emission inventories together with the methane, ethane and propane data and transport data to interrogate the observation of a bimodal character to the ethane/methane ratio (3-4 or 7-8%). The premise is that the inventory data will spatially describe the distribution of the propane/ethane/methane ratios. The transport model and time series will be used first to potentially explain the bimodal observations and ultimately inform the accuracy of the emission magnitude.
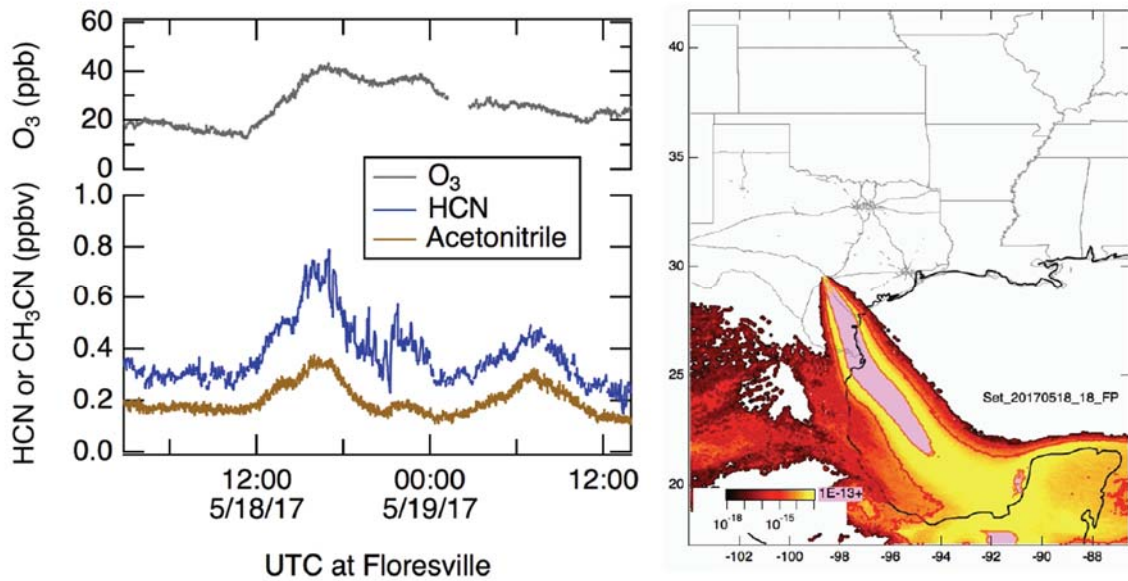
Figure 1. *Fire Emission Impact. The left-hand panel shows a time series of ozone (grey), hydrogen cyanide (blue) and acetonitrile (brown). The right-hand panel indicates a HYSPLIT calculated sampling footprint. Taken together, these suggest that the observed enhancements of the biomass burning tracers (HCN and CH₃CN) are due to fires from the Yucatan.*
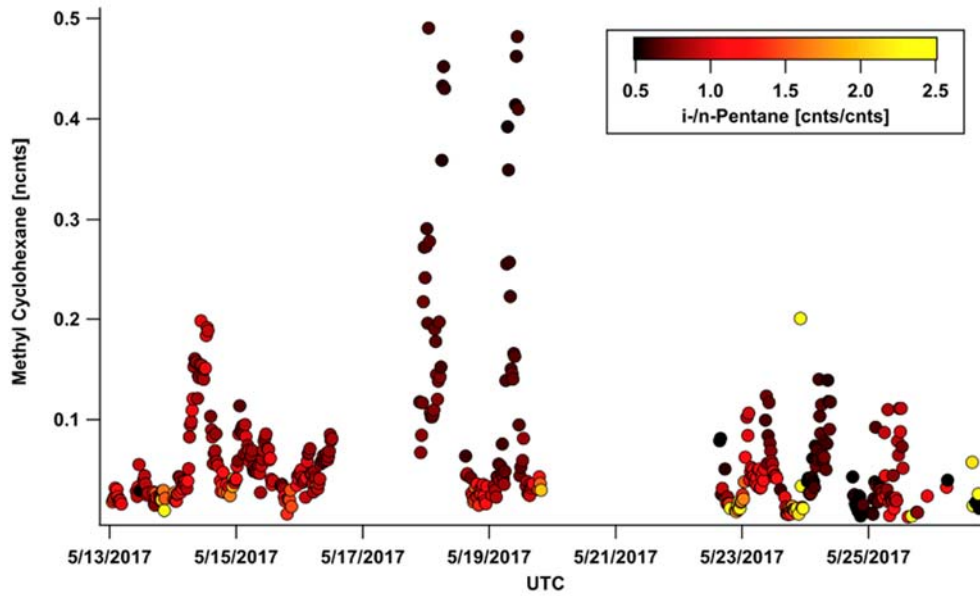
Figure 2. *Methyl cyclohexane time series colored by ratio of iso- to normal- pentane. The dark colored circles 5/18-5/20 were collected at Floresville and the 5/24 dark colored points were collected at Corpus Christi State Park with transport from the north.*

Project Update
Project 17-053 is complete. The final report is approved and all invoices have been paid. Project data has been submitted to the AQRP.

Project 17-SAFS   STATUS: Active – April 13, 2017
                                           Completed – October 31, 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   Expended Amount: $35,999.96

Amount Returned to AQRP: $10,000.04

Executive Summary
Under this project, a successful air quality study involving several research teams was carried out in and around San Antonio, TX, during the month of May, 2017, with ancillary meteorological measurements continuing through October 2017. Equipment installation, connection to electric service, and data transfer instrumentation were elements of this project. At project end, a permanent extension of electric power service installed at the UTSA campus under this project will allow construction of new teaching and research facilities.

Project Update
Project 17-SAFS is complete. The final report is approved and all invoices have been paid.

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. On September 4, 2017, the AQRP contract was renewed for the FY 2018/2019 biennium and additional funding of $750,000 per year was awarded. For each year, the funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

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

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

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

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

Program Administration

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

During the reporting period several staff members were involved, 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 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 25% 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.

In February 2018, FY 2016 and FY 2017 Administration funds were rebudgeted to allow for the most efficient utilization of the funds. All FY 2016-17 Administrative funds were expended at the end of the quarter.

Table 1: Administration Budgets

Administration Budget (includes Council Expenses)
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$74,376.95	$73,027.36	$147,404.31	$147,404.31	$0.00
Fringe Benefits		$18,118.37	$18,695.22	$36,813.59	$36,813.59	$0.00
Travel		$34.00	$0.00	$34.00	$34.00	$0.00
Supplies		$32.98	$974.69	$1,007.67	$1,007.67	$0.00
Equipment						
Total Direct Costs		$92,562.30	$92,697.27	$185,259.57	$185,259.57	$0.00
Authorized Indirect Costs 10% of Salaries and Wages		$7,437.70	$7,302.73	$14,740.43	$14,740.43	$0.00
Total Costs		**$100,000.00**	**$100,000.00**	**$200,000.00**	**$200,000.00**	**$0.00**

Administration Budget (includes Council Expenses)
FY 2018/2019

Budget Category		FY18 Budget	FY19 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$53,700.00	$53,700.00	$107,400.00	$11,956.20	$95,443.80
Fringe Benefits		$12,930.00	$12,930.00	$25,860.00	$3,324.98	$22,535.02
Travel		$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$3,000.00	$3,000.00	$6,000.00	$100.14	$5,899.86
Equipment						
Total Direct Costs		$69,630.00	$69,630.00	$139,260.00	$15,381.32	$123,878.68
Authorized Indirect Costs 10% of Salaries and Wages		$5,370.00	$5,370.00	$10,740.00	$1,195.62	$9,544.38
Total Costs		**$75,000.00**	**$75,000.00**	**$150,000.00**	**$16,576.94**	**$133,423.06**

ITAC

All ITAC expenses for FY 2016 were accounted for by the end of September 2016. During this reporting period the remaining FY 2016-17 ITAC funds were rebudgeted to Research Projects (91.5%) and Project Management (8.5%).

Table 2: ITAC Budgets

ITAC Budget
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary						
Fringe Benefits						
Travel		$4,076.57	$0.00	$4,076.57	$4,076.57	$0.00
Supplies		$1,079.20	$0.00	$1,079.20	$1,079.20	$0.00
Total Direct Costs		$5,155.77	$0.00	$5,155.77	$5,155.77	$0.00
Authorized Indirect Costs						
10% of Salaries and Wages						
Total Costs		**$5,155.77**	**$0.00**	**$5,155.77**	**$5,155.77**	**$0.00**

ITAC Budget
FY 2018/2019

Budget Category		FY18 Budget	FY19 Budget	Total	Expenses	Remaining Balance
Personnel/Salary						
Fringe Benefits						
Travel		$7,500.00	$7,500.00	$15,000.00	$0.00	$15,000.00
Supplies		$1,500.00	$1,500.00	$3,000.00	$0.00	$3,000.00
Total Direct Costs		$9,000.00	$9,000.00	$18,000.00	$0.00	$18,000.00
Authorized Indirect Costs						
10% of Salaries and Wages						
Total Costs		**$9,000.00**	**$9,000.00**	**$18,000.00**	**$0.00**	**$18,000.00**

Project Management

In February, FY 2016 Project Management funds were rebudgeted and FY 2017 Project Management funds were both increased and rebudgeted. The $638 increase was from a rebudget of ITAC funds that were split between Project Management and Contractual/Research Project funds.

Table 3: Project Management Budgets

Project Management Budget
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$53,470.31	$51,912.00	$104,988.00	$93,441.31	$11,546.69
Fringe Benefits		$11,337.17	$12,535.00	$23,691.43	$20,814.38	$2,877.05
Travel		$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$23.72	$500.00	$500.00	$163.62	$336.38
Other		$0.00	$5,000.00	$5,000.00	$0.00	$5,000.00
Total Direct Costs		$64,31.20	$69,947.00	$134,179.43	$114,419.31	$19,760.12
Authorized Indirect Costs 10% of Salaries and Wages		$5,347.03	$5,191.00	$10,498.80	$9,344.13	$1,154.67
Total Costs		**$70,178.23**	**$75,138.00**	**$144,678.23**	**$123,763.44**	**$20,914.79**

Project Management Budget
FY 2018/2019

Budget Category		FY18 Budget	FY19 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$38,060.00	$38,060.00	$76,120.00	$0.00	$76,120
Fringe Benefits		$9,134.00	$9,134.00	$18,268.00	$0.00	$18,268
Travel		$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$1000.00	$1,000.00	$2,000.00	$0.00	$2,000.00
Other		$2,500.00	$2,500.00	$5,000.00	$0.00	$5,000.00
Total Direct Costs		$50,694.00	$50,694.00	$101,388.00	$0.00	$101,388.00
Authorized Indirect Costs 10% of Salaries and Wages		$3,806.00	$3,806.00	$7,612.00	$0.00	$7,612.00
Total Costs		**$54,500.00**	**$54,500.00**	**$109,000.00**	**$0.00**	**$109,000.00**

Research Projects

For FY 2016/2017, 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. In February 2018, FY 2017 Contractual/Research Project funds were increased by $6,862 from the rebudget of unused ITAC funds.

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.

It should be pointed out that Table 4 does not indicate funding for the State of the Science Assessment project, which was awarded for $26,000. The funds for this project will be made available from remaining FY 2016 and FY 2017 project funds. Program Administration did not know the amount of FY 2016 funds available until all FY 2016 projects submitted final invoices and close-out documents. This information is now available and the State of the Science Assessment will be funded during the next quarter. This process allows the most efficient use of the available funding and will ensure that all FY 2016 funds are expended within the funding period.

For FY 2018/2019, a total of $1,223,000 is budgeted for research projects. A Request For Projects (RFP) is expected to be announced within the next 30 to 45 days.

Table 4: Contractual/Research Project Budget

Contractual Expenses				
FY 16 Contractual Funding		**$815,000**		
FY 16 Contractual Funding Transfers		**$9,666**		
FY 16 Total Contractual Funding		**$824,666**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
16-008	University of Houston	$191,366	$189,684.87	$1,681.13
16-010	Sonoma Technology, Inc.	$69,075	$69,075.00	$0.00
16-011	Ramboll Environ	$158,134	$158,127.36	$6.64
16-019	Univ. of Texas - Austin	$118,019	$117,551.39	$467.61
16-019	Ramboll Environ	$62,622	$62,618.81	$3.19
16-031	UNC - Chapel Hill	$225,000	$223,493.53	$1,506.47
FY 16 Total Contractual Funding Awarded		$824,216		
FY 16 Contractual Funds Expended (Init. Projects)			$820,550.96	
FY 16 Contractual Funds Remaining to be Spent				$4,115.04
FY 16 Additional Expenditures				
	State of the Science	$0	$0	$0.00
			$820,550.96	
FY 16 Contractual Funds Remaining to be Spent				$4,115.04

Table 4: Contractual/Research Project Budget (continued)

		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
FY 17 Contractual Funding		**$815,000**		
FY 17 Contractual Funding Transfers		**$9,862**		
FY 17 Total Contractual Funding		**$824,862**		
Project Number				
17-007	Univ. of Texas - Austin	$205,500	$202,348.21	$3,151.79
17-024	Atmospheric and Environmental Research, Inc.	$170,039	$170,039.00	$0.00
17-032	Drexel University	$59,000	$58,958.17	$41.83
17-039	Univ. of Alabama - Huntsville	$149,227	$149,226.81	$0.19
17-053	Aerodyne Research, Inc.	$185,193	$185,193.00	$0.00
17-SAFS	Univ. of Texas - Austin	$46,000	$35,999.96	$10,000.04
FY 17 Total Contractual Funding Awarded		$814,959		
FY 17 Contractual Funding Expended (Init. Projects)			$801,765.15	
FY 17 Contractual Funds Remaining to be Spent				$23,096.85
FY 17 Additional Expenditures				
	State of the Science	$0.00	$0.00	$0.00
	Data Storage	$0.00	$0.00	$0.00
FY 17 Contractual Funds Expended			$801,765.15	
FY 17 Contractual Funds Remaining to be Spent				$23,096.85
Total Contractual Funding		$1,649,528		
Total Contractual Funding Awarded		$1,639,175		
Total Contractual Funding Remaining to be Awarded		$10,353		
Total Contractual Funds Expended to Date			$1,622,316.11	
Total Contractual Funds Remaining to be Spent				$27,211.89