AIR QUALITY RESEARCH PROGRAM

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

Quarterly Report

December 1, 2014 through February 28, 2015

Submitted to

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

Prepared by

David T. Allen, Principal Investigator
The University of Texas at Austin
10100 Burnet Rd. MC R7100
Austin, TX 78758

March 10, 2015

Texas Air Quality Research Program

Annual Report

December 1, 2014 – February 28, 2015

Overview

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

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

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

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

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

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

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

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

After the TCEQ issued Amendment 9 to renew the grant, the AQRP developed the FY 2014/2015 research priorities and submitted them to the ITAC for input and to the TCEQ for review. Funding of $1,000,000 for FY 2014 and $1,000,000 for FY 2015 was awarded via Amendment 10 in October 2013. A call for proposals was released and by the November 22, 2013 due date, 31 proposals requesting $5.8 million in research funding were received. In December and January the ITAC and the TCEQ reviewed the proposals. On February 21, the Advisory Council selected 15 projects for funding, with one project on hold while TCEQ completed their review. These projects were funded with a combination of FY 2013, 2014, and 2015 funds.

In early March 2014, project Principal Investigators (PIs) were notified of the decision of the Advisory Council. AQRP Project Managers and TCEQ Project Liaisons were assigned to each funded project. A kick-off call was held with each project team to discuss the development of the Work Plans which consist of the project scope of work, budget and justification, and quality assurance project plan (QAPP). The TCEQ completed their review of the final projects to be recommended for funding and the Council approved the final project on April 2, 2014.

All projects began work as their Work Plans were approved. In August, the AQRP was notified by the PI of Project 14-023 that the site where the project work was to take place was no longer able to participate in the project and an alternate site could not be located. A decision was made to end Project 14-023 and return the unspent funds to the Research Program account. The TCEQ then performed a relevancy review of the projects that were not funded in the first round, and forwarded a ranking to the AQRP Review Panel, with a recommendation to fund 5 additional projects. The Review Panel concurred with that recommendation. The Advisory Council then reviewed the proposals and approved funding for the 5 additional projects recommended by the Review Panel.

During the period covered by this report, the AQRP approved the Work Plans of the 5 additional projects. Task Orders have been executed with each of the parties performing research, with the exception of the University of Alabama – Huntsville and George Mason University in the performance of Project 14-022. A Task Order has been submitted to the University of Alabama-Huntsville for signature. Work will begin as soon as it is executed. George Mason University was the only entity that did not already have a Master Agreement in place. This agreement is in the final stages of negotiation.

BACKGROUND

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

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

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

RESEARCH PROJECT CYCLE

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

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

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

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

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

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

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

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

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

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

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

Steps 1 – 9 have all been completed for both the 2010-2011 and 2012 - 2013 biennia. For the 2014-2015 biennium Steps 1 through 6 have been completed. Steps 7 and 8 are in progress.

PROJECT TIMELINE

During the project period covered by this report (December 1, 2014-February 28, 2015), three primary activities took place:

- Work Plans for the 5 additional project were approved
- A Master Agreement was submitted to George Mason University for signature
- Task Orders were executed for 4 of the 5 additional projects, with 1 Task Order out for signature and the final task order awaiting the execution of the Master Agreement

During this period, the AQRP Project Managers, the AQRP QAPP Manager, and the TCEQ Liaisons reviewed and approved the project Work Plans for the 5 new projects. A Master Agreement was submitted to George Mason University for review. Final terms are being negotiated. Task Orders have been fully executed for 4 of the 5 projects. A Task Order is at the University of Alabama-Huntsville awaiting signature and the final Task Order to George Mason University will be issued as soon as the Master Agreement is fully executed.

Funding for the 5 new projects is from FY 14 and FY 15 funds, as these projects have an end date of September 30, 2015. The funds that were made available when Project 14-023 ended were FY 13 funds. Several projects that were previously assigned to FY 14 or FY 15 funds were split between that FY and FY 13 in order to ensure the most efficient use of the research funds.

RESEARCH PROJECTS

FY 2014- 2015 research project activities are described below for all active projects. Some projects are analyzing the results of the Discover AQ program. A brief description of that program is provided for reference:

Discover AQ

In September of 2013, the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program deployed NASA aircraft to make a series of flights with scientific instruments on board to measure gaseous and particulate pollution in the Houston, Texas area. The purpose, for NASA, of this campaign was to better understand how satellites could be used to monitor air quality for public health and environmental benefit.

To complement the NASA flight-based measurements, and to leverage the extensive measurements being funded by NASA to better understand factors that control air quality in Texas, ground-based air quality measurements were made simultaneously by researchers from collaborating organizations, including research scientists and engineers funded wholly or in part by the AQRP and the TCEQ. Because of the opportunity to leverage NASA measurements, projects related to DISCOVER-AQ were a high priority for the 2012-2013 biennium.

FY 2014 – 2015 Projects

Project 14-002	STATUS: Active – June 6, 2014

Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC4RS Campaigns

University of Colorado - Boulder – Alan Fried
University of Maryland – Christopher Loughner

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

Funding Amount: $199,895
($150,508 UC-Boulder, $49,387 U of Maryland)

Executive Summary

During summer months the greater Houston-Galveston-Brazoria Metropolitan Area (HGBMA) often experiences elevated levels of ozone exceeding federal standards, particularly during hot and stagnant wind conditions. Although significant progress has been achieved understanding the major causes of these events over the past 10 years, there are still major unanswered questions related to sources of ozone from highly reactive volatile organic compounds (HRVOC's) emitted by large petrochemical facilities throughout the HGBMA. The toxic trace gas formaldehyde (CH_2O) is produced as an intermediate when these HRVOC's breakdown in the atmosphere, and ozone and radicals are formed when CH_2O further breaks down. Therefore a comprehensive understanding of CH_2O emissions, photochemical production rates, and transport processes is needed. Unfortunately, despite extensive efforts and advances from past studies, there are still major gaps in understanding related to the importance of directly emitted CH_2O from sources such as petrochemical flaring operations and automotive emissions relative to secondarily produced CH_2O from HRVOC's produced downwind, affecting large geographic areas far removed from the petrochemical facilities. Updating the emission inventories and temporal trends for CH_2O and its HRVOC precursors are two additional areas requiring attention.

To address these issues, a collaborative team, comprised of scientists from the University of Colorado, the University of Maryland, and the NASA Goddard Space Flight Facility, will analyze ambient measurements of CH_2O they acquired on the NASA P3 and DC-8 aircraft during the 2013 DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) and 2013 SEAC^{4}RS (Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys) studies, respectively.

The analysis will rely on the Community Multiscale Air Quality (CMAQ) model with Process Analysis, in very high-resolution mode (1 km resolution), driven by the WRF (Weather Research and Forecasting) meteorological model. The analysis will begin by identifying favorable time periods, such as Sept. 25, 2013, when sampling large petrochemical and refinery plumes under favorable meteorological conditions as well as other clearly identifiable sources (e.g., ship plumes, etc.) close to their source and downwind. The high resolution WRF-CMAQ model results will be compared with observations downwind at various times to arrive at updated emission rates for CH_2O and to help in validating the model meteorology and chemistry. The CMAQ model will be run in the Process Analysis Mode to quantify the relative importance of the major CH_2O sources. The analysis will conclude with an effort to compare select airborne CH_2O measurements with 24-hour averaged cartridge measurements acquired by The Texas Commission on Environmental Quality (TCEQ) every 6th day at the Clinton, Deer Park and Channelview sites as a means to further validate and/or provide error bounds, for such long-term CH_2O data in the greater HGBMA.

Project Update

Team members continued to coordinate, review progress, and update plans multiple times each month by telecoms. The CU team continued with their efforts in identifying favorable time periods and spatial domains for their initial analysis. Because of the large and dynamic pollution levels trapped in a shallow boundary layer, the CU team identified Sept. 25 for the initial analysis. Figure 1 shows the CH_2O distributions observed on the P3 during the 2nd circuit (starting around noon local time) from this flight overlaid on a map of the Houston sampling sites. The CH_2O color scale has been restricted here to 20 ppbv to allow small changes to be seen on subsequent plots even though CH_2O levels attained values as high as 33 ppbv over the ship channel in Galveston Bay and values as high as 26 ppbv near the Exxon-Mobil Baytown facility during the 1st circuit. For comparison, the entire DISCOVER-AQ data set from September 4 to September 26 has been analyzed in a similar fashion, and Fig. 2 plots the data for all circuits without Sept. 25 to emphasize the anomalously high CH_2O levels observed on Sept. 25. Starting with Sept. 25, the CU team has identified 4 specific airmass types for further study: 1) dominant petrochemical refinery emissions near the Baytown Exxon Mobil petrochemical complex; 2) dominant biogenic isoprene emissions near Conroe; 3) dominant CH_2O photochemical

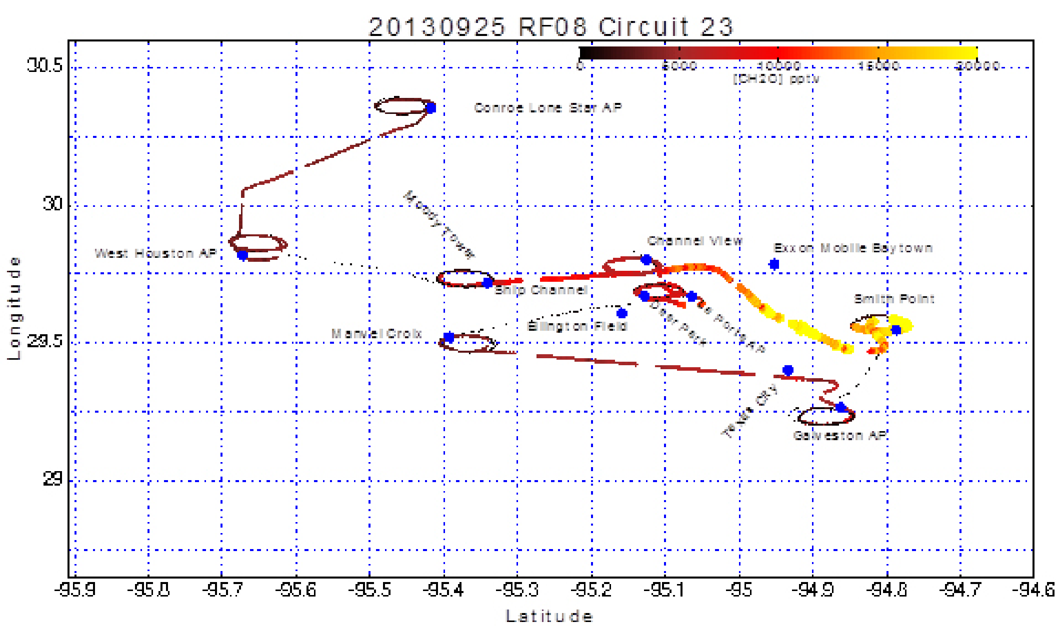

Figure 1: CH_2O distributions measured on the NASA P3 aircraft during the 2nd circuit of the Sept. 25 flight. The color scale here has been restricted to 20 ppbv even though CH_2O as high as 33 ppbv have been observed over Galveston Bay.

production downwind of the Baytown complex over Galveston Bay down to Smith Point; and 4) dominant urban sources over the center of Houston over Moody Tower. Regression plots of CH_2O as a function of CO for these 4 domains have been generated and are being studied. Because of the unique conditions on Sept. 25, the UMD/NASA Goddard team has directed their initial WRF-CMAQ model analysis to this day.

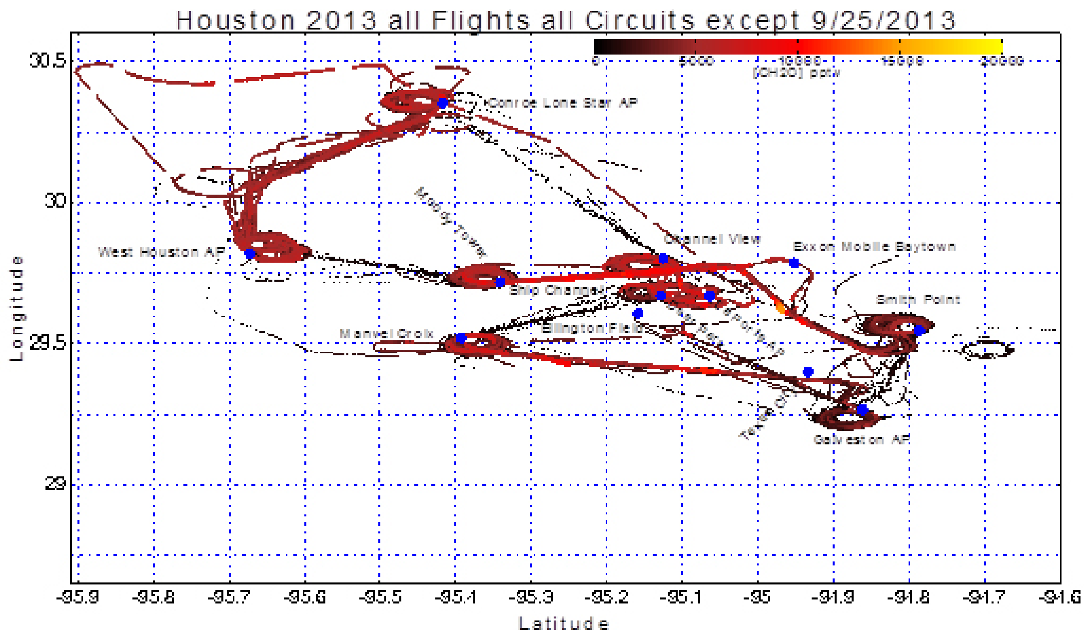

Figure 2: CH_2O distributions measured on the NASA P3 aircraft during the entire DISCOVER-AQ study from Sept. 4 to Sept. 26 with the exception of the 3 circuits on Sept. 25. A comparison of Fig. 1 with Fig. 2 shows the anomalously high CH_2O levels observed on Sept. 25.

Initial WRF-CMAQ simulations performed under project 14-004 at horizontal resolutions of 36, 12, and 4 km produced a weaker bay breeze than observed on September 25 that resulted in lower ozone concentrations along the western coastline of Galveston Bay and points inland to the north and west. The WRF modeling technique and inputs were revised under project 14-004 and a fourth modeling domain with a horizontal resolution of 1 km was added under this project to improve the model representation of the sea and bay breezes. The new run used the North American Mesoscale (NAM) 12 km model for initial and boundary conditions, nudged all domains, and employed an iterative technique where an initial WRF run performed analysis nudging based on the NAM 12 km and a second WRF run performed analysis nudging based on the previous WRF simulation. The iterative modeling technique prevented the relatively coarse NAM 12 km model from degrading the high-resolution WRF modeling domains (4 km and 1 km modeling domains). The new WRF run simulated a stronger bay breeze along the western coastline of Galveston Bay that is in better agreement with observations than our initial simulation (Figure 3).

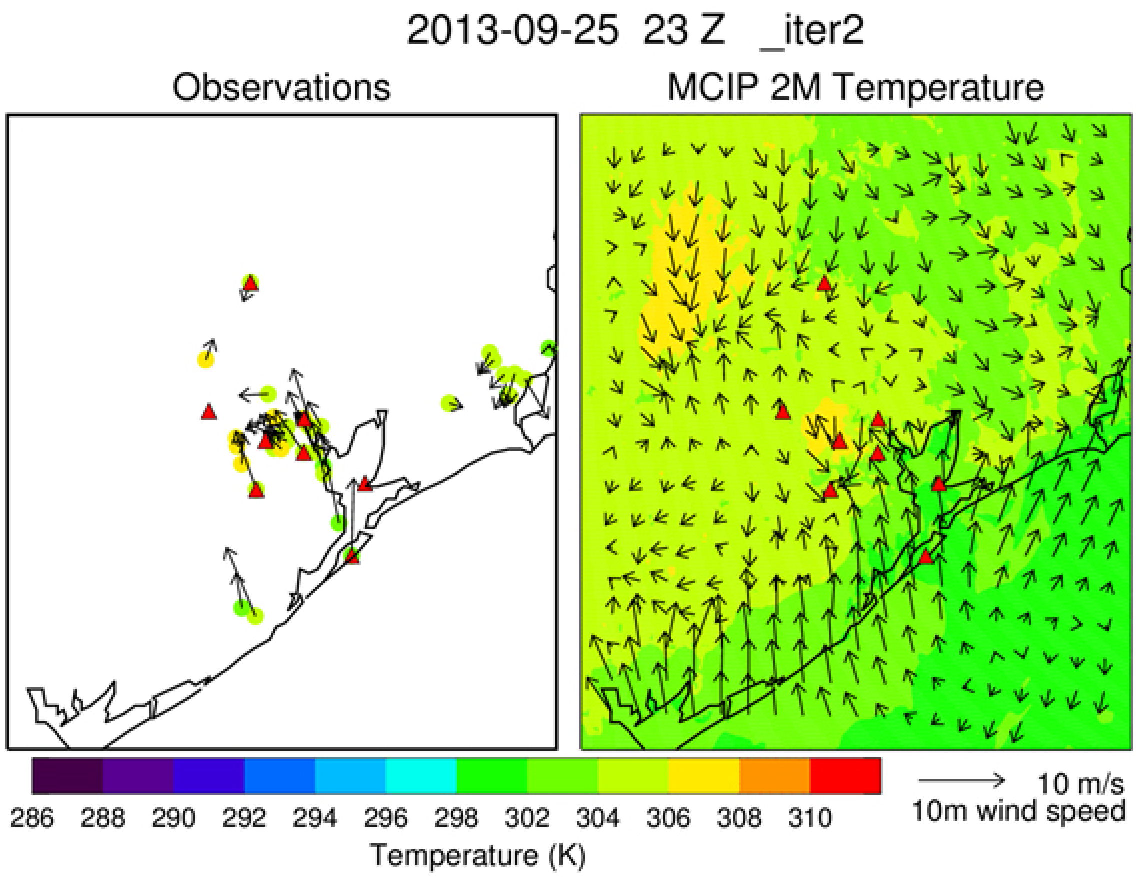

Figure 3: Observed (left) and WRF diagnosed (right) 2 m temperature and 10 m wind velocity at 23 UTC 25 September 2013 from the new 1 km WRF simulation.

New CMAQ simulations based on the new and improved WRF simulation have been completed for the 36, 12, and 4 km domains under project 14-004, and the CMAQ simulation for the 1 km domain is currently underway for this project. Project 14-004 found that overall, the new 4 km CMAQ simulation is in better agreement with ozone observations than the original simulation. Under this project (14-002), we performed a preliminary analysis of the CMAQ 4 km CH_2O model output (20 minute averages) with 1 minute averaged aircraft observations. On September 25, the model has a low bias relative to measurements throughout the boundary layer over Channelview (CV) during the 1st and 2nd circuits and over Deer Park (DP) during all three circuits (Figure 4). This will be further evaluated with the 1 km CMAQ simulation.

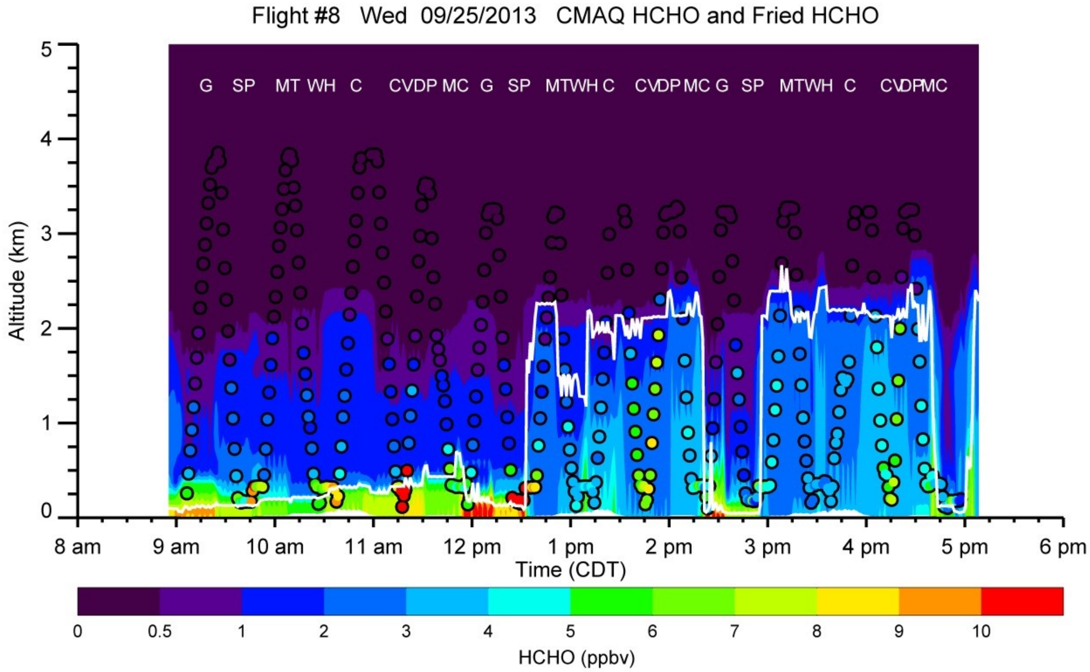

Figure 4: CMAQ simulated (background) and observed (overlay) formaldehyde concentrations along a flight track on 25 September 2013. The white line shows the location of the top of the boundary layer as calculated by the WRF model. The white letters at the top of the figure, “G”, “SP”, “MT”, “WH”, “C”, “CV”, “DP”, and “MC” stand for the spiral locations Galveston, Smith Point, Moody Tower, West Houston, Conroe, Channelview, Deer Park, and Manvel Croix, respectively. CMAQ results are from the new 4 km horizontal resolution domain performed under project 14-004.

Project 14-003	STATUS: Active – May 28, 2014

Update and evaluation of model algorithms needed to predict Particulate Matter from Isoprene

University of North Carolina – Chapel Hill – William Vizuete

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

Funding Amount: $200,000

Executive Summary

Terrestrial vegetation emits into the atmosphere large quantities (~500 teragrams C) of the reactive di-olefin isoprene (C_5H_8). Isoprene emissions in eastern Texas and northern Louisiana are some of the largest in the United States. Photochemical oxidation of isoprene leads to significant yields of gas-phase intermediates that contribute to fine particulate matter (PM2.5). The production of isoprene-derived PM2.5 is enhanced when mixed with anthropogenic emissions from urban areas like those found in Houston. To predict PM production from isoprene requires fundamental parameters needed to describe the efficiency with which gas phase intermediates react on the surface of atmospheric particles. Recently, EPA updated a regulatory chemical mechanism to include the formation of these new gas-phase isoprene-derived intermediates. Furthermore, the project investigators recently collaborated with the EPA to update the CMAQ model to predict isoprene-derived PM explicitly across the eastern US. This updated gas- and aerosol-phase framework found in CMAQ remains to be validated against systematically conducted chamber experiments. Thus, we first will conduct a series of new experiments at UNC to quantitatively measure the reactive uptake of the two predominant isoprene-derived gas phase intermediates to PM of different inorganic compositions. By providing these new fundamental measurements, we will be able to more directly evaluate the aerosol-phase processes added to the model. This work will produce a model evaluation of isoprene SOA formation against existing UNC outdoor smog chamber experiments. This project will also deliver performance data needed to bound uncertainties in key parameters used by CAMx to predict isoprene derived PM. This work directly addresses the stated priority area of investigating the transformation of gas-phase pollutants to particulate matter that impact Texas air quality.

Project Update

Progress on Project 14-003 is summarized below by Task:

1. Integration of Gas-Phase Epoxide Formation and Subsequent SOA Formation into UNC MORPHO Box Model

We have completed this task and generated the data necessary for QA of the code. Further, we have simulated bulk SOA formation in our indoor chamber. Based on our analysis we are confident in the QA/QC testing of the algorithms for the predicted gas phase precursors and the uptake of gaseous IEPOX onto an aerosol of variable acidity, temperature, and relative humidity.

Our first analysis with our model focused on the evaluation of a gas phase mechanism against chamber data. This resulted in the following manuscript currently in press in Atmospheric Environment entitled "Assessment of SAPRC07 with Updated Isoprene Chemistry against Outdoor Chamber Experiments."

This analysis focused on the latest addition of gas phase reactions for the formation of SOA precursors from isoprene oxidation. To keep up with the recent advance on isoprene oxidation chemistry, including the identification of isoprene epoxydiols (IEPOX) as a precursor to secondary organic aerosol (SOA), Xie et al. (2013) updated the SAPRC (Statewide Air Pollution Research Center)-07 chemical mechanism. It is currently unknown how the Xie modification of SAPRC07 impacts the ability of the model to predict O3. In this work we evaluated the Xie mechanism with simulations of 24 isoprene experiments from the UNC gas-phase chamber. Our results suggest that the new mechanism increases NOX (nitrogen oxides) inter-conversion and produces more O3 than SAPRC07 for all experiments. In lower NOX experiments, the new mechanism worsens O3 performance increasing bias as shown in Table 1. We found increased NOX recycling from PANs accounts for that. This could be explained by more PANs made due to increased first generation VOC products and OH production.

Table 1. Summary of O3 peak model performance statistics.

Experiment	Condition	Mechanism	NMB (%)	R^2
N=8	High NOX	SAPRC07	-5.45	0.02
		Xie	-16.00	0.03
N=16	Low NOX	SAPRC07	-22.12	0.76
		Xie	-30.60	0.68

2. Synthesis of Isoprene-derived Epoxides and Known SOA Tracers

We have completed all syntheses needed for the project. This includes generating the QA/QC data. There were some purification issues in the synthesis of the organosulfate standards, but these have been addressed.

3. Indoor Chamber Experiments Generating SOA Formation Directly from Isoprene-Derived Epoxides

For the last quarter we have begun generating experimental data to be evaluated by the model. These data will include wall-loss experiments (including for IEPOX and MAE), as well as actual experiments outlined in the work plan. Table 2 shows the experiments proposed.

Table 2. Indoor experiments to be conducted at UNC.

Expt. #	Epoxide	[Epoxide] (ppb)	Seed Aerosol Type	Initial Seed Aerosol (μg/m³)	RH (%)	T (°C)
1	IEPOX	300	$(NH_4)_2SO_4$	~20-30	~50-60	~20-25
2		300	$(NH_4)_2SO_4$ + H_2SO_4	~20-30	~50-60	~20-25
3	MAE	300	$(NH_4)_2SO_4$	~20-30	~50-60	~20-25
4		300	$(NH_4)_2SO_4$ + H_2SO_4	~20-30	~50-60	~20-25
5	none		$(NH_4)_2SO_4$	~20-30	~50-60	~20-25
6	none		$(NH_4)_2SO_4$ + H_2SO_4	~20-30	~50-60	~20-25
7	IEPOX	300	none	none	~50-60	~20-25
8	MAE	300	none	none	~50-60	~20-25

0.6 M (NH4)2SO4 + 0.6 M H2SO4

We expect the next 1-2 months will yield enough experimental data to be evaluated with the model. This will mean completing all experiments outlined in Table 2.

4. Modeling of Isoprene-derived SOA Formation From Environmental Simulation Chambers

We have completed our first modeling analysis that has resulted in a manuscript currently in press with Environmental Science & Technology Letters entitled "Heterogeneous Reactions of Isoprene-Derived Epoxides: Reaction Probabilities and Molar Secondary Organic Aerosol Yield Estimates."

In this study a combination of flow reactor studies and smog chamber modeling were used to constrain two uncertain parameters central to secondary organic aerosol (SOA) formation from isoprene-derived epoxides: (1) the rate of epoxide heterogeneous reaction with the particle phase and (2) the molar fraction of epoxides absorbed and that go on to contribute to the SOA burden – the SOA yield (α_{SOA}). Flow reactor measurements of the *trans*-β-isoprene epoxydiols (IEPOX) and methacrylic acid epoxide (MAE) aerosol reaction probability (ɣ) were performed on 1 – 2 component atomized aerosols with similar compositions as smog chamber SOA studies. Observed ɣ ranges for IEPOX and MAE were $6.5x10^{-4}$ – 0.021 and $4.9x10^{-4}$ – $5.2x10^{-4}$. A range in α_{SOA} for varying aerosol compositions is then estimated through the use of a time-dependent 0-D chemical box model initialized with chamber conditions and the ɣ measurements. The resulting α_{SOA} for the two epoxides were estimated between 0.03 and 0.22.

Table 3 summarizes the ɣ results for *trans*-β-IEPOX and MAE including the 1σ error for each measurement. Importantly, the aerosol and RH conditions chosen for the flow reactor was representative of conditions that produced notable SOA growth in the chamber experiments. Table 3 also includes estimates of aerosol acidity obtained from the Extended AIM Aerosol Thermodynamics Model III (E-AIM – http://www.aim.env.uea.ac.uk/aim/aim.php) using the atomizer solution composition and RH as inputs.[22] As there is no input for magnesium ion concentrations in E-AIM, we instead used 2 sodium ions for the calculations involving $MgSO_4$. The largest reaction probability for *trans*-β-IEPOX (ɣ = 0.021) was observed on $(NH_4)_2SO_4$ + H_2SO_4 aerosol under dry conditions. The ɣ values are similar to previous measurements for *trans*-β-IEPOX showing a general increase in ɣ with higher aerosol acidity, consistent with particle phase acid-catalyzed epoxide ring opening reactions. Moreover, for the same aerosol type at higher RH, decreases in ɣ are likely attributable to dilution from additional aerosol water. To our knowledge these are the first reaction probability measurements of MAE. ɣ's for MAE were significantly lower than those for *trans*-β-IEPOX and likely responsible for the generally smaller observed SOA production. Only at acidities closer to neutral ($[H^+] \sim 8x10^{-5}$) are the IEPOX and MAE ɣ's of similar magnitude with values on the order of $5x10^{-4}$.

As with the atomizer solutions, the RH used in the flow reactor studies were chosen to match the aforementioned chamber studies. In this way the ɣ's measured in the flow reactor experiments capture the appropriate ɣ that one would expect during the chamber experiments thus providing a reliable constraint for epoxide uptake rates in the chamber. However, in order to properly assess the overall SOA production, the α_{SOA} is needed in addition to ɣ. To this end a 0-D time-dependent box model was used to simulate the chamber experiments and estimate α_{SOA}. The model was initialized with ɣ's from the flow reactor measurements, the amount of epoxide injected into the chamber, the chamber-measured aerosol surface area and mass concentrations, the estimated chamber wall-loss rate from epoxide injections in the absence of seed particles, and the user-chosen α_{SOA}. Chemical rate equations for gas and aerosol-phase epoxide concentrations were integrated over the duration of the chamber experiment to determine time-dependent concentrations. The only losses of gas-phase epoxide were to particle surface area and to the chamber walls, and the only source of aqueous-phase epoxide was the reaction of gas-phase epoxide on the particle surface area. The aqueous-phase epoxide formation rate was scaled by α_{SOA} in order to match the chamber-observed aerosol mass loadings. Aerosol surface area was held constant over the course of a model run despite that the SOA formation does contribute to the surface area. This is less of an issue for MAE given the modest SOA growth compared to *trans*-β-IEPOX. For the *trans*-β-IEPOX experiments the additional SOA resulted in at most a 40% increase in surface area. It is not clear how this additional surface area would affect the modeled SOA growth. Based on previous studies, the presence of aerosol phase semi-oxidized organics in the form of polyethylene glycol tended to inhibit *trans*-β-IEPOX uptake, thereby slowing the SOA growth. Indeed we observed that the modeled SOA growth rate tended to be faster than that observed in the chamber experiments. However, this effect could also be in part a result of the instantaneous mixing assumed by the box model.

As shown in Figure 2, α_{SOA} was adjusted in the model to bracket the observed chamber SOA mass growth and obtain an upper and lower estimate of α_{SOA}. These ranges are reported in Table 3. α_{SOA} for *trans*-β-IEPOX and MAE varied for the different aerosol compositions from 0.03 – 0.16 and 0.05 – 0.22, respectively, with the slightly larger α_{SOA} observations for the ammonium sulfate seed types compared to magnesium sulfate. In general, we would expect aerosol conditions that influence ɣ – high aerosol acidity, the concentration of general acids like bisulfate, and the concentrations of nucleophiles – to influence α_{SOA} similarly. While ɣ was largest for the acidified aerosols, α_{SOA} seems to be largely independent of acidity with the largest α_{SOA} for *trans*-β-IEPOX (α_{SOA} = 0.16) observed on the pure ammonium sulfate aerosol. Therefore it appears that even in the absence of a substantial concentration of acid catalyst the same ultimate mass yield can be achieved provided the timescale is sufficiently long. Model outputs for IEPOX showed good agreement with the chamber observations especially considering that the characteristic leveling off of the SOA mass growth was well represented in the model output (see Figure 2a). This was not the case for the MAE experiments as seen in Figure 2b where the model outputs fail to capture any leveling off in aerosol mass. As a result α_{SOA} estimates for MAE may be less robust compared to *trans*-β-IEPOX. An underestimation of the MAE γ – and therefore an overestimation of the α_{SOA} – could result in such differences. That said, MAE γ measurements were reproducible and the modest SOA growth coupled with the low-time resolution of the mass concentration data make modeling the MAE experiments inherently more difficult.

It should be stated that the molecular weight of the SOA is assumed to be the same as *trans*-β-IEPOX or MAE, depending on which epoxide was investigated, while the majority of SOA tracers have a molecular weight larger than the parent epoxide. As a result, the α_{SOA} reported here are likely biased high. As an upper limit example, IEPOX-derived organosulfate (216 g/mole) has been shown to be a primary component of isoprene-derived SOA with a molecular weight almost twice that of IEPOX (118 g/mole). If we assume all of the SOA mass is made up of these organosulfates our reported α_{SOA} would be biased high by about 50%.

As we state above, it is not clear how γ and the α_{SOA} are affected when a significant fraction of the aerosol surface area is represented by epoxide-derived SOA. This warrants further investigation as it could be quite relevant in regions like the southeastern United States during summer where isoprene SOA can account for a substantial portion of the $PM_{2.5}$ mass and therefore surface area. The results presented here which constrain all reactions that contribute to IEPOX- and MAE-derived SOA could be beneficial in regional and/or global models to help constrain predictions in total IEPOX- and MAE-derived SOA, especially since current models only constrain the model with a few known aqueous phase reaction rates.

Table 3. Summary of Experiments and Results.

epoxide	aerosol	RH	aerosol $[H^+]$ (M)[a]	$\gamma \pm 1\sigma$	modeled α_{SOA} range
IEPOX	$(NH_4)_2SO_4$	0.50	7.74E-05	6.5e-4 ± 6.4e-4	0.13 - 0.16
IEPOX	$MgSO_4 + H_2SO_4$	0.08	0.04	0.011 ± 0.003	0.04 - 0.06
IEPOX	$MgSO_4 + H_2SO_4$	0.53	0.73	0.0094 ± 0.003	0.03 - 0.05
IEPOX	$(NH_4)_2SO_4 + H_2SO_4$	0.05	2.78	0.021 ± 0.001	0.09 - 0.11
IEPOX	$(NH_4)_2SO_4 + H_2SO_4$	0.59	2.01	0.019 ± 0.002	0.05 - 0.07
MAE	$MgSO_4 + H_2SO_4$	0.03	0.73	4.9e-4 ± 1e-4	0.05 - 0.11
MAE	$(NH_4)_2SO_4 + H_2SO_4$	0.03	2.78	5.2e-4 ± 1.1e-4	0.14 - 0.22

[a]Estimated from E-AIM model calculation of moles H^+ and total volume of aqueous phase. E-AIM RH input must be ≥0.1, so the same $[H^+]$ is estimated for like aerosol compositions despite differences in experimental RH.

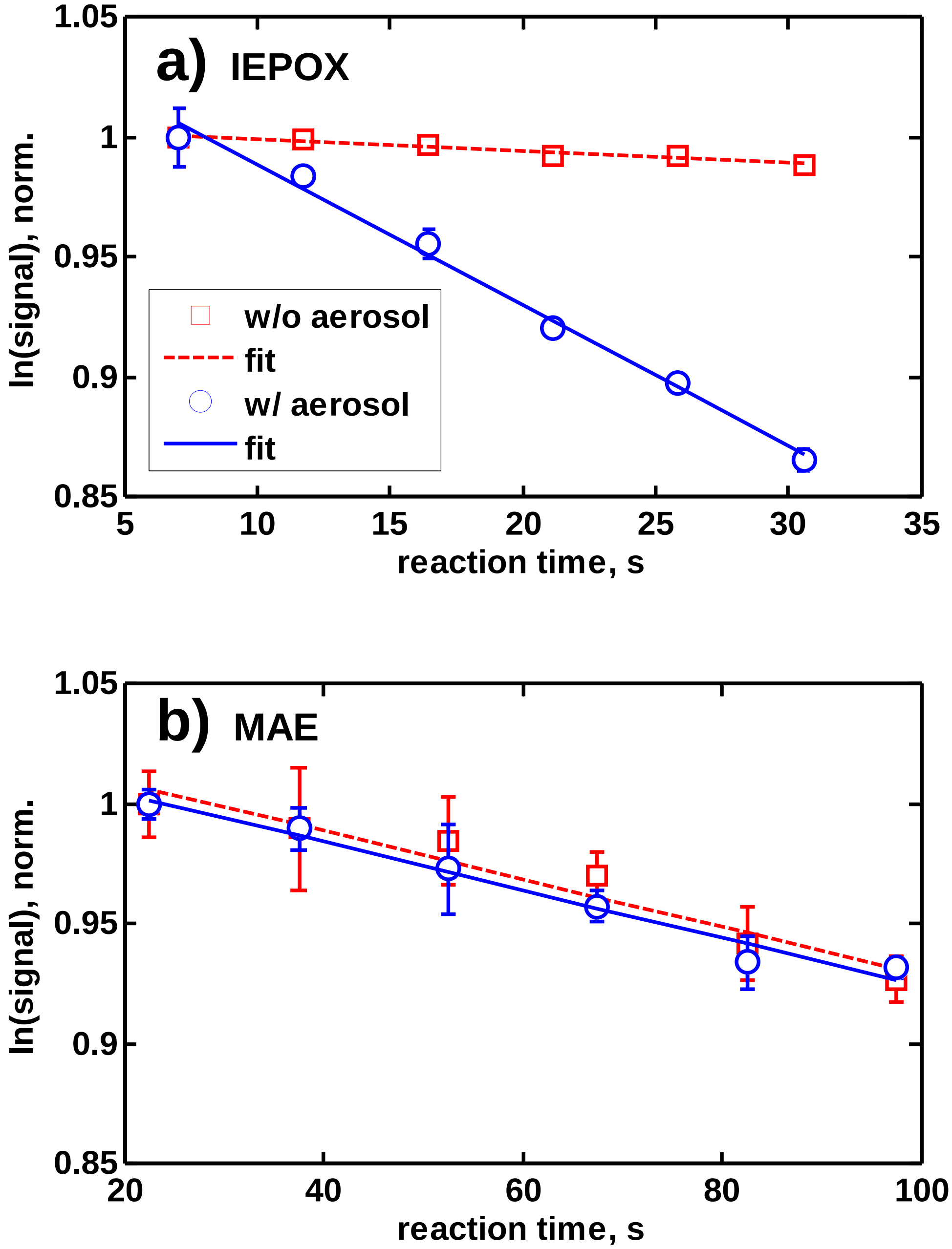

Figure 1. The average of the log of the epoxide signal versus reaction time and associated linear fit without aerosols (red squares, red dashed line is the fit) and with aerosols present in the flow reactor (blue circles, blue solid line is the fit) for (a) *trans*-β-IEPOX and (b) MAE on $(NH_4)_2SO_4$ + H_2SO_4 aerosol. Error bars represent the 2x the standard deviation of the averages. Values have been normalized to 1 for ease of comparison.

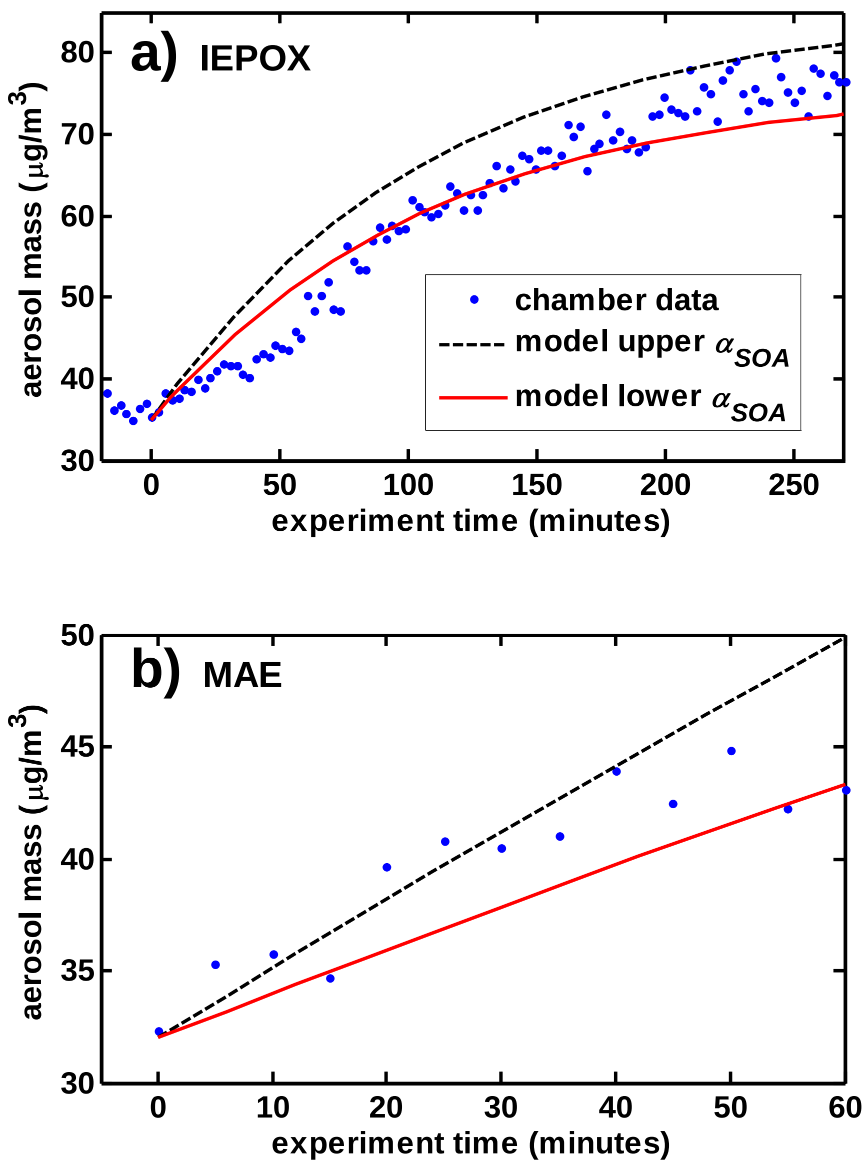

Figure 2. Chamber measured (blue dots) and modeled (black dashed line, red solid line) SOA mass loadings for (a) *trans*-β-IEPOX with $(NH_4)_2SO_4$ seed and (b) MAE with $(NH_4)_2SO_4$ + H_2SO_4 seed. The black dashed lines represent the model upper estimate of molar SOA yield, and the red solid lines represent the model lower estimate.

Project 14-004	STATUS: Active – June 20, 2014

Emission Source region contributions to a high surface ozone episode during DISCOVER-AQ

University of Maryland – Christopher Loughner
Morgan State University – Melanie Follette-Cook
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Doug Boyer

Funding Amount: $109,111
($55,056 Univ. of Maryland, $54,055 Morgan State Univ.)

Executive Summary

The highest ozone air pollution episode in the Houston, TX region in 2013 occurred September 24-26, which coincided with the DISCOVER-AQ (Deriving Information on Surface Conditions and Vertically Resolved Observations Relevant to Air Quality) field campaign. The maximum 8-hour average ozone peaked on September 25 at LaPorte Sylvan Beach reaching 124 ppbv. We will analyze this air pollution episode to quantify how emissions from various source regions (i.e., Houston, Dallas, Beaumont/Port Arthur, Lake Charles, LA, Oklahoma, etc.) contributed to Houston's poor air quality. This work will examine the importance of regional emissions and transport on local air quality.

The investigators will use a combination of model simulations and space-, aircraft-, and ground-based observations to investigate the roles of both regional transport and local emissions on air quality in Houston, TX for this event. This work will improve understanding of ozone formation and accumulation by examining the spatial patterns of emissions within and outside of Texas and the transport processes that contributed to high ozone in Houston.

The investigators will use Weather Research and Forecasting (WRF) and Community Multi-scale Air quality (CMAQ) model output along with ground- and aircraft-based observations obtained during the DISCOVER-AQ field campaign to identify plumes that entered the Houston metropolitan area and contributed to high surface ozone concentrations. The investigators will identify the origins of plumes by calculating back trajectories from the WRF simulation. CMAQ simulations performed with source apportionment will be analyzed to determine the contributions of various source regions on surface ozone concentrations in the Houston metropolitan area. In addition, satellite observations (Ozone Monitoring Instrument (OMI) tropospheric nitrogen dioxide, OMI ozone profiles, Measurement Of Pollution In The Troposphere (MOPITT) carbon monoxide, and Moderate Resolution Imaging Spectrometer (MODIS) and Visible Infrared Imaging Radiometer Suite (VIIRS) aerosol optical depth) will be analyzed to determine if they were able to detect the regional transport of air pollution and subsequent buildup in the Houston metropolitan area.

Project Update

Initial WRF-CMAQ simulations at horizontal resolutions of 36, 12, and 4 km produced a weaker bay breeze than observed on September 25 that resulted in lower ozone concentrations along the western coastline of Galveston Bay and points inland to the north and west. We re-ran WRF with a revised technique to improve the model representation of the sea and bay breezes. In addition, a fourth modeling domain was added with a horizontal resolution of 1 km under project 14-002. The new run used the North American Mesoscale (NAM) 12 km model for initial and boundary conditions instead of the North American Regional Reanalysis (NARR), which has a horizontal resolution of 40 km. We nudged all domains, whereas previously we only nudged the 36 km domain. In addition we used a WRF iterative technique, where we first ran WRF performing analysis nudging based on the NAM 12 km, and then re-ran WRF performing analysis nudging based on the previous WRF simulation. This modeling technique prevented the relatively coarse NAM 12 km model from degrading the high resolution WRF modeling domains (4 km and 1 km modeling domains).

New CMAQ simulations based on the new and improved WRF simulation have been completed for the 36, 12, and 4 km domains. Overall, the new 4 km CMAQ simulation is in better agreement with the observations of maximum 8 hour average ozone concentrations than the original simulation (Figures 1-3). For September 24, the new CMAQ simulation is in agreement while the original CMAQ simulation has a high bias compared to observations (Figure 1). For September 25, the new CMAQ simulation generally improves the representation of surface ozone concentrations than the original run (Figure 2). However, a high model bias is present at Galveston and a low model bias is present at LaPorte Sylvan Beach in both the original and new CMAQ simulations. The new 4 km CMAQ simulation did not capture the observed high ozone over Channelview and Deer Park during the 2nd and 3rd circuits and Moody Tower on the 3rd circuit (Figure 4). For September 26, both the new and original CMAQ simulations accurately capture the magnitude and spatial distribution of ozone concentrations throughout the Houston metropolitan area (Figure 3).

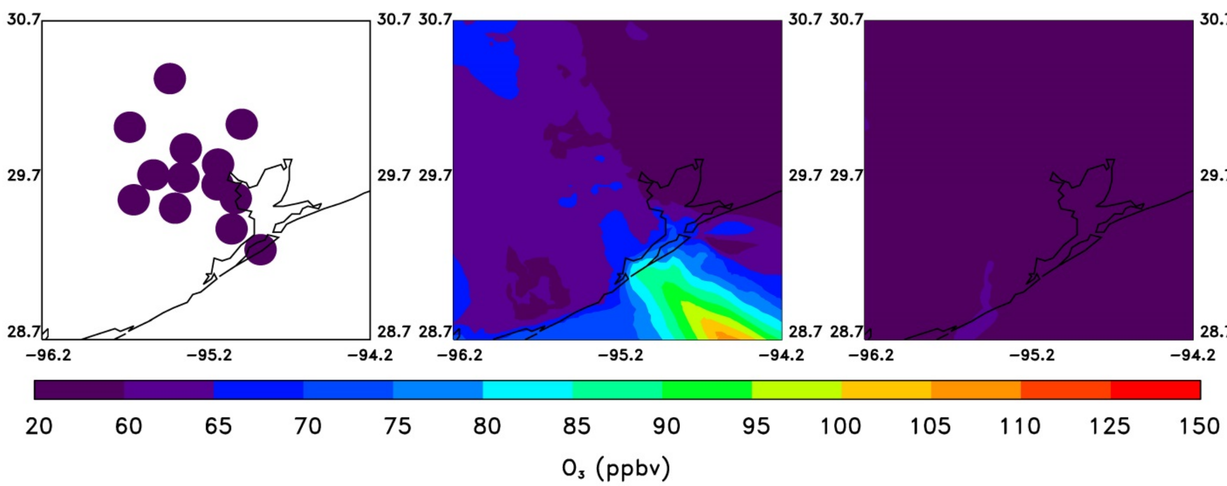

Figure 1: Eight hour average ozone maximum from observations (left), original 4 km CMAQ simulation (middle), and new 4 km CMAQ simulation on 24 September 2013.

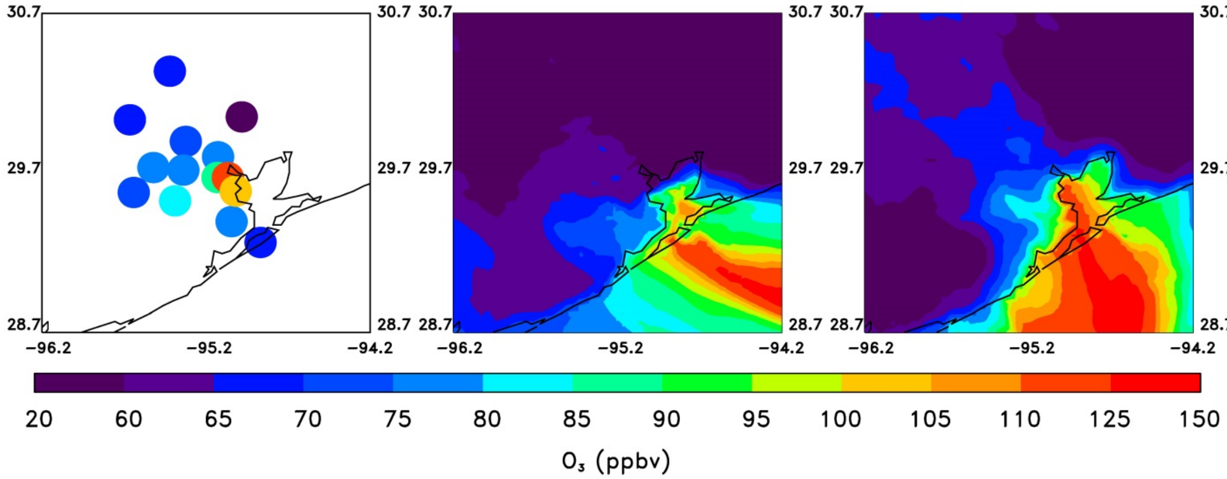

Figure 2: Eight hour average ozone maximum from observations (left), original 4 km CMAQ simulation (middle), and new 4 km CMAQ simulation on 25 September 2013.

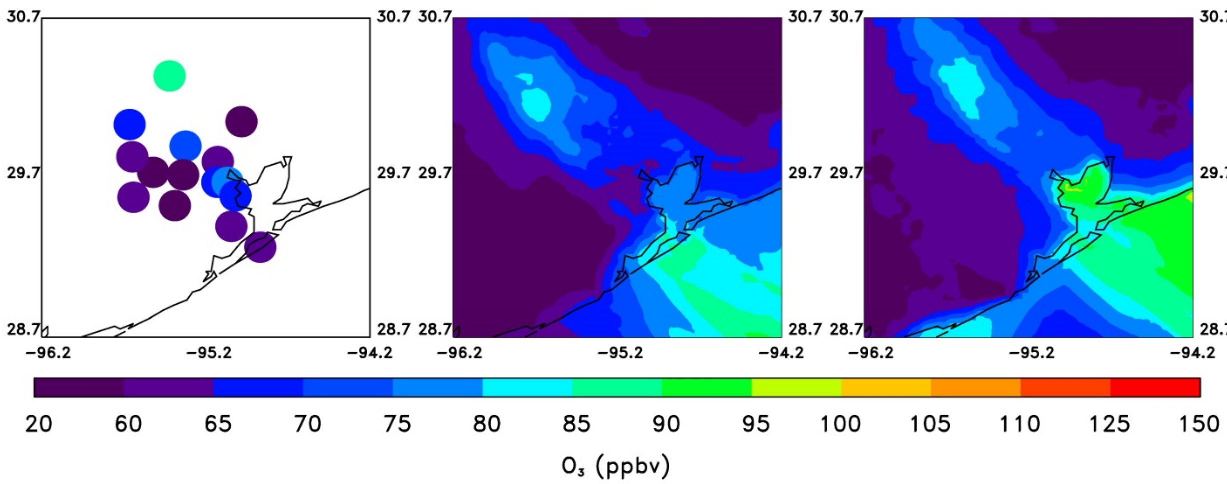

Figure 3: Eight hour average ozone maximum from observations (left), original 4 km CMAQ simulation (middle), and new 4 km CMAQ simulation on 26 September 2013.

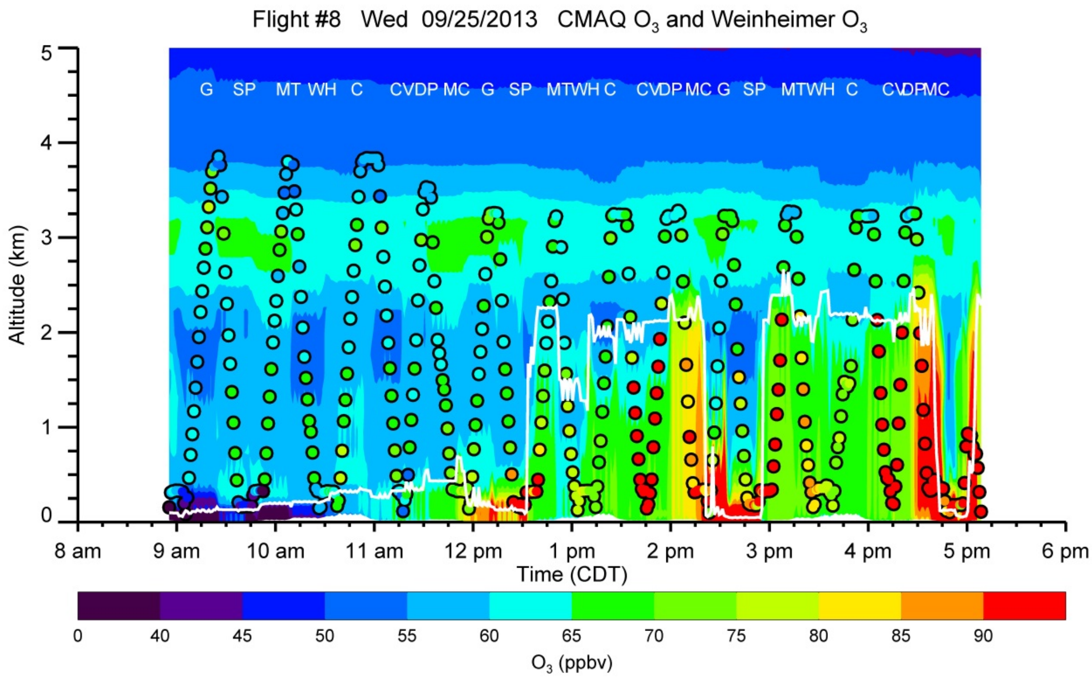

Figure 4: CMAQ simulated (background) and observed (overlay) ozone concentrations along a flight track on 25 September 2013. The white line shows the location of the top of the boundary layer as calculated by the WRF model. The white letters at the top of the figure, "G", "SP", "MT", "WH", "C", "CV", "DP", and "MC" stand for the spiral locations Galveston, Smith Point, Moody Tower, West Houston, Conroe, Channelview, Deer Park, and Manvel Croix, respectively. CMAQ results are from the new 4 km horizontal resolution domain.

Project 14-005	STATUS: Active – February 15, 2015

Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation

Texas A&M – Sarah Brooks

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

Funding Amount: $103,890

Executive Summary

Tropospheric air quality is degraded by local aerosol sources and gas phase precursors as well as aerosol transported over long distances. While the availability of recent satellites such as the Moderate-resolution Imaging Spectroradiometer (MODIS) and the Cloud-Aerosol Lidar with Orthogonal Polarization (CALIOP) offer improved accuracy and global coverage of aerosol, such measurements still rely on broad assumptions in determination of aerosol source and composition. During the fall of 2013, the Houston area was the site of the 2nd field intensive of the NASA Deriving Information on Surface conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign. During DISCOVER-AQ, this project's research team operated a new scattering instrument, the Cloud and Aerosol Spectrometer with Polarization (CASPOL), which measures the depolarization ratio of individual particles in the aerosol population. The polarization capabilities of CASPOL facilitate an effective approach to validate spaceborne aerosol retrieval, particularly CALIOP aerosol type classification. The CASPOL was operated on top of the 60 m tall Moody Tower (MT) on the University of Houston campus, a central urban location and site of many complementary measurements during DISCOVER-AQ. In this study, the CASPOL data set will be analyzed to determine the concentration, size distribution, and optical properties of aerosol from the wide variety of sources, including urban pollution sources from downtown Houston, the industrial Ship Channel, and transported aerosol. Combined with additional measurements of organic carbon, black carbon and ozone, the CASPOL data set provides an opportunity to determine the primary aerosol sources and impacts of aging due to ozone modified aerosol optical properties. These in-situ data will be compared to MODIS and CALIOP aerosol measurements to determine the sensitivity of remote sensing to changes in surface aerosol properties and air quality. Results from the project will improve the linkage between column observations provided by satellite instruments and near-surface atmospheric composition, which is relevant to air quality and human health in the short term and the relationship between future air quality and climate.

Project Update

The Cloud and Aerosol Spectrometer with Polarization (CASPOL) manufactured by Droplet Measurement Technology, Inc. (DMT) measures particle-by-particle aerosol optical properties and was operated in the field for the first time as a part of NASA's Deriving Information of Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ). The CASPOL was mounted on top of the 70 meter tall Moody Tower, located on the University of Houston's campus, and took continuous samples during the fall of 2013. The work presented here lays the groundwork for assessment of the feasibility of using CASPOL observations of optical properties of urban aerosols to create a new tool to be used to differentiate aerosol source. Results show that observed aerosol optical properties depend on source, and sources can be distinguished using the CASPOL particle-by-particle data by using the newly developed scattering signature technique. The results indicate that when aerosol concentrations are greater than 100 L^{-1}, the CASPOL can distinguish aerosol source with only a few hours of data.

1. CASPOL Data Collection and Quality Control.

From August 28 through October 4, 2013, the CASPOL was located on top of the Moody Tower. The Moody Tower is located at 29.7176° N, -95.3414° W, approximately four kilometers south of downtown Houston, Texas. The inlet was located on top of the building which is ~70 meters tall. The height of the tower is low enough that the aerosols being sampled are representative of the aerosols at the surface, but tall enough so that any intermittent point sources will not interfere with the measurements. This tower has been the location of many previous and current field campaigns (Brooks et al., 2010; Lefer et al., 2010; Rappenglück et al, 2010; Wong et al., 2011). The CASPOL inlet was specially designed to rotate so that it always points into the wind. The inlet was connected to a heated stainless-steel pipe (1.5 m in length), to maintain constant relative humidity and avoid condensation (Quinn et al., 1998), by a 3/4 inch outer diameter piece of non-conductive tubing that was 2.5 meters long. Beyond the heated pipe, the sample flow was split between the CASPOL (1.2 L min^{-1}) and a dump line (10 L Min^{-1}), and behind the CASPOL was a thermocouple, relative humidity meter (ROTRONIC H290D), HEPA filter, another thermocouple and then another relative humidity meter (ROTRONIC H290D), as seen in Figure 2. The inlet line was changed, and the other tubing was changed or dried at least twice a week. Data was removed if rainfall amounts exceeded three fourths of an inch in the six hours before and during any time period due to the likelihood of the majority of particles being removed via the wet deposition process. At the time of this report all CASPOL data collected during DISCOVER-AQ has been quality controlled. Data collected during and after precipitation events has been eliminated, as will any periods during which the CASPOL was operating offline for maintenance, drying, or flow testing.

2. Separation of All Data-Controlled CASPOL Data According to Source Location.

Air masses over the Moody Tower are likely to have been influenced by one of four major aerosol sources. The Ship Channel source, which is a heavily industrialized area on the east side of Houston. An Urban source, which consists of the densely populated, urban center of Houston. A marine source, which consists of transported aerosols from the Gulf of Mexico and potentially further (Goudie and Middleton, 2001). Lastly the Semi-Urban/Rural source, which consists of transported aerosols from the west and passes over the less densely populated zones of the greater Houston area. Conveniently, these sources come from four different wind directions relative to the Moody Tower. Time periods of when these sources potentially occurred were determined using the NOAA, Atmospheric Resources Laboratories Hybrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Draxler and Hess, 1997, 1998; Draxler et al., 1999) to create five day back trajectories with one hour intervals using Global Data Assimilation (GDAS) model data with 0.5 degree resolution. Ten cases were found in the data when HYSPLIT back trajectories were consistent, indicating the wind direction was from one of the four sources. These cases range from six to thirty hours in length. The Ship Channel case was sampled when the HYSPLIT showed the wind was from 45° to 135°, the Ocean case from 135° - 225°, the Semi-Urban/Rural case from 225° - 315°, and the Urban case from 315° to 45°. In total, five Ship Channel cases, three Urban cases, and two Ocean cases were identified for further analysis of the scattering properties. No Semi-Urban/Rural cases were identified during the time period of the campaign.

A technique for identifying particle type by the patterns in plotted optical properties for ensembles of sampled particle was developed by Glen and Brooks (2013). To create the patterns, or scattering signatures, the backscatter intensity and depolarization ratio are first discretized. Then the depolarization ratio is plotted on the x axis, and the backscatter intensity on the y axis. Next, the frequency of particles that have intersecting values of depolarization ratio and backscatter intensity are placed at each intersection. In Figure 2, the composite scattering signatures of all of the data from each of the three sources are shown. The color of each intersecting value indicates the percentage of particles at that intersecting value. The Ocean case has the strongest backscatter intensity, approaching 400, and is the most depolarizing. The data collected under the Ship Channel conditions (Figure 2) is slightly depolarizing but the backscatter intensity is around half of the Ocean data at around 210. The Urban data has an even lower backscattering intensity of 200 and is the least depolarizing at approximately 0.1 (Figure 1).

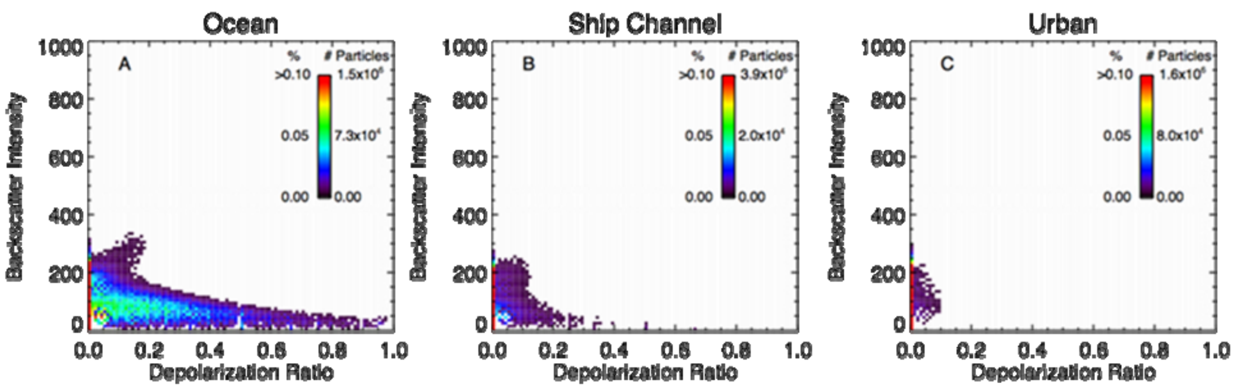

Figure 1. The scattering signatures for all of the data in the Ocean, Ship Channel, and Urban sources.

Each of these scattering signatures, or patterns, is unique in shape from the others. By using this scattering signature technique, the CASPOL can distinguish aerosol source regions in the Houston area. The CASPOL's ability to distinguish aerosol source shows that a potential exists for the CASPOL to be a useful tool in air quality monitoring. However, it should be noted that these signatures of each regime are a composite of several cases which span multiple hours. For the CASPOL to be effective as an air quality monitoring and diagnostic tool, it must be able to distinguish aerosol sources using scattering signatures created from a short time frame of data. We next explore scattering signatures of data collected during briefer periods of time.

Task 1 Deliverables:
A file has been produced for each day which contains for all quality controlled data collected that day CASPOL time, total particle number, size distribution.

Next, the data was classified according to source location. For each period in which the CASPOL continuously sampled under constant source conditions, a file was created containing single particle backscattering, and depolarization data, which was used to generate optical signature plots in Task 2 below.

Task 2 Deliverable:
HYSPLIT back trajectories have been run for all quality controlled CASPOL DATA. Based on the back trajectories, all CASPOL data has been sorted into categories, i.e. urban pollution, industrial pollution from the Ship Channel, or transported aerosol. From these files, CASPOL data from has been used to generate optical signature plots (backscattering vs. depolarization) for each time period of data of 6 or more continuous hours of CASPOL data collected in a single category.

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Project 14-006	STATUS: Active – June 12, 2014

Characterization of Boundary-Layer Meteorology during DISCOVER-AQ Using Radar Wind Profiler and Balloon Sounding Measurements

Sonoma Technology, Inc. – Clinton MacDonald
Valparaiso University – Gary Morris

AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Dave Westenbarger

Funding Amount: $65,588
($49,979 Sonoma Technology, $15,609 Valparaiso)

Executive Summary

As part of the DISCOVER-AQ (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality) program in August and September 2013, Sonoma Technology, Inc. and the National Oceanic and Atmospheric Administration, with support from the AQRP, operated radar wind profilers (RWPs) at four sites in the greater Houston area to collect boundary layer wind data. In addition, a permanent network of three RWPs also provided data during this study. Also, Pennsylvania State University and the Valparaiso University/University of Houston team conducted daily meteorological and ozone soundings on most days during DISCOVER-AQ. The combination of these data offers a rich source of boundary layer meteorological data and can be used to provide insight into the processes that influence the air quality in Houston.

To address questions about meteorological conditions during the DISCOVER-AQ study and to provide useful information to other researchers, this project will (1) characterize boundary layer meteorological processes on all aircraft flight days and high ozone days during the DISCOVER-AQ study period; (2) provide context to the DISCOVER-AQ boundary layer characteristics by comparing them to characteristics observed on high ozone days during the TexAQS-II project in 2005 and 2006 and over the past 10 years for the month of September; and (3) provide continuous daytime boundary layer height data at the seven RWP sites for the entire study period. The results from this project will be documented in a final report, distributed to other researchers, and presented at an end-of-project meeting in Austin in 2015.

Project Update

This report summarizes project activities that were completed for AQRP # 14-006 from December 2014 through February 2015. Over this period, the project team

- Completed the assessment of meteorological and air quality conditions on DISCOVER-AQ flight days and other days with high ozone levels in the Houston area;
- Compared meteorological conditions observed during the DISCOVER-AQ study period to those observed during the 2006 TexAQS program;
- Determined September average meteorological conditions for Houston;
- Attended a project team meeting at the Texas Commission for Environmental Quality in Austin in January 2015;
- Delivered wind and temperature data from the seven radar wind profilers in operation during the DISCOVER-AQ program;

- Documented analyses and findings in a draft report.

No additional data were gathered during this quarter. Work and analysis performed during this quarter included completing the characterization and summarizing of weather and air quality conditions in the Houston-area during the DISCOVER-AQ program (Task 1 of this project), and continued comparison of meteorological conditions observed during the DISCOVER-AQ period to those observed during the 2006 TexAQS program (Task 2).

Over the next quarter, work will focus on completing the analysis for Task 2, completing and submitting the Draft Final Report and Final Report, submitting mixing height data for the University of Houston Coastal Center radar wind profiler, and preparing a presentation for the end of project meeting in Austin.

Project 14-007	STATUS: Active – June 23, 2014

Improved Analysis of VOC, NO2, SO2 and HCHO data from SOF, mobile DOAS and MW-DOAS during DISCOVER-AQ

Chalmers University – Johan Mellqvist
University of Houston – Barry Lefer

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – John Jolly

Funding Amount: \$97,260
(\$74,179 Chalmers, \$23,081 UH)

Executive Summary

Mobile optical remote sensing measurements by the SOF and mobile DOAS techniques were carried out in the Houston area during September 2013 as part of the NASA Discover Air Quality experiment. Atmospheric gas column measurements of SO_2, NO_2, HCHO and VOCs were carried out in a box around the Houston Ship channel, in parallel with flights by two aircraft from NASA. In this project the collected optical remote sensing data will be reanalyzed, improved and compared to other data. In particular, the investigators will work with radiative transfer modeling to minimize cloud effects.

In addition, during the 2013 field campaign a new VOC sensor was used to map ratios of the ground concentrations of alkanes and aromatic VOCs downwind of various industries. In this project the investigators will refine the spectral analysis for measurements of the aromatic VOCs from this sensor and compare the data to parallel measurements with other techniques and write a scientific paper.

This project will support the AQRP priority research area: "Improving the understanding of ozone and particulate matter (PM) formation, and quantifying the characteristics of emissions in Texas through analysis of data collected during the DISCOVER-AQ and SEAC4RS campaigns."

Project Update

The main activity during the reporting period has been a detailed analysis of the multi-angle DOAS measurements that was performed at the end of the DISCOVER-AQ campaign, coinciding with the most interesting period from a photochemical perspective, September 24-26. These measurements provide a potential to quantify absolute concentration columns, as opposed to relative columns retrieved from standard measurements, and to control for long term drift in the measurement series. While relative column measurements are well-suited for emission flux calculations for local plumes, they may be less useful for studying air quality in ambient conditions and more aged and less well-defined plumes. Although the multi-angle DOAS measurements could potentially overcome this problem, the method is less straightforward and has not been applied in this configuration before and hence require extensive data treatment and careful analysis.

As a first step a radiative transfer model has been setup to simulate the pathways of the measured light through the atmosphere. The DOAS measurement are based on absorption spectroscopy of ultraviolet light scattered in the atmosphere. The absorption of light is dependent on both the amount of the molecular species of interest in the atmosphere and on the length of the pathway of the light through the atmosphere. To quantify the molecular species the pathway must be known and this will be dependent on the solar angle, the measurement direction and a number of atmospheric properties, most importantly the aerosol loadings and their scattering properties. Hence the model was supplied with aerosol data and other atmospheric properties compiled from in-situ measurements made from the P-3B aircraft as part of DISCOVER-AQ. Based on the results from the radiative transfer model, the relationship between the result from the spectroscopic analysis of the measurements and the absolute vertical column (the total amount of a molecular species from top to bottom of the atmosphere) could be determined as a function of solar angle and measurement angle, which also made it possible to determine what angles were more suitable for this analysis. Measurements with an azimuthal angle relative to the sun as close to 180° as possible were best-suited while those close to 0° were the worst. Additional parameters could also be derived from the model which allow for some verification of the model to the measurements, such as the amount of inelastically scattered light, which causes the so called Ring effect in the measured spectra.

The spectroscopic evaluation of the measurements had been performed previously, but it was determined that it would be beneficial to apply a spectral averaging approach to reduce the noise in the results. Four consecutive sideway-looking spectra were averaged and as a reference spectrum the average of eight zenith-looking spectra measured during approximately the same time period was used. This meant that each spectral evaluation typically corresponded to a measurement period of approximately 30 seconds.

To apply the results from the radiative transfer model to the results from the spectroscopic analysis it proved to be important to know the exact measurement direction for each measured spectrum. This was derived based on the driving direction of the measurement vehicle, which was calculated from the GPS data which was continuously logged throughout the campaign. This information together with the solar angle, which was simply calculated based on latitude, longitude and time of day, allowed a relationship between the columns derived from the spectroscopic analysis and the absolute vertical columns to be established for each measurement. This allowed for a conversion to vertical columns for the more suitable measurement angles. This was done for both formaldehyde (HCHO) and nitrogen dioxide (NO_2), which are both of key interest in the DISCOVER-AQ campaign. This also allowed for verification of the model results based on for instance Ring effect results.

Since the relationships between measured columns and vertical columns as derived from the model results are based on a number assumptions and idealizations, such as a horizontally homogenous atmosphere, this interpretation is sensitive to some deviations from these assumptions, such as horizontal gradients of the molecular species of interest and the aerosol loadings. This makes the derived absolute vertical columns significantly more noisy than the relative columns normally derived. For this reason it is desirable to try to combine results from the two methods to produce a data set of absolute vertical columns with the precision of the relative measurements. Some ways of doing this has been tested with promising results, but some question marks still remain regarding what is the most suitable method.

During the DISCOVER-AQ campaign the P-3B regularly flew in spiral patterns which allows for vertical profiles of molecular species measured to be established as well as corresponding vertical columns. These vertical columns are available from the campaign data archive and have been downloaded and the ones corresponding to spirals performed close to Houston Ship Channel have been qualitatively compared to the multi-angle DOAS results described above. These comparisons are promising although some questions remain. When a final data set has been produced for the DOAS measurements, these comparisons will be remade in a more systematic way. Comparisons to DOAS measurements made from the P200 aircraft during the campaign has been started, but some questions have been raised about these measurements. This work will continue in more detail.

Project 14-008	STATUS: Active – April 17, 2014

Investigation of Input Parameters for Biogenic Emissions Modeling in Texas during Drought Years

The University of Texas at Austin – Elena McDonald-Buller

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Barry Exum

Funding Amount: $175,000

Executive Summary

The role of isoprene and other biogenic volatile organic compounds (BVOCs) in the formation of tropospheric ozone has been recognized as critical for air quality planning in Texas. In the southwestern United States, drought is a recurring phenomenon and, in addition to other extreme weather events, can impose profound and complex effects on human populations and the environment. Understanding these effects on vegetation and biogenic emissions is important as Texas concurrently faces requirements to achieve and maintain attainment with the National Ambient Air Quality Standard (NAAQS) for ozone in several large metropolitan areas. Previous research has indicated that biogenic emissions estimates are influenced by potentially competing effects in model input parameters during drought and that uncertainties surrounding several key input parameters remain high. The primary objective of the project is to evaluate and inform improvements in the representation of one of these key input parameters, soil moisture, through the use of simulated and observational datasets. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) will be used to explore the sensitivity of biogenic emission estimates to alternative soil moisture representations.

Project Update

Progress on Project 14-008 is summarized below by Task:

Task 1. Investigation and Evaluation of Soil Moisture Datasets

Work continued on retrieval and processing of the North American Land Data Assimilation System-Phase II (NLDAS-2) datasets. Activities during the previous quarter were primarily focused on soil moisture predictions provided by the Noah and Mosaic Land Surface Models (LSMs). During the current quarter, hourly predictions of soil moisture for years 2006-2013 from the Noah with multi-parameterization (NoahMP) and Variable Infiltration Capacity (VIC) NLDAS-2 LSMs were obtained and interpolated to the 12-km grid domain that covers Texas and surrounding areas. Analysis of these additional NLDAS-2 datasets was initiated with the goal of describing the seasonal and inter-annual variability of soil moisture by depth among the four NLDAS-2 datasets.

Task 2. Comparison of Simulated and Observed Soil Moisture

In-situ measurements of soil moisture from two networks [Soil Climate Analysis Network (SCAN) and the U.S. Climate Reference Network (USCRN)] were used to evaluate the simulation of soil moisture by the NLDAS-2 Mosaic and Noah LSMs. The evaluations were performed within the 12km grid domain that covers Texas and surrounding states for years 2006-2013. Because of the sometimes large biases between NLDAS-2 simulations and in-situ measurements, a soil moisture anomaly was calculated to better compare the interannual variability in soil water contents. Overall, the Noah and Mosaic predictions had similar directional seasonal variability compared to the available soil moisture observations. In general, agreement was better for Mosaic compared to Noah that tended to underestimate soil moisture in the eastern half of the 12km grid domain and overestimate soil moisture in the west, especially in the top soil layers. Observed soil moisture exhibits a gradual increase with increasing soil depth in the east; however, the predicted NLDAS-2 soil moisture contents show lower variability leading to a large underestimation of soil moisture at 50 and 100cm depths. Across the 12km grid domain and all soil depths, soil moisture values during the 2006-2013 growing seasons were generally lowest during 2011 for both observations and NLDAS-2 predictions.

Task 3. Preparation of MEGAN Simulations
In consultation with TCEQ, MEGANv2.1 simulations were generated to predict isoprene emissions for years 2006 2007, and 2011 during March through October on the 4km grid domain at 1km horizontal spatial resolution. Datasets processed for input to MEGAN included National Centers for Environmental Predictions North American Regional Reanalysis (NCEP-NARR) meteorological data (temporal/spatial resolution: 3 h/32 km), MODIS 4-day LAI product (MCD15A3; spatial resolution: 1 km), Photosynthetically Active Radiation (PAR) produced using solar insolation data from the Geostationary Operational Environmental Satellites (GOES; temporal/spatial resolution: 1 h/4 km) that were obtained from the University of Alabama in Huntsville, and the TCEQ land cover products. Emission factors were those specified by the default MEGAN gridded maps.

Task 4. Sensitivity of Biogenic Emission Estimates to Soil Moisture
MEGAN simulations to predict hourly isoprene emissions were performed for a basecase (impact of soil moisture not considered) in addition to simulations to estimate the impact of reduced soil moisture availability during drought that utilized the NLDAS-2 soil moisture databases: Noah, NoahMP, Mosaic, and VIC. The primary geographic focus of the simulations is on five eastern Texas climate regions: North Central, South Central, East, Upper Coast, and eastern portions of Edwards Plateau. During periods of drought, the Noah and NoahMP simulations estimated the lowest changes in predicted isoprene emissions relative to the basecase; for example, region-averaged emissions reductions relative to the basecase during summer 2011 were -5.8% for Noah and -9.1% for NoahMP; in contrast, Mosaic and VIC had substantially greater reductions that averaged -67.9% and -84.1%, respectively. Surprisingly, VIC predicted consistently large emissions reductions during 2007, a year that was not characterized by drought conditions in eastern Texas. Crucially, the Mosaic and VIC wilting point values were found to be factors of approximately two and four, respectively, greater than those for Noah and NoahMP. The difference in wilting points between the NLDAS-2 LSMs is significant because the wilting point value is the threshold value below which isoprene emissions are set to zero. Preliminary analysis suggests that the majority of differences in predicted emissions between the Noah/NoahMP and Mosaic/VIC simulations are driven by differences in wilting points as opposed to differences in predicted soil moisture values. Analyses of results from the isoprene simulations are on-going.

Project 14-009	STATUS: Active – July 1, 2014

Analysis of Surface Particulate Matter and Trace Gas Data Generated during the Houston Operations of DISCOVER-AQ

Rice University – Robert Griffin
University of Houston – Barry Lefer

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $219,232
($109,867 Rice, $109,365 UH)

Executive Summary
In recent years, the National Aeronautics and Space Administration (NASA) has placed considerable emphasis on the use of satellite remote sensing in the measurement of species such as O_3 and PM that constitute air pollution. However, additional data are needed to aid in the development of methods to distinguish between low- and high-level pollution in these measurements. To that end, NASA established a program titled Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ). DISCOVER-AQ began in summer 2011 with work in the Mid-Atlantic Coast that featured satellite, airborne, and ground-based sampling. The DISCOVER-AQ program conducted operations in and near Houston in September 2013.

During the Houston operations of DISCOVER-AQ, there was a need for ground-based measurement support. The predecessor to this project filled that need by providing quantitative measurements of sub-micron particle size and composition and mixing ratios of volatile organic compounds (VOCs) and other photochemically relevant gases such as O_3 and oxides of nitrogen (NO_x = nitric oxide (NO) plus nitrogen dioxide (NO_2)). The instrumentation for these measurements was deployed using the University of Houston (UH) mobile laboratory. The current project focuses on the analysis of data generated during the mobile laboratory operations during DISCOVER-AQ. To date, work has focused simply on contracting issues and development of a work plan and a quality assurance plan.

Project Update
Preliminary analysis of the organic aerosol (OA) dataset generated during DISCOVER-AQ with the HR-ToF-AMS was conducted using positive matrix factorization (PMF) using PMF2 (version 4.2, available from the Environmental Protection Agency) running in robust mode. The main factors contributing to the organic fraction of the submicron aerosol were identified in a sub-dataset corresponding to a period where elevated sub-micron PM concentrations were observed (near the end of the field campaign in northwest Houston). Preliminary results indicate that three main factors explain most of the variance in the dataset: a component corresponding to hydrocarbon-like OA (thought to be a proxy for primary OA) and two oxygenated OA components that differ in the level of oxidation (thought to be secondary OA of various atmospheric ages). Factor analysis of the size-resolved OA composition is being performed currently using a model named PARAFAC, as PMF does not consider particle size as a variable. The variation in the degree of oxidation of the submicron OA (again indicative of secondary material) across Houston during DISCOVER-AQ was examined based on different metrics as

well. The atomic hydrogen to carbon, atomic oxygen to carbon, and organic mass to organic carbon ratios and the average carbon oxidation state were analyzed in terms of spatial distribution. Results suggest that secondary OA with different degrees of processing depending on location is the major component of submicron OA in Houston. These metrics are being considered in terms of "zones" around Houston to more easily consider spatial variability.

Additional efforts have been made to identify secondary processes of relevance to the inorganic sub-micron PM measured as part of DISCOVER-AQ. To start, the DISCOVER-AQ inorganic PM data have been formatted such that they easily can be input into a freely available inorganic aerosol thermodynamic model to allow estimation of the various forms of inorganic material present (for example, sulfate versus bisulfate), liquid water content, and hydrogen ion concentration. Datasets of precursor gas mixing ratios (sulfur dioxide and ammonia) have been downloaded from the NASA archive and formatted for analysis with regard to sulfate and ammonium aerosol from the HR-ToF-AMS. The split between organic and inorganic nitrate has been estimated using techniques available from the literature, and it appears organic nitrate dominates.

Because biogenic volatile organic carbon data are not available for all periods of the MAQL operation, alternative data sources have been identified. The University of Houston Air Quality Forecasting group ran Community Multi-scale Air Quality (CMAQ) model simulations for every day during the campaign. The model ran at a 4-kilometer spatial resolution with 1-hour time steps over southeast Texas. Isoprene, isoprene oxidation products, and monoterpene data have been extracted for the MAQL locations during DISCOVER-AQ. For this process, the CMAQ model cell was identified for each location reported by the MAQL global positioning system. The model concentrations at the surface level were extracted for the closest model time step. It appears that monoterpene oxidation by nitrate radical leads to enhanced OA at night in the northwest part of Houston.

The FACSIMILE model is being utilized to evaluate ozone and radical production rates and to provide an estimate of their uncertainty by using multiple chemical mechanisms. Efforts on these tasks focus on development of the necessary hydrocarbon inputs to allow FACSIMILE modeling to be performed at each location and time of the MAQL. One method will be to construct biogenic hydrocarbon data from the CMAQ modeling output. A second method is to use hydrocarbon data from the Moody Tower and the flights. After removing outliers, hydrocarbon data have been regressed against either carbon monoxide (CO) or nitrogen oxides (NO_x) when sectored by wind direction (to characterize different air mass source regions). The resulting relationship for a source region can be used when the MAQL was downwind of that region, and the measured CO or NO_x (whichever provides a stronger correlation) from the MAQL can be used to estimate the hydrocarbon level at the MAQL. The standard deviations of the regression fits provide additional input for a sensitivity analysis. These regressions are complete. Because it is recognized that local instantaneous wind direction is not the only relevant metric to determine air mass history, back trajectory modeling is being used to determine more appropriate air mass source regions for the MAQL at every sampling time and location. Multiple elevations within the troposphere have been simulated to assure that the air mass regions assigned to each time and location of the MAQL are appropriate. These trajectory simulations are complete, and the next step is to match the regression relationships with the trajectory outputs in order to estimate hydrocarbon concentrations for the MAQL.

Nitrogen dioxide was measured in situ aboard the NASA P-3B and remotely sensed from the King Air B200 using the Airborne Compact Atmospheric Mapper (ACAM) during the flights of DISCOVER-AQ. For these flights, the NO_2 measurements were compared to the NO_2 column measurements from the network of Pandora spectrometers in Houston when coincidences occurred. The spatial footprint of the ACAM and Pandora measurements are much more similar than when compared to available satellite data. The biggest deviations from a one-to-one relationship (with ACAM being in excess of Pandora) are in the more polluted regions (Channelview, Moody Tower, and Deer Park). In order to compare Pandora measurements to P-3B data, the in situ data was binned and integrated to produce a lower tropospheric column. Nitrogen dioxide was measured aboard the aircraft at one-second temporal resolution. Aircraft spiral data are averaged in 100-meter bins through the height of the profile and summed to derive a lower tropospheric column density (that is, data from above 5 kilometers height are not included). To fill in gaps of missing data, interpolation was used. Profiles missing more than five bins were excluded from this analysis. Coincident Pandora measurements were averaged through the time of the spiral and the monthly averaged stratosphere (from satellite) was subtracted to give a tropospheric estimate. These efforts also showed that deviations from a one-to-one relationship were larger in polluted regions.

Project 14-010	STATUS: Active – July 1, 2014

Impact of large-scale circulation patterns on surface ozone concentrations in HGB

Texas A&M Galveston – Yuxuan Wang

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Mark Estes

Funding Amount: $79,325

Executive Summary

The Bermuda High (BH) is a key driver of large-scale circulation patterns in Southeastern Texas in summer. The variations in the location and strength of the Bermuda High are expected to influence surface ozone concentrations and cause high- or low-ozone years in HGB through modulating the southerly flows that bring marine air with lower ozone background from the Gulf of Mexico. This project aims at establishing a statistical relationship from historical observations to quantify the impact of the BH variations on the variability of surface O_3 in HGB during the ozone seasons. Such a relationship will then be used to improve the GEOS-Chem simulation of background ozone inflow from the Gulf of Mexico through development of a bias correction scheme. The more than decade-long observational record of ozone and meteorology (1998 – 2012) during the ozone season (April 1 – October 31) will be analyzed to characterize the complex effects of the BH on surface ozone variations in HGB. The ozone variability will be defined for maximum daily 8-h average (MDA8) at the monthly and interannual time scales (i.e., the timescale of determining air quality attainment or nonattainment). A variety of indices to define the location and strength of the Bermuda High (BH Index; BHI) will be adopted from the literature and new BHI of better relevance to Texas air quality will be proposed. Statistical relationships between the variability of surface ozone concentrations and BHI will be constructed based on observations. The observed relationship will then be used as a mechanistic basis to design a bias correction scheme in the GEOS-Chem global CTM to improve its simulation of background O_3 associated with maritime inflow to HGB. The results will benefit the regulatory models of TCEQ through improved boundary conditions at the Gulf of Mexico model domain.

Project Update

Progress on Project 14-010 is summarized below by Task:

Task 1: The project team has collected the MDA8 ozone concentrations over HGB at continuous ambient monitoring stations (CAMS) during the study period (1998-2013), monthly gridded Global Historical Climatology Network (GHCN) data, National Centers for Environmental Prediction/National Center for Atmospheric Research (NCEP/NCAR), European Centre for Medium Range Forecast Re-analysis Interim (ERA-Interim) and North American Regional Reanalysis (NARR) reanalysis data.

Data collected includes:

Observational Data

- Daily maximum 8-hour ozone concentrations from 1998 to 2013 at CAMS sites over HGB region;
- Monthly gridded GHCN temperature data and monthly GHCN in situ temperature data

Reanalysis data:

- NCEP/NCAR reanalysis data (monthly mean surface temperature and relative humidity, sea level pressure, surface and 850hPa wind field; daily surface temperature and sea level pressure);

- ERA-Interim reanalysis data (monthly mean surface temperature and relative humidity, sea level pressure, surface and 850hPa wind field);

- NARR reanalysis data (monthly mean surface temperature, relative humidity, sea level pressure and surface wind field).

Using this data, we have started preliminary analyses of the MDA8 ozone variability over HGB (Fig 1), interannual variations of the longitude of the west edge of the Bermuda High (BH) (Fig 2) and Bermuda High index (BHI) (Fig 3. The longitude of the BH west edge is defined as the cross point of the adjusted 1560-gpm isoline and the 850 hPa wind ridge line; BHI is defined as the difference of regional mean SLP between the Gulf of Mexico (25.3°-29.3°N, 95°-90°W) and the southern Great Plains (35°-39°N, 105.5°-100°W) (Zhu et al., 2012).

The ozone-season (May to October) mean ozone surface concentration over HGB is shown in Figure 1. The detrended time series are obtained by subtracting the linear trend (dashed line; determined by least-square fit) from the raw data time series.

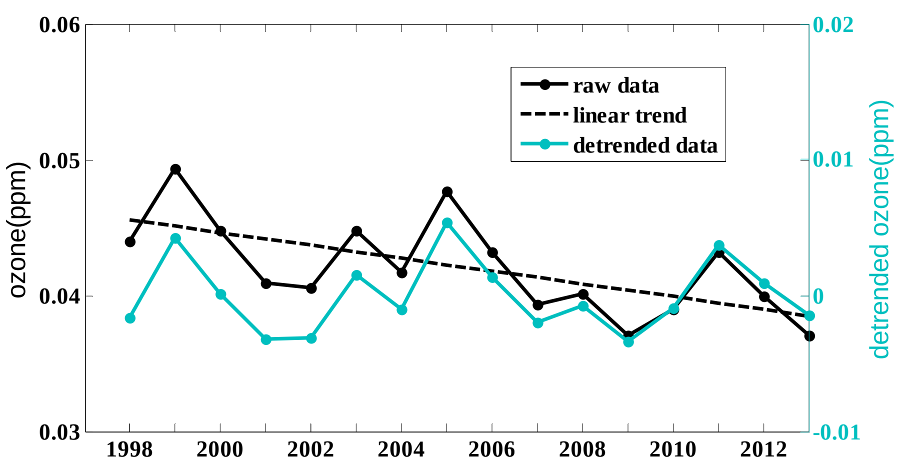

Figure 1.Time series of HGB spatial mean surface ozone concentrations (ppm) and detrended surface ozone concentration during the ozone season.

The following Figures 2-3 display the interannual variability of two different indices relating to the Bermuda High variability according to the definitions described above. The NCEP reanalysis data are used to generate these plots. The detrended time series in Figures 2-3 are obtained by subtracting the linear trend (dashed line; determined by least-square fit) from the raw data time series.

Preliminary analysis of Figure 1 to Figure 3 reveals that a higher surface ozone concentration is often companied with a more eastern location of the west edge of Bermuda High (e.g., 1999, 2005 and 2011). The BHI has a smaller value in 1999 and 2005, indicating a weaker Bermuda High of these two years, but the BHI in 2011 has a large value. In-depth analysis will be conducted in the succeeding report.

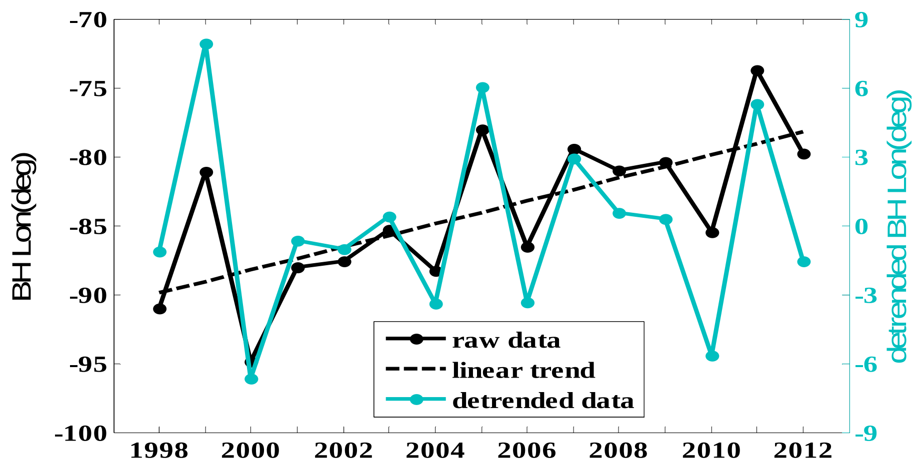

Figure 2.Time series of the longitude of the west edge of Bermuda High (raw data and detrended data; unit: degree longitude).

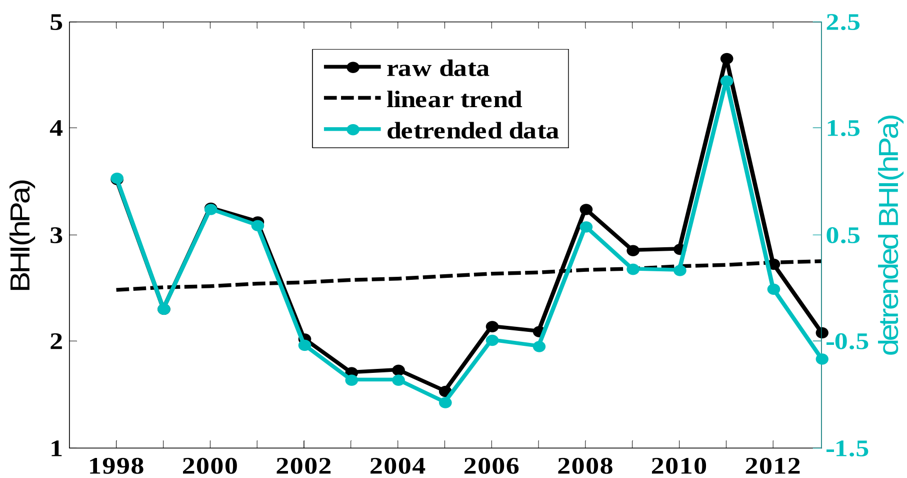

Figure 3.Time series of BHI (raw data and detrended data; unit: hPa).

Other reanalysis data and observational data mentioned in the work plan including Modern Era Retospective-analysis for Research and Applications (MERRA) reanalysis and GHCN daily observational data and other meteorological variables of potential importance to the project will be downloaded.

Further analyses will be done in Task 2.

In task 3, four sets of GEOS-Chem runs will be conducted, all at a spatial resolution of 2^{o} x 2.5^{o}. In preparation, we will set up the GEOS-Chem model for the full-chemistry simulation and tagged-ozone simulation.

Project 14-011	STATUS: Active – June 23, 2014

Targeted Improvements in the Fire Inventory from NCAR (FINN) Model for Texas Air Quality Planning

The University of Texas at Austin – Elena McDonald-Buller
Environ – Christopher Emery

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

Funding Amount: $179,586
($151,167 UT-Austin, $28,419 Environ)

Executive Summary
Wildland fires and open burning can be substantial sources of ozone precursors and particulate matter. The influence of fire events on air quality in Texas has been well documented by observational studies. During the 2012-2013 fiscal year of the Air Quality Research Program (AQRP), Dr. Elena McDonald-Buller, Dr. Christine Wiedinmyer, and Mr. Chris Emery led a project (#12-018) that evaluated the sensitivity of emissions estimates from the Fire INventory from NCAR (FINNv1; Wiedinmyer et al. 2011) to the variability in input parameters and the effects on modeled air quality using the Comprehensive Air Quality Model with Extensions (CAMx; ENVIRON, 2011). The project included an analysis of the climatology of fires in Texas and neighboring regions, comparisons of fire emission estimates between the FINN and BlueSky/SmartFire (Larkin 2009; Chinkin et al., 2009) modeling frameworks, evaluation of the sensitivity of FINN emissions estimates to key input parameters and data sources, and assessment of the effects of FINN sensitivities on Texas air quality. Among the many findings of the study were the needs for targeted improvements in land cover characterization, burned area estimation, fuel loadings, and emissions factors. These needs were particularly pronounced in areas with agricultural burning. This project addresses specific improvements in FINN that will support fire emissions estimates for Texas and the next public release of the FINN model. Fire emissions and air quality modeling will focus on 2012 to support TCEQ's air quality planning efforts.

Project Update
Progress on Project 14-01 is summarized below by Task:

Task 1. Regional Land Cover Characterization
Land cover characterization is a critical element in the estimation of fire emissions, as it is used to establish emission factors and fuel loadings. The Moderate Resolution Imaging Spectroradiometer (MODIS) Land Cover Type (LCT) product is used to characterize vegetation types in the default FINN v.1 configuration. For this study, alternative land cover representations are being developed using other global and U.S. national and regional land cover products. These include the European Space Agency's (ESA's) Climate Change Initiative Land Cover (CCI-LC) product released in 2014, the Global Land Cover – SHARE (GLC-SHARE) database released in 2014 by the UN Food and Agriculture Organization (FAO), the Fuel Characteristic Classification

System (FCCS) database and National Agricultural Statistical Service (NASS) Cropland Data Layer (CDL) both of which are available for the continental United States, and a high resolution regional land use/land cover database for Texas and surrounding states developed by Popescu et al. (2011).

The team presented a poster on early findings from the study at the American Geophysical Union Fall Meeting in San Francisco, California during December 15-19, 2014. Land cover classes for the GLC-SHARE, FCCS, and CDL databases were mapped to fourteen FINN land cover categories and compared with the default MODIS LCT product (see Figure 1). Estimates of CO emissions from fire events during 2012 (see Figures 2 and 3) were generated using various combinations of land cover products. A particular focus has been on the use of the NASS CDL for cropland characterization.

Work with the ESA CCI-LC product is on-going; it may be a promising alternative to either the MODIS LCT or GLC-SHARE products as it includes data on vegetation coverage. Currently, the MODIS Vegetation Continuous Fields (VCF) product is used to identify the density of the vegetation at each active fire location because the MODIS LCT product does not include such information.

The team will work to identify a suite of final land cover scenarios based on individual or combined datasets that are most relevant to TCEQ needs for regulatory air quality modeling. FINN estimates of CO, NOx, and $PM_{2.5}$ emissions will be produced.

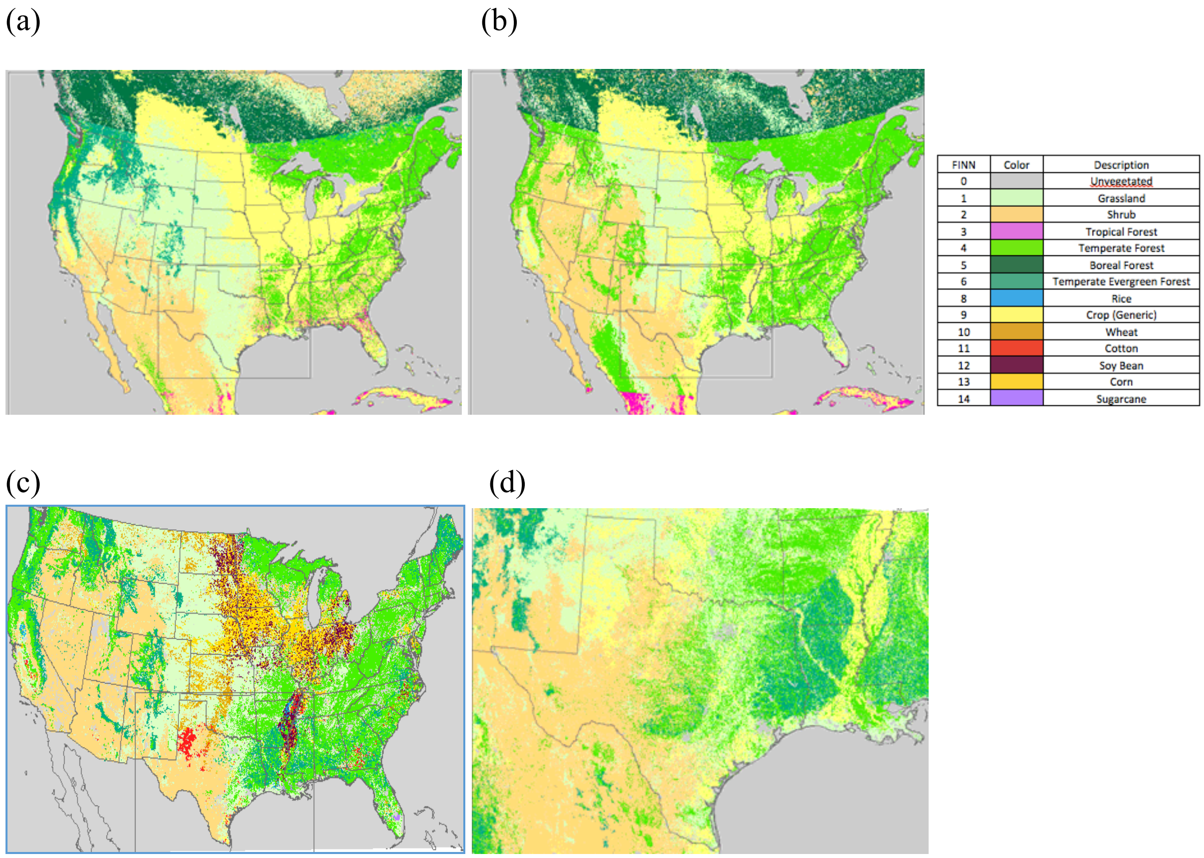

Figure 1. Mapping of fourteen FINN land cover types from the (a) MODIS LCT, (b) GLC-SHARE, (c) merged FCCS and NASS CDL products, and (d) high resolution (30 m) regional data developed by Popescu et al. (2011) for Texas and neighboring states for the Texas Commission on Environmental Quality (TCEQ).

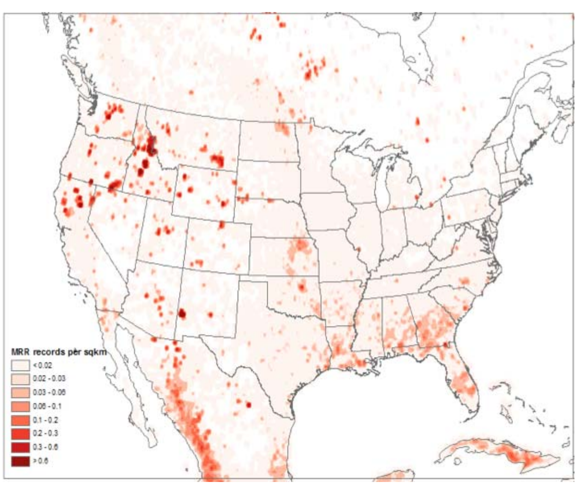

Figure 2. Annual total MODIS Rapid Response (MRR) fire counts in 2012 (detection confidence estimate ≥ 20%).

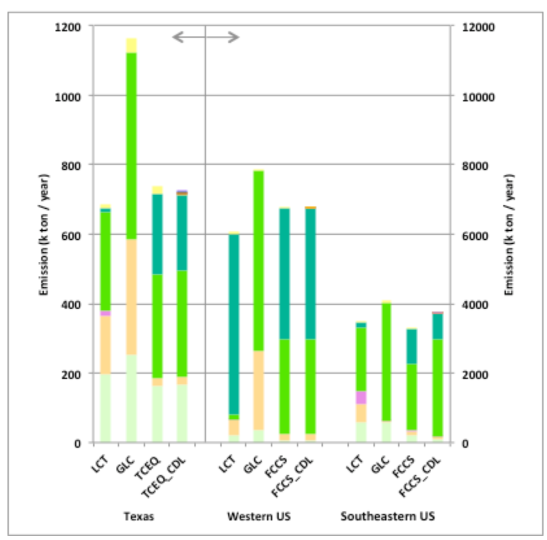

Figure 3. Example of annual total CO emissions from fires by land cover type (Fig. 1 legend) in Texas and U.S regions for selected land cover databases.

Task 2. Mapping of Croplands Data
Cropland data has been obtained from the NASS CDL database, as described above. Crop-specific emission factors, developed by Jessica McCarty at Michigan Technological University, for sugarcane, wheat, cotton, soy, corn, and sorghum (on-going) have been added to the FINN default configuration. Sensitivity studies have been developed that explore the influence of using the NASS CDL, which has the most detailed characterization of crop types, on emission estimates.

Task 3. Estimation of Burned Area
Much of the work with FINN has centered on improvements to the algorithm used for quantification of burned area. The 2012 MRR data for North America was obtained from the U.S. Forest Service Remote Sensing Applications Center (RSAC) (http://activefiremaps.fs.fed.us/data/fireptdata/modisfire_2012_na.htm) and is being used for all FINN simulations. The team has worked to modify how point fire detections from the MRR product are processed to quantify burned area, to improve the estimation of whether or not multiple point detections constitute the same fire event, and to improve the ability of the algorithm to capture the diversity of land cover over the burned area.

Task 4. Sub-grid scale Partitioning of NO_x Emissions to NO_z in Fire Plumes
This task has not yet been initiated.

Task 5. Comprehensive Air Quality Model with Extensions (CAMx) Sensitivity Studies
This task relies on receipt of the 2012 CAMx air quality modeling episode currently under development by the TCEQ. The full episode is not ready for release, but the TCEQ is sharing the emissions inventories for fires and other sources with our team. Our initial objective is to compare TCEQ's current fire emission estimates with those from our FINN simulations.

Project 14-014	**STATUS: Active – January 27, 2015**

Constraining NO_X Emissions Using Satellite NO_2 and HCHO Column Measurements over the Southeast Texas

University of Houston – Yunsoo Choi

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Dave Westenbarger

Funding Amount: $84,927

Executive Summary

Ozone production depends not only on availability of Volatile Organic Compounds (VOCs) and Nitrogen Oxides (NO_x) but also on their relative concentrations, which can be expressed as a VOC/NO_x ratio. Over or under prediction of either component in an air quality model changes the VOC/NO_x ratio and limits the capability of an air quality model to predict ozone properly. Additionally, accurate predictions of meteorological variables are crucial to simulate atmospheric chemistry and consequently properly simulate ozone concentrations. In addition to ground and aircraft measurements obtained in Houston during the Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign in September 2013, remote sensing data of NO_2 are available from Aura Ozone Monitoring Instrument (OMI). NO_2 column data products and can be used as a proxy for NO_x and their values in air quality models can be quantified and thus constrained. In this project, an analysis of the archived in-situ aircraft and ground measurements will be performed and satellite measurements of NO_2 will be utilized to improve the bottom-up NO_x emission inventories and study the impact of these improved emissions on ozone predictions. Objective analysis (OA) of meteorological simulations will be applied to improve predictions of meteorological parameters as well as ozone predictions.

The primary objectives of this project are to: (1) utilize satellite measurements of tropospheric NO_2 columns to quantify surface NO_x anthropogenic and soil emissions using inverse modeling; (2) evaluate model-simulated formaldehyde and isoprene concentrations (key drivers for ozone) using in-situ ground and/or aircraft measurements; (3) examine how the ratio of model-simulated NO_2/HCHO in Air Quality Forecasting system at UH (AQF-UH) varies and corresponds to remote sensing NO_2/HCHO column measurements, and (4) perform objective analysis (OA) of meteorological predictions to improve their predictions, and consequently, ozone predictions. The Air Quality Forecasting System will use the Community Multiscale Air Quality (CMAQ) Model with a 4 km resolution for Southeast Texas. The meteorological inputs will be provided by the Weather Research and Forecasting (WRF) model.

Project Update

The project team has finished WRF simulation for the 2013 DISCOVER-AQ Texas period, which is the whole month of September. To test the impact of different nudging settings, three sets of simulations are performed, with differences in the observation nudging, which is all referred as objective analysis (OA).

The first case, “No-OA” does not employ observational nudging or objective analysis. The second case, “3Hr-OA” runs observational nudging at 3-hr interval. The third case, “1Hr-OA” runs observational nudging at 1-hr interval.

Modeling domain

The WRF domains are shown in Figure 1 as two nested domains: 12-km (red) and 4-km (blue). The domain sizes are: 161x145 for the outer domain and 97×79 for the inner domain. Both WRF and CMAQ share the same vertical structure since no layer collapsing has been employed in Meteorology-Chemistry Interface Processor (MCIP). The vertical structure is listed in Table 1.

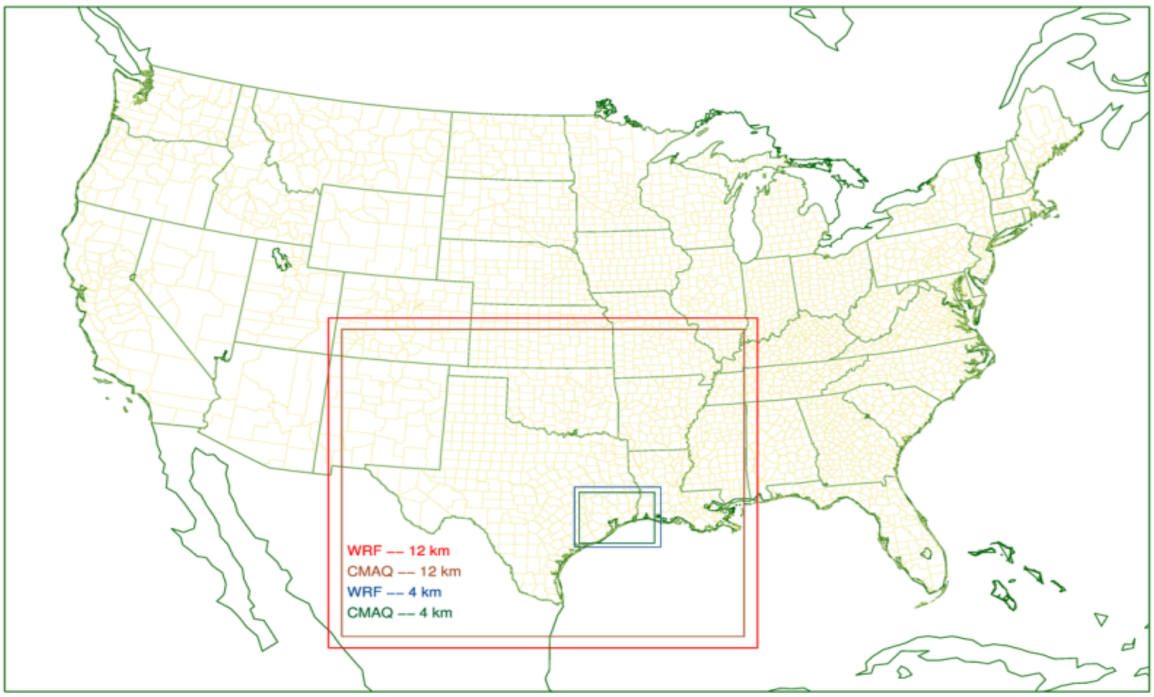

Figure 1: WRF (thick lines) domains used for the UH Air Quality Forecasting (AQF) System. There are two domains: the 12-km Texas domain and the 4-km Houston-Galveston-Brazoria (HGB) domain.

Table 1. Vertical layer structures of WRF.

Layer	**AGL (m)**	**Layer**	**AGL (m)**
1	32.4	15	1517.8
2	81.2	16	1751.4
3	163.1	17	1990
4	245.9	18	2233.9
5	329.5	19	2534.7
6	413.7	20	3164.8
7	498.4	21	4193.1
8	583.8	22	5415.3
9	669.7	23	6964.2
10	756.2	24	9083.3
11	887.2	25	11444.6
12	1019.6	26	14549.2
13	1153.4	27	16540.7
14	1288.8		

The domain projection employs Lambert conformal conic projection (LCC) which is commonly used in the WRF modeling community for mid-latitude regions. Projection parameters are shown in Table 2.

Table 2. Projection Parameters

First True Latitude (Alpha)	33°N
Second True Latitude (Beta)	45°N
Central Longitude (Gamma)	-97°W
Projection Origin	(31.55113°N, -98.13650 °W)

WRF Physics Options

The WRF physics parameters are listed in Table 3. Among the various schemes, the choices of boundary layer scheme and cumulus cloud option are especially important. YSU has been well tested in our prior studies and generally outperforms others. The Kain-Fritsch (K-F) cumulus scheme is a relatively "dry" scheme compared to other popular schemes like Grell-Freitas (GF) or Betts-Miller-Janjic (BMJ). K-F is desired in our tests as it produced less artificial thunderstorms than GF.

Table 3. WRF physics

WRF Version	V3.6.1, latest
Microphysics	Lin et al. Scheme
Long-wave Radiation	Rapid Radiative Transfer Model for GCMs (RRTMG)
Short-wave Radiation	New Goddard scheme
Surface Layer Option	Monin-Obukhov with Carslon-Boland viscous sublayer scheme
Land-Surface Option	Unified Noah LSM (Land Surface Model)
Urban Physics	None
Boundary Layer Scheme	Yonsei University (YSU)
Cumulus Cloud Option	Kain-Fritsch

WRF Input Analysis Data

The analysis input will be from the North American Regional Reanalysis (NARR) dataset. The NARR data are based on an Eta 221 grid at 29 pressure levels. Its horizontal resolution is 32 km and the frequency is 3 hours. The initial and boundary conditions will be generated from the NCEP NARR input by WRF model.

Besides the standard grid nudging using the "met_em" files, the project team also performed observation nudging in attempt to correct certain model errors. Observation nudging is regarded as a low-cost and effective method in improving meteorological model performance, it requires additional observational data. In this study, we acquire the input observation data and generated files in little_r format using UH in-house developed codes. Observational data come from the Meteorological Assimilation Data Ingest System (MADIS) and the Continuous Ambient Monitoring Station (CAMS) network. MADIS is a National Oceanic and Atmospheric Administration (NOAA) program that collects, integrates, performs quality checks on, and distributes observations from NOAA and non-NOAA organizations. The four MADIS datasets used for the obs-nudging are NOAA Profiler Network (NPN), Cooperative Agency Profilers (CAP), Aviation Routine Weather Report (METAR) and NOAA Radiosonde (RAOB). CAMS is a surface-based monitor network measuring air pollutants, meteorological data, and other parameters. It is maintained by the Texas Commission on Environmental Quality (TCEQ).

The UH implementation is shown in Figure 2. First MADIS data were downloaded from MADIS FTP site and decompressed. The METAR / NPN / CAP / RAOB data streams were then extracted and processed, along with the CAMS data. The output were subsequently combined into little-r formatted data files ready for OBSGRID, a WRF component which generates necessary input for observation nudging. Since there are two horizontal domains, the extraction and processing will repeat twice, once for each domain.

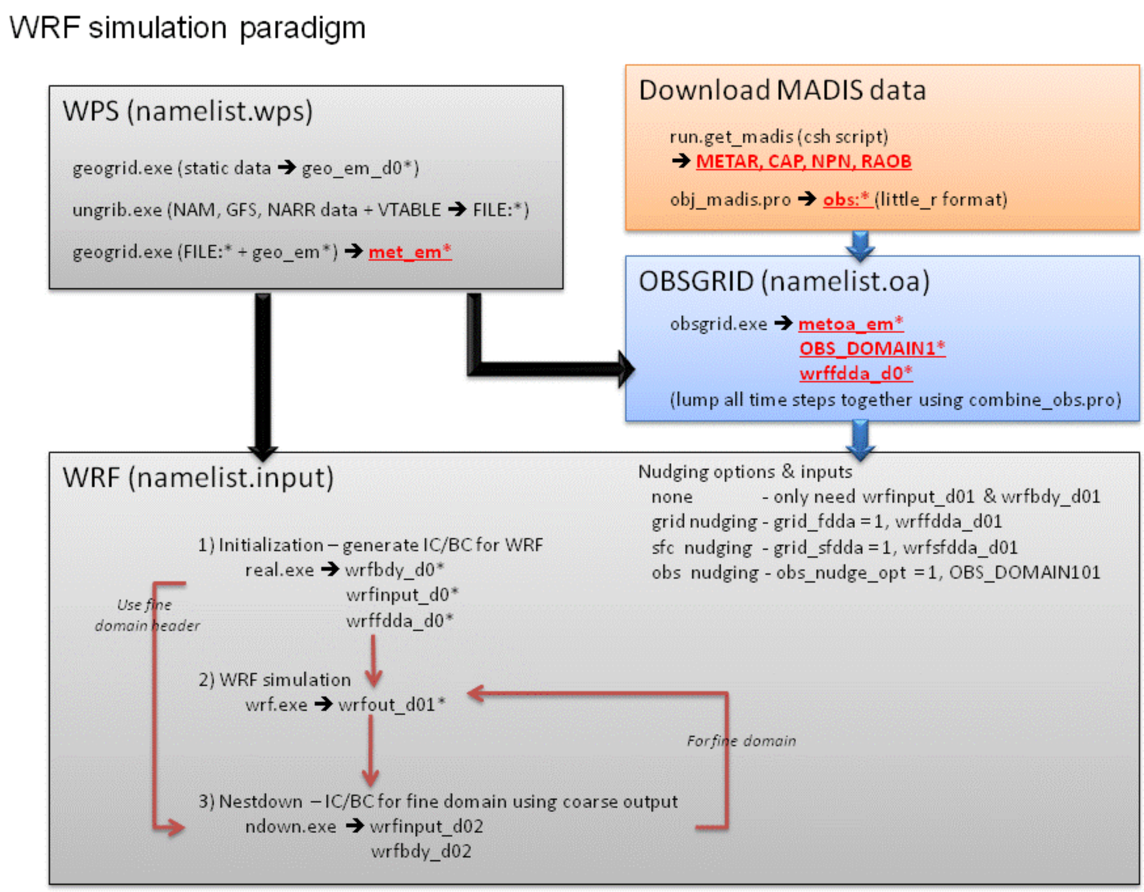

Figure 2. Implementation of UH observation nudging

There is one set of output files for each domain. Therefore our implementation actually utilized observations twice. For the OBSGRID, we adopted mostly the default options in the namelist file, with the exception in nudging frequency.

Since most analysis input has a temporal resolution of 3-hours, the default time-interval for output nudging files (OBS_DOMAIN) in OBSGRID is 3-hours (10800 seconds). On the other hand, most of the observations are hourly, hence it is desirable to use all of them for the nudging. To test the impact of different nudging time-interval, we have two cases: one uses the default 3-

hour (case “3Hr-OA”) while another uses the 1-hour (case “1Hr-OA”). To see the effect of OA, another case “No-OA” with no observation nudging is run for comparison.

In WRF, there are a few namelist variables controlling the frequency of grid nudging and observation nudging. The first one is “interval_seconds”, which should match the interval of 3D grid nudging files (“met-em”). In our simulation, it is “10800” seconds”. The second one is “sgfdda_interval_m”, matching the interval of surface grid nudging files (“sgfdda”). The third one is “auxinput11_interval”, controlling the updating interval for observation nudging files (“OBS_DOMAIN”). The last one, “obs-ionf”, determines the nudging frequency relative to internal integration time-step. For example, if time-step for the coarse domain is 30 seconds, setting “obs_ionf” to 1 means performing OA every 30 seconds, while setting "obs_ionf" to 3 means performing OA every 90 seconds. In our simulation, “obs_ionf” is set to 1. There are other namelist variables in “fdda” section controlling the nudging behaviour. We usually adhere to the default settings.

To evaluate the performance of WRF simulations, we used following statistics. All of them are frequently used in the modeling community. Observational CAMS data are used to validate model results.

1) Correlation (r) between model values and observed values

$$r = \frac{\sum_{t=1}^{n}[(x_t - \bar{x})(y_t - \bar{y})]}{\sqrt{\sum_{t=1}^{n}(x_t - \bar{x})^2 * \sum_{t=1}^{n}(y_t - \bar{y})^2}}$$

n – number of data points, x – observed values, y - model values, values with an over bar indicate the mean.

2) Index of Agreement (IOA) between model values and observed values

$$IOA = 1 - \frac{\sum_{t=1}^{n} e_t^2}{\sum_{t=1}^{n}(|y_t - \bar{x}| + |x_t - \bar{x}|)^2}$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values, values with an over bar indicate the mean.

3) Root Mean Square Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{t=1}^{n} e_t^2}$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

4) Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_{t=1}^{n}|e_t|$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

5) Mean Bias (MB)

$$MB = \frac{1}{n}\sum_{t=1}^{n}e_t$$

n – number of data points, $e_t = y_t - x_t$, x – observed values, y - model values

General Meteorological Conditions

The weather during the September 2013 simulation period was relatively dry with mostly southerly, easterly or southeasterly winds. From 09/05 to 09/19, there was a lack of influence of strong synoptic weather systems. Shifting wind patterns were observed during the period: light northeasterly in the early morning gradually turned clockwise to southeasterly in the afternoon and evening hours. The only cold front arrived in early 09/21. There are three time-periods showing a temperature dip: 09/07 to 09/09, 09/21 to 09/24, and and 09/28 to 09/30. The first and the last one are caused by cloudy sky while the second one is due to cold front. Rain events occurred on 09/02, 09/10, 09/16, 09/19 to 09/21 and 09/28 to 09/30. However, none of these was a significant event. The 09/20 and 09/21 events consisted of widespread light to medium showers. Besides above-mentioned dates, there are a few other days with sporadic drizzles.

To examine cloud cover, we obtained both visible and infrared satellite images from NASA's GOES satellite. A majority of the days between 09/01 and 09/20 were mostly sunny to mostly cloudy. The periods from 09/08 to 09/10 and 09/18 to 09/20 had more clouds than other days. The period from 09/21 to 09/30 was influenced by the cold front passage. The days between 09/22 and 09/25 were sunny and cool, after which the wind direction reversed in mid 09/25 and brought clouds back from 09/26 to 09/30.

Although not very significant to photochemistry, temperature drop is usually a good proxy for the critical factors affecting ozone production or transport such as cloudiness, wind, and precipitation. Table 4 presents the statistics of hourly surface temperature. It shows that the OA cases clearly outperform the no-OA case, with correlation coefficient increased by about 10%, IOA improved by 7%-8%. The biases for all the cases are low, indicating excellent energy budget in the model. On the other hand, the two OA cases have similar statistics, with "1Hr-OA" slightly ahead.

Table 4 Statistics of hourly surface temperature

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
No-OA	41058	0.84	0.9	1.8	1.3	0.7	27.4	28.1	3.1	2.8
3Hr-OA	41058	0.93	0.96	1.2	0.9	0	27.4	27.4	3.1	3.1
1Hr-OA	41058	0.94	0.97	1	0.8	0	27.4	27.4	3.1	3.1

- N – data points; Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M – Model Mean; SD – Standard Deviation
- Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD: degree C

Compared to temperature, hourly winds at local scale are harder to predict by meteorological models, including WRF. The performance of the model is also greatly influenced by the quality of input analysis data. Running the model at a finer resolution can provide more local meteorological details than at coarser resolution. A fine resolution run usually does not alter the average winds inherited from the coarse resolution run unless objective analysis is performed. Therefore, when the large-scale winds from the input analysis differ from observation, there is little chance that the model can get winds correctly. One remedy is to add objective analysis (observation nudging) during the WRF run.

Wind statistics are computed for U and V components. Statistics for U-wind are displayed in Table 5, while statistics for V-wind are shown in Table 6. An alternative approach for calculating wind statistics is to compute statistics for wind speed and wind direction. The drawback for this approach is that wind direction is measured by degrees. A direction of 5 degrees is actually close to the direction of 355 degrees. But by statistics, 5 and 355 are far apart.

Model winds generally have lower correlation with observation than model temperature. Evaluating wind statistics needs extra caution as correlation can be misleading for days with light winds. Specifically, a low correlation in a day with light winds does not necessarily mean poor model performance since wind direction in a light wind day can vary from hour to hour somewhat randomly at a given site, and it is usually hard for the model to capture these local changes.

Table 5 Statistics of hourly surface U wind

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
No-OA	43246	0.74	0.74	2.2	1.8	-1.4	-1.3	-2.7	1.6	2.5
3Hr-OA	43246	0.79	0.88	1.1	0.8	-0.3	-1.3	-1.6	1.6	1.6
1Hr-OA	43246	0.81	0.89	1	0.8	-0.3	-1.3	-1.6	1.6	1.6

Table 6 Statistics of hourly surface V wind

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
No-OA	0.73	0.76	2.4	1.9	1.4	0.4	1.8	2	2.8	0.73
3Hr-OA	0.77	0.88	1.3	1	-0.1	0.4	0.4	2	2	0.77
1Hr-OA	0.8	0.89	1.2	0.9	-0.1	0.4	0.4	2	2	0.8

- N – data points; Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M – Model Mean; SD – Standard Deviation
- Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD: m/s

The pattern for U, V statistics are similar to that of temperature, i.e, OA cases outperform no-OA case while the differences between the two OA cases are smaller. It is interesting that the model performance on U and V are quite consistent, each case has almost identical IOA values for both U and V.

The results show that OA improves the statistics of surface temperature significantly and winds to a lesser scale while different OA frequencies only bring small changes in performance.

Other activities

Besides the WRF modeling, we also worked on downloading and analyzing remote-sensing data, as well as emission preparation.

Remote Sensing

OMI NO_2 daily observations (level 2) from NASA with a nadir spatial resolution of 13×24km for September of 2013 were downloaded. The pixels having high uncertainties have been filtered out by defining the following tests: total columns < 1.5×10^{15}, a cloud fraction > 20%, a root mean squared error of fit > 0.0003, a solar zenith angle > 85^o and without a good quality flag. In order to grid the daily granules to our model domain, the most recent algorithm has been implemented in python and been compiled. In order to compare directly the output of the model and OMI, the influences of priori profiles from OMI observations should be considered. Consequently, a MATLAB code has been developed by the group to perform the task. The input of the algorithm is CMAQ NO_2 and pressure profiles, OMI NO_2, Air Mass Factor and its corresponding flags, scattering weights and other variables. The updated OMI NO_2 (by considering the AMF of the model) will be provided, and subsequently will be re-gridded for our domain.

Emissions Preparation
Four sectors of emission inventories of NOx from the Sparse Matrix Operator Kernel Emissions (SMOKE) model are prepared. We are currently working on the National Emissions Inventory of 2011 (NEI2011). Until the model-ready emissions are ready, we will be working on the NEI of 2008 for the test of inverse modeling. They contain 24-hour values averaged over September, 2013 for our 4-km CMAQ model domain covering Southeast Texas. The snapshot of surface level soil, area, mobile, and point NOx emissions at 20:00Z is shown in Fig. 3.

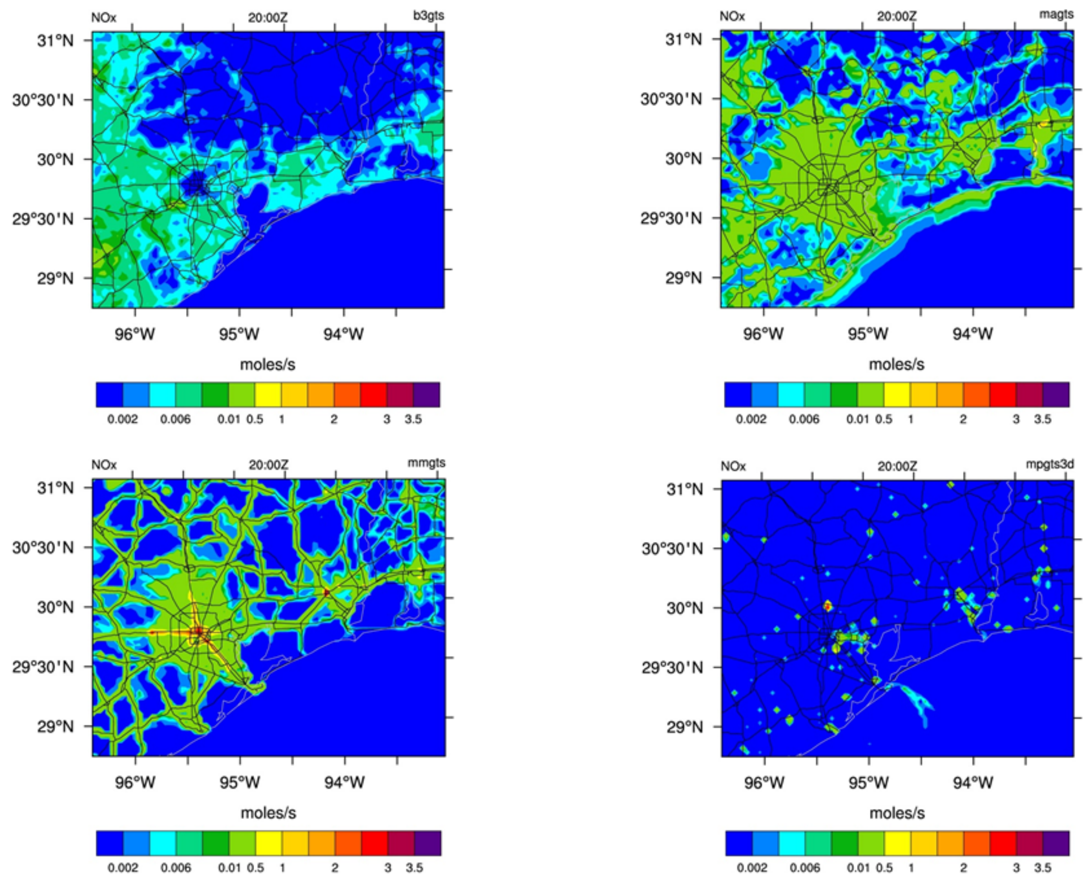

Figure 3. Mean soil, area, mobile, and point NO_x emissions over Houston at 20:00 Z during the period of September 2013 from SMOKE.

Surprisingly, the highest peak point source appears around Houston intercontinental IAH airport region (from the right bottom). The reason that the peak location is at IAH is because SMOKE assigns airport-related area-source emissions as point sources at airport locations, as opposed to spatially allocating them to grid cells using spatial surrogates (https://www.cmascenter.org/smoke/documentation/2.1/html/ch02s09s08.html). The project team has further examined the point source distribution, and found a local peak around Hobby airport due to the area-to-point conversion of emissions by the SMOKE process at airport locations. This issue will be checked again when we produce a new emission inventory based on the NEI2011.

Project 14-016	STATUS: Active – June 4, 2014

Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations

Environ – Greg Yarwood

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

Funding Amount: $271,911

Executive Summary

The exchange of gases and aerosols between the Earth's surface and the atmosphere is an important factor in determining atmospheric composition and regional air quality. Accurate quantification of emission fluxes is a necessary step in developing air pollution control strategies. In some cases emissions can be directly measured (e.g., point sources with continuous emission monitors) or can be estimated with reasonable confidence (e.g., point sources that have well-defined operating parameters). In contrast, large uncertainties are associated with area sources including emissions from vegetation, and in particular, emissions of biogenic volatile organic compounds (BVOCs). Vegetation is the largest source of VOC emissions to the global atmosphere. The oxidation of BVOCs in the atmosphere affects ozone, aerosol and acid deposition. Current BVOC emission estimates are based on measurements for individual plants that must be scaled up to represent landscapes and adjusted for environmental conditions. There is a critical need for independent BVOC emission inputs for air quality models.

AQRP Project 14-016 will use aircraft observations from the 2013 Southeast Atmosphere Study (SAS) and the 2006 Texas Air Quality Study (TexAQS) to assess and reduce uncertainties associated with a widely-used BVOC emissions model, namely the Model of Emissions of Gases and Aerosol from Nature version (MEGAN). The eddy covariance technique will be used to directly quantify BVOC emission fluxes for all suitable aircraft observations from the SAS study. Using the relationship between BVOC fluxes and concentrations derived from this subset of SAS aircraft data, BVOC emission fluxes will be estimated for 2013 SAS and 2006 TexAQS flights in the southeastern U.S. and Texas, respectively. In addition, the investigators will improve the land cover and emission factor input data sets that are considered the major uncertainties associated with BVOC emission estimates. The overall benefit of this project will be more accurate BVOC emission estimates that can be used in Texas air quality simulations that are critical for scientific understanding and the development of effective regulatory control strategies that will enhance efforts to improve and maintain clean air.

Project Update

Progress on Project 14-016 is summarized below by Task:

Task 1: Estimation of Terpenoid Emission Fluxes from Aircraft Data

NOAA continued work on using the measurements of isoprene onboard the NOAA WP-3D and NCAR C-130 during SAS to estimate isoprene emission fluxes using the mass balance approach published previously [Warneke et al., 2010]. The results were compared vs. the eddy fluxes determined from the C-130 measurements. Good agreement was obtained in some cases. In other cases, the mass balance approach yields higher values than the eddy fluxes. Research is in progress to understand the differences between those cases. Work continued on comparing the fluxes according to the mass balance approach with the emissions according to the BEIS 3.13 and MEGAN 2.0 inventories using the aircraft measured temperature and photoactive radiation. Preliminary findings include that (1) BEIS 3.13 captures the variability in emissions better than MEGAN 2.0, (2) BEIS 3.13 gives lower emissions than estimated from the measurements, and (3) MEGAN 2.0 gives higher emissions than those estimated from the measurements. These findings qualitatively agree with those from a previous study that used data from the SOS99, TexAQS 2000 and 2006, and ICARTT 2004 campaigns. Work was started to compare the isoprene fluxes derived from the measurements with those calculated from chemical transport models.

NOAA also worked on the validation of one of the main assumptions in our work so far: what is the relation between isoprene and hydroxyl (OH) radical concentrations in the planetary boundary layer (PBL), and can isoprene concentration measurements be used to derive isoprene emissions? To answer this question, we used the results from a large eddy simulation (LES) model that were previously published [*Kim et al.*, 2012]. This model describes the turbulent mixing and chemical removal of isoprene in a planetary boundary layer capped by fair-weather cumulus clouds as is typical for Texas and the Southeast U.S. First, we verified that the variance in measured isoprene agrees with the modeled variance, and we found good agreement for different NOx regimes. Next, we studied the dependence of average isoprene mixing ratios in the model versus the average OH (Figure 1). It was found that there is a simple inverse relationship between mean isoprene and mean OH. Moreover, the factor between mean isoprene and the inverse of mean OH agrees within 10% with the assumed isoprene emissions in the model. This validates our use of measured isoprene mixing ratios ([ISOP]) to derive isoprene emissions $ISOP_{em}$, following the equation [*Warneke et al.*, 2010]:

$$[ISOP] = \frac{ISOP_{em}}{BL_{height} \times k_{OH} \times [OH]} \quad (1)$$

where BL_{height} is the height of the PBL, [OH] is the OH radical concentration estimated according to a parameterization that includes measured NO_2, ozone and J-values [*Ehhalt and Rohrer*, 2000], and k_{OH} is the rate coefficient for the reaction between isoprene and OH.

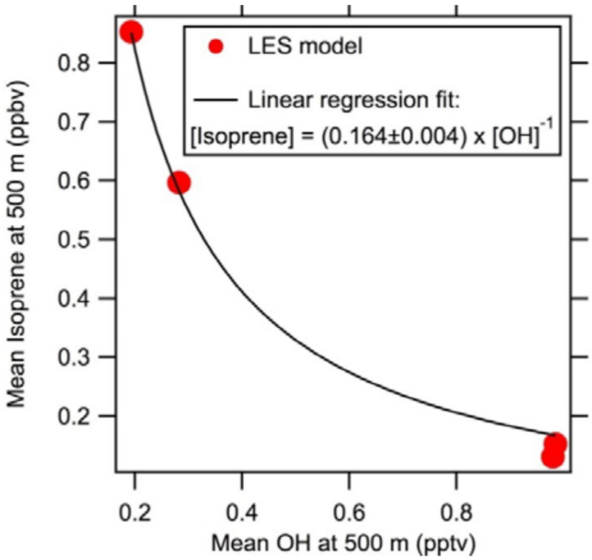

Figure 1: Mean isoprene as a function of mean OH at 500 m altitude in the mid-afternoon boundary layer calculated from the large eddy simulation (LES) results published previously

Task 2: Development of High Resolution Land Cover Data for MEGAN Modeling in Texas and the Southeastern U.S.

PNNL updated the LAIv dataset for the North America based on updated maximum fractional vegetation cover data from USGS.

Task 3: Emission Factor Database Development

PNNL continued work on developing high resolution land cover database for the continental US. The database was developed by combining MEGAN v2.1 land cover, LandFire vegetation cover, National Land Cover Database 2011, Forest Inventory and Analysis (FIA) survey and Cropland Data Layer (CDL) data.

PNNL developed 30 meter resolution PFT dataset for the continental US by integrating MEGANv2.1 grass and shrub land cover, LandFire vegetation cover, National Land Cover Database 2011, Forest Inventory and Analysis (FIA) survey and USGS maximum vegetation cover data. In addition, PNNL has also developed an emission factor dataset for the continental US and evaluated the product against MEGANv2.1 dataset. PNNL continues working on improving the emission factor dataset by incorporating aircraft observations.

Task 4: Development of MEGAN Biogenic Emission Inventories and Inventory Evaluation using Regional Photochemical Modeling

ENVIRON completed development of software to perform CAMx model performance evaluation along aircraft flight tracks and merged the TCEQ 2013 emission inventory with the new MEGAN emission inventory based on default inputs. ENVIRON ran CAMx for the June 1-July 15, 2013 period using MEGAN emissions developed using default inputs and the final WRF run. We evaluated the model against ozone surface observations from the CASTNet monitoring network and the TCEQ's CAMS network as well as against aircraft observations of isoprene, ozone and other species along the C-130 aircraft flight tracks. Model performance for ozone at surface monitoring sites was reasonably good given the 12 km model resolution, but there was a positive bias for ozone overall. CAMx concentrations of isoprene and ozone were well-correlated with the C-130 observations, but showed an overall high bias for both species (Figure 2). Next, ENVIRON will prepare MEGAN emissions using updated MEGAN inputs provided by PNNL under Tasks 2 and 3 and will run CAMx with the updated MEGAN emissions. Performance in the two CAMx runs will be compared.

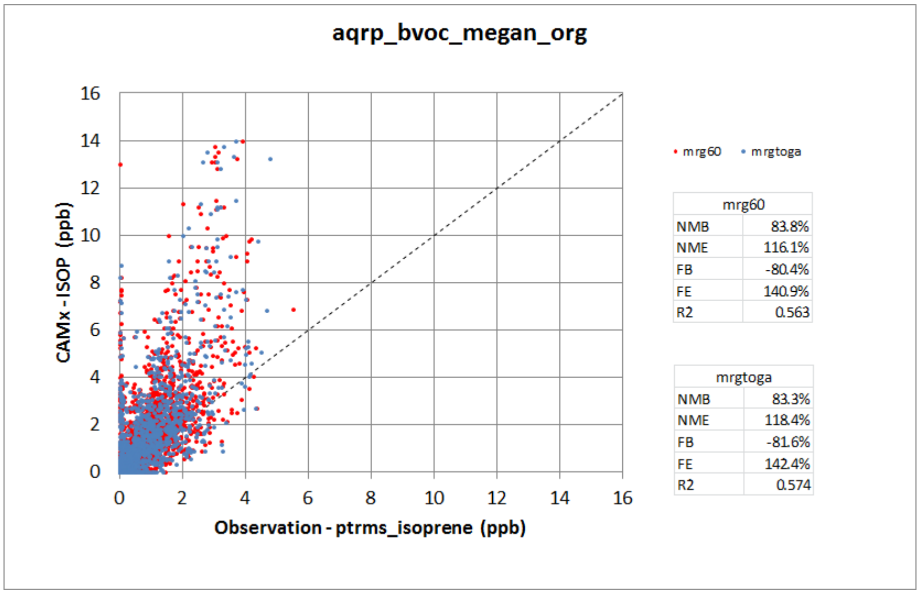

Figure 2: Comparison of CAMx modeled isoprene and isoprene measured by PTRMS along the C-130 flight tracks during the period June 1-July 14, 2013. mrg60 data are 1-minute averages of observed data, and mrgTOGA data are 2-minute averages.

Task 5: Project Management

ENVIRON, NOAA and PNNL/Battelle prepared an outline of the final report.

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Project 14-017	STATUS: Active – July 8, 2014

Incorporating Space-borne Observations to Improve Biogenic Emission Estimates in Texas

University of Alabama - Huntsville – Arastoo Pour Biazar
Rice University – Daniel Cohan

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

Funding Amount: $199,982
($137,003 UAH, $62,979 Rice)

Executive Summary

One of the challenges in understanding the Texas air quality has been the uncertainties in estimating the biogenic hydrocarbon emissions. Biogenic volatile organic compounds, BVOCs, play a critical role in atmospheric chemistry, particularly in ozone and particulate matter (PM) formation. In southeast Texas, BVOCs (mostly as isoprene) are the dominant summertime source of reactive hydrocarbon. Despite significant efforts by the State of Texas in improving BVOC estimates, the uncertainties in emission inventories remain a concern. This is partly due to the diversity of the land use/land cover (LU/LC) over southeast Texas coupled with a complex weather pattern, and partly due to the fact that isoprene is highly reactive and relating atmospheric observations of isoprene to the emissions source (vegetation) relies on many meteorological factors that control the emission, chemistry, and atmospheric transport.

BVOC estimates depend on the amount of radiation reaching the canopy (Photosynthetically Active Radiation, PAR), and temperature. However, the treatment of temperature and PAR is not uniform across emissions models and still poses a problem when evaluating the inventories. Recent studies show that the largest uncertainty comes from the model solar radiation estimates and that using satellite-based PAR would be preferable. Emissions from soils also remain as one of the poorly quantified sources of NOx (nitrogen oxides) in most air quality models. Soils can be the largest source of NOx in rural regions where low-NOx conditions make ozone production efficiency especially high, contributing to background ozone levels.

The overall objective of the current activity is to advance our understanding of Texas Air Quality by utilizing satellite observations and the new advances in biogenic emissions modeling to improve biogenic emission estimates. This work specifically addresses a priority area in Texas AQ studies by improving biogenic emission estimates. In particular, the objectives are:

(1) To provide satellite-based PAR estimates for Texas during selected periods of 2006 and the Discover-AQ period (September, 2013).

(2) To produce an improved biogenic emission estimate for Texas and help in the evaluation of biogenic emission inventories over Texas by providing the best model representation of the atmospheric condition during the observations used for evaluation.

(3) To prepare and use a new soil NOx scheme that provides more mechanistic representation of how emissions respond to nitrogen deposition, fertilizer application, and changing meteorology.

The University of Alabama in Huntsville (UAH) currently generates a set of products from the Geostationary Operational Environmental Satellite (GOES) that includes surface incident short-wave radiation as well as cloud albedo and cloud top temperature. Under this activity, UAH will produce the Photosynthetically Active Radiation (PAR) needed in the estimation of biogenic hydrocarbon emissions. Satellite-derived PAR will be evaluated against previous satellite-based products as well as surface observations for the summer of 2006 and also during Texas Discover-AQ campaign. Furthermore, the new PAR retrievals will be used in MEGAN (the Model of Emissions of Gases and Aerosols from Nature) to generate BVOC emissions.

The new soil NOx scheme to be used is an implementation of the Berkeley-Dalhousie Soil NOx Parameterization (BDSNP) within MEGAN. A series of sensitivity simulations will be performed and evaluated against Discover-AQ observations to test the impact of satellite-derived PAR and the new soil NOx emission model on air quality simulations.

Project Update

The following activities took place in the past three months.

Satellite-based PAR estimates

An algorithm for producing satellite-based PAR was finalized and PAR estimates for September 2013 (Discover-AQ period) were produced. The estimates were evaluated against surface observations obtained from Surface Radiation Budget Network (SURFRAD) operated by NOAA (http://www.esrl.noaa.gov/gmd/grad/surfrad/), which is the only available direct continuous measurement of PAR at seven sites nationwide, and the Soil Climate Analysis Network (SCAN), operated by the US Department of Agriculture (http://www.wcc.nrcs.usda.gov/scan/), which has continuous solar radiation measurements collected by pyranometers at more than 100 stations located in 40 states. Performing a bias correction on satellite-derived insolation before arriving at PAR estimates improved performance statistics for this time period.

Since 2013 evaluation of PAR products were satisfactory, we proceeded to generate PAR for the summer of 2006 (to be evaluated against University of Maryland PAR product). PAR for 2006 has been generated and the evaluation work is ongoing.

Figure 1 shows satellite retrievals of insolation compared to SCAN pyranometer data after applying bias correction. While there is still some scatter in the data, the overall pattern shows a good correlation between pyranometer and GOES retrievals.

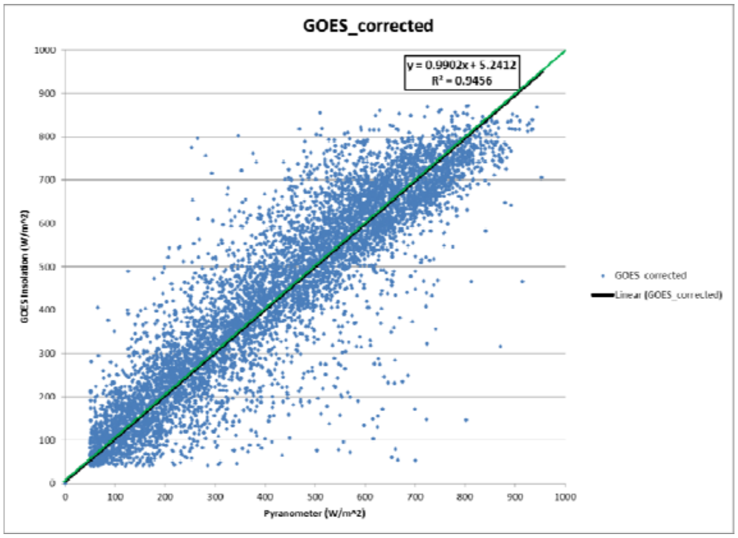

Figure 1. Scatter plots showing GOES insolation retrievals against Soil Analysis Climate Network (SCAN) data for September 2013. The figure shows the data after applying bias correction to GOES retrievals.

Biogenic VOC emission estimates in MEGAN

For the biogenic VOC emission modeling, we are testing the sensitivity of MEGAN simulations of biogenic VOCs in the year 2006 to four cases of meteorological and Photosynthetically Active Radiation (PAR) inputs: base case WRF, WRF with satellite-based PAR from the University of Maryland, WRF with the new satellite-based PAR from University of Alabama-Huntsville, and a new WRF simulation with clouds assimilated by UAH. Comparisons of these simulations will enable us to evaluate the impact of these alternate inputs. We are also evaluating the performance two sets of PAR or insolation satellite retrievals by comparing with the ground measurement data.

Figure 2 shows the comparison between MEGAN BVOC emission outputs for isoprene (ISOP, upper panel) and monoterpenes (TERP, lower panel) with the two types of radiation input. The base cases with WRF inputs are shown on the left, and the percent changes caused by satellite-based PAR are shown on the right. The estimated ISOP emission rate is much larger than TERP, with hotspots appearing at Southeast states with the typical value of 30 mol/s/gridcell while the corresponding typical value for TERP is only 5 mol/s/gridcell during the evaluation period. However, due to the different plant functional types and different temperature response curve between ISOP and TERP, there is less spatial heterogeneity for TERP compared with ISOP. Isoprene emission is more sensitive to PAR inputs with the highest increase in Northeast (> 30%) and decrease in the Northwest (> 20%). The relative change for monoterpene emission is modest (-10% to 5%). As expected, the south and Southeast region is the largest contributor to BVOC emission. Emission rate estimates using satellite PAR data is projected to increase at Northeast by 4%, Southeast by 1% but decrease at Northwest by 7%, West in 7%, and South region in 8% for both isoprene and monoterpene.

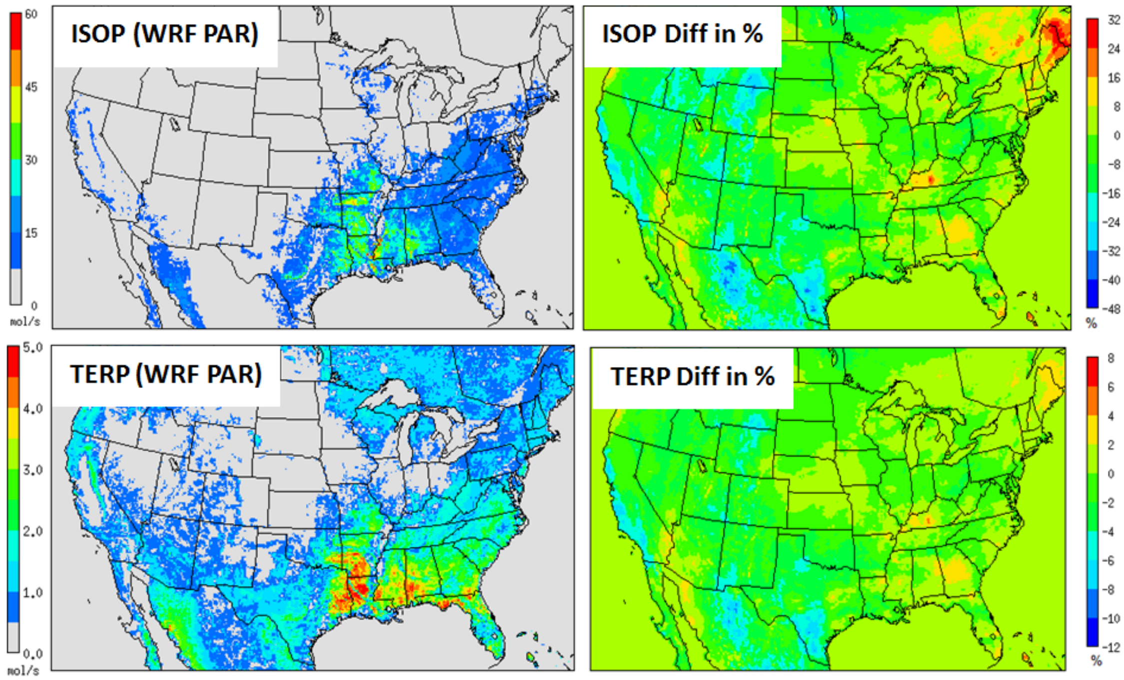

Figure 2. Spatial distribution of estimated ISOP and TERP emission rate by MEGAN using different PAR inputs data (WRF versus UAH satellite retrievals)

<u>Developing offline BDSNP module for soil NOx emission estimates</u>
The Rice team has adapted its implementation of the Berkeley Dalhousie Soil NO Parameterization (BDSNP) emission scheme from CMAQ into a stand-alone version that can be used for more efficiently estimating soil NO emissions for other modeling platforms, such as CAMx. Testing has been conducted to confirm that the stand-alone version yields soil NO emissions estimates similar to those produced by the CMAQ inline version. We are now generating a new biome spatial map based on finer resolution land cover data and climate zone classification to link with published estimates for biome-specific base emission rates to produce more detailed NO emission estimates over the continental U.S.

Figure 3 provides the comparison of the soil NOx emission estimates with the inline and offline option. It is obvious that with the nearly identical inputs files, the two options yield a quite similar result in terms of general spatial pattern and peak values. However, CMAQ N deposition fields are needed to run the offline version. One approach would be to use 2005 CMAQ deposition results as a surrogate (since full year simulation is available) and assume that the corresponding date N deposition pattern in 2005 is comparable with the situation for the date being simulated.

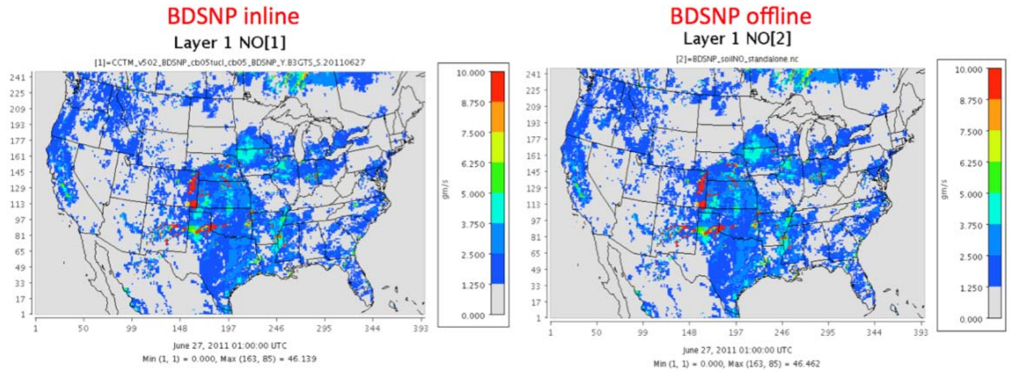

Figure 3. Comparison of soil NOx emission estimates using the inline (left) and offline (right) BDSNP scheme on Jun 28, 2011

<u>WRF simulations with cloud assimilation for 2013</u>

Performing cloud assimilation requires a base (control) simulation to quantify model errors with respect to cloud simulation. Base WRF simulations for 2013 were performed. Also, the necessary satellite observations were collected and a secondary data quality check was performed. Furthermore, the data were processed and mapped to the WRF domain configuration. We are currently in the process of performing assimilation simulations.

Project 14-020	STATUS: Active – February 2, 2015

Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC4RS

University of Maryland – Xinrong Ren

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

Funding Amount: $70,000

Executive Summary

Despite great efforts undertaken in the past decades to address the problem of high ozone concentrations, our understanding of the key precursors that control tropospheric ozone production remains incomplete and uncertain. Sensitivity of ozone production to nitrogen oxides (NO_x) and volatile organic compounds (VOCs) represents a major uncertainty for oxidant photochemistry in urban areas and is expected to vary from location to location and from time of a day. Understanding of the non-linear relationship between ozone production and its precursors is critical for the development of an effective ozone control strategy.

The DISCOVER-AQ campaign in Houston in August/September 2013 provided rich data sets to examine and improve our understanding of atmospheric photochemical oxidation processes related to the formation of secondary air pollutants like ozone and particulate matter (PM). In this project, an analysis of ozone production and its sensitivity to NO_x and VOCs will be performed. An observation-constrained box model based on Carbon Bond mechanism, Version 5 (CB05) will be used to study the photochemical processes along the NASA P-3B flight track, as well as at eight surface sites where the P-3B conducted spiral profiles. Ozone (O_3) production rates will be calculated at different locations and at different times of day and its sensitivity to NO_x and VOCs will be investigated. Spatially and temporally resolved ozone production and its sensitivity will also be investigated.

This project specifically addresses one of the AQRP priority research areas: Improving the understanding of ozone and particulate matter (PM) formation, and quantifying the characteristics of emissions in Texas through analysis of data collected during the DISCOVER-AQ campaign. The following tasks will be performed in this project:

(1) An investigation of spatial variations of ozone production and its sensitivity to NO_x and VOCs in Houston during DISCOVER-AQ.

(2) An investigation of temporal variations of ozone production and its sensitivity to NO_x and VOCs in Houston during DISCOVER-AQ.

(3) Investigate non-uniform emission reduction of O_3 pollution in Houston using spatial and temporal variations of ozone production and its sensitivity to NO_x and VOCs.

(4) Calculation of ozone production efficiency (OPE) at different locations using the ratio of ozone production rate to the NO_x oxidation rate calculated in the box model.

These activities will strengthen our understanding of O_3 production, which is essential to meet the primary and secondary National Ambient Air Quality Standards (NAAQS) for ozone.

Project Update

During the period from February 2, 2015 (starting date of Project 14 -020) to February 28, 2015, the team at University of Maryland College Park has accomplished the following tasks:

(1) We have upgraded the software FACSIMILE to the latest version and multiple users. FACSIMILE will be used as the platform to run the box model. We purchased a laptop computer and have FACSIMILE installed on it. We will use the laptop computer to run the box model and conduct some data analysis.

(2) We have run the box model using the Regional Atmospheric Chemistry Mechanism Version 2 (RACM2). We have plotted the P-3B data against the RACM2 mechanism on the September 25th case.

(3) RACM2 box model has been used to simulate ozone production rates under different NOx and VOC levels. Results from these model runs have been analyzed to created ozone production empirical kinetic modeling approach (EKMA) diagram (Figure 1). This diagram clearly shows the sensitivity of ozone production to NOx and VOCs.

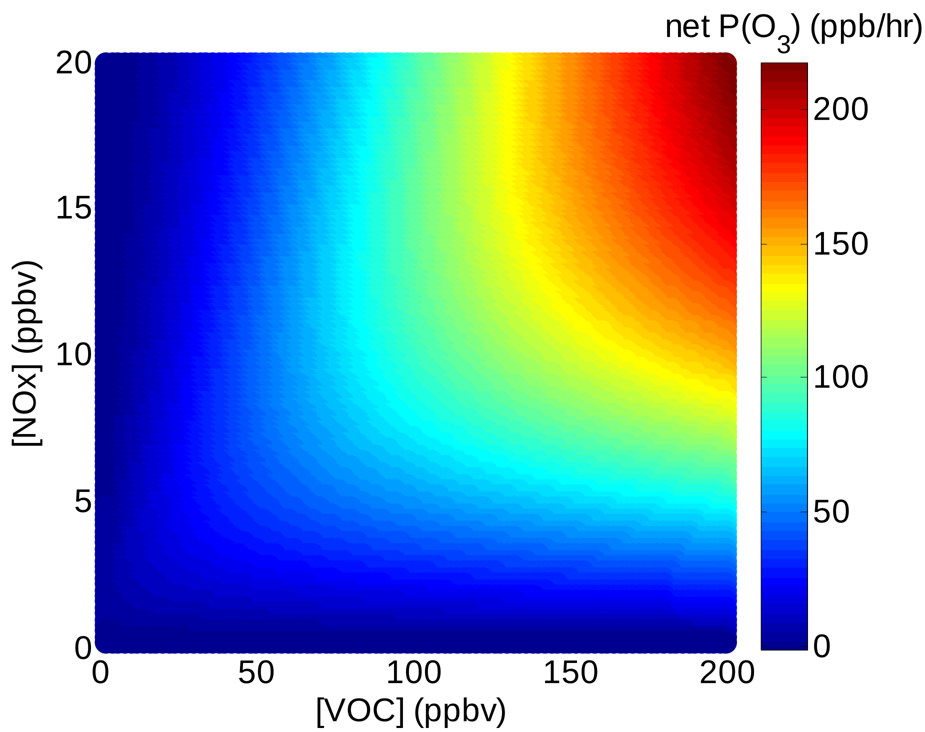

Figure 1. Ozone production empirical kinetic modeling approach (EKMA) diagram using the RACM2 box model results with NOx levels varying from 0-20 ppbv and VOC levels from 0-200 ppbv while the mean concentrations of other species observed during DISCOVER-AQ in Houston in 2013 were used to constrain the box model.

(4) WRF-CMAQ simulations and model evaluations performed under project 14-004 were reviewed. The improved modeling methodology and inputs used in performing these simulations will be implemented in future WRF-CMAQ simulations with process analysis.

During the next quarter, the following tasks are anticipated to be accomplished:

(1) We will work on getting the input files set up for the Carbon Bond Version 5 (CB05) mechanism for the box model runs.

(2) We will run the CB05 box model for the DISCOVER-AQ study in Houston in 2013.

(3) We will use the box model results to calculate ozone production and its sensitivity to NOx and volatile organic compounds (VOCs) along the NASA P-3 flight track during the DISCOVER-AQ study in Houston in 2013.

(4) Our next steps involve running CMAQ with process analysis in order to map the ozone production efficiency (OPE) and nitrogen oxides (NOx) and VOC limited areas throughout the Houston metropolitan area. CMAQ model output will be extracted for use in the box model.

Project 14-022	STATUS: Active – February 19, 2015

Use of satellite data to improve specifications of land surface parameters

University of Alabama-Huntsville – Richard McNider
George Mason University – Daniel Tong

AQRP Project Manager – Vincent Torres
TCEQ Project Liaison – Bright Dornblaser

Funding Amount: $116,000
($71,004 UAH, $44,996 GMU)

Executive Summary

Land surface processes play a critical role in air quality model performance. Land surface temperatures impact boundary layer heights and turbulent mixing. Temperature gradients can also produce local wind patterns. For example in Houston the land-sea temperature gradient drives both the daytime sea breeze and nighttime land breeze. This growing temperature contrast in the morning is responsible for physical features such as a dead zone ahead of the sea breeze front, which develops as the land sea pressure gradient force opposes the large scale weather pattern. This dead zone allows the accumulation of precursors that are part of the peak ozone levels later in the day as this dead zone moves northward with the sea breeze front. Surface temperatures also impact air quality levels through temperature dependence of evaporative emissions and biogenic emissions. Temperatures also control the thermal decomposition of nitrogen species, which in turn impacts the efficiency of ozone production per NO molecule emitted. Thus, not only can temperatures affect ozone production, they can impact the efficacy and efficiency of control strategies.

It is the purpose of this project to evaluate and improve the performance of the land surface models used in the meteorological model (WRF) by the use of satellite skin temperatures to better specify physical parameters associated with land use classes. While considerable work has been done by the national community and especially in Texas to develop improved land use classifications, land use classes themselves are not directly used in models. Rather, physical parameters such as heat capacity, thermal resistance, roughness, surface moisture availability, albedo etc. associated with a land use class are actually used in the land surface model. Many of the land use class associated parameters such as surface moisture availability are dynamic and ill-observed depending on antecedent precipitation and evaporation, soil transport, the phenological state of the vegetation, irrigation applications etc. Other parameters such as heat capacity, thermal resistance or deep soil temperature are not only difficult to observe they are often unknowable *a priori.* This project will use satellite data to retrieve or adjust these critical land surface parameters.

The project will first develop skin temperature data sets from geostationary satellites and polar orbiting platforms and make direct comparisons to the skin temperatures from the WRF land surface model. This will be done for intensive field programs such as the recent DISCOVER-AQ and SEAC4RS campaigns. Second, techniques to use satellite observed skin temperatures to adjust land surface parameters such as surface moisture and surface thermal resistance will be tested to improve WRF skin and air temperatures. Extensive evaluation of model performance will be made against standard National Weather Service observations, special observations made

during the DISCOVERY-AQ field campaign in September 2013 and other independent satellite observations.

Project Update

This project formally started February 19, 2015 so this is not a full quarterly report period. The beginning of this project has largely concentrated on two activities. The first is data collection and initial evaluation for the satellite data to be utilized in the project. The second is initial runs of the WRF model for the Discovery AQ period. These are described below. Acronyms are explained at the end of the report.

Data Collection

Satellite Insolation Data: The first data set to be utilized in the WRF model is a satellite-derived insolation product (incoming solar energy). To correctly characterize the land surface it is most important to provide the correct incoming energy from the sun since during the day this is the largest component in the land surface energy budget. Models may have clouds in the wrong place and at the wrong time. Since later in this project we will be using satellite measured skin temperatures, it is important that correct energy input is specified otherwise we might attribute differences in skin temperature to another term in the energy budget such as soil moisture or heat capacity. In the past the UAH group has utilized an insolation data set that it produces in conjunction with NASA SPoRT (Haines et al. 2003 and McNider et al 1995). This product is based on the physical retrieval technique developed by George Diak at the University of Wisconsin (Gautier and Diak 1980) and has been produced in real-time by UAH and NASA SPoRT since the late 1990's. As part of other funded activities we are implementing upgrades to the retrieval including the addition of variable atmospheric water vapor. We will be processing this data for the Discovery AQ period under this project using the new updated retrieval method. However, while waiting for this reprocessing in order to begin the WRF model simulations we decided to try a new NOAA GCIP insolation product. Thus, we have downloaded this data from the National Climatic Data Center (NCDC) CLASS data archive for the Discovery AQ period and processed it for use in the WRF model. The modeling section below describes the first use of this new (to us) insolation product.

The second data we have acquired and are quality assuring is the satellite skin temperature data set. We have downloaded and mapped the GCIP skin temperature data (see Wan and Dozier 1996 and updates) and have made an initial comparison to a second skin temperature data set generated by NASA MSFC which is a physical split window technique (Jedlovec 1987, Guillory et al. 1993). Figure 1 shows the difference between the two products. The differences are much larger than we expected in the Western U.S. A full report on these data sets will be provided for a deliverable on April 15, 2015. We are in discussions with developers of both products about the differences.

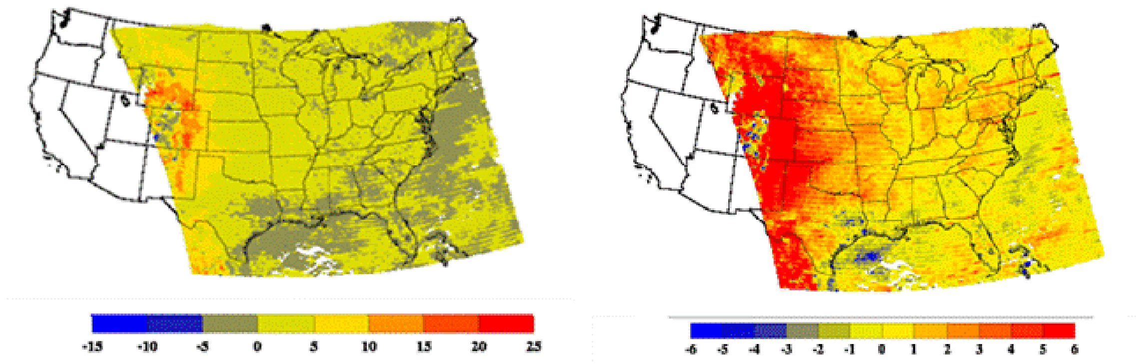

Figure 1 - Average daytime difference of GCIP skin temperature minus SPoRT skin temperature for the period 1-10 September 2013. The left panel shows the full range of differences, while the right panel shows the differences truncated to ± 6 K to show more detail.

Model Insolation Runs

We have begun the process of setting up the WRF model for the Discovery AQ period (2-29 September 2013). For the results summarized in this report two consecutive 5.5 day 12-km WRF simulations were performed with a 12-h overlap. The first run covers the period 0000 UTC 1 September 2013 through 1200 UTC 6 September 2013. The second run covers the period 0000 UTC 6 September 2013 through 1200 UTC 11 September 2013. The principal physics choices are summarized in Table 1. These runs use a consistent choice of the "Pleim-Xiu" package for the surface layer, land surface, and boundary layer choices. Three dimensional nudging is performed with a corresponding time scale of about 55 min for temperature and wind but with a smaller water vapor nudging impact with a corresponding time scale of about 28 h. The nudging of soil moisture within the Pleim-Xiu land surface model is activated which uses the 2-m observed analysis produced by the WPS program "OBSGRID". Version 3.6.1 of the WPS/WRF package is being used.

We have run WRF with the NOAA GCIP insolation data replacing the model insolation for the first ten days of the Discovery AQ period. Figure 2 shows the difference. We will provide a full report as part of the first deliverable on this project (March 1, 2015) describing the difference and impact on the model 2 m temperatures and skin temperatures of the model insolation versus satellite observed insolation. Since the NOAA GCIP insolation is a new product for our assimilation we will be comparing the GCIP product to the Sport product. We will also make comparisons to National Weather Service observables such as 2 m temperatures.

Table 1. Summary of Principal WRF Model Namelist Parameters

Category	Namelist Variable	Namelist Value	Description
Microphysics	MP_PHYSICS	8	New Thompson scheme
Longwave Radiation	RA_LW_PHYSICS	4	RRTMG scheme
Shortwave Radiation	RA_SW_PHYSICS	4	RRTMG scheme
Surface Layer	SF_SFCLAY_PHYSICS	7	Pleim-Xiu surface layer
Land Surface	SF_SURFACE_PHYSICS	7	Pleim-Xiu Land Surface Model
Planetary Boundary Layer	BL_PBL_PHYSICS	7	ACM2 PBL:
Cumulus Parameterization	CU_PHYSICS	1	Kain-Fritsch scheme
3D Analysis Nudging	GRID_FDDA	1	turned “on”
Wind Nudging	GUV	$3.0 \times 10^{-4}\ s^{-1}$	time scale of about 55 min
Temperature Nudging	GT	$3.0 \times 10^{-4}\ s^{-1}$	time scale of about 55 min
Water Vapor Nudging	GQ	$1.0 \times 10^{-5}\ s^{-1}$	time scale of about 28 h
Pleim-Xiu Soil Nudging	PXLSM_SOIL_NUDGE	1	

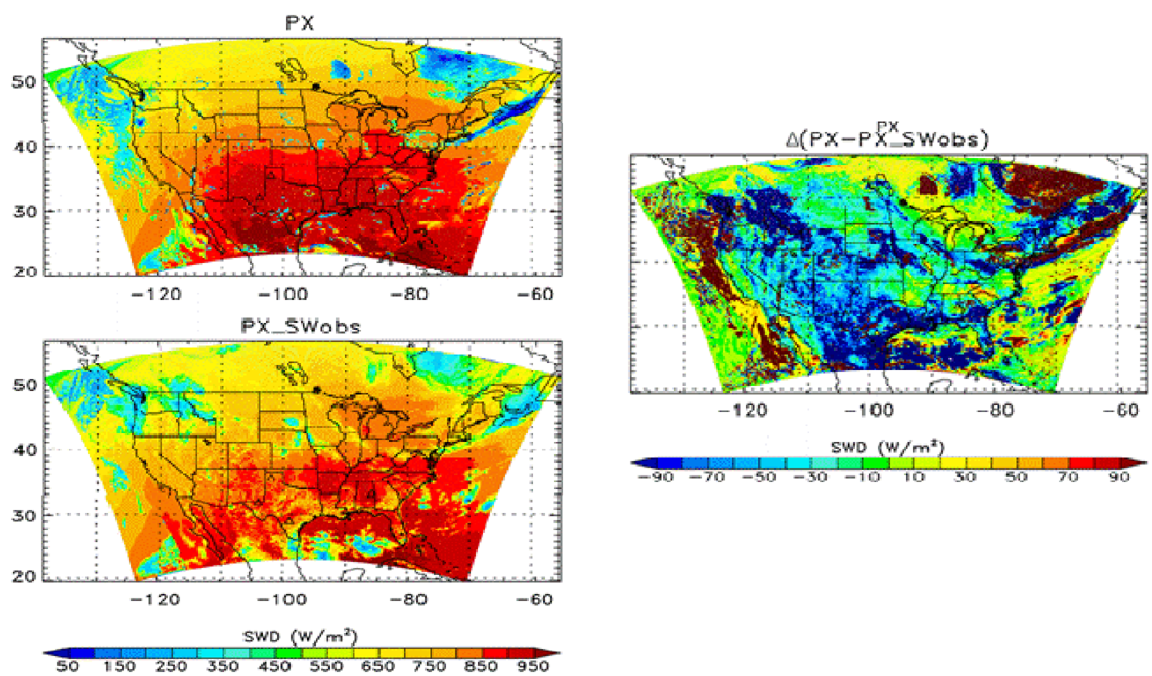

Figure 2 - Difference in insolation in the WRF model between model and satellite observed insolation (NOAA GCIP insolation product). Top left is the insolation computed by the model and bottom left the insolation from the NOAA GCIP data. Right middle gives the difference in insolation. Note PX refers to the Pleim-Xiu scheme and SWobs refers to satellite derive insolation.

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Pleim, J., and A.Xiu, 2003: Development of a land surface model. Part II: Data assimilation. J. Appl. Meteor., 42, 1811–1822.

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Acronyms

WRF	The Weather Research and Forecasting (WRF) Model
WPS	WRF Preprocessing System
UAH	The University of Alabama in Huntsville
NASA	National Aeronautics and Space Administration
SPoRT	Short-term Prediction Research and Transition Center (http://weather.msfc.nasa.gov/sport/)
NOAA	National Oceanic and Atmospheric Administration
GEWEX	Global Energy and Water Cycle Experiment
GCIP	GEWEX Continental-Scale International Project
NCDC	National Climatic Data Center
CLASS	Comprehensive Large Array-Data Stewardship System

Project 14-023	STATUS: Active – May 23, 2014 Ended – August 31, 2014

Assessment of Two Remote Sensing Technologies to Control Flare Performance

The University of Texas at Austin – Vincent Torres
Aerodyne Research, Inc. – Scott Herndon
Leak Surveys, Inc. – Joshua Furry
Providence Photonics, LLC – Yongshen Zeng

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Russell Nettles

Original Funding Amount: $480,741
($239,773 UT-Austin, $157,066 Aerodyne, $26,716 Leak Survey, $57,186 Providence Photonics)

Final Funding Amount: $36,587.11 ($25,874.37 UT-Austin, $10,712.74 Aerodyne)

Executive Summary
Industrial flares are devices used at industrial facilities to safely dispose of relief gases in an environmentally compliant manner through the use of combustion. Recent studies of industrial air- and steam-assisted flares have shown that merely complying with federal regulations like the Environmental Protection Agency's 40CFR § 60.18 and 40CFR § 63.11, do not ensure the flare will operate with at high combustion efficiency when combusting hydrocarbons over the entire range of operating scenarios for dual service flares. For vent gas streams containing hydrocarbons, the combustion efficiency (CE) is the percentage of the total hydrocarbon stream entering the flare that burns completely to form only carbon dioxide and water. It is desirable to have high combustion efficiency at all times to maximize flare performance.

The purpose of the proposed project was to conduct a series of field tests using an operational, full-scale industrial flare at a Petrologistics, LLC plant in Houston, Texas, to determine the technical, economic and operational feasibility of two approaches designed to maximize flare performance. These approaches continuously measure or determine the flare's combustion efficiency and would use this information to adjust the steam assist to the flare to adjust the flare's performance. To assess the technical performance of the approaches, the combustion efficiency measurements of each approach will be compared to an independent direct sampling measurement (the reference measurement) of the flare's combustion efficiency to determine the accuracy and completeness of the measurements obtained from the two approaches. For the field tests, the performance of the flare will not be controlled by either of the two approaches so that the prescribed test plan can be conducted with the flare. After the test series, the economic and operational feasibility will be evaluated based on the operational and safety characteristics observed during the tests and the estimated cost to implement each approach.

Project Update
On August 15, 2014, notice was sent to the AQRP Project Manager that the project would need to be ended and all unspent funds returned to the AQRP due to the plant where the testing was to be done no longer being able to participate.

No further work will be performed or costs incurred on this project.

Project 14-024	STATUS: Active – June 18, 2014

Sources of Organic Particulate Matter in Houston: Evidence from DISCOVER-AQ Data, Modeling and Experiments

The University of Texas at Austin – Lea Hildebrandt Ruiz
Environ – Greg Yarwood
University of California – Riverside – Gookyoung Heo

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $300,000
($163,282 UT-Austin, $101,404 Environ, $35,314 UC – Riverside)

Executive Summary

The United States Environmental Protection Agency recently lowered the annual National Ambient Air Quality Standard (NAAQS) for particulate matter smaller than 2.5 μm in diameter ($PM_{2.5}$) from 15 to 12 μg m^{-3}. This new annual standard brings the Houston region near to non-attainment for $PM_{2.5}$, underlining the importance of understanding the composition and sources of $PM_{2.5}$ in Houston. Recent measurements made during the month of September indicate that a majority of $PM_{2.5}$ in the Houston region is composed of organic material. An improved understanding of Houston organic aerosol is therefore essential and will directly benefit the Texas Commission on Environmental Quality (TCEQ) in understanding how to manage Houston's air quality.

Project 14-024 will focus on improving our understanding of the contributions of intermediate volatility organic compounds (IVOC) to formation of secondary organic aerosol (SOA). IVOCs, specifically large alkanes and polycyclic aromatic hydrocarbons, are largely excluded from current emission inventories because these compounds fall between the definitions of volatile organic compounds (VOC) and primary organic $PM_{2.5}$. Emissions of IVOC are expected to be high in Houston, due to the combination of petrochemical industry and mobile source emissions, and the contributions of IVOC to SOA appear to be important but underestimated. Work will include analysis of recently collected ambient data during DISCOVER-AQ on PM concentration and composition, new environmental chamber experiments on the SOA formation potential of IVOC, and photochemical modeling of the Houston region. Modeling of the formation of SOA from VOC and IVOC precursors will use a new state of the art approach based on the Volatility Basis Set (VBS) that has recently been implemented in the Comprehensive Air-quality Model with extensions (CAMx).

Project Update

In this quarter the UT Austin team set up the thermodenuder which will be used in environmental chamber experiments to measure the volatility of secondary organic aerosol. The valve controller is now coupled to the Aerosol Chemical Speciation Monitor which enables automatic and synchronized valve switching. UT Austin also conducted trial experiments to evaluate the wall losses of the IVOCs studied in these experiments – the IVOCs were injected into the environmental chamber and their concentrations were measured 4-5 times over the course of 2-3 hours. UT Austin also continued analysis of DISCOVER-AQ data, including improving the positive matrix factorization (PMF) analysis of the organic aerosol data. Filter samples collected at Conroe were sent to the Dessert Research Institute (DRI) for analysis of inorganic ions.

ENVIRON developed the CAMx model inputs (meteorology and natural emissions) for simulations of the DISCOVER-AQ period. Anthropogenic emissions for the on-road, off-road, non-road, area, and elevated source sectors were obtained from TCEQ. Emission inventory data was analyzed to estimate emissions of organic compounds from different source types (gasoline and diesel vehicles, meat cooking, biomass burning, etc.) which are needed for the VBS modeling.

Project 14-025	STATUS: Active – May 21, 2014

Development and Evaluation of an Interactive Sub-Grid Cloud Framework for the CAMx Photochemical Model

Environ – Christopher Emery
Texas A&M University – John Nielson-Gammon
AQRP Project Manager – Gary McGaughey
TCEQ Project Liaison – Khalid Al-Wali

Funding Amount: $256,261
($135,735 Environ, $120,526 TAMU)

Executive Summary

The US Environmental Protection Agency (EPA) requires the use of photochemical models to demonstrate that emission control plans will achieve the federal standard for ground-level ozone (EPA, 2007). The TCEQ uses the Comprehensive Air quality Model with extensions (CAMx) for research and regulatory photochemical modeling. Previous research conducted for the TCEQ has concluded that improvements to the CAMx modeling system, including a sub-grid cloud convection treatment, are necessary to reduce model under prediction biases in oxidized nitrogen compounds in the upper troposphere. Cloud convection at sub-grid scales is an important mechanism for exchanging boundary layer air with the free troposphere and for chemical processing. The current sub-grid cloud approach within CAMx influences photolysis rates, scavenging by rainfall, and aqueous chemistry at grid scale, but does not explicitly treat these processes at cloud scale and does not include sub-grid convective transport.

Small-scale clouds are often widespread but they are not explicitly resolved by the grid scales employed in regional meteorological and photochemical modeling applications. The physical effects from these sub-grid clouds are difficult to characterize accurately, but they can substantially influence many different atmospheric processes, including: boundary layer mixing, ventilation, and deep vertical transport of heat, moisture, and chemical tracers; radiative transfer and surface heat budgets; spatio-temporal precipitation patterns, intensity and wet scavenging rates; chemistry via photolysis and aqueous reactions; and certain environmentally-sensitive emission sectors (e.g., biogenic). Cloud convection is also an important component for long-range transport of ozone, PM, and precursors. The effects of sub-grid clouds on vertical transport, chemistry, and wet scavenging are addressed to varying degrees in off-line photochemical models (i.e., models like CAMx that operate separately from meteorological models that supply environmental inputs). However, the spatio-temporal distributions of such clouds, and all the processes that occur within them, must be re-diagnosed because meteorological models do not export necessary information from their sub-grid cloud parameterizations. This leads to potentially large inconsistencies between the models.

Under this AQRP Project, ENVIRON and collaborators at the Texas A&M University (TAMU) will incorporate and extensively evaluate an explicit sub-grid cloud model within CAMx. The primary goal of this work is to introduce shallow and deep convective cloud mixing at sub-grid scales. Further, the investigators will develop an approach to improve interactions with chemistry and wet deposition to operate explicitly at sub-grid scales in tandem with the cloud mixing scheme. The approach will tie into recent updates implemented in the Weather Research and

Forecasting (WRF) model by researchers at EPA, whereby specific sub-grid cloud fields will be passed to CAMx to define their spatio-temporal distributions and mixing rates for the new sub-grid cloud algorithm. This will yield a more consistent cloud-mixing-chemistry system across the WRF and CAMx models. The new CAMx treatment will be tested for three convective episodes that occurred during the September 2013 Houston DISCOVER-AQ field study and the Spring 2008 START08 field study, particularly addressing tropospheric profiles of NOx, ozone, and other chemical tracers by comparing to in situ profiles from aircraft measurements. The new model will be provided to TCEQ to support future regulatory and research-oriented ozone and PM modeling.

Project Update

A summary of activities for the period December 1, 2014 through February 28, 2015 is presented below.

In November, ENVIRON completed modifications and testing of the WRFCAMx interface and CAMx model to use data generated by EPA's interim version of WRF that includes an improved coupling between its Kain-Fritsch (K-F) sub-grid convection and radiative transfer modules. At that time we contacted EPA on the status of their latest version of WRF, which includes a new "multi-scale" Kain-Fritsch (MSKF) module that allows for sub-grid convective treatment down to grid scales of 1 km. This was considered important for CAMx, which is anticipated to be run on nested 36/12/4 km grids over Texas. However, this version of WRF was delayed as EPA worked with NCAR's WRF experts to address various bugs and implementation issues.

In December, ENVIRON collected existing modeling datasets to support WRF/CAMx model testing over the September 2013 DISCOVER-AQ and 2008 START08 periods. Data were compiled on a hard disk drive and transferred to Texas A&M (TAMU).

EPA transferred their MSKF version of WRF to ENVIRON in January. We reviewed the new WRF code, and implemented additional modifications to support the transfer of convective model fields to CAMx. However, our testing of WRF (with and without our additional modifications) resulted in model crashes. This issue was discussed with EPA's developers, but no solution could be identified.

As a result, the team decided to use EPA's interim version of WRF for the remainder of the project. In February, the interim version of WRF and new WRFCAMx and CAMx codes supporting the new CAMx convection treatment were transferred to Texas A&M (TAMU) to begin model applications over the DISCOVER-AQ and START08 episodes.

The EPA version of WRF/MSKF exhibited runtime crashes. We were able to isolate the crashes to EPA's MSKF code updates. Discussions with EPA developers did not yield any clear solutions, but we believe we isolated the problem to incompatibilities among compiler options and MPICH libraries. We decided to move the project forward by using the EPA's interim version of WRF that we successfully employed this past fall to develop and test the CAMx convection algorithm (as documented in previous progress reports).

The project remains on budget, but the schedule is roughly one month behind. Project completion and delivery of the final AQRP-reviewed report is scheduled for June 30, 2015.

Project 14-026	**STATUS: Active – May 21, 2014**

Quantifying ozone production from light alkenes using novel measurements of hydroxynitrate reaction products in Houston during the NASA SEAC4RS project

Environ – Greg Yarwood
(NOAA – Thomas Ryerson)

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

Funding Amount: \$165,562 (Reduced from 231,182)
(\$165,562 increased from \$135,782 Environ, \$0 reduced from \$95,400 CalTech)

Executive Summary

The objective of this project is to improve and quantify our understanding of ozone (O_3) and formaldehyde (HCHO) production from industrial emissions of Highly Reactive Volatile Organic Compounds (HRVOCs) in the Houston area. Aircraft flights during the National Aeronautics and Space Administration (NASA) Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys ($SEAC^4RS$) project encountered plumes with enhanced O_3 downwind of petrochemical facilities in Houston. For example, on 25 September 2013, ground monitoring downwind of the Ship Channel showed 5-minute average O_3 values peaking at 165 ppb and are associated with elevated concentrations of the oxidation products of HRVOCs. HRVOCs, specifically ethene, propene, butenes and 1,3-butadiene, have been implicated in these types of high ozone events but quantifying the relative contributions of individual HRVOCs to O_3 formation has been difficult.

The project objective will be accomplished by a combination of data analysis and reactive plume modeling. Data taken aboard the NASA DC-8 research aircraft during the 2013 $SEAC^4RS$ project in Houston will be analyzed. Chemical compounds called β-hydroxynitrates are formed when HRVOCs react in the atmosphere in the presence of nitrogen oxides (NOx). Measurements of the C_2-C_4 hydroxynitrates aboard the DC-8 provide a novel means to link observed enhancements of O_3 and HCHO to reactions of specific HRVOCs. Analyzing the data will provide a robust first-order attribution of observed O_3 and HCHO enhancements to the oxidation of individual HRVOCs emitted from the Houston Ship Channel. The plumes of HRVOCs and O_3 that the DC-8 intercepted will be analyzed further to estimate what emissions of HRVOCs and NOx gave rise to each plume. A reactive plume model (SCICHEM) will be used to model these plumes and test chemical reaction mechanisms for individual HRVOCs. The model sensitivity to plume expansion rates will be evaluated to test how plume dilution influences chemical processing and therefore how grid model resolution can influence assessments for HRVOC sources. The benefits of this project to the TCEQ will be a data-driven assessment of the contributions of individual HRVOCs to O_3 and HCHO enhancements downwind of the Houston ship channel and improved modeling tools for assessing the air quality impacts of HRVOC emissions in the Texas State Implementation Plan (SIP).

Project Update

This AQRP project is being performed by ENVIRON International Corporation (ENVIRON), NOAA, and Dr. David Parrish. Both NOAA and Dr. Parrish will conduct their tasks under subcontract to ENVIRON. A summary of activities for the period December 1, 2014 through February 28, 2015 is presented below.

Task 1: QA/QC Alkene Hydroxynitrate Measurements by the Caltech TOF-CIMS aboard the DC-8 during SEAC^{4}RS and Generate Final Data

The QA/QC'd Caltech hydroxynitrate data were downloaded from the SEAC^{4}RS data archive. Dr. Parrish completed the review of the alkene hydroxynitrate measurements and extracted the meteorological and chemical information required for data analysis (Task 2) and modeling (Task 3) for the DC-8 flight of primary interest (18 Sep 2013). The identification of additional potential SEAC^{4}RS flights that appear to have fortuitously intercepted ship channel plumes has also been completed; trajectory analysis of these plumes will be conducted to independently identify likely sources (see Task 2 below).

Task 2: Analysis of DC-8 airborne data to quantify plume initial conditions, production rates, and yields of O_3 and HCHO from parent alkenes

The preliminary kinetics scheme for the HRVOC chemistry that was developed by Dr. Parrish in the previous reporting period has been refined and finalized after discussions with ENVIRON and Caltech. The analysis of the alkene hydroxynitrate data for the 18 Sep 2013 flight has been completed. Trajectory analysis of the plumes intercepted on this flight has also been completed. Trajectory analysis for the other potential flights of interest has been started and is in progress, and will help identify the flights that will be selected for further analysis and modeling.

Task 3: Photochemical plume modeling to assess effects of hydroxynitrate sinks and 2nd-generation reaction products on inferred plume ozone production

ENVIRON has started implementing the final kinetics scheme for the HRVOC chemistry in SCICHEM. Meteorological input files for the 18 Sep 2013 flight have been prepared using routine observations as well as meteorological measurements from the DC-8. ENVIRON is using the plume measurements near the ship channel to develop input files that characterize ship channel emissions.

Project 14-029	STATUS: Active – July 10, 2014

Spatial and temporal resolution of primary and secondary particulate matter in Houston during DISCOVER-AQ

Baylor University – Rebecca Sheesley

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Shantha Daniel

Funding Amount: $178,679

Executive Summary

This project builds on a previously-funded AQRP project tasked at the initial elemental carbon (EC), organic carbon (OC), and optical black carbon (BC) characterization of particulate matter (PM) at Moody Tower and Manvel Croix during DISCOVER-AQ Houston Texas 2013 (AQRP 12-032). Under the original framework of PIs Sheesley and Usenko's AQRP ECOC Project, samples were to be collected over the entire DISCOVER-AQ sampling period at two primary sites in Houston: Moody Tower (urban) and Manvel Croix (southern suburb). Collaborations developed during the early stages of this project increased the sampling intensity at the two primary sites and expanded PM sampling efforts to Conroe (far north suburb) and La Porte (urban industrial).

The overall goals of this project are to analyze the filter samples collected in the previous project and to quantify the strength of PM formation and PM emission sources, including shipping emissions, motor vehicle exhaust, biomass burning and biogenic emissions, across the Houston metropolitan area. This work builds on the strengths of DISCOVER-AQ, specifically the spatial and temporal sampling strategies (i.e. multiple ground-based sites sampled for approximately 28 days). These strategies allow for the examination of both regional and long-range transport as well as anthropogenic and biogenic influences on air quality. The project will characterize PM through the quantification of water-soluble OC, organic tracers, EC, OC, ^{14}C, select inorganic ions, and elemental tracers from PM filters collected from four DISCOVER-AQ anchor sites including Moody Tower, Manvel Croix, Conroe, and La Porte. The PIs will apply a combination of radiocarbon source apportionment of organic and elemental carbon with source-specific organic and inorganic molecular tracers to tightly constrain urban and regional, fossil and biomass burning/biogenic sources.

Progress Report

The major focus of this quarter (December 2014 through February 2015) was to finalize filter plans of analysis of quartz fiber filters collected during DISCOVER-AQ and ship filter aliquots out for analysis to independent contract laboratories. A filter plan is a systematic strategy that specifies the amount or area of filter to be dedicated for each type of analysis. It is imperative that each set of analyses has a fully vetted filter plan. This will ensure that no analysis goes forward at the detriment of another. Deciding factors in filter area apportionment include: bulk carbon analysis, sampled air volume, analytical detection limits and co-located measurements. Filter plans were created during this period for inorganic ions, metals (51 elemental tracers), organic tracers, and radiocarbon. Filter plans needed to be created for all four ground-based sites (Moody Tower, Manvel Croix, Conroe, and La Porte) as well as for different quartz fiber filters size fractions; specifically total suspended particulates (TSP) and particulate matter 2.5 µm ($PM_{2.5}$). A filter plan for the Conroe $PM_{2.5}$ quartz fiber filters was created in the previous quarter and implemented in December to help support AQRP project (14-024).

Baylor students cut and shipped filters to Desert Research Institute (DRI) for inorganic ion analysis (quartz fiber filters from Moody Tower and Conroe) and for metals analysis (Teflon filters from Moody Tower). Baylor PIs (principal investigators) and students have been in close communication with DRI (specifically, Steven Kohl) in the past month to insure that Moody Tower and Conroe samples are analyzed in a timely manner for inorganic ion and metals (Teflon filters) as part of the project deliverables. Based on DRI turnaround estimates Baylor should receive inorganic ion and metals data by the end of the February or early March. The invoice for both analyses will be submitted after receiving inorganic ion data. Teflon filters ($PM_{2.5}$) were collected only at Moody Tower and will be used for metal analysis. No filter plan was needed as the entire Teflon filter is consumed in the analysis. Metal daily concentrations will be measured on $PM_{2.5}$ Teflon filters collected at Moody Tower.

Filter Plans

Inorganic Ion. Filter plans were created for inorganic ion analysis at Moody Tower. Baylor PIs and student shipped 26 samples and 4 blanks (following project's approved QAQC plan) to DRI for inorganic ion analysis. Based on DRI turnaround estimates, Baylor should receive inorganic ion data by the end of the February or early March. The percentage dedicated for inorganic ion analysis was approximately 8 to 16% of the quartz fiber filter. The DRI quote cost for inorganic ion analysis was $4750. Conroe filters dedicated for inorganic ion analysis were shipped earlier on in the project to help support AQRP project (14-024). Inorganic ions analysis was not a deliverable for Manvel Croix or La Porte. Inorganic ion analysis for Conroe is a deliverable for 14-024; Baylor graduate students cut and shipped Conroe filters to DRI in December, 2014.

Metals (Elemental Tracers). Metals are only to be measured at Moody Tower and only on Teflon filters. Baylor PIs and student shipped 25 samples and 3 blanks (following project's approved QAQC plan) to DRI for metal analysis in February. Based on DRI turnaround estimates, Baylor should receive inorganic ion data by the end of the February or early March. The entire Teflon filter was dedicated to the analysis of 51 metals using DRI and XRF. The DRI quote cost for metal analysis was $2342.

Radiocarbon. Filter plans were created for radiocarbon analysis at Moody Tower, Manvel Croix, Conroe, and La Porte. Baylor PIs and student shipped samples and blanks (following project's approved QAQC plan) to National Ocean Sciences Accelerator Mass Spectrometry Facility (NOSAMS) for radiocarbon analysis in February. Based on NOSAMS turnaround estimates, Baylor should receive inorganic ion data by the end of the April or early May. Samples and blanks were shipped in batches to help improve turnaround time for the submission of invoices. A total of 48 filters (including samples and blanks) were shipped to NOSAMS. The NOSAMS cost for radiocarbon analysis is approximately $26,000. Exact final costs are dependent upon factors in the analysis process and will not be determined until final invoicing.

Organic Tracers. Filter plans were created for organic tracer analysis at Moody Tower, Manvel Croix, Conroe, and La Porte. Baylor PIs and student will cut and analyze aliquots of quartz fiber filter for organic tracers for each site. Organic tracer analysis will follow QAQC criteria described in the project's QAPP. Approximately 50 plus samples and blanks will be analyzed for organic tracers. Filter plans were finalized using relationship between bulk organic carbon and organic tracer concentrations. Note: Organic carbon, elemental carbon, and water soluble organic carbon concentrations were measured earlier on in the project and was discussed and compared with other DISCOVER-AQ PIs at the December 2014 American Geophysical Union conference in San Francisco. Organic tracer concentrations were measured on a subset of representative samples. These two datasets were used to explore the relationship between bulk organic carbon and organic tracer concentrations. These tracer to organic carbon relationships were correlated with an R squared of greater than 0.97. Baylor PIs used these relationships to help determine the mass of organic carbon needed to measure organic tracers, while consuming the least amount of filter. The mass of organic carbon needed was converted into a percentage of the filter that would be dedicated for organic tracer analysis. The mass of organic carbon was measured on every filter, which allowed Baylor PIs to calculate the percentage dedicated for organic tracers analysis for each filter. This is extremely important because the overall loading varied by the duration of the sampling effort as well as from day to day and from site to site. Typically, the percentage dedicated for organic tracer analysis was approximately 10 to 60% of the quartz fiber filter. This preliminary effort is designed to reduce the number of non-detects for organic tracer analysis while potentially allowing preservation of more filter for future analysis.

Results for the project's organic carbon, elemental carbon, and water soluble organic carbon concentrations as well as the method for organic tracers were presented at the December 2014 American Geophysical Union conference in San Francisco.

Poster Presentations for American Geophysical Union

- Poster titled "Spatial trends in surface-based carbonaceous aerosol, including organic, water-soluble and elemental carbon, during DISCOVER-AQ in Houston, TX"
- Poster titled "A Pressurized Liquid Extraction Technique for the Analysis of Pesticides, PCBs, PBDEs, OPEs, PAHs, Alkanes, Hopanes, and Steranes from Atmospheric Particulate Matter".

Manuscript submission

- The manuscript titled "Pressurized Liquid Extraction Technique for the Analysis of Pesticides, PCBs, PBDEs, OPEs, PAHs, Alkanes, Hopanes, and Steranes in Atmospheric Particulate Matter".
- Manuscript was subsequently submitted for publication to the *Chemosphere*

Delays or Issues Report
After review of potential contract laboratories, Drs. Sheesley and Usenko determined that DRI was the best choice for metals analysis. This was based reviewing: (1) the contracted Scope of Work, (2) timeline for completing deliverables and (3) a consideration of intercomparison with previous TCEQ datasets. This decision was formally submitted to AQRP and TCEQ on 2/4/15 and was approved on 2/10/15. This will also be discussed in the February monthly report.

Project 14-030	STATUS: Active – June 25, 2014

Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation

Texas A&M University – Qi Ying

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

Funding Amount: $176,109

Executive Summary

Isoprene emitted from biogenic sources plays an important role in atmospheric chemistry that leads to the formation of ozone and secondary particulate matter (PM). Although drought has been thought to affect biogenic emissions, the capability of the current drought parameterization to adjust the impact of soil moisture on isoprene emissions has not been critically evaluated, especially under severe drought conditions in Texas. The impact of this change in isoprene emissions on regional ozone concentrations is also unclear. In this study, biogenic isoprene emissions during two seven-month episodes, one representing a relatively wet year (2007) and one representing a severe drought year (2011) will be estimated using the most recent version of the MEGAN biogenic emission model (MEGAN v2.1). Emissions during the severe drought year 2011 will be estimated using several different soil moisture parameterization schemes, including one that will be developed in this study based on additional field and climate-controlled laboratory measurements of isoprene emissions at leaf-level for selected Texas tree species. The Community Multiscale Air Quality Model (CMAQ) will be used to simulate isoprene, isoprene oxidation products and ozone concentrations during the dry and wet episodes. The predicted concentrations will be evaluated against all available measurements to evaluate the ability of different drought parameterization schemes and quantify the impact of drought on biogenic isoprene emission and ozone concentrations in Texas. Optimal configuration of the WRF model that is most appropriate for meteorology and soil moisture simulations during the drought seasons will also be investigated.

Project Update

Progress on Project 14-030 is summarized below by Task:

Task 1: Meteorology simulation with WRF.

We completed WRF simulation for both 2007 and 2011 using data from a number of sources, including the 3-h resolution North American Regional Reanalysis (NARR), satellite-based daily sea surface temperature, gridded soil moisture from North America Land Data Assimilation System (NLDAS) and MODIS-based, year-specific Leaf Area Index (LAI) and land use/land cover classification. Model performance analyses suggested that soil moisture predictions generally agree with available observations with a mean bias (MB) of approximately 0.1-0.15. The model performance of other variables such as temperature, wind speed, relative humidity and precipitation are within model performance criteria or comparable to those found in other studies using WRF.

Task 2: Perform field and laboratory measurements on common Texas tree species.
During the 3rd quarter of this project, no more measurements on potted oak tree seedlings in the greenhouse in College Station were undertaken, because the growing season had reached its end in November and most leaves had senesced and been dropped. We have since monitored the seedlings for photosynthetic activity if they still bore green leaves, or monitored for new growth if they did not. The results form measurements so far were assembled into a spreadsheet, its format discussed and modified based on sponsor feedback. Winter dormancy was used to carry out laboratory testing on the effectiveness of our sampling method, and to evaluate the need for new seedlings. We confirmed that our sampling method is unbiased under conditions of timely analysis (within 48 hours), and decided to acquire and pot a series of new seedlings that showed first signs of leaf development end of February. New measurements are expected as early as March 2015.

Task 3: Evaluate drought parameterization for isoprene emissions.
This work is currently on going.

Task 4: Perform regional BVOC modeling using MEGAN.
In the past quarter, we completed two set of MEGAN simulations of BVOC emissions for 2007 and 2011. One set of emissions (base case) was based on the original MEGAN model obtained from Dr. Alex Guenther without considering the soil moisture effect (drought effect) on BVOC emissions. The second set of emissions (soil moisture case 1) were based on our modified MEGAN with drought effect parameterization based on Dr. Guenther's original parameterization as documented in his MEGAN papers. The following figure shows the predicted monthly average emissions of isoprene in the 12-km domain from the base case and the differences between the soil moisture case 1 and the base in July 2011.

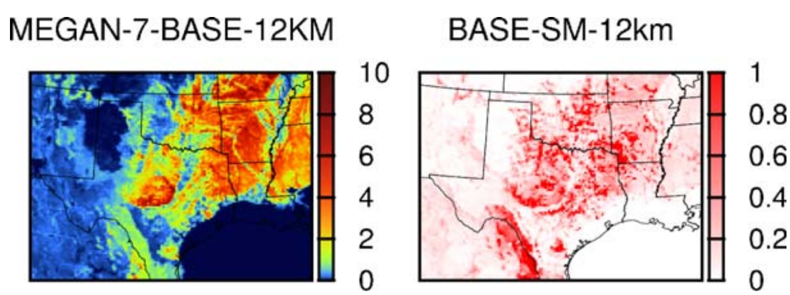

Figure 1. Predicted base case monthly emissions of isoprene in July 2011 (left) and the decrease of isoprene emissions due to drought effect (right). Units are mol s^{-1}.

Task 5: Perform regional air quality simulations.
In the past quarter, we have accomplished the following items. 1) All anthropogenic emissions for 2011 were regenerated due to several problems in the first set of emissions we generated in the previous quarter. 2) Preliminary air quality model simulations using the Community Multiscale Air Quality (CMAQ) model for April to July 2011. We found that 1) predicted isoprene concentrations are significantly higher than observations, even when the drought effect

was considered; We plan to investigate if this was caused by over-predictions of Photosynthetically Active Radiation (PAR) in the WRF model; 2) ozone concentrations were also over-predicted, especially on some days in summer times; and the days with ozone predictions are associated with over-predictions of NOx. In most stations, ozone predictions are not sensitive to isoprene reductions, suggesting that other meteorological factors, such as mixing height might play a role here. This will be further investigated in several sensitivity analyses that we planned to do.

FINANCIAL STATUS REPORT

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

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

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

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

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

FY 2012 funds were fully expended at the end of April 2014. FY 2013 funds are expected to be fully expended by April/May 2015.

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

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

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

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

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

Program Administration

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

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

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

As discussed in previous Quarterly Reports, the AQRP Administration requested and received permission to utilize funds in future fiscal years. This is for all classes of funds including Administration, ITAC, Project Management, and Contractual. As of the writing of this report, the FY 2010, FY 2011, and FY 2012 funds have been fully expended. This same procedure will be followed for the FY 2013, FY 2014, and FY 2015 funds.

In May 2014, UT-Austin received a Contract Extension for the AQRP. This extension will continue the program through April 27, 2016.

Table 1: AQRP Administration Budget

Administration Budget (includes Council Expenses)
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$202,816.67	$172,702.06	$375,518.73	$375,518.73	$0.00	$0.00
Fringe Benefits		$38,665.65	$33,902.95	$72,568.60	$72,568.60	$0.00	$0.00
Travel		$346.85	$0	$346.85	$346.85	$0.00	$0.00
Supplies		$15,096.14	$101.25	$15,197.39	$15,197.39	$0.00	$0.00
Equipment		$0	$0	$0			$0.00
Total Direct Costs		$256,925.31	$206,706.26	$463,631.57	$463,631.57	$0.00	$0.00
Authorized Indirect Costs		$20,281.69	$17,270.20	$37,551.89	$37,551.89	$0.00	$0.00
10% of Salaries and Wages							
Total Costs		**$277,207.00**	**$223,976.46**	**$501,183.46**	**$501,183.46**	**$0.00**	**$0.00**
Fringe Rate		22%	22%		19%		

Administration Budget (includes Council Expenses)
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$74,238.65	$257,404.00	$331,642.65	$307,561.38	$0.00	$24,081.27
Fringe Benefits		$17,068.38	$58,503.95	$75,572.33	$70,809.73	$0.00	$4,762.60
Travel		$339.13	$0.00	$339.13	$339.13		$0.00
Supplies		$3,560.62	$8,532.05	$11,912.67	$11,912.65	$0.00	$0.02
Equipment		$0.00	$0.00	$0			$0
Total Direct Costs		$95,206.78	$324,260.00	$419,466.78	$390,622.89	$0.00	$28,843.89
Authorized Indirect Costs		$7,423.86	$25,740.00	$33,163.86	$30,756.13	$0.00	$2,407.73
10% of Salaries and Wages							
Total Costs		**$102,630.64**	**$350,000.00**	**$452,630.64**	**$421,379.02**	**$0.00**	**$31,251.62**
Fringe Rate		22%	22%		23%		

Administration Budget (includes Council Expenses)
FY 2014/2015

Budget Category		**FY14 Budget**	**FY15 Budget**	**Total**	**Expenses**	**Pending Expenses**	**Remaining Balance**
Personnel/Salary		$70,000.00	$70,000.00	$140,000.00	$0.00	$0.00	$140,000.00
Fringe Benefits		$15,150.00	$15,150.00	$30,300.00	$0.00	$0.00	$30,300.00
Travel		$350.00	$350.00	$700.00	$0.00	$0.00	$700.00
Supplies		$7,500.00	$7,500.00	$15,000.00	$0.00	$0.00	$15,000.00
Equipment							
Total Direct Costs		$93,000.00	$93,000.00	$186,000.00	$0.00	$0.00	$186,000.00
Authorized Indirect Costs		$7,000.00	$7,000.00	$14,000.00	$0.00	$0.00	$14,000.00
10% of Salaries and Wages							
Total Costs		**$100,000.00**	**$100,000.00**	**$200,000.00**	**$0.00**	**$0.00**	**$200,000.00**
Fringe Rate		22%	22%		0%		

ITAC

No ITAC activities occurred during this period.

Table 2: ITAC Budget

ITAC Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$16,378.86	$6,292.97	$22,671.83	$22,671.83	$0.00	$0
Supplies		$1,039.95	$284.67	$1,324.62	$1,324.62	$0.00	0
Total Direct Costs		$17,418.81	$6,577.64	$23,996.45	$23,996.45	$0.00	$0
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$17,418.81**	**$6,577.64**	**$23,996.45**	**$23,996.45**	**$0.00**	**$0**

ITAC Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$5,323.31	$0.00	$5,323.31	$5,323.31	$0	$0.00
Supplies		$231.86	$0.00	$231.86	$231.86		$0.00
Total Direct Costs		$5,555.17	$0.00	$5,555.17	$5,555.17	$0	$0.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$5,555.17**	**$0.00**	**$5,555.17**	**$5,555.17**	**$0**	**$0.00**

ITAC Budget
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary							
Fringe Benefits							
Travel		$7,000.00	$7,000.00	$14,000.00	$0.00	$0.00	$14,000.00
Supplies		$500.00	$500.00	$1,000.00	$0.00	$0.00	$1,000.00
Total Direct Costs		$7,500.00	$7,500.00	$15,000.00	$0.00	$0.00	$15,000.00
Authorized Indirect Costs							
10% of Salaries and Wages							
Total Costs		**$7,500.00**	**$7,500.00**	**$15,000.00**	**$0.00**	**$0.00**	**$15,000.00**

Project Management

During this quarter, Project Managers continued to work with the project teams to ensure all reporting requirements were met and projects were moving forward as described in the Work Plans. Vince Torres was named as the Project Manager for the 5 new projects. Cyril Durrenberger assisted with the QAPP review as a part of the new project Work Plan approval process.

Table 3: Project Management Budget

Project Management Budget
FY 2010/2011

Budget Category		FY10 Budget	FY11 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$145,337.70	$121,326.64	$266,664.34	$266,664.34	$0	$0
Fringe Benefits		$28,967.49	$23,102.60	$52,070.09	$52,070.26	$0	($0.17)
Travel		$0	$0	$0	$0		$0
Supplies		$778.30	$207.98	$986.28	$986.22	$0	$0.06
Total Direct Costs		$175,083.49	$144,637.22	$319,720.71	$319,720.82	$0	($0.11)
Authorized Indirect Costs		$14,533.77	$12,132.66	$26,666.43	$26,666.32	$0	$0.11
10% of Salaries and Wages							
Total Costs		**$189,617.26**	**$156,769.88**	**$346,387.14**	**$346,387.14**	**$0**	**$0.00**

Project Management Budget
FY 2012/2013

Budget Category		FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$53,384.46	$123,314.00	$176,698.46	$172,680.86	$0.00	$4,017.60
Fringe Benefits		$10,991.04	$23,841.00	$34,832.04	$33,841.75	$0.00	$990.29
Travel		$0.00	$0.00	$0.00	$0.00		$0.00
Supplies		$967.98	$487.00	$1,454.98	$1,452.52		$2.46
Total Direct Costs		$65,343.48	$147,642.00	$212,985.48	$207,975.13	$0.00	$5,010.35
Authorized Indirect Costs		$5,338.44	$12,332.00	$17,670.44	$17,268.09	$0.00	$402.35
10% of Salaries and Wages							
Total Costs		**$70,681.92**	**$159,974.00**	**$230,655.92**	**$225,243.22**	**$0.00**	**$5,412.70**

Project Management Budget
FY 2014/2015

Budget Category		FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary		$52,000.00	$52,000.00	$104,000.00	$10,327.15	$0.00	$93,672.85
Fringe Benefits		$9,300.00	$9,300.00	$18,600.00	$2,206.63	$0.00	$16,393.37
Travel							
Supplies		$1,000.00	$1,000.00	$2,000.00	$587.25	$0.00	$1,412.75
Total Direct Costs		$62,300.00	$62,300.00	$124,600.00	$13,121.03	$0.00	$111,478.97
Authorized Indirect Costs		$5,200.00	$5,200.00	$10,400.00	$1,032.71	$0.00	$9,367.29
10% of Salaries and Wages							
Total Costs		**$67,500.00**	**$67,500.00**	**$135,000.00**	**$14,153.74**	**$0.00**	**$120,846.26**

Research Projects

FY 2010-2011

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

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

Table 4 on the following 2 pages illustrates the 2010-2011 Research Projects, including the funding awarded to each project and the total expenses reported on each project through the expiration of the FY 2011 funds on June 30, 2013.

FY 2012-2013

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

Funds that were not expended by the FY 2012 – 2013 research projects totaling $1,662,870.99 have been allocated to projects from the FY 2014-2015 RFP. Table 5 illustrates the 2012-2013 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of February 28, 2015. FY 2013 funding will be fully expended by June 30, 2015.

FY 2014-2015

The FY 2014 and 2015 Research/Contractual budgets were originally funded at $825,000 each. Research projects have been awarded to FY 2013, 2014, and 2015 funds.

Table 4: 2010/2011 Contractual Expenses

Contractual Expenses

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

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

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

Table 5. 2012/2013 Contractual Expenses

Contractual Expenses

FY 12 Contractual Funding		$815,000.00		
FY 12 Contractual Funding Transfers		$32,438.67		
FY 12 Total Contractual Funding		**$847,438.67**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
12-004	UT-Austin (Torres)	$20,174.10	$20,174.10	$0.00
12-006	UC-Riverside	$101,765.00	$101,765.00	$0.00
12-006	TAMU/TEES	$44,494.00	$42,134.22	$2,359.78
12-011	Environ International	$77,420.00	$77,410.16	$9.84
12-012	UT-Austin (Hildebrandt)	$79,463.00	$79,173.94	$289.06
12-012	Environ International	$69,374.00	$69,372.64	$1.36
12-013	Environ International	$59,974.00	$59,960.93	$13.07
12-018	UT-Austin (McDonald-Buller)	$85,282.00	$85,197.80	$84.20
12-018	Environ International	$21,688.00	$21,686.26	$1.74
12-028	University of Houston	$19,599.00	$16,586.51	$3,012.49
12-028	UCLA	$17,944.00	$17,709.51	$234.49
12-028	Environ International	$44,496.00	$44,496.00	$0.00
12-028	UNC - Chapel Hill	$35,230.00	$35,230.00	$0.00
12-032	Baylor	$45,972.00	$43,642.21	$2,329.79
12-TN1	Maryland	$64,994.00	$64,537.12	$456.88
12-TN2	Maryland	$69,985.00	$68,362.27	$1,622.73
FY 12 Total Contractual Funding Awarded		$847,438.67		
FY 12 Contractual Funds Expended to Date			$847,438.67	
FY 12 Contractual Funds Remaining to be Spent				$0.00

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

FY 13 Contractual Funding		$835,000		
FY 13 Contractual Funding Transfers		$2,209,000		
FY 13 Total Contractual Funding		**$3,044,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
13-004	UT-Austin (Torres)	$1,555,770	$805,228.06	$750,541.84
13-005	Chalmers University of Tech	$129,047	$129,047.00	$0.00
13-005	University of Houston	$48,506	$44,928.24	$3,577.76
13-016	Valparaiso	$46,652	$46,652.10	$0.00
13-016	University of Houston	$19,846	$14,101.40	$5,744.60
13-022	Rice University	$89,912	$75,881.86	$14,030.14
13-022	University of Houston	$116,903	$116,122.47	$780.53
13-024	Maryland	$90,444	$89,658.88	$785.12
FY 13 Total Contractual Funding Awarded		$2,097,080		
FY 13 Contractual Funds Expended (Init. Projects)			$1,321,620.01	
FY 13 Contractual Funds Remaining Unspent				$1,722,379.99
FY 13 Additional Expenditures				
	DATA Storage	$5,535	$5,535	$0.00
FY 13 Contractual Funds Expended			$1,327,155.01	
FY 13 Contractual Funds Remaining Unspent				$1,716,844.99

Note:
After all FY13 projects were completed contractual funds in the amount of $1,716,844.99 remained. The funds will be utilized for FY14 projects and will be accounted for on the following page.

FY 13 Remaining Contractual Funding		**$1,716,844.99**		
FY 13 Remaining Contractual Funding Transfers		**($53,974.00)**		
FY 13 Total Remaining Contractual Funding		**$1,662,870.99**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-003	UNC Chapel Hill	$180,000.00	$41,196.31	$138,803.69
14-006	Sonoma Technology	$48,985.00	$26,184.50	$22,800.50
14-006	Valparaiso	$3,578.11	$3,578.11	$0.00
14-006	St. Edwards	$11,025.00		$11,025.00
14-007	Chalmers Univ.	$65,233.00	$55,880.00	$9,353.00
14-007	Univ. of Houston	$10,000.00	$10,000.00	$0.00
14-008	UT-Austin (McDonald-Buller)	$156,500.00	$107,511.32	$48,988.68
14-009	Rice University	$60,000.00	$42,774.84	$17,225.16
14-011	UT-Austin (McDonald-Buller)	$131,166.00	$75,768.81	$55,397.19
14-011	Environ	$6,000.00	$733.77	$5,266.23
14-016	Environ	$240,000.00	$124,285.29	$115,714.71
14-017	Univ. of Alabama-Huntsville	$25,000.00	$17,909.48	$7,090.52
14-017	Rice University	$25,000.00	$9,369.28	$15,630.72
14-023	UT-Austin (Torres)	$25,874.37	$25,874.37	$0.00
14-023	Aerodyne	$10,712.74	$10,712.74	$0.00
14-024	UT-Austin (Hildebrandt Ruiz)	$143,282.00	$108,040.32	$35,241.68
14-024	Environ	$25,000.00	$25,000.00	$0.00
14-024	UC Riverside	$33,270.50	$33,270.50	$0.00
14-025	Environ	$80,000.00	$68,659.34	$11,340.66
14-025	TAMU	$20,000.00	$20,000.00	$0.00
14-026	Environ	$80,000.00	$68,819.12	$11,180.88
14-029	Baylor University	$150,000.00	$45,859.82	$104,140.18
14-030	TEES	$132,227.43	$67,666.93	$64,560.50

FY 13 Total Remaining Contractual Funding Awarded	$1,662,854.15		
FY 13 Remaining Contractual Funds Expended		$989,094.85	
FY 13 Remaining Contractual Funds Remaining to be Spent			$673,776.14
Total Contractual Funding	$3,837,465		
Total Contractual Funding Awarded	$3,837,448		
Total Contractual Funding Remaining to be Awarded	$17		
Total Contractual Funds Expended to Date		$3,163,688.53	
Total Contractual Funds Remaining to be Spent			$673,776.14

Table 6. 2014/2015 Contractual Expenses

Contractual Expenses

FY 14 Contractual Funding		**$825,000**		
FY 14 Contractual Funding Transfers		**$0**		
FY 14 Total Contractual Funding		**$825,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-002	CU - Boulder	$150,508.00	$105,328.78	$45,179.22
14-002	Univ. of Maryland	$49,387.00		$49,387.00
14-003	UNC Chapel Hill	$20,000.00	$0.00	$20,000.00
14-004	Univ. of Maryland	$55,056.00	$33,189.44	$21,866.56
14-004	Morgan State Univ.	$54,055.00	$21,255.60	$32,799.40
14-009	Rice Univ.	$49,867.00	$6,465.76	$43,401.24
14-009	Univ. of Houston	$109,635.00	$14,389.53	$95,245.47
14-014	Univ. of Houston	$0.00	$0.00	$0.00
14-026	Environ	$85,782.00	$15,419.16	$70,142.84
14-030	TAMU/TEES	$43,881.57		$43,881.57
				$0.00
				$0.00
FY 14 Total Contractual Funding Awarded		$617,951.57		
FY 14 Contractual Funding Remaining to be Awarded		$207,048.43		
FY 14 Contractual Funds Expended to Date			$196,048.27	
FY 14 Contractual Funds Remaining to be Spent				$628,951.73

FY 15 Contractual Funding		**$825,000**		
FY 15 Contractual Funding Transfers		**$0**		
FY 15 Total Contractual Funding		**$825,000**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-005	TAMU	$103,890.00	$0.00	$103,890.00
14-006	Sonoma Technology	$2,000.00	$0.00	$2,000.00
14-007	Chalmers University	$8,946.00	$0.00	$8,946.00
14-007	Univ. of Houston	$13,081.00	$5,001.79	$8,079.21
14-008	Univ. of Texas - Austin	$18,500.00		$18,500.00
14-010	TAMU	$79,325.00		$79,325.00
14-011	Univ. of Texas - Austin	$20,001.00		$20,001.00
14-011	Environ	$22,419.00		$22,419.00
14-016	Environ	$31,911.00	$0.00	$31,911.00
14-017	Univ. of Alabama - Huntsville	$112,003.00		$112,003.00
14-017	Rice University	$37,979.00		$37,979.00
14-023	Aerodyne Research	$0.00	$0.00	$0.00
14-024	Univ. of Texas - Austin	$20,000.00	$0.00	$20,000.00
14-024	Environ	$76,404.00	$6,839.40	$69,564.60
14-025	Environ	$55,735.00	$6,923.09	$48,811.91
14-025	TAMU	$100,526.00	$16,770.43	$83,755.57
14-029	Baylor University	$28,679.00		$28,679.00
FY 15 Total Contractual Funding Awarded		$801,399.00		
FY 15 Contractual Funding Remaining to be Awarded		$23,601.00		
FY 15 Contractual Funds Expended to Date			$35,534.71	
FY 15 Contractual Funds Remaining to be Spent				$789,465.29

Total Contractual Funding	$1,650,000		
Total Contractual Funding Awarded	$1,419,351		
Total Contractual Funding Remaining to be Awarded	$230,649		
Total Contractual Funds Expended to Date		$231,582.98	
Total Contractual Funds Remaining to be Spent			$1,418,417

Table 7. Breakdown of Project Funding Across Fiscal Years

Project	Final Approved Budget by Entity	FY 13	FY 14	FY 15	
14-002 - UC Boulder	150,508.00		150,508.00		$150,508.00
14-002 - Maryland	49,387.00		49,387.00		$49,387.00
14-003 - UNC - CH	200,000.00	180,000.00	20,000.00		$200,000.00
14-004 - Maryland	55,056.00		55,056.00		$55,056.00
14-004 - Morgan State	54,055.00		54,055.00		$54,055.00
14-005 - TAMU	103,890.00			103,890.00	$103,890.00
14-006 - Sonoma Tech	50,985.00	48,985.00		2,000.00	$50,985.00
14-006 - Valpo	3,578.11	3,578.11			$3,578.11
14-006 - St. Edwards	11,025.00	11,025.00			$11,025.00
14-007 - Chalmers	74,179.00	65,233.00		8,946.00	$74,179.00
14-007 - UH	23,081.00	10,000.00		13,081.00	$23,081.00
14-008 - UT Austin	175,000.00	156,500.00		18,500.00	$175,000.00
14-009 - Rice	109,867.00	60,000.00	49,867.00		$109,867.00
14-009 - UH	109,635.00		109,635.00		$109,635.00
14-010 - TAMU	79,325.00			79,325.00	$79,325.00
14-011 - UT	151,167.00	131,166.00		20,001.00	$151,167.00
14-011 - Environ	28,419.00	6,000.00		22,419.00	$28,419.00
14-014 - UH	84,927.00		84,927.00		$84,927.00
14-016 - Environ	271,911.00	240,000.00		31,911.00	$271,911.00
14-017 - UAB	137,003.00	25,000.00		112,003.00	$137,003.00
14-017 - Rice	62,979.00	25,000.00		37,979.00	$62,979.00
14-020 - Maryland	70,000.00			70,000.00	$70,000.00
14-022 - UAB	71,004.00		71,004.00		$71,004.00
14-022 - George Mason U	44,996.00		44,996.00		$44,996.00
14-023 - UT	25,874.37	25,874.37		0.00	$25,874.37
14-023 - ARI	10,712.74	10,712.74		0.00	$10,712.74
14-023 - Leak Sys	0.00				$0.00
14-023 - Provid	0.00				$0.00
14-024 - UT	163,282.00	143,282.00		20,000.00	$163,282.00
14-024 - Environ	101,404.00	25,000.00		76,404.00	$101,404.00
14-024 - UC-Riverside	33,270.50	33,270.50			$33,270.50
14-025 - Environ	135,735.00	80,000.00		55,735.00	$135,735.00
14-025 - TAMU	120,526.00	20,000.00		100,526.00	$120,526.00
14-026 - Environ	165,562.00	80,000.00	85,562.00		$165,562.00
14-026 - CalTech	0.00		0.00		$0.00
14-029 - Baylor	178,679.00	150,000.00		28,679.00	$178,679.00
14-030 - TAMU	176,109.00	132,227.43	43,881.57		$176,109.00
Amt in Projects	3,283,131.72	1,662,854.15	818,878.57	801,399.00	
Available Funding		1,662,870.99	825,000.00	825,000.00	
Funding Remaining		16.84	6,121.43	23,601.00	

Appendix A

Financial Reports by Fiscal Year

FY 10 and 11

(Expenditures reported as of November 30, 2014.)

Administration Budget (includes Council Expenses)

FY 2010

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

Administration Budget (includes Council Expenses)

FY 2011

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

ITAC Budget

FY 2010

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

ITAC Budget

FY 2011

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

Project Management Budget
FY 2010

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

Project Management Budget
FY 2011

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

AQRP Budget

FY 2010

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

AQRP Budget

FY 2011

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

Appendix B

Financial Reports by Fiscal Year

FY 12 and 13

(Expenditures reported as of November 30, 2014.)

Administration Budget (includes Council Expenses)

FY 2012

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

Administration Budget (includes Council Expenses)

FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$257,404.00	$233,322.73		$24,081.27
Fringe Benefits		$58,503.95	$53,741.35		$4,762.60
Travel		$0.00	$0.00		$0.00
Supplies		$8,352.05	$8,352.03		$0.02
Equipment					
Other		$0.00			
Total Direct Costs		$324,260.00	$295,416.11	$0.00	$28,843.89
Authorized Indirect Costs		$25,740.00	$23,332.27		$2,407.73
10% of Salaries and Wages					
Total Costs		**$350,000.00**	**$318,748.38**	**$0.00**	**$31,251.62**

ITAC Budget

FY 2012

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

ITAC Budget

FY 2013

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

Project Management Budget
FY 2012

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

Project Management Budget
FY 2013

Budget Category		FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$123,314.00	$119,296.40		$4,017.60
Fringe Benefits		$23,841.00	$22,850.71		$990.29
Travel					
Supplies		$487.00	$484.54		$2.46
Equipment					
Other					
Contractual					
Total Direct Costs		$147,642.00	$142,631.65	$0	$5,010.35
Authorized Indirect Costs		$12,332.00	$11,929.65		$402.35
10% of Salaries and Wages					
Total Costs		**$159,974.00**	**$154,561.30**	**$0.00**	**$5,412.70**

AQRP Budget

FY 2012

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

AQRP Budget
FY 2013

Budget Category		**FY13 Budget**	**Cumulative Expenditures**	**Pending Expenditures**	**Remaining Balance**
Personnel/Salary		$257,404.00	$233,322.73	$0.00	$24,081.27
Fringe Benefits		$58,503.95	$53,741.35	$0.00	$4,762.60
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$8,352.05	$8,352.03	$0.00	$0.02
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$2,990,026.00	$2,316,249.86	$0.00	$673,776.14
ITAC		$0.00	$0.00	$0.00	$0.00
Project Management		$159,974.00	$154,561.30	$0.00	$5,412.70
Total Direct Costs		$3,474,260.00	$2,766,227.27	$0.00	$708,032.73
Authorized Indirect Costs		$25,740.00	$23,332.27	$0.00	$2,407.73
10% of Salaries and Wages					
Total Costs		**$3,500,000.00**	**$2,789,559.54**	**$0.00**	**$710,440.46**

Appendix C

Financial Reports by Fiscal Year

FY 14 and 15

(Expenditures reported as of November 30, 2014.)

Administration Budget (includes Council Expenses)
FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment					
Other					
Total Direct Costs		$93,000.00	$0.00	$0.00	$93,000.00
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$0.00**	**$0.00**	**$100,000.00**

Administration Budget (includes Council Expenses)
FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment					
Other					
Total Direct Costs		$93,000.00	$0.00	$0.00	$93,000.00
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$100,000.00**	**$0.00**	**$0.00**	**$100,000.00**

ITAC Budget

FY 2014

Budget Category		**FY14 Budget**	**Cumulative Expenditures**	**Pending Expenditures**	**Remaining Balance**
Personnel/Salary					
Fringe Benefits					
Travel		$7,000.00	$0.00	$0.00	$7,000.00
Supplies		$500.00	$0.00	$0.00	$500.00
Equipment					
Other					
Total Direct Costs		$7,500.00	$0.00	$0.00	$7,500.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$7,500.00**	**$0.00**	**$0.00**	**$7,500.00**

ITAC Budget

FY 2015

Budget Category		**FY15 Budget**	**Cumulative Expenditures**	**Pending Expenditures**	**Remaining Balance**
Personnel/Salary					
Fringe Benefits					
Travel		$7,000.00	$0.00	$0.00	$7,000.00
Supplies		$500.00	$0.00	$0.00	$500.00
Equipment					
Other					
Total Direct Costs		$7,500.00	$0.00	$0.00	$7,500.00
Authorized Indirect Costs					
10% of Salaries and Wages					
Total Costs		**$7,500.00**	**$0.00**	**$0.00**	**$7,500.00**

Project Management Budget
FY 2014

Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$52,000.00	$10,327.15	$0.00	$41,672.85
Fringe Benefits		$9,300.00	$2,206.63	$0.00	$7,093.37
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$1,000.00	$0.00	$0.00	$1,000.00
Equipment					
Other					
Total Direct Costs		$62,300.00	$12,533.78	$0.00	$49,766.22
Authorized Indirect Costs		$5,200.00	$1,032.71	$0.00	$4,167.29
10% of Salaries and Wages					
Total Costs		**$67,500.00**	**$13,566.49**	**$0.00**	**$53,933.51**

Project Management Budget
FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$52,000.00	$0.00	$0.00	$52,000.00
Fringe Benefits		$9,300.00	$0.00	$0.00	$9,300.00
Travel		$0.00	$0.00	$0.00	$0.00
Supplies		$1,000.00	$587.25	$0.00	$412.75
Equipment					
Other					
Total Direct Costs		$62,300.00	$0.00	$0.00	$61,712.75
Authorized Indirect Costs		$5,200.00	$0.00	$0.00	$5,200.00
10% of Salaries and Wages					
Total Costs		**$67,500.00**	**$0.00**	**$0.00**	**$66,912.75**

AQRP Budget

FY 2014

Budget Category		**FY14 Budget**	**Cumulative Expenditure s**	**Pending Expenditures**	**Remaining Balance**
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$825,000.00	$196,048.27	$0.00	$628,951.73
ITAC		$7,500.00	$0.00	$0.00	$7,500.00
Project Management		$67,500.00	$13,566.49	$0.00	$53,933.51
Total Direct Costs		$993,000.00	$209,614.76	$0.00	$783,385.24
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$209,614.76**	**$0.00**	**$790,385.24**

AQRP Budget
FY 2015

Budget Category		FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary		$70,000.00	$0.00	$0.00	$70,000.00
Fringe Benefits		$15,150.00	$0.00	$0.00	$15,150.00
Travel		$350.00	$0.00	$0.00	$350.00
Supplies		$7,500.00	$0.00	$0.00	$7,500.00
Equipment		$0.00	$0.00	$0.00	$0.00
Other		$0.00	$0.00	$0.00	$0.00
Contractual		$825,000.00	$35,534.71	$0.00	$789,465.29
ITAC		$7,500.00	$0.00	$0.00	$7,500.00
Project Management		$67,500.00	$587.25	$0.00	$66,912.75
Total Direct Costs		$993,000.00	$36,121.96	$0.00	$956,878.04
Authorized Indirect Costs		$7,000.00	$0.00	$0.00	$7,000.00
10% of Salaries and Wages					
Total Costs		**$1,000,000.00**	**$36,121.96**	**$0.00**	**$963,878.04**