## AIR QUALITY RESEARCH PROGRAM

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

Quarterly Report September 1, 2014 through November 30, 2014

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

**December 15, 2014** 

1

**Texas Air Quality Research Program** 

#### **Annual Report**

September 1, 2014 – November 30, 2014

## Overview

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

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

On April 30, 2010, the Texas Commission on Environmental Quality (TCEQ) contracted with the University of Texas at Austin to administer the AQRP. For the 2010-2011 biennium, the AQRP had approximately \$4.9 million in funding available. Following discussions with the TCEQ and an Independent Technical Advisory Committee (ITAC) concerning research priorities, the AQRP released its first request for proposals in May, 2010. Forty-five proposals, requesting \$12.9 million in research funding were received. After review by the ITAC for technical merit, and by the TCEQ for relevancy to the State's air quality research needs, the results of the reviews were forwarded to the AQRP's Advisory Council, which made final funding decisions in late August, 2010. A total of 15 proposals were selected for funding. 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, project Principal Investigators (PIs) were notified of the decision of the Advisory Council. AQRP Project Managers and TCEQ Project Liaisons were assigned to each project. A kick-off call was held with 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.

The PIs of the 5 additional projects have been notified and are now in the process of developing their Work Plans.

#### BACKGROUND

Section 387.010 of HB 1796 (81<sup>st</sup> 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 <u>http://aqrp.ceer.utexas.edu/</u>.
- 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 (September 1, 2014-November 30, 2014), three primary activities took place:

- Last contracts executed with University of Colorado-Boulder and Texas A&M
- AQRP Review Panel met
  - Approved change in scope and funding for Project 14-026
  - o Recommended 5 additional projects for funding
- Advisory Council approved funding for 5 additional projects

During this period, contracts were finalized with the University of Colorado at Boulder and Texas A&M University. Project managers continued to work with principal investigators to ensure that all project goals were met, as well as all reporting and invoicing requirements. Two projects underwent significant changes:

Project 14-026, led by Environ International, was authorized to begin work in May, even though contract negotiations were still on-going with the project partner, the California Institute of Technology (Cal Tech). In August, Environ notified AQRP that Cal Tech was terminating contract negotiations with the AQRP and would no longer be involved with the project. Cal Tech's contract negotiations office confirmed this with AQRP's contract negotiations office. Environ submitted a revised Work Plan to the AQRP to modify the scope and budget of the project in light of the change in participants. The change included bringing on David Parrish as a consultant. The revised Work Plan was reviewed by the AQRP Review Panel in September and these changes were approved. Because this resulted in a reduction of funds for this project, Advisory Council approval was not needed; however, the Council was notified of this change.

Project 14-023, led by The University of Texas at Austin, began work in May. In July, the host of the site where the work was to be performed notified the PI that the company was being sold, and the new owners would not allow the project to take place on that site. The PI tried to locate an alternate site for the project, but was unable to find a host. In August, the PI officially notified the AQRP that the project could not be completed. The project was ended and all unspent funds were returned to the AQRP Research Projects fund.

The changes in the two projects listed above resulted in approximately \$511,000 being returned to the AQRP Research Projects fund.

As significant funding was now available for additional research projects, the TCEQ performed a relevancy review of the proposals that were submitted in response to the FY 14-15 RFP, but

were not selected for funding in the initial round of reviews. During the September call, the Review Panel identified 5 alternate projects for funding based on that relevancy review. Due to the limited amount of time available to complete the projects, a recommendation was also made to reduce the scope and budget by approximately 30%, so that the work could be completed by October 2015. These proposals were then submitted to the Advisory Council along with the recommendations for the scope and budget changes. The Council approved the funding for all 5 projects, at the level recommended by the AQRP and the Review Panel.

The additional projects are:

14-005 PI: Sarah Brooks, Texas A&M Sources and Properties of Atmospheric Aerosol in Texas: DISCOVER-AQ Measurements and Validation

14-010 PI: Yuxuan Wang, Texas A&M Galveston Impact of large-scale circulation patterns on surface ozone concentrations in HGB

14-014 PI: Yunsoo Choi, University of Houston Constraining NOX and HCHO Emissions Using Satellite NO2 and HCHO Column Measurements over the Southeast Texas

14-020 PI: Xinrong Ren, University of Maryland Analysis of Ozone Formation Sensitivity in Houston Using the Data Collected during DISCOVER-AQ and SEAC4RS

14-022 PI: Richard McNider, University of Alabama-Huntsville Use of satellite data to improve specifications of land surface parameters

The PIs of the 5 additional projects have all been notified and are currently developing the Work Plan for their projects. Work is expected to begin in January.

## **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: Work Plan Approved Master Agreement Negotiations Pending

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

University of Colorado - Boulder – Alan Fried University of Maryland – Christopher Loughner AQRP Project Manager – Gary McGaughey TCEQ Project Liaison – Jim Smith

#### Funding Amount: \$199,895

(\$150,508 UC-Boulder, \$49,387 U of Maryland)

#### **Executive Summary**

During summer months the greater Houston-Galveston-Brazoria Metropolitan Area (HGBMA) often experiences elevated levels of ozone exceeding federal standards, particularly during hot and stagnant wind conditions. Although significant progress has been achieved understanding the major causes of these events over the past 10 years, there are still major unanswered questions related to sources of ozone from highly reactive volatile organic compounds (HRVOC's) emitted by large petrochemical facilities throughout the HGBMA. The toxic trace gas formaldehyde (CH<sub>2</sub>O) is produced as an intermediate when these HRVOC's breakdown in the atmosphere, and ozone and radicals are formed when CH<sub>2</sub>O further breaks down. Therefore a comprehensive understanding of CH<sub>2</sub>O 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<sub>2</sub>O from sources such as petrochemical flaring operations and automotive emissions relative to secondarily produced CH<sub>2</sub>O from HRVOC's produced downwind, affecting large geographic areas far removed from the petrochemical facilities. Updating the emission inventories and temporal trends for CH<sub>2</sub>O 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<sub>2</sub>O 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<sup>4</sup>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 6<sup>th</sup> day at the Clinton, Deer Park and Channelview sites as a means to further validate and/or provide error bounds, for such long-term  $CH_2O$  data in the greater HGBMA.

#### **Project Update**

The Work Plan for Project 14-002 was approved on June 5, 2014. Contract negotiations between the University of Colorado-Boulder and UT Austin were not finalized until September 2014. The project start date was backdated to the date the project Work Plan was approved; however, work did not begin until September. For this reason, the end date was extended to September 30, 2015.

During this quarter, team members coordinated and reviewed by telecoms the specific tasks assigned to each group. The UMD/NASA Goddard Group started their efforts in running WRF down to 1 km resolution. The CU team initiated their efforts to identify P3 and DC8 aircraft sampling periods arising from clearly identifiable sources. These periods will then be used for further study by WRF and CMAQ. Because of the large and dynamic pollution levels trapped in a shallow boundary layer, the CU team identified Sept. 25 for the initial analysis. This team started this analysis by quantifying CH2O/CO slopes from the final DISCOVER-AQ data for 4 specific events where: 1) petrochemical refinery emissions were dominant over the Baytown Exxon Mobil petrochemical complex; 2) biogenic isoprene emissions were dominant near Conroe; 3) where an unknown source, possibly from CH<sub>2</sub>O photochemical production downwind of the Baytown complex, were dominant over Smith Point; and 4) where automotive sources were dominant over the center of Houston over Moody Tower. These events will be used as starting points to arrive at updated emissions.

WRF model output will be used to run CMAQ and calculate back trajectories with the Read/Interpolate/Plot (RIP) program. The CU team will provide to the UMD/Goddard team interesting time periods for further analysis. Initial efforts will focus on P3 sampling on September 25, 2013.

The AQRP task order was executed over 4 months after the anticipated start date established in the Work Plan. Although we don't anticipate issues that will retard progress, the late start will necessitate pushing back the accomplishments of each Milestone.

## 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:

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

We have generated simulations necessary for QA of data from the model including the predicted bulk SOA formation in our indoor chamber using reactive uptake coefficients we recently derived in flow tube studies (Gaston et al., 2014, ES&T). Based on our analysis we are confident in the QA/QC testing of the algorithms for the predicted uptake of gaseous IEPOX onto an aerosol of variable acidity, temperature, and relative humidity.

#### Task 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.

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

We have begun our experiments and expect over the next 2-3 months that we will generate enough experimental data to be evaluated by the model. These will include wall-loss experiments (including for IEPOX and MAE), as well as actual experiments outlined in the work plan. Table 1 shows the experiments proposed.

	[Epoxide]			Initial Seed	RH	—
<b>Ехр</b> τ. <i>#</i>	Epoxide	(ppb)	Seed Aerosol Type	Aerosol (µg/m <sup>3</sup> )	(%) 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	

#### Table 1. Indoor experiments to be conducted at UNC.

#### 0.6 M (NH4)2SO4 + 0.6 M H2SO4

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

We have been able to model some of our flow tube experiments. We used a combination of flow reactor studies and smog chamber modeling to constrain two uncertain parameters central to epoxide-derived secondary organic aerosol (SOA): the rates of epoxide heterogeneous reactions with the particle phase and the molar fraction of these uptaken epoxides that go on to contribute to the SOA burden – which we define as the SOA yield ( $\alpha_{SOA}$ ).

As shown in the table below, flow reactor measurements of epoxide-aerosol reaction probability  $(\gamma)$  were performed on atomized aerosols. Heterogeneous reactions are often thought of in terms of the reaction probability as it is can be efficiently incorporated into regional and global models. We fit the log of the epoxide decay in the presence and absence of aerosol particles to obtain a pseudo first order rate coefficient for the wall loss and the sum of the wall loss and aerosol loss reactions which can then be converted to  $\gamma$  given the aerosol surface area concentration in the flow reactor. We chose aerosol compositions and flow reactor relative humidities to mimic previous smog chamber epoxide SOA experiments. In this way we can use both the flow reactor data and the SOA growth measured in the chamber experiments to constrain  $\alpha_{SOA}$ .

As shown in the table below a range in  $\alpha_{SOA}$  is estimated through the use of a time-dependent 0-D chemical box model designed to simulate the chamber experiments. We initialize the model with  $\gamma$ 's from the flow reactor measurements and epoxide mixing ratios, aerosol surface area and mass concentrations from the chamber experiments. Then we vary  $\alpha_{SOA}$  in the model to bracket the chamber-measured SOA mass growth and estimate the  $\alpha_{SOA}$  range. This range provides an approximation of the fraction of aqueous phase epoxide reactions that produce SOA relative to the total number of aqueous phase reactions. Given these two constraints coupled with ambient measurements of epoxide concentrations and aerosol composition, we can place bounds on the epoxide contribution to SOA in the atmosphere.

epoxide	aerosol	RH	aerosol [H⁺] (M)*	γ±1σ	modeled $lpha_{SOA}$ range
IEPOX	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	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	$0.011 \pm 0.003$	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	$0.021\pm0.001$	0.09 - 0.11
IEPOX	$(NH_4)_2SO_4 + H_2SO_4$	0.59	2.01	$0.019 \pm 0.002$	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

 Table 2. Modeling results from chamber experiments.

\*Estimated from E-AIM model calculation of moles  $H^{\star}$  and total volume of aqueous phase.

E-AIM RH input must be  $\geq 0.1$ . Hence the same estimated [H<sup>+</sup>] for same aerosol and RH<0.1.

All funds allocated to the project are intended to be utilized by June 30, 2015.

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 groundbased 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 Multiscale 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**

WRF and CMAQ model simulations were performed with nested domains with horizontal resolutions of 36, 12, and 4 km. Read/Interpolate/Plot (RIP) meteorological back trajectories were performed from the 4 km WRF model output to suggest transport from Dallas impacted surface ozone concentrations in the Houston metropolitan area on September 25 and 26 (Figure 1). WRF simulated weaker sea and bay breezes than observed on September 25 (Figure 2). This caused the model to simulate maximum surface ozone concentrations over the water and

Galveston, whereas observations show peak ozone along the western shore of Galveston Bay (Figure 3). Observed southeasterlies along the western shore of the Galveston Bay likely caused high air pollution levels over the Galveston Bay to be transported onshore resulting in peak maximum 8 hour average ozone concentrations to be located along the western shore of the Galveston Bay. WRF simulated northerlies near the western coastline of Galveston Bay, causing CMAQ to transport the pollutants over Galveston Bay southward toward Galveston, which was near the model simulated sea breeze convergence zone.

We are currently re-running WRF with different model inputs and options to try to improve the model representation of the sea and bay breezes. We are now using 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 are also nudging all domains, whereas previously we only nudged the 36 km domain. In addition we are now using a WRF iterative technique, where we first run WRF performing analysis nudging based on the NAM 12 km, and then re-run WRF performing analysis nudging based on the previous WRF simulation. This modeling technique prevents the relatively coarse NAM 12 km model from degrading the high resolution WRF modeling domains (4 km and 1 km modeling domains).

Once the WRF model simulation is refined to more accurately represent the sea and bay breeze circulations observed during this air pollution episode, RIP and CMAQ will be re-run to determine the contributions of various source regions on surface ozone concentrations in the Houston metropolitan area. In addition, satellite observations will be analyzed to determine if space-based observations observed regional transport into Houston during this air pollution episode.



Figure 1. Back trajectories from 4 km WRF model output initialized at La Porte Sylvan Beach at 20 UTC at 0.5 km (red), 1 km (green), and 2 km (blue) AGL. The letter 'D' shows the location of Dallas, TX.



Figure 2. Observed (left) and WRF diagnosed (right) 2 m temperature and 10 m wind velocity at 21 UTC 25 September 2013.



Figure 3. Observed (left) and CMAQ simulated (right) maximum 8 hour average ozone on 25 September 2013.

## 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**

Over this quarter, the project team held internal project progress meetings to discuss project roles, assignments, and deadlines; continued gathering meteorological and air quality data from the DISCOVER-AQ program necessary to complete the analysis; calculated and delivered mixing heights from radar wind profilers and ozonesondes operated in the Houston area during DISCOVER-AQ, and assessed meteorological and air quality conditions on DISCOVER-AQ flight days and other days with high ozone levels in the Houston area.

Additional surface and upper-level meteorological data were gathered for this project during September-November 2014. Work and analysis performed during this quarter included characterizing and summarizing weather and air quality conditions in the Houston-area during the DISCOVER-AQ program (Task 1 of this project), and calculating and delivering mixing heights from six of the seven radar wind profilers (Task 3). Raw data files from these six radar wind profilers were also provided.

Over the next quarter, work will focus on concluding the calculation of mixing heights from the seventh radar wind profiler (Task 3), completing the characterization of weather and air quality conditions in the Houston-area during the DISCOVER-AQ program (Task 1), and comparing the results found in Task 1 to weather and air quality conditions observed during the 2006 TexAQS program (Task 2).

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<sub>2</sub>, NO<sub>2</sub>, HCHO and VOCs were carried out in a box around the Houston Ship channel, in parallel with flights by two aircraft from NASA. In this project the collected optical remote sensing data will be reanalyzed, improved and compared to other data. In particular, the investigators will work with radiative transfer modeling to minimize cloud effects.

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

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

#### **Project Update**

During the period September 1 to November 30 the activities below have been carried out with the aim to improve the data set measured in Houston during Discover AQ. The work has been carried out in collaboration between Chalmers University of Technology and University of Houston.

Optical measurements (DOAS) carried out at multiple angles during Discover-AQ have been evaluated and the results have been examined. The spectral retrieval of the measurements seems good, but interpreting the evaluated slant columns will require input from radiative transfer modeling.

Input data sets for running a radiative transfer model have been produced, corresponding to atmospheric profiles of absorbing species and aerosol optical parameters from various measurements. Also other relevant parameters needed for the model have been investigated.

A cloud filter based on color index has been developed and tested on test measurements made during September. The filter has shown good results and it is possible to qualitatively distinguish between clear sky and clouds. An investigation of the spectral structures in clouds has led to the conclusion that clouds do not appear to cause significant residual spectral structures in the evaluations. Instead the changes in evaluated columns associated with clouds appear to be the result of changed paths of the measured light due to scattering in the clouds. This precludes the possibility of improving measurements in cloudy and partly cloudy conditions by modifications to the spectral retrieval. Instead the cloud filter will be used to filter out the cloud-affected measurements during partly cloudy conditions.

In the process of investigating cloud effects, a spectral artifact caused by changing temperature has been discovered and characterized. A software routine has been developed to correct for these artifacts which greatly improves the quality of the measurements.

Archived data from the Discover-AQ aircraft have been downloaded and initial work has been done to read this data and visualize it to be able to compare it to Mobile DOAS measurements. We have also tried to obtain comparative continuous emission monitoring data for the measurements period, September 2013, through TCEQ but unfortunately this data is not available for this period.

# 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

A primary focus of work during the quarter was the retrieval and processing of North American Land Data Assimilation System-Phase II (NLDAS-2) datasets. NLDAS-2 is an offline modeling system running various land models (e.g., Mosaic, Noah, Variable Infiltration Capacity (VIC), Noah with multi-parameterization); models such as Noah and Mosaic are of particular interest because they have been developed within the surface-vegetation-atmosphere transfer scheme community. Hourly NLDAS-2 predictions of soil moisture for years 2006-2013 were obtained and interpolated to the 12-km MEGAN grid domain that covers Texas and surrounding areas. Analysis of the 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 as well as tracking the rate of change in spatial gradients of soil moisture during representative drought periods.

## Task 2. Comparison of Simulated and Observed Soil Moisture

Daily observations of soil moisture measurements were gathered at Soil Climate Analysis Network (SCAN) and Climate Research Network (CRN) observational locations to support a comparison of region-wide observed and NLDAS-2 soil moisture values. An initial comparison of observed and Mosaic/Noah predictions of soil moisture at monitoring locations in eastern Texas show that NLDAS-2 often captures the abrupt increases in soil moisture associated with precipitation events; however, the relative changes with respect to depth are often different. The NLDAS-2 predictions generally replicated the seasonal (i.e., long-term) changes in observed soil moisture; however, a baseline offset is evident. Unlike observations, Noah had little variability with respect to soil depth. Both Mosaic and especially Noah tended to be too wet in the nearsurface layer and too dry at deeper depths compared to observations.

## Task 3. Preparation of MEGAN Simulations

An additional focus of work this quarter has been towards modifying the existing MEGAN modeling configuration so that in-situ (observed) and NLDAS-2 soil moisture datasets can be used as inputs to MEGAN in order to predict region-wide isoprene emissions. Preparation and processing of various environmental datasets (e.g., shortwave radiation, temperature, leaf area index) has been performed for portions of years 2006, 2007, and 2011.

## Task 4. Sensitivity of Biogenic Emission Estimates to Soil Moisture

A modified MEGAN configuration was developed so that simulations could be conducted at three Texas soil moisture monitoring locations: Palestine, Prairie View, and Port Aransas. Similar to the comparison results for soil moisture values, isoprene predictions that used observations had better agreement with Mosaic compared to Noah. Predicted emissions had substantial sensitivity to the input soil moisture dataset; for example, Noah predictions were the same as baseline while Mosaic emissions at Port Aransas were lower by >60%. These results will be presented in a poster presentation at the 2014 American Geophysical Union (AGU) annual meeting in San Francisco during December 15-19, 2014.

All funds allocated to the project are intended to be utilized by June 30, 2015.

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<sub>3</sub> 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**

Considerable effort was placed on determination of organic aerosol (OA) emission factors (EFs) from the Houston vehicle fleet. Through use of the the MOtor Vehicle Emission Simulator emissions model from the United States Environmental Protection Agency and a ratio technique using observed data, EFs for OA ranged from 0.14 to 13.74 g of OA per mile driven. To further characterize differences that cause this large range, a targeted motor vehicle emissions study will be performed using the MAQL in early 2015.

Efforts also focused on large PM concentration events that are short in temporal duration (order minutes). Analysis of the submicron PM peak events observed and identification of the probable sources responsible for these events (based on time, location, and video footage) were finalized. Twenty-six statistically defined peak events were observed during the MAQL mobile-mode operations, associated with traffic activity, industrial sources (specifically chemical and petrochemical facilities), and biomass burning activities (cooking and lawn refuse burning). The

increases in OA (up to ~100  $\mu$ g per cubic meter) or sulfate (up to ~30  $\mu$ g per cubic meter) concentration compared with local background levels were calculated. Preliminary characterization of the PM during these peak events using metrics such as the ratios of oxygen to carbon (O/C), hydrogen to carbon (H/C), and organic mass to organic carbon (OM/OC) of the OA also was performed as a reality check for when contributions from primary or secondary OA (SOA) were expected.

Data from the MAQL were shared with collaborators from The University of Texas (UT) at Austin (Hildebrandt-Ruiz) and Baylor University (Sheesley). Comparison of shared data was performed. The focus of the comparison was the HR-ToF-AMS being operated by the Rice group using the MAQL and the aerosol chemical speciation monitor (ACSM) data from UT at times when the mobile laboratory was co-located with the UT measurements in Conroe. Three PM species were considered: bulk OA, nitrate aerosol, and sulfate aerosol. For all three species, regression of the HR-ToF-AMS (y-variable) and the ACSM (x-variable) data shows a high degree of linearity. Slopes of 1.17 for OA and 0.89 for nitrate aerosol are well within the uncertainties associated with each instrument. However, the slope of 1.61 for sulfate is higher than that deemed acceptable so current efforts focus on rectifying this difference in the sulfate aerosol measurements.

The temporal variation of the submicron PM concentration was studied using the data obtained during stationary operations of the MAQL. The diurnal character of different PM constituents at Conroe, Spring Creek Park, and Manvel Croix has been evaluated. All diurnal profiles are strongly location dependent and show considerable variability, likely due to the non-consecutive nature of the datasets that are being used to generate the diurnal profiles from the HR-ToF-AMS.

The spatial variation in PM loading and composition also was investigated, primarily using data from stationary mode operations, but including mobile operations within pre-defined geographic areas. A wide range of average submicron PM concentration was observed, from  $\sim 3 \mu g$  per cubic meter in upwind locations to  $\sim 12 \mu g$  per cubic meter in downwind locations likely to be subject to photochemical processing and formation of secondary PM. In all locations, except for Galveston, OA constituted, on average, more than half of the observed PM. In Galveston, sulfate was the largest contributor to the PM. However, it should be stressed that this observation is based on one location for a relatively short period of time. The OA metrics (O/C, H/C, and OM/OC) confirm the relative importance of primary OA and SOA in upwind and downwind locations, respectively.

Determination of the role that biogenic volatile organic compounds (VOCs) play in ozone and SOA formation is of great interest. Based on comparison to previous literature, it appears that nitrate radical-initiated oxidation of biogenic VOCs is a critical process leading to nocturnal formation of SOA in downwind areas of the city. However, because of the lack of speciated VOC measurements, considerable effort has been placed on acquisition of modeled VOC profiles for comparison to MAQL data.

Pandora nitrogen dioxide column retrievals and in situ surface data were compared. Directly comparing surface concentrations (x-axis) to Pandora column measurements (y-axis) indicates a time-dependent relationship, with a larger slope during the middle of the day during peak periods of photochemistry. However, if the in situ nitrogen dioxide mixing ratio is integrated over the

height of the boundary layer, the time dependence disappears, and the strength of this linear relationship improves ( $R^2 = 0.53$ ), though the resulting slope of 0.41 indicates that assuming the nitrogen dioxide mixing ratio is constant up to the boundary layer height is inappropriate. Nitrogen dioxide data from the Pandora spectrometer instrument also were compared to data derived from the OMI satellite. Cloudy conditions during this time period (September 2013) led to fewer data points for comparison than expected. OMI data were filtered by the row anomaly and cloud fractions greater than 20%. Pandora data were only considered valid for clear sky direct-sun measurements, if normalized root mean squared values of the spectral fit were less than 0.01, and if nitrogen dioxide column measurement errors were less than 0.05 DU. Based on the valid data, the relationship between Pandora and OMI changes spatially in Houston. In some locations, the data cluster around a one-to-one line; in others, one technique consistently outputs larger column concentrations than the other, with southern locations exhibiting higher OMI values and northern locations exhibiting higher Pandora values. These data are being investigated in the context of relative levels of air pollution.

A zero-dimensional model has been prepared for evaluation of ozone production rates and different radical production rates via various chemical pathways. The model to be used was received from NASA Langley. The model has been installed and is in good working order. All input data for the model are available from the MAQL, except the full suite of VOCs. Efforts continue to use regression analyses from VOCs measured on the Moody Tower to estimate VOCs for the MAQL (e.g., a relationship between a VOC and nitrogen oxide at Moody Tower is assumed to also hold for the MAQL). Once these relationships have been determined, it will be possible to generate all necessary input files for this effort.

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

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

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

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

#### **Executive Summary**

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

## **Project Update**

Progress on Project 14-011 is summarized below by Task:

#### Task 1. Regional Land Cover Characterization

The Moderate Resolution Imaging Spectroradiometer (MODIS) Land Cover Type (LCT) product is used to characterize vegetation type in the default FINN v.1 configuration. For this study, alternative land cover representations have been developed using other global and U.S. national and regional land cover products including 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 (Figure 1) developed by Popescu et al. (2011). Land cover classes for each product have been mapped to fifteen FINN land cover categories (i.e., unvegetated, grassland, shrub, tropical forest, temperate forest, boreal forest, temperate evergreen forest, rice, cropgeneric, wheat, cotton, soy bean, corn, sorghum, and sugar cane) that are associated with emission factors and fuel loadings. FINN simulations with different land cover representations, shown in Table 1, are being conducted to explore the sensitivity in estimates of CO, NOx, and  $PM_{2.5}$  emissions.

Simulation ID	Objective	Texas and CONUS within 12-km Domain	Portion of Mexico within 12-km Domain	Remainder of CONUS	Remainder of Mexico and Canada
LCT	FINN global default	MODIS LCT	MODIS LCT	MODIS LCT	MODIS LCT
GLC	Alternative global product	GLC- SHARE	GLC- SHARE	GLC- SHARE	GLC- SHARE
FCCS	Fuel loadings for CONUS; generic crop class	FCCS	MODIS LCT	FCCS	MODIS LCT
FCCS_CDL	Fuel loadings for CONUS; crop- specific classes	FCCS/CDL	MODIS LCT	FCCS/CDL	MODIS LCT
TCEQ	High resolution Texas regional	TCEQ	TCEQ	FCCS	MODIS LCT
TCEQ_CDL	All CONUS updates	TCEQ/CDL	TCEQ	FCCS/CDL	MODIS LCT

Table 1. FINN simulations conducted with the default land cover product (MODIS LCT) and alternative land cover representations. The 12-km domain is shown in Figure 1.



Figure 1. Nested domains for Texas air quality modeling (Source: <u>https://www.tceq.texas.gov/assets/public/implementation/air/am/maps/GoogleMap/domain/rider8\_modeling\_domains.pdf</u>). Land cover data for the 12-km domain was developed by Popescu et al. (2011) for the Texas Commission on Environmental Quality.

## Task 2. Mapping of Croplands

Crop-specific emission factors from McCarty et al. (2011) for sugarcane, wheat, cotton, soy, corn, and sorghum have been added to the FINN default configuration. Sensitivity studies (Table 1) have been developed that explore the influence of the NASS CDL for crop characterization on emissions estimates.

### Task 3. Estimation of Burned Area

A preliminary comparison of the Monitoring Trends in Burn Severity (MTBS), Visible Infrared Imaging Radiometer Suite (VIIRS) Active Fire, and MODIS Rapid Response (MRR) product detections of large fires in Texas during 2012 was conducted. Interestingly, the VIIRS AF product missed a number of fires that were detected by the MRR. Because MTBS has a size constraint on fires that are reported (>1000 acres), at this time the team is moving forward with the MODIS RR product for 2012 but will continue to review the evolution of the VIIRS algorithms and products. 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.

Task 4. Sub-grid scale Partitioning of  $NO_x$  Emissions to  $NO_z$  in Fire Plumes This task has not yet been initiated. Task 5. CAMx Sensitivity Studies This task has not yet been initiated.

Dr. Wiedinmyer had an invited presentation that included some of the fire emissions work in Texas at American Association for Aerosol Research 33<sup>rd</sup> Annual Conference in Orlando during October 20-24, 2014. A copy of her presentation is available upon request.

The team is currently preparing a poster on early findings from the study for presentation at the American Geophysical Union Fall Meeting in San Francisco, California during December 15-19, 2014.

All funds allocated to the project are intended to be utilized by June 30, 2015.

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

Aircraft measurement data, as well as PTR-MS VOC measurement data from the 2013 Southeast Atmosphere Study (SAS) field campaign (NCAR C-130 and NOAA P-3 aircraft), and the 2006 Texas Air Quality Study (NOAA P-3 aircraft), were collected. PNNL also developed, improved,

and evaluated scripts that calculate biogenic VOC flux at given aircraft flight tracks using wavelet based techniques, based upon code and data provided by Dr. Thomas Karl (Karl et al, 2013) and Lisa Kaser (NCAR). Comparisons against flux results from traditional FFT (Fast Fourier transform) techniques show reasonable agreement. Preliminary flux results are available and PNNL is performing QA/QC tasks on the results.

Figure 1 shows an example racetrack in research flight # 1, and Figure 2 shows estimated isoprene flux for the example racetrack. The ratio of mean wavelet/FFT flux is 0.99 for the example racetrack. While FFT based flux analysis provide only one flux value for the entire racetrack, wavelet based analysis provides flux data in much higher resolution.



**Figure 1.** 3D plot of an example racetrack from research flight (RF) #1 of SAS campaign. The entire flight track of RF1 is shown in black line. The example racetrack is shown in red line.



**Figure 2.** Estimated isoprene flux for the example racetrack shown in Figure 1. Mean wavelet/FFT flux is 0.99

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

PNNL compiled a database of LAIv values at 1 km spatial resolution and 8 day temporal resolution, covering all of North America, for April to September of 2013. For this task, LAI data retrieved from the MODIS (MOderate Resolution Imaging Spectroradiometer) satellite (product MCD15A2.005) were used, and fractional vegetation land cover (fc) data from MEGAN v2.1 database were applied. To efficiently handle MODIS LAI data, a Python script was written. This script will download MODIS data from a remote server, extract LAI data from the retrieved files, and merge the extracted data into a single file. Another Python script was written to calculate LAIv data based on input LAI and fc data, with an upper limit of 10 set for LAIv to eliminate high values due to uncertainties in low fc values in some grid cells.

Several alternative fractional vegetation land cover datasets were also tested for this project and compared with the existing MEGAN v2.1 fc database, including vegetation cover data from the SPOT-VEGETATION satellite. It was determined that that SPOT data could be a useful data source for future efforts but there some data quality issues and it was decided that further examination was beyond the scope of this task and the existing MEGAN v2.1 fc database for 2008 was used to quantify vegetation cover fraction for this project. The LAIv data developed for this project were compared against previously calculated MEGANv2.1 LAIv data, for previous years, for QA/QC purposes.

Figure 3 shows LAIv data for four selected time periods for 2013 (April 7th, June 10th, August 5th and September 30th). Progressively increasing values of LAIv were observed for the majority of North America from April to August, and decreasing LAIv was observed beyond August. The spatial pattern and temporal variations of LAIv follow expected patterns and are also consistent with previously calculated MEGAN v2.1 LAIv data.

It should be recognized that the fractional vegetation land cover data used here are based on satellite data for the year 2008, even though we are estimating LAIv for 2013. However we do not expect substantial changes in vegetation cover fraction from 2008 to 2013.



Figure 3. The calculated LAIv data for selected time periods from April to September 2013.

## Task 3: Emission Factor Database Development

Several additional data sources that can be used to develop high resolution PFT database for Texas were identified. PNNL is evaluating these data for their applicability in this project.

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

ENVIRON completed evaluation of Weather Research and Forecast (WRF) Model (Skamarock et al. 2008) 12 km grid output fields for the period June 1-July 15, 2013 against CAMS station data within Texas and ds472 airport station wind, temperature and humidity data within and outside of Texas and the PRISM precipitation product. The precipitation evaluation showed the presence of an artifact around the 4 km grid focused on Houston. The 4 km grid was present in this WRF run so it could also be used by AQRP Project 14-024. The precipitation artifact was caused by the use of the 2-way nesting option on the 4 km grid. WRF was run a second time without the nested 4 km grid, and the model performance evaluation was completed. No precipitation artifact was present in the second run. An example of the resulting precipitation field for a 24-hour period is shown in Figure 4. In general, the WRF model was able to reproduce the large-scale patterns of precipitation across the 12 km domain seen in the PRISM analysis, but often overestimated the intensity of the precipitation. Overestimates of precipitation are often noted in WRF runs, especially over the southeastern U.S. (e.g., Alapaty et al., 2014).

WRF surface performance was assessed using the METSTAT program to generate statistics and graphical model-observation comparisons for winds, temperature and humidity. Bias and error statistics for wind speed, direction, temperature, and humidity were tabulated, with averages

taken across geographical regions (Figure 5). Each statistical metric was compared to performance benchmarks to evaluate how well the model performed. An example of a soccer plot display containing performance benchmarks and daily and monthly model performance statistics for wind speed is shown in Figure 6.



**Figure 4.** July 10-11, 2013 accumulated precipitation from PRISM analysis (left panel) and WRF model (right panel).



Figure 5. Subdomains for surface meteorological field model performance evaluation.



**Figure 6.** WRF model run soccer plot showing wind speed performance for East Texas inland region (G1) shown in Figure 5. Small icons represent performance for individual days, and large icons show monthly average performance.

ENVIRON continued development of software to perform CAMx model performance evaluation along aircraft flight tracks and began configuring the CAMx model for the baseline run using the default MEGAN emission inventory.

### Task 5: Project Management

ENVIRON, NOAA and PNNL/Battelle finalized subcontracting agreements for NOAA and PNNL/Battelle for work to be done under Tasks 1-3.

Delays or Technical Issues during the Reporting Period

The development of subcontracting agreements progressed more slowly than expected, but was completed during this quarter. We expect that the schedule for Tasks 1-3 will be extended by 3-4 months. However, sufficient progress on all Tasks has been made that the project remains on schedule for completion with delivery of the final AQRP-reviewed report by June 30, 2015.

We intend to use all funds allocated to the project by 06/30/2015.

#### References

Alapaty, K., J.S. Kain, J. A. Herwehe, O. R. Bullock Jr., and M. S. Mallard. 2014. Multiscale Kain-Fritsch Scheme: Formulations and Tests. CMAS presentation. https://www.cmascenter.org/conference/2014/slides/jerry\_herwehe\_evaluation\_developments\_2 014.pdf.
Guenther, A. B., X. Jiang, C. L. Heald, T. Sakulyanontvittaya, T. Duhl, L. K. Emmons, and X. Wang (2012), The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions, Geosci. Model Dev., 5(6), 1471-1492.

Karl, T., P. K. Misztal, H. H. Jonsson, S. Shertz, A. H. Goldstein, and A. B. Guenther. 2013. Airborne flux measurements of BVOCs above Californian oak forests: Experimental investigation of surface and entrainment fluxes, OH densities and Dahmköhler numbers. J. Atmos. Sci., 70, 3277–3287.

Sakulyanontvittaya, T., G. Yarwood and A. Guenther. 2012. Improved Biogenic Emission Inventories Across the West. Final Report. Prepared for: Western Governors' Association, 1600 Broadway, Suite 1700, Denver, CO 80202. http://www.wrapair2.org/pdf/WGA\_BiogEmisInv\_FinalReport\_March20\_2012.pdf.

Skamarock, W. C., J. B. Klemp, J. Dudhia, D. O. Gill, D. M. Barker, W. Wang, and J. G. Powers, 2008. A description of the Advanced Research WRF Version 3. NCAR Tech Notes-475+STR. <u>http://www.mmm.ucar.edu/wrf/users/docs/arw\_v3.pdf</u>.

**Project 14-017** 

#### 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**

#### SATELLITE-BASED PAR - Initial Algorithm

Currently, UAH collaborates with the IR group at the NASA/MSFC to generate and archive several GOES derived products. The retrieval system, GOES Product Generation System (GPGS), provides routine near real-time retrievals of skin temperature, total precipitable water, cloud top temperature/pressure, cloud albedo, surface albedo and surface insolation for the use in meteorological and air quality models (Haines et al., 2003). Over the years these products have been evaluated and used in many air quality studies (Pour-Biazar et al., 2007; Mackaro et al., 2011; McNider et al., 1998; Haines et al., 2003).

The algorithm used for the retrieval of albedo and surface insolation is the implementation of Gautier et al. (1980) method complemented by the improvements from Diak and Gautier (1983). The method uses the information from GOES Imager visible channel (.52-.72  $\mu$ m) at 1km resolution, and employs a clear and a cloudy atmosphere to explain the observed upwelling radiant energy. The model applies the effects of Rayleigh scattering, ozone absorption, water vapor absorption, cloud absorption, and cloud reflection. The effects of Rayleigh scattering are modeled after Coulson (1959) and Allen (1963) for the GOES visible band (radiant flux as viewed by the satellite) and for the bulk solar flux incident at the surface. Ozone absorption is modeled after Lacis and Hansen (1974). Water vapor absorption is assumed to be negligible in both the surface and cloud albedo calculations (explaining the observed radiance in the GOES visible band), but accounted for when applying the total solar flux in the surface insolation calculation. Water vapor absorption coefficients are obtained from Paltridge (1973), and total column water vapor is assumed to be 25 mm and adjusted for solar zenith angle. Cloud absorption is assumed to be a constant 7% of the incident flux at the top of the cloud (Diak and Gautier, 1983). The products are aggregated to 4-km and archived at UAH.

In this project, we are using GOES visible channel observations to generate PAR. PAR is defined as:

$$PAR = \int_{A}^{7} I(\lambda) d\lambda \quad (W m^{-2}) = \frac{1}{hc} \int_{A}^{7} I(\lambda) d\lambda \quad (quanta m^{-2} s^{-1})$$
(1)

Therefore, in principle, insolation can be scaled to produce PAR. This means that we can define a conversion factor (*CF*) to convert insolation to PAR:

$$CF = \frac{PAR}{Insolation} \tag{2}$$

Frouin and Pinker, 1995 and Pinker and Laszelo, 1992, documented the dependency of such conversion factor on several relevant atmospheric parameters such as water vapor, total overhead ozone, optical depth (representing aerosol/cloud impact), and zenith angle. The largest variations are caused by water vapor, optical depth, and solar zenith angle (Figure 1).



**Figure 1.** Variation of PAR conversion factor with respect to solar zenith angle, optical depth, and water vapor (adapted from Frouin and Pinker, 1994).

This variation is mostly due to the difference in the impact of direct and diffused light. Meaning that in the presence of water vapor and aerosols, a modest increase in diffused light increases the conversion factor. However, one must note that the largest increase in CF is when the insolation is drastically reduced (for optical depths greater than 10-15). This means that in the presence of opaque clouds, the sizeable reduction in surface incident radiation will offset such marginal increases in CF. The practical variation of conversion factor hovers around .5. In fact many of the models used in agricultural applications use the .5 factor. A review of the MEGAN code also revealed that MEGAN uses CF=.5 when model estimates of solar radiation is used. Guenther et al., 2012, argue that the largest uncertainty comes from the model solar radiation estimates and that using satellite-based PAR would be preferable.

Our approach is to construct a conversion factor that encapsulates the impact of environmental variables on PAR. Our initial algorithm was based on a simple parameterization for calculating a variable conversion factor for generating PAR from the current insolation product at UAH. We devised the following relationship that takes into account the impact of optical depth and zenith angle on conversion factor:

$$CF = \frac{PAR}{Insolation} = .48 + .17 * Cfactor * Zfactor$$

$$Where \quad Cfactor = \sqrt{1 - (\alpha_c - 1)^2}$$
and 
$$\alpha_c = cloud \ albedo$$
(3)

This relationship assumes a conversion factor of .48 for a completely cloud free atmosphere. At the time we did not consider zenith angle dependency (Zfactor=1). Note that in Figure 1, CF=.48 can be obtained for overhead sun when aerosol optical depth is .23. The conversion factor gradually increases for increased clouds.

After initial testing and evaluation of the product, we incrementally improved the functional form of the conversion factor and implemented the zenith angle dependency.

#### Final Conversion Factor

After several iterations we finally converged on the following functional form of conversion factor that encapsulates the properties demonstrated in Figure 1. The relationship, offered above, used cloud albedo as a surrogate for optical depth without offering a justification. In this alternate approach we arrive at a best fit for CF as a function of optical depth based on the data offered in Pinker and Laszlo (1992) and Frouin and Pinker (1995) as described above. Then, we estimate optical depth from cloud albedo by the relationship yielded by a simple model similar to Stephens 1978 and Joseph 1976 (implemented in RADM, CAMx and CMAQ). The optical depth can be estimated as:

$$\tau = \frac{8\alpha_c}{(1 - \alpha_c)^2}$$
where  $\alpha_c = cloud \ albedo$ 
and  $\tau = Optical \ Depth(OD)$ 
(4)

C-albedo is cloud albedo plotted against OD as in Fischer et al. and Eduardo. OD-1 is OD estimated as a function of cloud albedo similar to Chang et al. (1987) used in RADM, CAMx and CMAQ. OD-2 and OD-3 are two best fit curves for C-albedo. OD-3 will be used in our estimation of PAR.

Then, using the estimated optical depth, we devised the following fit to Frouin and Pinker, 1994 and Pinker and Laszelo, 1991 (as described in method 1):

$$CF = \frac{PAR}{Insolation} = .42 + .28 * Cfactor * Zfactor$$

$$Where \quad Cfactor = (1 - 1.8^{-\sqrt{.1\tau}})$$

$$and \quad Zfactor = (1.1 - .1\sqrt{\cos(Z)})^{-\tau}$$
(5)



Figure 2 shows the old and new conversion factors against the data presented in Figure 1.

**Figure 2.** New and old conversion factors plotted against the data presented in Figure 1 as a function of optical depth for overhead sun (zenith angle set to zero).

Figure 3 demonstrates how the new functional form of conversion factor performs as a function of optical depth for two different zenith angles as presented in Figure 1. The new functional form of conversion factor seems to be fitting the data well and is taken as our final form of conversion factor to be used to produce PAR.



**Figure 3.** Conversion factor as a function of optical depth for two different zenith angles as presented in Figure 1.

#### Bias Correction for Insolation Product

Since our PAR product is based on the satellite insolation retrievals, any error in insolation retrieval carries over to the PAR product. During our initial evaluation of PAR product we noticed a systematic bias for clear-sky satellite-based PAR against surface pyranometer observations. Further investigation of this problem revealed that the issue is related to a source of uncertainty in the insolation retrieval. The insolation retrieval is currently using a constant correction factor when accounting for the impact of percipitable water on insolation. Due to the large spatial variation of precipitable water over the continental United States from east to west, using a constant correction factor is under-estimating insolation in the west and overestimating insolation in the eastern U.S.

Figure 4 shows the progression of over-estimations from west to east. The figure demonstrates paired pyranometer observations versus GOES insolation retrievals for several locations representing western, central and eastern United States. The red dots and the corresponding best linear fit for the data indicated by the red line, show the scatter plot for a Soil Climate Analysis Network (SCAN) site in Virginia. The blue dots and the corresponding blue line are for the

SCAN sites in Iowa, Tennessee, and Kansas. The green dots and the corresponding green line exhibit the scatter plot for Nebraska, Wisconsin, and Colorado. As demonstrated in the figure, the bias reduces as we move from east to west.



**Figure 4.** Scatter plots and the corresponding best linear fit showing GOES insolation retrievals versus pyranometer observations from Soil Analysis Climate Network (SCAN) for the month of September 2013.

We are working with George Diak from the University of Wisconsin-Madison to implement a dynamic moisture adjustment in the retrieval code to alleviate this issue. However, as a workaround for the immediate needs of this project we apply a bias correction to the insolation data before retrieving satellite-based PAR.

Figure 5 shows all the data as compared to SCAN pyranometer data before and after applying bias correction. While there is still some scatter in the data, the overall pattern shows a good correlation between pyranometer and GOES retrieval data with a negligible bias after bias correction.



**Figure 5.** Scatter plots showing GOES insolation retrievals against Soil Analysis Climate Network (SCAN) data for September 2013. The top figure shows the data before applying bias correction to GOES retrievals, and the bottom figure shows the scatter plot after applying bias correction.

#### Satellite-Based PAR for September 2013

Using the final version of conversion factor we re-processed GOES data for September 2013 to produce a revised version of satellite-based PAR. Figure 6 shows a snap shot of GOES observed insolation and PAR at 19:45 GMT. PAR is produced in units of W/m<sup>2</sup> and micro-mol/m<sup>2</sup>/s.



**Figure o.** A snap snot of saterine-derived insolation and FAK at 19.43  $(W/m^{-2})$ , september 1, 2013. PAR is produced in units of W/m<sup>2</sup> as well as micro-mol/m<sup>2</sup>/s.

A detailed description of the evaluation work is documented in the next sections.

#### Evaluation of PAR Products

As a trial run, the whole month of September 2013 coinciding with the DISCOVER-AQ Houston period was chosen to evaluate the product of PAR satellite retrievals by comparing with the available ground observations. Two networks were chosen for evaluation. One is the 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. The other is 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. For this trial run, 40 sites from the SCAN network and 7 sites from the SURFRAD network were chosen for evaluation. The locations of these sites are shown in Figure 7.



Figure 7. Location of SCAN and SURFRAD sites used for PAR/insolation evaluation

The time series of PAR/insolation product at each evaluation site were pin-pointed at the nearest satellite pixel/grid (with horizontal resolution 4 km) containing the pyranometer and were interpolated to the value to the end of each hour since the GOES data were instantaneous observations at 45 minutes after the hour reported on GMT time. As a reference, a 12 km CONUS WRF simulation during September 2013 was also conducted to show the typical weather model radiation performance without data assimilation from GOES satellite. Details of the WRF model configurations can be found in Table 4.

Figure 8 provides time series plot comparisons between observed PAR (blue scatter) and PAR results from WRF model simulation (black line) or satellite retrievals (blue line) at different SURFRAD sites. The comparisons show that the PAR satellite retrieval product tends to systematically decrease the positive bias of the WRF model for the peak values during the daytime. This can be seen most clearly for periods such as Sep 17 at BON site, Sep 8 at DRA site, Sep 11-13 at PSU site, Sep 15-18 at SXF site, and Sep 13 at TBL site. The overestimation of PAR by the WRF model might be due to the incapability of its current cumulus physics module to resolve enough subgrid clouds, and because meteorological models often underpredict the amount of thin clouds.

Table 1 gives more detailed evaluation of PAR product at each SURFRAD site by listing the values of widely used statistic metrics, including observation mean (OBS\_AVE), simulation mean (SIM\_AVE), index of agreement (IA), correlation coefficient (R), root mean square error (RMSE), mean bias (MB), mean aggregate gross error (MAGE), normalized mean bias (NMB), and normalized mean error (NME). The satellite-based PAR products show high correlation and good agreement with ground observations with the typically R value of 0.97-0.98 at each site. On average, the satellite retrieval tends to overestimate the PAR value by 18% (MB: 6.6%-28%) and deviate from the observation by 15.6 W/m2. This over-estimation could have been reduced by our bias correction in which insolation was reduced by an average of 12%.

Table 2 gives the summary of statistics of PAR results either from satellite retrieval or WRF simulation against SUFRAD observations. The satellite-based PAR product systematically outperforms WRF in simulating the observed PAR, improving the correlation from 0.94 to 0.98 and decreasing the bias from 28.8% to 18% (this could be even more with the revised product).

	OBS_AVE	SIM_AVE	IA	R	RMSE	MB	MAGE	NMB	NME
Site	(W/m2)	(W/m2)			(W/m2)	(W/m2)	(W/m2)	(%)	(%)
BON	81.8	111.2	0.97	0.97	45.5	23.1	26.2	28.0	31.9
DRA	110.8	119.0	0.99	0.99	30.1	7.4	18.2	6.6	16.3
FPK	73.7	87.8	0.98	0.98	31.1	13.5	19.4	18.2	26.2
GCM	93.5	115.0	0.97	0.98	44.7	21.5	27.2	22.9	28.9
PSU	84.0	95.3	0.98	0.98	32.4	14.6	20.2	17.3	24.0
SXF	76.2	90.9	0.98	0.98	30.3	13.1	18.4	17.2	24.0
TBL	83.3	93.2	0.98	0.97	38.2	13.1	21.6	15.7	26.0
Average	86.2	101.8	0.98	0.98	36.0	15.2	21.6	18.0	25.3

#### Table 1 Statistics of UAH PAR products compared with SURFRAD network sites

Table 2 Summary of statistics for PAR results evaluation at SURFRAD network

	OBS_AVE	SIM_AVE	IA	R	RMSE	MB	MAGE	NMB	NME
Site	(W/m2)	(W/m2)			(W/m2)	(W/m2)	(W/m2)	(%)	(%)
WRF	86.2	110.7	0.94	0.94	60.3	24.2	32.8	28.8	38.8
UAH	86.2	101.8	0.98	0.98	36.0	15.2	21.6	18.0	25.3



# Figure 8 Time series comparison between PAR measurements and satellite retrievals (UAH) or simulation results (WRF)

The satellite retrievals also outperform WRF in simulating observations of insolation at SCAN network sites. The quality of PAR satellite product is closely depended on the quality of GOES insolation retrievals, since PAR is generated from overall solar insolation by applying a conversion factor (CF). Table 3 gives the summary of statistics for those comparisons. It can be seen that on average the WRF results tend to overestimate the insolation during September 2013 by 36.5 W/m<sup>2</sup> at SCAN network sites and the satellite product decrease the bias to 23.6 W/m<sup>2</sup>.

The satellite retrievals outperform WRF for simulating observed insolation as measured by each of the statistic metrics considered, with correlation improving from 0.94 to 0.96, the RMSE from 113.8 W/m<sup>2</sup> to 86 W/m<sup>2</sup>, and NMB from 21.8% to 14.4%. In Figure 9, the scatter plots between SCAN observations and WRF simulation (black, left) or UAH retrievals (red, right) as well as their liner fit results are shown side by side for comparison. The UAH product produces a more compact scatter distribution pattern, with the fitted slope approaching the 1:1 ratio (1.06 versus 1.08) and a much smaller intercept value (6.4 versus 15.8). As mentioned earlier, the corrected insolation should perform even better as it reduces the bias.

Despite the improvements, there is still a substantial amount of scatter between satellite-based and ground-observed insolation, with a sizeable number of points differing by a factor of two or more. There are two possible reasons that need to be considered in the next step evaluation work. One is the navigation error. Currently, we use the nearest pin-pointed grid value to compare with the specific site observations by matching the lat/lon coordinate of the grid with the site location. Depending on the projection of the location, the actual pyranometer may fall into the nearby grids with one grid cell off. Therefore, instead of using the center grid pinpointed value, we may need to fetch all the nearby 9 satellite grid values and find the best match with observation. The other reason is that the insolation retrievals used in this comparison use a constant precipitable water value for the clear sky moisture correction. We will update our evaluation result in next quarterly report using the updated data.

 Table 3. Summary of statistics for insolation results evaluation at SCAN network

	OBS_AVE	SIM_AVE	IA	R	RMSE	MB	MAGE	NMB	NME
Site	(W/m2)	(W/m2)			(W/m2)	(W/m2)	(W/m2)	(%)	(%)
WRF	186.9	225.5	0.95	0.94	113.8	36.5	59.6	21.8	33.8
UAH	186.9	212.2	0.97	0.96	86.0	23.6	48.1	14.4	27.1



Figure 9. Scatter plot of WRF (left) and UAH (right) insolation results with SCAN network observations

Spatially (Figure 4), the satellite-derived insolation product achieved less bias in the western part of United States (with NMB -10%-10%) than in the central and southeastern part of the country (with typical NMB ~20%). There are two SCAN sites (site 2042 at Vermont and site 2039 at Virginia) that had much higher bias than the others (NMB ~50%) in the current evaluation. This is partly due to the insolation bias as described in section 2.3. Detailed investigation is needed to decide whether to keep those two sites for further comparison, after assuring that they will not be substantially affected by bias correction.



### Figure 10. Spatial distribution of normalized mean bias at each SCAN site during September 2013.

In the next quarterly report, we will include the detailed evaluation of the updated satellite-based PAR products with local Texas radiation data.

#### **BVOC and Soil NOx Emission Estimates in MEGAN**

The WRF-MEGAN modeling framework was implemented to quantify the sensitivity of BVOC emission estimates to different PAR inputs (WRF versus UAH satellite-based). The September 2013 period on the 12km CONUS domain was used for the initial testing. Details of the WRF model configurations are provided in Table 4.

By default, the MEGAN model scales the insolation data from WRF uniformly by half (CF=0.5) to represent the PAR value. MEGAN simulations with the UAH satellite retrievals can directly use its PAR estimates, which had already been computed by condition-specific conversion factors. Data from the UAH retrievals were aggregated from nine 4km pixels to represent one PAR value on the 12km grid used in the MEGAN simulations. We compare MEGAN BVOC emission outputs for isoprene (ISOP, upper panel) and monoterpenes (TERP, lower panel) with the two types of radiation input in Figure 11. 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.

In terms of magnitude, 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, the geographic distribution of TERP emission is wider than ISOP; in

other words, there is less spatial heterogeneity for TERP compared with ISOP. Isoprene emission is more sensitive to PAR inputs with the highest increase region at Northeast (> 30%) and decrease at the Northwest (> 20%). The relative change for monoterpene emission is modest (-10% to 5%).

If we focus on Texas region only, the eastern part of Texas is projected to increase biogenic emissions by using the satellite radiation data and the southern part of Texas is projected to decrease. However, it is important to note that these results are for an initial test with preliminary satellite retrievals, and that the impact of the retrievals on BVOC emissions will change as the data product is finalized and additional periods are tested.

WRF			
Version:	ARW V3.5	Shortwave radiation:	RRTMG scheme
Horizontal resolution:	12kmX 12 km(471X311)	Surface layer physic:	Pleim-Xiu Surface Model
Vertical resolution:	36 layer, first layer height ~ 37 m,	PBL scheme:	ACM2
	10 layer within 1km	Microphysics:	Morrison double-moment scheme
Boundary Condition:	NARR 32km	Cumulus Parameterization:	Kain-Fritsch scheme
Initial condition:	NECP-ADP	Analysis nudging:	NECP-ADP
Longwave radiation:	RRTMG scheme		Temp, wind, moisture above boundary layer
MEGAN			
Version:	V2.10	Emission factor:	CONUS 12km default
Horizontal resolution:	12kmX 12 km(396X246)	Leaf area index:	MODIS 8 day average
Plant function type:	16 types, MODIS 8 day average	Gas-phase mechanism:	CB6

#### Table 4 Configuration of WRF-MEGAN used in this study



Figure 11. Spatial distribution of estimated ISOP and TERP emission rate by MEGAN using different PAR inputs data (WRF versus UAH satellite retrievals)

Figure 12 provides the domain-wide sum of ISOP and TERP emission rates based on different climate regions using different PAR inputs. As expected the south and Southeast region is the biggest 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 12. Total ISOP (left) and TERP (right) emission rate estimates by MEGAN using different PAR inputs data (WRF versus UAH satellite retrievals) at different climate region in United States

The Rice group has implemented the Berkeley Dalhousie soil NOx parameterization scheme (BDSNP) as an alternate option to the old Yienger-Levy parameterization (YL95) in CMAQ to better represent the soil NOx process response to nitrogen deposition, fertilizer application and changing meteorology. Figure 13 demonstrates the daily mean difference of soil NO emission estimates by using the BDSNP scheme at one test case in July 2011 at 12 km CONUS domain. It can be seen that for most part of agricultural land in United States the soil NO emission is projected to increase more than 5 mg/s/grid with the highest increase appearing at Kansas and Northern Texas.

We are in the final stages of coding the BDSNP scheme into a stand-alone emission model that would not require inline calculation of emissions within a time-consuming air quality model simulation and would allow BDSNP soil NO emissions to be used in models other than CMAQ. Instead of using the N deposition inline from CMAQ, we will first assume that a certain fraction of soil NO emissions originate due to N deposition, determined based on previous N deposition fields generated by either CMAQ or CAMx.

Our next step for Task 3 will focus more on the Texas region to test the temporal and spatial heterogeneity dependence on different PAR inputs for MEGAN biogenic VOC estimates. We will also use the standalone BDSNP soil NOx emission model to develop new estimates of soil NO emissions over Texas.



Figure 13. Demonstration of spatial different of soil NO emission rate estimates using BDSNP or YL95 scheme

References

- Allen, C.W. (1963). Astrophysical Quantities, 291 pp., Athlene Press, London, England, 1963.
   Allen, David, Elena McDonald-Buller, and Gary McGaughey, 2012: AQRP State of the Science Report, 2012, <u>http://aqrp.ceer.utexas.edu/docs/FY12-13/State of the Science</u> 2012\_06042012.pdf
- Coulson, K.L. (1959). Characteristics of the radiation emerging from the top of a Rayleigh atmosphere, 1 and 2, *Planet Space Science*, Vol. 1, pp. 256-284, 1959.
- Diak, G. R. and C. Gautier (1983). Improvements to a simple physical model for estimating insolation from GOES data. *J. Appl. Meteor.*, **22**, 505–508.
- Frouin, R. and R. T. Pinker (1995): Estimating photosynthetically active radiation (PAR) at the earth's surface from satellite observations. *Remote Sen. Environ.*, 51, 98–107.
- Gautier, C., G.R. Diak, S. Mass, 1980: A simple physical model for estimating incident solar radiation at the surface from GOES satellite data. *J. Appl. Meteor.*, **19**, 1005-1012.
- Guenther, A.B., X. Jiang, C.L. Heald, T. Sakulyanontvittaya, T. Duhl, L.K. Emmons, and X. Wang (2012). The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): An extended and updated framework for modeling biogenic emissions. *Geoscientific Model Development*, 5, 1471-1492, DOI: <u>10.5194/gmd-5-1471-2012</u>.
- Haines, S. L., G. J. Jedlovec, and R. J. Suggs (2003). The GOES Product Generation System. NASA Technical Memorandum, Marshall Space Flight Center.

- Lacis, A.A., and J.E. Hansen (1974). A parameterization for absorption of solar radiation in the Earth's atmosphere, *J. Atmospheric Science*, Vol. 31, pp. 118-133, 1973.
- Mackaro, S., R. McNider, and A. Pour Biazar (2011), Some physical and computational issues in land surface data assimilation of satellite skin temperatures, *Pure and Appl. Geophys.*, 1-14, *Doi:* 10.1007/s00024-011-0377-0.
- McNider, R. T., W. B. Norris, D. M. Casey, J. E. Pleim, S. J. Roselle, and W. M. Lapenta (1998). Assimilation of satellite data in regional air quality models XII. Edited by Gryning, Chaumerliac, and Plenum Press, pp. 25-35. 1998.
- Paltridge, G.W. (1973). Direct measurement of water vapor absorption of solar radiation in the free atmosphere, *J. Atmospheric Science*, Vol. 30, pp. 15-160, 1973.
- Pinker, R. T. and I. Laszlo (1992). Global distribution of photosynthetically active radiation as observed from satellites. *J. Climate*, 5, 56–65.
- Pour-Biazar, A., K. Doty, Y-H Park, R.T. McNider (2011). Cloud assimilation into the Weather and Research and Forecast (WRF) model. Submitted to Thomas C. Ho, Lamar University, Prepared for Bright Dornblaser, Texas Commission on Environmental Quality (TCEQ), 2011.
- Pour-Biazar, Arastoo, Richard T. McNider, Shawn J. Roselle, Ron Suggs, Gary Jedlovec, Soontae Kim, Daewon W. Byun, Jerry C. Lin, Thomas C. Ho, Stephanie Haines, Bright Dornblaser, Robert Cameron. (2007), Correcting <u>photol<sup>y</sup>sis rates on the basis of satellite</u> <u>observed clouds</u>, J. *Geophys. Res*, 112, D10302, doi:<u>10.1029/2006JD007422</u>.

#### **Project 14-023**

#### STATUS: Active – May 23, 2014

#### Assessment of Two Remote Sensing Technologies to Control Flare Performance

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

#### **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.

#### 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  $\mu$ m in diameter (PM<sub>2.5</sub>) from 15 to 12  $\mu$ g m<sup>-3</sup>. This new annual standard brings the Houston region near to non-attainment for PM<sub>2.5</sub>, underlining the importance of understanding the composition and sources of PM<sub>2.5</sub> in Houston. Recent measurements made during the month of September indicate that a majority of PM<sub>2.5</sub> 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<sub>2.5</sub>. 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 designed, built and set-up a heated injector which will be used to inject IVOCs in laboratory chamber experiments (the heated injector was built at a machine shop at UT Austin). UT Austin also designed, ordered and has received the body of the thermodenuder (built by Swagelok®) and the temperature and valve controller of the thermodenuder (built by Aerodyne Research, Inc.). The team is now ready to set up the thermodenuder and use it in laboratory chamber experiment to measure the volatility of organic

aerosol formed. UT Austin also developed gas chromatography and mass spectrometry methods to analyze the IVOCs used in these experiments and adjusted the thermal desorption program to analyze the compounds with Tenax-TA tubes. Trial analyses of the compounds were successful and calibration curves were developed. UT Austin also continued analysis of DISCOVER-AQ data, including positive matrix factorization (PMF) of the organic aerosol data. The team has shared preliminary data with investigators of AQRP projects 14-009 and 14-029.

ENVIRON worked on developing meteorological input data to the Comprehensive Air-quality Model with Extensions (CAMx) for simulations of the DISCOVER-AQ period. Model configuration of Weather Research and Forecast (WRF) model simulations was determined based on model performance evaluation for wind speed/direction, temperature and humidity data within and outside of Texas. The latest version of CAMx (v6.10) was updated with the 1.5-D Volatility Basis Set (VBS) organic aerosol module.

We intend to use all funds allocated to the project by June 30, 2015.

**Project 14-025** 

STATUS: Active – May 21, 2014

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

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

#### Funding Amount: \$256,261

(\$135,735 Environ, \$120,526 TAMU)

#### **Executive Summary**

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

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

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

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

#### **Project Update**

WRF version 3.6.1 was modified to pass additional entrainment/detrainment fluxes and precipitation water profiles from the EPA-modified sub-grid cloud scheme to the variable output registry. Modifications were completed for the WRFCAMx interface program to read new WRF output fields and to process them as new variables in the CAMx cloud/rain input file. Functional testing on a sample set of WRF data was completed. Quality assurance (QA) procedures were conducted to ensure that new code was correctly implemented and was properly processing new cloud data and generating the CAMx data files. These QA steps revealed certain aspects of the technique that required slight modifications to a few details, and also revealed issues in the original diagnostic option that led us to improve the robustness of that approach as well. WRFCAMx speed was not impacted by the addition of the sub-grid cloud option or by any subsequent modifications from the QA procedures.

Work was completed on CAMx modifications to incorporate a Cloud-in-Grid (CiG) module, which includes convective cloud mixing using data ingested from WRF, wet scavenging within the cloud and in the "ambient" fraction of the grid column, and aqueous PM chemistry within the cloud and the ambient fractions. Combining the implementation of convective transport together with chemistry and wet deposition has proven to be a more efficient approach for coding and testing than implementing these functions in separate tasks (as originally planned).

Functional testing on a sample WRF/CAMx dataset was completed. Model configuration, emissions, and initial/boundary conditions were taken from previous projects conducted for TCEQ. Extensive QA testing was conducted to ensure that new code was correctly implemented and was properly processing convective transport, wet scavenging, and aqueous chemistry. Particular attention was given to testing for mass conservative and positive-definite solutions, both of which have been attained. These QA steps revealed certain aspects of the technique that required modifications to a few details, but the approach as described in the design document remains intact. CAMx tests with single processor versus multi-processor parallelization (OMP and MPI) verified that identical results are achieved with 1 and 8 CPUs, with consistent speed improvements as the original CAMx code.

#### Delays or Technical Issues During the Reporting Period

Establishment of an AQRP sub-contract with co-principal investigators at Texas A&M was delayed until September.

We contacted EPA on the status of their latest version of WRF, which includes a new "multiscale" Kain-Fritsch (MSKF) module that allows for sub-grid convective treatment down to grid scales of 1 km. This will be important for CAMx/CiG, which is anticipated to be run on nested 36/12/4 km grids over Texas. Code delivery has been delayed as EPA is addressing bugs related to running MSKF on nested grids. EPA is unclear on when the WRF code will be made available, but based on EPA's response we expect to receive it in December. This delay may affect the project schedule by about 1 month.

Other than addressing routine technical details in the implementation and debugging of the subgrid cloud system in CAMx, no major technical issues have been encountered during the reporting period.

We intend to use all funds allocated to the project by 6/30/2015.

**Project 14-026** 

STATUS: Active – May 21, 2014

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

Environ – 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<sup>4</sup>RS) project encountered plumes with enhanced  $O_3$  downwind of petrochemical facilities in Houston. For example, on 25 September 2013, ground monitoring downwind of the Ship Channel showed 5minute 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 1,3butadiene, 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<sup>4</sup>RS project in Houston will be analyzed. Chemical compounds called β-hydroxynitrates are formed when HRVOCs react in the atmosphere in the presence of nitrogen oxides (NOx). Measurements of the C<sub>2</sub>-C<sub>4</sub> hydroxynitrates aboard the DC-8 provide a novel means to link observed enhancements of O<sub>3</sub> and HCHO to reactions of specific HRVOCs. Analyzing the data will provide a robust first-order attribution of observed O<sub>3</sub> and HCHO enhancements to the oxidation of individual HRVOCs emitted from the Houston Ship Channel. The plumes of HRVOCs and O<sub>3</sub> 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<sub>3</sub> 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**

Progress on Project 14-026 is summarized below by Task: <u>Task 1: QA/QC Alkene Hydroxynitrate Measurements by the Caltech TOF-CIMS aboard the</u> <u>DC-8 during SEAC<sup>4</sup>RS and Generate Final Data</u> While this task was initially going to be conducted by Caltech, a contractual agreement between Caltech and AQRP could not be reached, and Caltech withdrew from the project. However, under a NASA contract, Caltech is still conducting the hydroxynitrate data QA/QC (that was to be conducted for Task 1) and the QA/QC'd data are available for the AQRP study. Dr. David Parrish, under subcontract to ENVIRON, will collaborate with Caltech in completing the remaining components of Task 1, as described in the revised Work Plan and QAPP submitted to AQRP by the ENVIRON study team. AQRP approved the revisions to the Work Plan on September 11, 2014 and notified ENVIRON of the approval on September 15, 2014.

Caltech uploaded the QA/QC'd hydroxynitrate data to the SEAC<sup>4</sup>RS data archive on 25 November 2014. These data will probably have another revision in the next few months, but the revisions are likely to only influence data in the remote regions. Since this project will focus on data in the immediate vicinity of the Houston Ship Channel, Task 1 can proceed.

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

This task is being conducted by NOAA with assistance from Dr. David Parrish (Caltech was initially going to assist NOAA in this task but has withdrawn from the AQRP study as indicated above). The bulk of this task will be conducted once Task 1 is completed. However, Dr. Parrish has developed a preliminary kinetics scheme for the HRVOC chemistry. This scheme will underpin both the data analysis (Tasks 1 and 2) and the modeling (Task 3). As Tasks 1 and 2 move forward, the details and specific parameters of this scheme will be refined.

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

This task is being conducted by ENVIRON. As part of this task, ENVIRON updated the chemical mechanisms in SCICHEM from CB05 to CB6r2 and will be conducting tests to ensure that the implementation has been done correctly. The remaining components of this task (updates to CB6r2 mechanism to include additional explicit reactions to represent hydroxynitrate production from individual HRVOCs; plume modeling) will require the products of Tasks 1 and 2 before the task can be completed.

#### Project Management

ENVIRON developed and finalized subcontracting agreements for NOAA and Dr. Parrish for work to be conducted under Tasks 1 and 2.

The release of the QA/QC'd data by Caltech was delayed by about 10 days. We do not expect any impacts from this delay on the overall project schedule.

We intend to use all funds allocated to the project by 06/30/2015.

**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, <sup>14</sup>C, select inorganic ions, and elemental tracers from PM filters collected from four DISCOVER-AQ anchor sites including Moody Tower, Manvel Croix, Conroe, and La Porte. The PIs will apply a combination of radiocarbon source apportionment of organic and elemental carbon with source-specific organic and inorganic molecular tracers to tightly constrain urban and regional, fossil and biomass burning/biogenic sources.

#### **Progress Report**

In Sept-Nov 2014, significant analytical progress was made for WSOC, organic tracer analysis and method improvements for radiocarbon capture. Preparations were begun on two manuscripts: organic tracer pressurized liquid extraction (PLE) methods paper and spatial and temporal trends in carbonaceous aerosol components during DISCOVER-AQ. Three graduate students, an undergraduate student and a post doc worked with the PIs to accomplish this work. The PLE methods paper is first authored by a graduate student and the carbonaceous aerosol paper is first authored by a graduate student and the carbonaceous aerosol paper is first authored by a graduate student and the first year graduate student.

In detail the following progress was made on the Task Order during Sept – Nov:

- Shared WSOC data for Conroe.
- Completed WSOC analysis for Conroe, Moody Tower, Manvel Croix and La Porte.
- Purchased and prepared standards for organic tracer analysis
- Began preliminary sample analysis for organic tracers and contaminants at Moody Tower and Manvel Croix
- Validated method for organic tracers and contaminants using NIST SRMs 1649b and 2585
- Preparation of posters for AGU
- Demonstrated organic tracer method using multiple days of Moody Tower and Manvel Croix particulate matter samples
- Method development to improve carbon capture efficiency on Sunset for radiocarbon sample preparation
- Near-final draft of organic tracer method paper completed
- Prepared filters for shipment to DRI for inorganic ion analysis
- Began manuscript preparation of carbon characterization across the four Houston sites during DISCOVER-AQ

No anticipated delays. All funds are expected to be expended by June 30, 2015.

**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 climatecontrolled 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:

<u>Task 1: Meteorology simulation with WRF.</u> A number of simulations were conducted to find the most appropriate model input data that can best reproduce the observed meteorology parameters and soil moisture content. It was determined that the following configuration leads to optimal results: 1) 3-h resolution North American Regional Reanalysis (NARR) dataset, 2) daily satellite-based sea surface temperature, 3) gridded soil moisture from North America Land Data Assimilation System (NLDAS), 4) Noah land surface scheme, 5) MODIS-based year specific Leaf Area Index (LAI) and land use/land cover classification. <u>All meteorology simulations have been completed and final meteorology fields in CMAQ model-ready format have been generated, and are currently undergoing final quality check.</u>

<u>Task 2: Perform field and laboratory measurements on common Texas tree species.</u> The activities of the first quarter of the project were focused on obtaining baseline responses for the

investigated trees seedlings. Equipment was deployed to the greenhouse, such as calibrated soil sensors (which were before deployment), a pyranometer, and temperature sensors, with data recorded on a CR1000 data-logger. In September isoprene emissions from post oak and water oak were measured under normal greenhouse conditions, and plants were watered every 2-3 days. Due to a forced change of greenhouse location earlier that summer, and other stress factors, the drought experiment did not start until the month of October. In October, however, the greenhouse was remodeled and lamps were installed, with the constant opening of the greenhouse door likely having caused pests entering the greenhouse. The plants then unfortunately suffered from an insect infestation, which was later controlled by applying the pesticide Conserve (spinosad).

Measurements were taken during that month, with plants in normal conditions watered every 2-3 days and plants under drought conditions watered every 10-15 days. At the same time, since ambient temperatures and light decreased substantially, artificial light and heaters were turned on. Measurements continued until the end of November, but the multitude of stressors and changes likely contributed to the inconsistent results obtained so far.

#### Task 3: Evaluate drought parameterization for isoprene emissions – Will start in December.

<u>Task 4: Perform regional BVOC modeling using MEGAN.</u> 1) The FORTRAN version of the MEGAN v2.1 model is updated to include the original drought parameterization. In the original MEGAN models (both 2.04 and 2.1), the soil moisture correction factor was set to unity. 2) The MCIP meteorology preprocessor has been updated to generate multi-layer soil moisture data that are needed by the updated MEGAN model. 3) The MEGAN model input preprocessor (megan\_bio\_emiss) was modified to generate input files that are compatible with the nested CMAQ domains, which are typically smaller than the WRF domains. 4) Preprocessing programs were developed to transform downloaded 2007 and 2011 MODIS LAI into MEGAN preprocessor acceptable format. 5) 1x1 km wilting point database was prepared for MEGAN based on Penn State CONUS-SOIL data base and the IGBP-DIS data from ORNL. 6) LAIs in urban areas were determined using the National Land Cover Database (NLCD) using the TCEQ method. 7) <u>CMAQ model ready biogenic emission files for both model years were generated.</u>

<u>Task 5: Perform regional air quality simulations.</u> 1) Anthropogenic emissions for the CMAQ model for 2011 have been generated. 2) Online dust emission module in CMAQ model modified to use the MODIS based land use/land cover data. 3) CMAQ simulation using default drought parameterization will start in December.

#### 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 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:

<u>Program Administration</u> – 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.

#### <u>ITAC</u>

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

<u>Project Management</u> – 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.

<u>Research Projects</u> / 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

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 2010/2011

#### Administration Budget (includes Council Expenses) FY 2012/2013

Budget Category	FY12 Budget	FY13 Budget	Total	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary	\$74,238.65	\$265,040.00	\$339,278.65	\$270,737.66	\$0.00	\$68,540.99
Fringe Benefits	\$17,068.38	\$47,706.00	\$64,774.38	\$61,732.37	\$0.00	\$3,042.01
Travel	\$339.13	\$750	\$1,089.13	\$339.13		\$750.00
Supplies	\$3,560.62	\$10,000	\$13,560.62	\$12,505.25	\$0.00	\$1,055.37
Equipment	\$0.00	\$0	\$0			\$0
Total Direct Costs	\$95,206.78	\$323,496.00	\$418,702.78	\$345,314.41	\$0.00	\$73,388.37
Authorized Indirect						
Costs	\$7,423.86	\$26,504.00	\$33,927.86	\$27,073.76	\$0.00	\$6,854.10
10% of Salaries and Wages						
Total Costs	\$102,630.64	\$350,000.00	\$452,630.64	\$372,388.17	\$0.00	\$80,242.47
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

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						
Total Costs	\$17,418.81	\$6,577.64	\$23,996.45	\$23,996.45	\$0.00	\$0

### ITAC Budget

#### 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. As 5 new projects are being added, Vince Torres was added as a Project Manager. \$53,974 in FY 13 research project funds were rebudgeted to project management to cover the costs associated with the additional project manager. At 5.4% of the research project funds, project management costs for FY 13 are well below the allowed 8.5%.

### 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

112012/2015						
Budget Category	FY12 Budget	FY13 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary	\$53,384.46	\$119,981.00	\$173,365.46	\$143,524.43	\$0.00	\$29,841.03
Fringe Benefits	\$10,991.04	\$26,995.00	\$37,986.04	\$27,922.93	\$0.00	\$10,063.11
Travel	\$0.00	\$0.00	\$0.00	\$0.00		\$0.00
Supplies	\$967.98	\$1,000.00	\$1,967.98	\$1,452.52		\$515.46
Total Direct Costs	\$65,343.48	\$147,976.00	\$213,319.48	\$172,899.88	\$0.00	\$40,419.60
Authorized Indirect						
Costs	\$5,338.44	\$11,998.00	\$17,336.44	\$14,352.44	\$0.00	\$2,984.00
10% of Salaries and Wages						
Total Costs	\$70,681.92	\$159,974.00	\$230,655.92	\$187,252.32	\$0.00	\$43,403.60

### Project Management Budget FY 2012/2013

### Project Management Budget FY 2014/2015

Budget Category	FY14 Budget	FY15 Budget	Total Budget	Expenses	Pending Expenses	Remaining Balance
Personnel/Salary	\$52,000.00	\$52,000.00	\$104,000.00	\$3,869.46	\$0.00	\$100,130.54
Fringe Benefits	\$9,300.00	\$9,300.00	\$18,600.00	\$785.46	\$0.00	\$17,814.54
Travel						
Supplies	\$1,000.00	\$1,000.00	\$2,000.00	\$587.25	\$0.00	\$1,412.75
Total Direct Costs	\$62,300.00	\$62,300.00	\$124,600.00	\$5,242.17	\$0.00	\$119,357.83
Authorized Indirect Costs	\$5,200.00	\$5,200.00	\$10,400.00	\$386.94	\$0.00	\$10,013.06
10% of Salaries and Wages						
Total Costs	\$67,500.00	\$67,500.00	\$135,000.00	\$5,629.11	\$0.00	\$129,370.89

### **Research Projects**

FY 2010-2011

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

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

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

### FY 2012-2013

The FY 2012 Research/Contractual budget was originally funded at \$815,000. Transfers to date have increased the budget by \$32,438.67. These funds were fully expended as of April 2014. The FY 2013 Research Contractual budget was originally funded at \$835,000. In June 2013, Amendment 9 increased this budget by \$2,100,000. (The remaining \$400,000 was allocated to Admin and Project Management.) Transfers to date have increased that by an additional \$55,026 for a total FY 2013 Research Contractual budget 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.

Total FY 2013 research project expenditures are \$1,321,620.01. Funds that were not expended by the FY 2012 – 2013 research projects totaling \$1,716,844.99 have been allocated to projects from the FY 2014-2015 RFP. Table 5 illustrates the 2012-2013 Research Projects, including the funding awarded to each project and the total expenses reported on each project as of November 30, 2014. This does not include the funding for the 5 new projects. 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.

Contractual E FY 10 Contractua	Expenses al Funding	\$2,286,000		
FY 10 Contractua FY 10 Total Cont	al Funding Transfers ractual Funding	\$1,827.93 <b>\$2,287,827.93</b>		
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 Contr	ractual Funding Awarded	\$2,286,000		
FY 10 Contractua	l Funding Expended (Init. Projects)		\$2,244,812.59	
FY 10 Contractua	I Funds Remaining Unspent after Project	t Completion		\$41,187.41
FY 10 Additional	Projects			
10-505	Data Storage State of the Science	\$7,015.34 \$36,000,00	\$7,015.34 \$36,000,00	\$0 \$0
10 303		\$30,000.00	\$30,000.00	ŶŬ
FY 10 Contractua	I Funds Expended to Date*		\$2,287,827.93	
FY 10 Contractua	l Funds Remaining to be Spent			\$0

Table 4: 2010/2011 Contractual Expenses

I

FY 11 Contractual Funding FY 11 Contractual Funding Transfers FY 11 Total Contractual Funding		\$1,736,063.00 \$116,377.62 <b>\$1,852,440.62</b>		
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 Contr	actual Funding Awarded	\$1,758,099		
FY 11 Contractua	l Funds Expended (Init. Projects)		\$1,713,287.06	
FY 11 Contractua	I Funds Remaining Unspent after Project	t Completion		\$44,811.94
FY 11 Additional I	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 Contractua	l Funds Expended to Date*		\$1,852,440.51	
FY 11 Contractua	l 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

Contractu	Contractual Expenses					
FY 12 Contractual Funding FY 12 Contractual Funding Transfers FY 12 Total Contractual Funding		\$815,000.00 \$32,438.67 <b>\$847,438.67</b>				
Project Numb	ber	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 C	ontractual Funding Awarded	\$847,438.67				
FY 12 Contrac	ctual Funds Expended to Date		\$847,438.67			
FY 12 Contrac	ctual 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 Contrac	ctual Funding Transfers	\$2,209,000	_	
FY 13 Total C	ontractual Funding	\$3,044,000		
Project Numt	ber	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 Co	ontractual Funding Awarded	\$2,097,080		
FY 13 Contrac	ctual Funds Expended (Init. Projects)		\$1,321,620.01	
FY 13 Contrac	ctual Funds Remaining Unspent			\$1,722,379.99
FY 13 Additio	nal Expenditures			
	DATA Storage	\$5,535	\$5,535	\$0.00
FY 13 Contrac	ctual Funds Expended		\$1,327,155.01	
FY 13 Contrac	ctual Funds Remaining Unspent			\$1,716,844.99
Note: After all FY13 funds will be	projects were completed contractual fun utilized for FY14 projects and will be acco	ds in the amount c unted for on the fo	of \$1,716,844.99 ollowing page.	remained. The

FY 13 Remaining Contractual Funding

\$1,716,844.99

FY 13 Remaining Cont FY 13 Total Remaining	ractual Funding Transfers g Contractual Funding	<mark>(\$53,974.00)</mark> \$1,662,870.99	-	
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
14-003	UNC Chapel Hill	\$180,000.00	\$0.00	\$180,000.00
14-006	Sonoma Technology	\$47,979.00	\$14,067.00	\$33,912.00
14-006	Valparaiso	\$15,609.00	\$0.00	\$15,609.00
14-007	Chalmers Univ.	\$15,233.00	\$15,233.00	\$0.00
14-007	Univ. of Houston	\$10,000.00	\$4,387.77	\$5,612.23
14-008	UT-Austin (McDonald-Buller)	\$175,000.00	\$55,281.52	\$119,718.48
14-011	UT-Austin (McDonald-Buller)	\$131,166.00	\$40,898.35	\$90,267.65
14-011	Environ	\$6,000.00	\$733.77	\$5,266.23
14-016	Environ	\$240,000.00	\$98,690.68	\$141,309.32
14-017	Univ. of Alabama-Huntsville	\$25,000.00		\$25,000.00
14-017	Rice University	\$25,000.00		\$25,000.00
14-023	UT-Austin (Torres)	\$76,773.00	\$25,874.37	\$50,898.63
14-023	Aerodyne	\$147,066.00	\$10,712.74	\$136,353.26
14-024	UT-Austin (Hildebrandt Ruiz)	\$143,282.00	\$69,433.78	\$73,848.22
14-024	Environ	\$25,000.00	\$17,201.59	\$7,798.41
14-024	UC Riverside	\$35,314.00	\$33,270.50	\$2,043.50
14-025	Environ	\$40,000.00	\$40,000.00	\$0.00
14-025	TAMU	\$20,000.00		\$20,000.00
14-029	Baylor University	\$150,000.00		\$150,000.00
14-030	TEES	\$132,227.43	\$38,994.58	\$93,232.85

FY 13 Total Remaining Contractual Funding Awarded	\$1,640,649.43		
FY 13 Remaining Contractual Funds Expended		\$464,779.65	
FY 13 Remaining Contractual Funds Remaining to be S	ntractual Funds Remaining to be Spent		
Total Contractual Funding	\$3,891,439		
Total Contractual Funding Awarded	\$3,815,243		
Total Contractual Funding Remaining to be Awarded	\$76,196		
Total Contractual Funds Expended to Date		\$2,639,373.33	
Total Contractual Funds Remaining to be Spent			\$1,252,065.34

Table 6. 2014/2015 Contractual Expenses

Contractual Expenses					
FY 14 Contractual Fur FY 14 Contractual Fur FY 14 Total Contractu	nding nding Transfers al Funding	\$825,000 \$0 \$825,000			
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance	
14-002	CU - Boulder	\$150,508.00		\$150,508.00	
14-002	Univ. of Maryland	\$49,387.00		\$49,387.00	
14-003	UNC Chapel Hill	\$20,000.00	\$0.00	\$20,000.00	
14-004	Univ. of Maryland	\$55,056.00		\$55,056.00	
14-004	Morgan State Univ.	\$54,055.00	\$10,812.95	\$43,242.05	
14-009	Rice Univ.	\$109,867.00	\$29,159.10	\$80,707.90	
14-009	Univ. of Houston	\$109,635.00	\$2,228.70	\$107,406.30	
14-026	Environ	\$135,782.00	\$69,613.44	\$66,168.56	
14-030	TAMU/TEES	\$43,881.57		\$43,881.57	
				\$0.00	
				\$0.00	
				\$0.00	
FY 14 Total Contractu	al Funding Awarded	\$728,171.57			
FY 14 Contractual Fun Awarded	ding Remaining to be	\$96,828.43			
FY 14 Contractual Fun	ds Expended to Date		\$111,814.19		
FY 14 Contractual Fun	ds Remaining to be Spent	_		\$713,185.81	

FY 15 Contractual Fund	ding	\$825,000				
FY 15 Contractual Fund	ding Transfers	\$0				
FY 15 Total Contractua	al Funding	\$825,000				
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance		
14-006	Sonoma Technology	\$2,000.00	\$0.00	\$2,000.00		
14-007	Chalmers University	\$58,946.00	\$20,617.00	\$38,329.00		
14-007	Univ. of Houston	\$13,081.00		\$13,081.00		
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	\$10,000.00	\$0.00	\$10,000.00		
14-024	Univ. of Texas - Austin	\$20,000.00	\$0.00	\$20,000.00		
14-024	Environ	\$76,404.00	\$0.00	\$76,404.00		
14-025	Environ	\$95,735.00	\$7,813.25	\$87,921.75		
14-025	TAMU	\$100,526.00		\$100,526.00		
14-029	Baylor University	\$28,679.00		\$28,679.00		
FY 15 Total Contractual Funding Awarded		\$629,684.00				
FY 15 Contractual Fund	\$195,316.00					
FY 15 Contractual Fund		\$28,430.25				
FY 15 Contractual Fund	ds Remaining to be Spent			\$796,569.75		

Total Contractual Funding	\$1,650,000		
Total Contractual Funding Awarded	\$1,357,856		
Total Contractual Funding Remaining to be Awarded	\$292,144		
Total Contractual Funds Expended to Date		\$140,244.44	
Total Contractual Funds Remaining to be Spent			\$1,509,756

Appendix A

# Financial Reports by Fiscal Year FY 10 and 11

(Expenditures reported as of November 30, 2014.)

## Administration Budget (includes Council Expenses)

Ff 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		

#### FY 2010

## 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		

### EV 2010

## 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.)

FY 2012

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

## Administration Budget (includes Council Expenses)

#### FY 2013

Budget Category	FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary	\$265,040.00	\$196,499.01		\$68,540.99
Fringe Benefits	\$47,706.00	\$44,663.99		\$3,042.01
Travel	\$750.00	\$0.00		\$750.00
Supplies	\$10,000.00	\$8,944.63		\$1,055.37
Equipment				
Other	\$0.00			
Total Direct Costs	\$323,496.00	\$250,107.63	\$0.00	\$73,388.37
Authorized Indirect Costs	\$26,504.00	\$19,649.90		\$6,854.10
10% of Salaries and Wages				
Total Costs	\$350,000.00	\$269,757.53	\$0.00	\$80,242.47

## 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	\$119,981.00	\$90,139.97		\$29,841.03
Fringe Benefits	\$26,995.00	\$16,931.89		\$10,063.11
Travel				
Supplies	\$1,000.00	\$484.54		\$515.46
Equipment				
Other				
Contractual				
Total Direct Costs	\$147,976.00	\$107,556.40	\$0	\$40,419.60
Authorized Indirect Costs	\$11,998.00	\$9,014.00		\$2,984.00
10% of Salaries and Wages				
Total Costs	\$159,974.00	\$116,570.40	\$0.00	\$43,403.60

## AQRP Budget

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 <i>,</i> 438.67	\$0.00	\$0.00
ITAC	\$5,555.17	\$5 <i>,</i> 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
	<u> </u>	67 400 0C		
Authorized Indirect Costs	\$7,423.86	\$7,423.86	\$0.00	\$0.00
10% of Salaries and Wages			4	4.4
Total Costs	\$1,026,306.40	\$1,026,306.40	\$0.00	\$0.00

FY 2012

AQRP Budget FY 2013

Budget Category	FY13 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary	\$265,040.00	\$196,499.01	\$0.00	\$68,540.99
Fringe Benefits	\$47,706.00	\$44,663.99	\$0.00	\$3,042.01
Travel	\$750.00	\$0.00	\$0.00	\$750.00
Supplies	\$10,000.00	\$8 <i>,</i> 944.63	\$0.00	\$1,055.37
Equipment	\$0.00	\$0.00	\$0.00	\$0.00
Other	\$0.00	\$0.00	\$0.00	\$0.00
Contractual	\$2,990,026.00	\$1,791,934.66	\$0.00	\$1,198,091.34
ITAC	\$0.00	\$0.00	\$0.00	\$0.00
Project Management	\$159,974.00	\$116,570.40	\$0.00	\$43,403.60
Total Direct Costs	\$3,473,496.00	\$2,158,612.69	\$0.00	\$1,314,883.31
Authorized Indirect Costs	\$26,504.00	\$19,649.90	\$0.00	\$6,854.10
10% of Salaries and Wages				
Total Costs	\$3,500,000.00	\$2,178,262.59	\$0.00	\$1,321,737.41

Appendix C

# Financial Reports by Fiscal Year FY 14 and 15

(Expenditures reported as of November 30, 2014.)

	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)

## 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		

FY 2014						
Budget Category		FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance	
Personnel/Salary						
Fringe Benefits						
Travel		\$7,000.00	\$0.00	\$0.00	\$7,000.00	
Supplies		\$500.00	\$0.00	\$0.00	\$500.00	
Equipment						
Other						
Total Direct Costs		\$7,500.00	\$0.00	\$0.00	\$7,500.00	
Authorized Indirect Costs						
10% of Salaries and Wages						
Total Costs		\$7,500.00	\$0.00	\$0.00	\$7,500.00	

## ITAC Budget

FY 2015

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

## Project Management Budget

FY 2014						
Budget Category	FY14 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance		
Personnel/Salary	\$52,000.00	\$3,869.46	\$0.00	\$48,130.54		
Fringe Benefits	\$9,300.00	\$785.46	\$0.00	\$8,514.54		
Travel	\$0.00	\$0.00	\$0.00	\$0.00		
Supplies	\$1,000.00	\$0.00	\$0.00	\$1,000.00		
Equipment						
Other						
Total Direct Costs	\$62,300.00	\$4,654.92	\$0.00	\$57,645.08		
Authorized Indirect Costs	\$5,200.00	\$386.94	\$0.00	\$4,813.06		
10% of Salaries and Wages						
Total Costs	\$67,500.00	5,041.86	\$0.00	\$62,458.14		

## Project Management Budget

FY 2015

Budget Category	FY15 Budget	Cumulative Expenditures	Pending Expenditures	Remaining Balance
Personnel/Salary	\$52,000.00	\$0.00	\$0.00	\$52,000.00
Fringe Benefits	\$9,300.00	\$0.00	\$0.00	\$9,300.00
Travel	\$0.00	\$0.00	\$0.00	\$0.00
Supplies	\$1,000.00	\$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

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	\$111,814.19	\$0.00	\$713,185.81				
ITAC	\$7,500.00	\$0.00	\$0.00	\$7,500.00				
Project Management	\$67,500.00	\$5,041.86	\$0.00	\$62,458.14				
Total Direct Costs	\$993,000.00	\$116,856.05	\$0.00	\$876,143.95				
Authorized Indirect Costs	\$7,000.00	\$0.00	\$0.00	\$7,000.00				
10% of Salaries and Wages								
Total Costs	\$1,000,000.00	\$116,856.05	\$0.00	\$883,143.95				

FY 2014

## 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	\$28,430.25	\$0.00	\$796,569.75
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	\$29,017.50	\$0.00	\$963,982.50
Authorized Indirect Costs	\$7,000.00	\$0.00	\$0.00	\$7,000.00
10% of Salaries and Wages				
Total Costs	\$1,000,000.00	\$29,017.50	\$0.00	\$970,982.50