AIR QUALITY RESEARCH PROGRAM

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

Quarterly Report

March 1, 2019 through May 31, 2019

Submitted to

Donna Huff
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

June 10, 2019

The preparation of this report was financed through a grant from the Texas Commission on Environmental Quality (TCEQ), administered by The University of Texas at Austin through the Air Quality Research Program (AQRP). The contents, findings, opinions, and conclusions are the work of the author(s) and do not necessarily represent findings, opinions, or conclusions of the TCEQ.

Texas Air Quality Research Program

Quarterly Report

March 1, 2019 – May 31, 2019

OVERVIEW

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

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

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

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

PROGRAM ACTIVITIES FOR THE QUARTER

Throughout the quarter, Project Managers worked with project teams to ensure all reporting requirements were met and assisted with project activities as needed. Program management communicated the invoicing and financial status report (FSR) requirements to each entity, and reviewed each invoice/FSR for compliance prior to submission for payment. All projects are in progress and progressing towards completion with no major delays reported.

In April, Maria Stanzione, AQRP Grant Manager, notified the TCEQ that she would be moving to a different unit within the University of Texas at Austin, and leaving the AQRP Program. She continued to support the AQRP on a half-time basis through the end of May. Vincent Torres has been named the new secondary designee as of June 1, 2019. In addition, a new AQRP Grant Manager, RoseAnna Goewey, has been named. Ms. Goewey will join the program on June 24, 2019. Maria Stanzione will continue to provide basic support to the AQRP during the interim, and will train Ms. Goewey through July 15, 2019.

BACKGROUND

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

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

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

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

RESEARCH PROJECT CYCLE

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

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

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

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

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

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

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

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

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

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

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

During this reporting period all Program activity concentrated on Steps 7 and 8 of the Research Project Cycle.

RESEARCH PROJECTS

FY 2018 – 2019 Projects

Project 18-005 **STATUS: Active – October 31, 2018**

Next steps for improving Texas biogenic VOC and NO emission estimates

University of California-Irvine – Alex Guenther
Ramboll – Greg Yarwood
AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Doug Boyer

Funded Amount: $168,146
(UC-Irvine $139,193, Ramboll $28,953)

Abstract
The emissions of gases and particles into the atmosphere are the primary drivers of regional air quality. There are a wide variety of emission sources including automobiles, factories, and biological organisms including vegetation and microbes. While emissions from combustion sources and industrial activities dominate in urban and industrial locations, biogenic emissions dominate on global scales and contribute to atmospheric composition in urban and nearby areas.

The overall goal of this project is to improve numerical model predictions of regional ozone and aerosol distributions in Texas by reducing uncertainties associated with quantitative estimates of biogenic volatile organic compound (BVOC) and biogenic nitric oxide (BNO) emissions from Texas and the surrounding region. Although there have been significant advancements in the procedures used to simulate these biogenic emissions, there are still major uncertainties that limit predictability of Texas air quality simulations. In this project, we will improve the capability of the Model of Emissions of Gases and Aerosols from Nature (MEGAN) framework to estimate emissions of these compounds for application in numerical air quality models. To accomplish this, we will conduct high quality measurements of speciated BVOC emission factors at eastern Texas field sites near San Antonio, Dallas, and Houston. These results and other recent advances, including an improved approach for modeling BNO emissions, will be integrated into MEGAN.

The primary output of the proposed research will be a more accurate approach for estimating BVOC and BNO emissions. The overall benefit of this project will be more accurate VOC and NO emission estimates for the Texas air quality simulations that are critical for scientific understanding and the development of regulatory control strategies that will enhance efforts to improve and maintain clean air.

Project Activities
AQRP 18-005 activities for this quarter focused on Task 1 (Measure Texas BVOC emission factors and their variability) and Task 2 (MEGAN model improvements). Work on Task 3 (MEGAN3.1 sensitivity analysis of Texas biogenic emissions) will begin in the next quarter.

Field measurements were conducted on the UC Irvine campus on common Texas tree species including Quercus virginiana (eastern live oak), Nyssa sylvatica (black gum), Taxodium distichum (baldcypress) and Liquidambar styraciflua using four enclosure systems. This activity provided both observations on important Texas plant species and an optimization of the approaches that will be used for the June 2019 field study in Texas. The approach was optimized

by replacing GC-PID analysis with GC-MS analysis which provides more sensitive and specific BVOC measurements. In addition, BVOC emission measurements using GCMS and PTR-TOF-MS analytical tools were made on 8 dominant Texas Crop species including Arachis hypogaea (peanuts), Cynodon dactylon (coastal bermuda grass), Glycine max (soybeans), Gossypium hirsutum (cotton), Medicago sativa (alfalfa), sorghum bicolor (sorghum), Triticum aestivum (wheat), and Zea mays (corn). All plant species studied emitted some BVOC but the total emission factors ranged from >30 to <0.3 nmol/m^2/s. Light oxygenated VOC (e.g., acetaldehyde, methanol, acetone) dominated emissions of most crops but the amounts and types of compounds varies. Corn had high emissions of DMS while peanuts emitted a large range of compounds that are not typically observed from other plants.

The specific coding tasks required for implementing the new soil NO emission algorithm were identified and coding strategies determined. Updates were made to the MEGAN-EFP python code and BVOC emission inputs. This included an improved framework for assigning default values to species with no measurements and landscapes with no tree data. BVOC emission inputs were developed for regions outside of the US (e.g., regions in Mexico that border the TCEQ domain).

The project is progressing as expected. All funds allocated to the project are expected to be used by 8/31/2019.

Project 18-007 **STATUS: Active – October 16, 2018**

DDM Enhancements in CAMx: Local Chemistry Sensitivity and Deposition Sensitivity

Ramboll – Greg Yarwood

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

Funded Amount: $150,000

Abstract
The Texas Commission on Environmental Quality uses the CAMx photochemical air quality model in planning activities for ground-level ozone. Estimating uncertainty in a model's predictions due to uncertainties in all the inputs and parameters, known as a global uncertainty analysis, is a challenge due to the hundreds or even thousands of inputs and parameters and the relatively long computer runtimes for photochemical models. This project will develop a new and efficient sensitivity analysis tool for CAMx called Chemistry Sensitivity Analysis (CSA) that is based on the decoupled direct method (DDM) for sensitivity analysis already present in CAMx. Then, we will use CSA to estimate the uncertainty range in ozone predictions in Texas due to chemistry uncertainty by creating alternative chemistry mechanisms with high and low ozone productivity. Also, we will extend the implementation of DDM in CAMx to calculate sensitivity to dry deposition velocity which has been identified as an important factor influencing ozone predictions. We will combine the effects of estimated uncertainty in the chemistry with uncertainty due to model emissions, boundary concentrations, and dry deposition velocity to estimate an overall uncertainty in CAMx ozone predictions for Texas.

Project Activities
This AQRP project is being performed by Ramboll in collaboration with Dr. Alan Dunker, an independent consultant. A summary of activities for the period March 1, 2018 through May 31, 2019 is provided below.

Task 1: Develop the Chemistry Sensitivity Analysis (CSA) Tool for CAMx

Ramboll developed setup routines for the new CSA probing tool in CAMx, including the new memory structures and output options required for CSA, and has started testing these routines. Ramboll implemented the algorithms for calculating reaction term sensitivity coefficients within the CSA tool.

Task 2: Apply CSA for Ozone in Texas to Investigate Chemical Mechanism Condensation and Uncertainty

Ramboll conducted base case CAMx simulations with process analysis (CPA) using the 2012 TCEQ modeling database to identify grid cells for CSA application and testing.

Task 3: Implement DDM for Dry Deposition in CAMx

Ramboll implemented the code to calculate the dry deposition sensitivities and compared the sensitivity coefficients with those derived from brute force runs. Dr. Dunker is reviewing the results of these tests.

Task 4: 3-D DDM Analysis

Ramboll has started the application of 3-D DDM for the June 2012 episode with the CB6r4 mechanism. The 3-D DDM first-order sensitivities are being calculated for the following parameters:

1. Ozone sensitivity to local emissions of anthropogenic NOx, anthropogenic VOC, and biogenic VOC
2. Ozone sensitivity to regional (i.e., outside of the selected local area) emissions of all species
3. Ozone sensitivity to dry deposition velocity of ozone
4. Ozone sensitivity to dry deposition velocities of all species but ozone
5. Ozone sensitivity to ozone boundary concentrations

Task 5: Reporting

This task has not yet been initiated.

Project Management

Ramboll submitted progress reports when required.

Ramboll received authorization to begin work on the project in October 2018. We do not expect this delay in initiating the study to impact the overall schedule for delivering the draft final report by August 1, 2019.

We intend to use all funds allocated to the project by 08/31/2019.

Project 18-010 **STATUS: Active – October 26, 2018**

A synthesis study of the role of mesoscale and synoptic-scale wind on the concentrations of ozone and its precursors in Houston

Texas A&M University – Qi Ying

AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Jonathan Steets

Funded Amount: $121,000

Abstract
While it is known that low synoptic-scale winds and mesoscale recirculation contribute to high ozone formation in Houston, a comprehensive synthesis of all relevant data and analyses to elucidate the interaction between the mesoscale and synoptic-scale winds and air pollutants is not yet available. An improved understanding of the roles of mesoscale and synoptic-scale processes would allow researchers and policy makers to distinguish between days dominated by local emissions and those dominated by regional contributions. The overall objective of this research is to synthesize existing data, previous analyses, and photochemical model experiments to provide a comprehensive and reconciled description of how mesoscale and synoptic-scale winds affects dispersion and accumulation of air pollutants emitted in the Houston area and from other regions, and how they contribute to high ozone events. The relationship between surface winds and boundary-layer mesoscale transport features will be clarified, and a novel source- and age-resolved regional air quality model will be applied to investigate selected high ozone events under the influence of mesoscale circulations. The results from this study will facilitate a better understanding of the interaction between the mesoscale and synoptic-scale winds and air pollutants and how they contribute to high ozone events in Houston. Such information is extremely useful for understanding high ozone events as they occur and for developing appropriate control strategies and policy options for the unique Texas meteorological environment.

Project Activities
Task 1 is on the synthesis of mesoscale wind structures in the synoptic-scale context. Nielsen-Gammon's group focused on tools and techniques for analyzing the radar wind profiler data. In particular, we are implementing techniques for automatically isolating the diurnal wind cycle from time-varying background winds. Previous analyses had operated on a somewhat different format of profiler data and had treated the background winds as static. This new implementation will separately identify the mean background wind, the gradual evolution in background wind over time, and the diurnal winds forced by the sea breeze and the low-level jet. Using this tool, we will investigate the extent to which changes in background wind are important in producing conditions highly favorable for wind recirculation and pollution concentration, and conversely the extent to which diurnal wind variations are sensitive to the temporal evolution of the background wind. Appropriate episodes will be selected for further CMAQ modeling investigation. For Task 2, Qi Ying's group continued to analyze the summer ozone episode in August and September 2000. Vertical distributions of aged and fresh ozone were analyzed using the age-resolved CMAQ model. Figure 1 shows that at Galveston aged ozone (> 8 hours) can be a significant contributor to total ozone at both surface and higher elevations. On August 30 and 31, higher aged ozone occurred at higher elevations about 250-500 m above the surface with

concentrations exceeding 30 ppb. In the afternoon and evening hours of September 4, the high concentration of aged ozone occurred throughout the boundary layer and lasted for more than 12 hours. Fractional contributions of aged ozone to total ozone exceeds 50% on these hours.

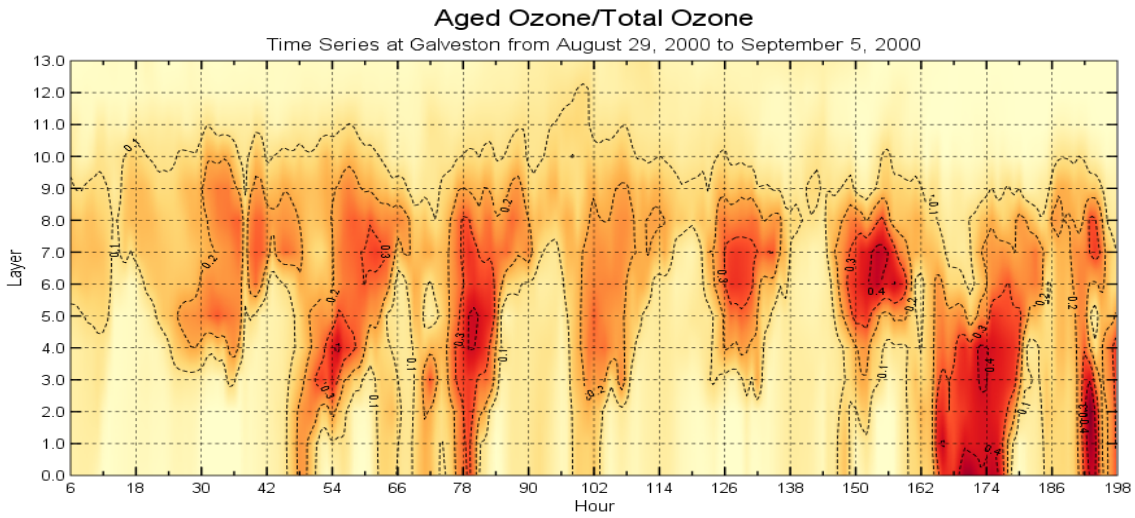

Figure 1 Time series of the vertical distribution of aged ozone (> 8 hrs) fraction at Galveston from August 29, 2000, to September 5, 2000. Hour 6 is the 0000 hours local time on August 29, 2000.

At this point, all funds allocated to the project is expected to be used by 8/31/2019.

Project 18-022 **STATUS: Active – September 1, 2018**

Development and Evaluation of the FINN v.2 Global Model Application and Fire Emissions Estimates for the Expanded Texas Air Quality Modeling Domain

University of Texas at Austin – Elena McDonald-Buller
Sonoma Technology, Inc. – Fred Lurmann

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Stephanie Shirley

Funded Amount: $172,114
(UT Austin $85,768, Sonoma Tech $86,346)

Abstract
Wildland fires and open burning can be substantial sources of ozone precursors and particulate matter. Air quality in Texas can be affected by fire events that occur locally, regionally, or across longer distances from within the United States or across its international borders. With this recognition, the Texas Commission on Environmental Quality's future air quality model domain has been extended to include all of Mexico and large parts of Central America and the Caribbean. The Fire INventory model from the National Center for Atmospheric Research (FINN) estimates daily emissions of trace gases and particles from open biomass burning. The objectives of this project are to leverage new findings and data products from ongoing laboratory studies, surface and airborne field measurement campaigns, and satellite-based sensors in the development of FINN and to produce a fully operational, next generation global FINN application. The new FINN application will be used to develop fire emissions estimates for 2012-2017, a time period that includes 2016, which is the base year for the U.S. Environmental Protection Agency's national air quality modeling platform. FINN performance will be assessed using a new satellite algorithm, the Multi-Angle Implementation of Atmospheric Correction (MAIAC), for aerosol optical depth (AOD) retrievals, with a focus on fire events that originate from within Mexico, Central America, or the Caribbean and influence Texas air quality. The project is a collaborative effort between the University of Texas at Austin, Sonoma Technology, Inc., and Dr. Christine Wiedinmyer.

Project Activities
The objective of this project is to complete the development of the next generation of the FINN modeling system that will be designated as FINNv2.2. The FINN modeling system consists of three primary components, including the preprocessor, emissions model, and chemical speciation code. The development of FINNv2.2 has been completed with quality assurance on-going as simulations are completed. During the quarterly period ending May 31, 2019, several refinements were made to the modeling system. These included screening of active fire data records from the Visible Infrared Imaging Radiometer Suite (VIIRS) to remove volcanic and anthropogenic stationary sources in the preprocessor, revisions to biomass (fire fuel) loadings and emissions factors in the emissions model, and development of the chemical speciation profile for non-methane organic compounds (NMOCs) for the MOZART-T1 chemical mechanism. FINNv2.2 simulations have been completed for North America for 2012-2017 with active fire detections products from VIIRS and the Moderate Imaging Spectroradiometer (MODIS), as well as for 2012 with MODIS fire detections only. Two global simulations for

2016 and 2018 with FINNv2.2 using MODIS and VIIRS active fire detections are on-going. The team has begun to document the methodology used in the FINNv2.2 development.

Predictions of air quality from the Comprehensive Air Quality Model with Extensions (CAMx) with FINNv2.2 fire emissions estimates for 2012 will be compared with the Multi-Angle Implementation of Atmospheric Correction (MAIAC) aerosol optical depth (AOD) product to assess FINN performance. CAMx simulations are being conducted with all fire emissions removed ("no fires") as a basis for reference, with processed FINNv2.2 emissions with MODIS and VIIRS active fire detections, and with processed FINNv2.2 emissions with only MODIS detections. A particular focus for the simulations has been on the vertical and temporal distributions of fire emissions and the effects on predicted ozone and $PM_{2.5}$ concentrations. Case studies have been analyzed for specific fire events in the 36-km and 4-km domains that exhibited large hourly peak concentrations of these compounds. The TCEQ shared the EPS3 processing stream for their FINNv1.x emission estimates which was a beneficial basis for comparison.

Dispersion modeling of smoke emissions from FINNv2.2 was begun during the period ending May 31, 2019, and runs are ongoing for March through September for years 2012 through 2017. The dispersion modeling uses Global Data Assimilation System (GDAS0P5) meteorological data, and runs are facilitated using the BlueSky modeling framework. Following completion of the runs, HYSPLIT results will be compared with the Multi-Angle Implementation of Atmospheric Correction (MAIAC) aerosol optical depth (AOD) product. MAIAC data for the relevant periods have been obtained in preparation for the assessment.

Two presentations will be given about the project on August 2, 2019, at the International Emissions Inventory Conference in Dallas, Texas. The project is on-schedule, and all funds allocated are intended to be utilized by August 30, 2019.

Project 19-023 **STATUS: Active – September 5, 2018**

Emission Inventory Development and Projections for the Transforming Mexican Energy Sector

University of Texas at Austin – Elena McDonald-Buller
Ramboll – Greg Yarwood

AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Michael Ege

Funded Amount: $158,309
(UT Austin $93,296, Ramboll $65,013)

Abstract
Within Texas, characterizing emission sources along its border and within Mexico has been recognized as essential for air quality modeling. Mexico's energy sector has been undergoing potentially transformational changes as part of Constitutional reforms ratified in 2013. A primary motivation is to encourage domestic and foreign investment and productivity growth in the oil, gas and power sectors. The reforms have the potential to significantly transform the magnitudes and spatial distributions of emissions from the oil and gas and power generation sectors over the next one to two decades. The overall objective of the proposed project is to apply new information to develop a bottom-up assessment of emissions for the upstream and midstream oil and gas sectors and power sector and to develop future emission projections based on likely outcomes of on-going bid rounds that are attracting new investment for exploration and production of oil and gas resources. Information and analytics for Mexico's upstream and midstream oil and gas sectors and power sector will be used to develop a 2016 base year emissions inventory, which coincides with the U.S. Environmental Protection Agency's national air quality modeling platform and will likely be the basis for future air quality modeling by the Texas Commission on Environmental Quality. Plans and results for the hydrocarbon bid rounds will be used as the basis for three future emissions projections that compare continued development of Mexico's onshore conventional and shallow water resources, which is consistent with historical practices, with expansion of its deep water and onshore shale regions that have been underdeveloped to date relative to their potential. The project is a collaborative effort between the University of Texas at Austin and Ramboll U.S Corporation.

Project Activities
During the quarter ending May 31, 2019, the team focused on development of the base year upstream and midstream emissions inventory components. These include on-shore oil and gas well site exploration and production (upstream sector), off-shore oil and gas exploration and production platforms (upstream sector), compressor stations (midstream sector), natural gas processing plants (midstream sector), and electric power plants.

Emissions estimates have been developed for onshore and offshore oil and gas drilling and producing well sites in Mexico's northern Burgos and Sabinas basins as well as the central and southern basins of Sureste, Tampico-Misantla, and Veracruz that were active during 2016. Emission factors for the Western Gulf Basin were used as the basis for the Burgos and Sabinas basins in northern Mexico, which primarily produce natural gas. Emission factors for the Palo Duro Basin were used for all other basins that typically have both oil and natural gas production

(e.g. Tampico-Misantla, Veracruz). Surrogates, such as oil or gas well counts, spud count, and oil or gas production by well type from Mexican government data resources were used to characterize activity. Quality assurance and documentation of the methodology and results is on-going.

Regulatory emission control requirements that would result in substantial flaring at Mexico upstream well sites are not required at this time. However, it is suspected that flaring controls may be used at upstream well sites as a safety measure. Projected estimates of flaring emissions in 2016 were developed during this reporting period.

For the midstream sector, emission estimates for natural gas compressor stations and natural gas processing plants in Mexico that were active during 2016 were completed along with documentation of the methodology and results for these sources.

An emissions inventory for Mexico's electric power sector was also completed, along with documentation of the methodology and results for these sources.

The project is on-schedule, and all funds allocated are intended to be utilized by August 30, 2019.

Project 19-025 **STATUS: Active – October 16, 2018**

Apportioning the Sources of Ozone Production during the San Antonio Field Study

Aerodyne Research, Inc. – Tara Yacovitch AQRP Project Manager – Elena McDonald-Buller
TCEQ Project Liaison – Bright Dornblaser

Funded Amount: $199,974

Abstract
Ozone high up in the stratosphere is protective against UV rays, but when it is present at ground-level, it is a pollutant that can cause shortness of breath and other respiratory health problems. With new federal ozone standards in effect, it is more important than ever to understand the causes of ozone in and around San Antonio.

Ozone is formed when volatile organic hydrocarbons (VOCs) react with nitrogen oxides (NOx, the primary component in smog). A wide variety of VOCs are present in the air around cities such as San Antonio; they stem from sources as varied as vehicle exhaust, oil and gas extraction, and trees and vegetation. This project aims to discover which sources contribute to the formation of ground-level ozone in and around San Antonio, and in what quantities.

Raw data from the 2017 San Antonio Field Study (SAFS) will be examined closely and analyzed in full to identify characteristic sets of VOCs associated with different source types. Computer modeling of air transport will help identify the broad geographic areas where the measured air originated. An ozone formation computer model, in which individual source categories can be turned on, off, or varied, will be used to understand how each source type contributes to ozone formation in and around San Antonio.

Project Activities
During the third quarter, much progress has been made on each of the project tasks. For Task 1, which consists of high-resolution analysis of raw data from three separate instruments followed by identification of any new chemical species of atmospheric importance, the high-resolution analysis of the mass spectral data (PTR and I-CIMS) has been completed. This will supplement and significantly expand the initial dataset provided in 2017. Analysis and interpretation of the GC-ToF data is ongoing. The new data is being incorporated into Positive Matrix Factorization (PMF) analysis. The PMF analysis (Task 2) of the I-CIMS data allows us to remove artifacts and suspect signals by excluding those that do not respond to instrument zeroes, and identify factors that vary across the three locations or diurnally. This ongoing analysis already reveals multiple diurnal factors.

We have developed and begun working with a 0D box model based upon the dynamically simple model for atmospheric chemical complexity (DSMACC), and incorporated the master chemical mechanisms version 3.3. We have identified initial artifacts in the model and have developed mitigation strategies based upon Edwards et al (2013). Initial work with this model is using a small set of species to optimize computation and streamline the incorporation of experimental data. Based upon these efforts we will build our workflow for the modeling using a much-expanded set of VOCs.

Finally, we have developed HYSPLIT footprint analyses (Task 4) that investigates overlap with different land use types in Texas. This included separating by various biogenic sources (e.g. oak trees for isoprene) and anthropogenic sources (e.g. oil and gas activity for alkanes). Ongoing analysis compares various I-CIMS, trace gas, GC-ToF, and PTR PMF factors (Task 2) to these footprint time series to connect potential emission sources with downwind VOC classes and related atmospheric processing.

During this quarter the primary challenges have been finishing high-resolution analysis of the mass spectral data, and optimizing both the 0D box model workflow and the HYSPLIT trajectory modelling. Regular project-wide meetings as well as smaller focused scientific discussions have been crucial in pushing these tasks forward. We expect in the next quarter to continue drawing connections among these tasks (PMF analysis, chemical modeling, and footprint analysis) to yield a more coherent picture of the drivers of ozone formation and VOC chemistry in San Antonio.

This project is currently on track to use all available funds and finish by 8/31/2019.

Project 19-031 **STATUS: Active – October 26, 2018**

Detecting events and seasonal trends in biomass burning plumes using black and brown carbon: (BC)2 El Paso

Baylor University – Rebecca Sheesley
University of Houston – James Flynn
AQRP Project Manager – David Sullivan
TCEQ Project Liaison – Erik Gribbin

Funded Amount: $131,294
(Baylor $98,087, UH $33,207)

Abstract
Recent efforts by the Texas Air Quality Research Program (AQRP) and TCEQ to monitor and study air quality in Texas cities has resulted in improved understanding of the processes and sources which control urban air quality in e.g. Houston. As highlighted in the AQRP Priority Research Areas 2018-2019, El Paso is near the National Ambient Air Quality Standards for particulate matter (PM) and ozone (O_3). Reductions in anthropogenic emissions through implementation of cleaner technologies for e.g. motor vehicle exhaust, coal-fired power plants, have refocused efforts to understand the contribution of biomass burning to urban air pollution. This is particularly relevant for El Paso, which can experience large impacts of periodic biomass burning/wildfire plumes transported from out-of-state. Black carbon (BC), a marker for combustion influences on air quality, has been shown to be decreasing in urban areas across the United States due to increased regulation and the use of cleaner fuels. As a result, biomass-burning contributions are likely becoming more important for BC and for urban air quality in general.

We will provide critical insight on the influence of biomass burning on the air quality in El Paso, TX through the characterization of BC and brown carbon (BrC). BrC is the carbon fraction of an aerosol that selectively absorbs short wavelengths of light. The $(BC)^2$ El Paso field campaign will include the deployment of the Baylor air quality trailer, which will be outfitted with a suite of specific technologies developed to assess biomass burning through the monitoring of BC and BrC. Biomass burning plumes will be identified using aerosol composition and light absorption properties, including BC and BrC concentrations, absorption Ångström exponents (AAE), and aerosol light absorption coefficients for specific ultraviolet (UV) and visible wavelengths. The newest technology for real-time monitoring of aerosol absorption is the tricolor absorption photometer (TAP). The TAP measures adsorption at UV, green and red wavelengths to more specifically target biomass burning. This inexpensive and continuous photometer was designed by the National Oceanic and Atmospheric Administration (NOAA) and is commercially produced by Brechtel to address issues with previous photometers, including cost, sensitivity, noise and effective scattering corrections. Although it was only recently available, Baylor and UH PIs have run this instrument successfully during the 2017 San Antonio field campaign (SAFS) in the Baylor air quality trailer. The two goals of $(BC)^2$ El Paso are to 1) address scientific air quality questions of frequency, seasonality, and optical properties of biomass burning plumes in El Paso and 2) to evaluate the TAP instrument suite for application in long-term monitoring at urban sites in Texas.

Project Activities

Progress in the quarter being reported has included a significant amount of field campaign data collection, additional field-based instrument testing, and several site visits to the University of Texas El Paso (UTEP) campus.

The UTEP site was modified by UTEP facilities and the Baylor University Air Quality Trailer was installed in March 2019. Measurements started Mar 22 and have been running continuously since that time. Instrumentation from both Baylor and the University of Houston (UH) is housed and being run remotely in the Baylor trailer. The real time instrumentation in the Baylor trailer includes two new Tricolor Absorption Photometers (TAPs) (aerosol absorption alternating every hour), aethalometer (black carbon), nephelometer (aerosol scattering), and trace-level CO and NO_x.

Baylor and UH personnel remotely check the data streams for the instruments daily. These data are archived continuously to redundant storage at UH. Nest cameras in the Baylor trailer are used to do remote visual checks on the instruments and gas cylinder pressures. Baylor and UH oversee UTEP students paid to conduct weekly site checks and filter changes on the TAP. Baylor students have done site visits in April and May to train UTEP students and to do routine maintenance. The site is on track to continue routine sampling.

Project 19-040 **STATUS: Active – September 18, 2018**

Analysis of Ozone Production Data from the San Antonio Field Study

Drexel University – Ezra Wood

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

Funded Amount: $130,264

Abstract
San Antonio is on the cusp of being in non-attainment of the U.S. Environmental Protection Agency's air quality standard for ozone, also known as photochemical smog. In order to mitigate potentially bad air quality in San Antonio, regulators will benefit from a full understanding of the sources of ozone and how future emissions can affect its concentration. During May 2017, a team of researchers from Drexel University, University of Houston, Rice University, and Aerodyne Research, Inc. conducted a field study focused on ozone air pollution in the greater San Antonio Area. The main goals were to collect data that would enable a determination of the rate at which ozone was being produced by chemical reactions in the air, to determine the relative importance of upwind and urban sources of ozone precursor emissions, and to determine the importance of different types of emissions (e.g., nitrogen oxides from fossil fuel combustion vs. biogenic volatile organic compounds from trees). The measurements from these field measurements were largely successful. In this project, the research team at Drexel University will analyze many aspects of the data in order to address the above goals. This research will consist of three tasks:

1. To characterize the relationship between the ozone production rate (calculated using measured concentrations of nitric oxide and total peroxy radicals) and the concentrations of other pollutants, including nitrogen oxides and volatile organic compounds,

2. To conduct zero-dimensional modeling of the photochemistry (in which spatial variations in pollutant concentrations are not considered) in order to determine if chemical models can successfully characterize the photochemistry, and

3. To conduct 3-dimensional air quality modeling, in which knowledge of emissions, meteorology, and the relevant chemistry are combined to predict spatially-resolved concentrations of ozone and other pollutants.

Project Activities
During the quarter ending 5/31/2019, the project team members focused on tasks 2 and 3 as task 1 is largely complete.

For Task 2 (conduct 0-D photochemical modeling of the dataset with several model chemical mechanisms to investigate ozone production rates at four SAFS measurement sites), we have mostly completed the modeling at the UTSA, Corpus Christi, Floresville, and Traveler's World measurement sites. The first three sites utilized the Aerodyne Mobile Laboratory data, and we were able to compare the peroxy radical concentrations (and ozone production rates) predicted by the models with the measured values. For Traveler's World, which is a more centrally located site subject to higher NOx concentrations, we used the combined Baylor U. / Rice U. / U. of Houston dataset. Interestingly, the Master Chemical Mechanism, which is the most explicit of all

the mechanisms used, produced the highest ozone formation rates – roughly a factor of two higher than the observed values.

Finally we have continued work on Task 3: Apportion ozone concentrations to location-specific emission sources using 3-D air quality modeling with the instrumented Community Multiscale Air Quality model (CMAQ). CMAQ version 5.2.1 was installed on the Drexel high performance computing cluster and in the last few weeks we have started to collect meaningful output with which to compare to measurements recorded at TCEQ-operated monitoring sites across the state and the SAFS data. In addition to comparing the ground-based concentrations predicted by CMAQ to measurements from the monitoring sites, we have also begun comparing the total NO_2 column predicted by the model to those measured by satellite spectrometers. If we are satisfied that the NOx emissions and chemistry are doing an adequate job, then we will continue with the rest of Task 3 which will entail determining the sensitivity of ozone formation to precursor emissions.

FINANCIAL STATUS REPORT

Initial funding for fiscal years 2016 and 2017 was established at $1,000,000 each, for a total award of $2,000,000 for the FY 2016/2017 biennium. On September 4, 2017, the AQRP contract was renewed for the FY 2018/2019 biennium and additional funding of $750,000 per year was awarded. For each year, the funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are:

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

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

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

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

Program Administration

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

During the reporting period several staff members were involved, at various levels of effort, in the administration of the AQRP. Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. Maria Stanzione, AQRP Program Manager, assisted Dr. Allen in the program administration. Shannon Thorne and Susan McCoy provided assistance with program organization and financial management.

Beginning September 1, 2018, The University of Texas at Austin switched to a federally negotiated fringe benefit rate. For fiscal year 2018/2019 the fringe rates are:

Full-time/Benefits Eligible (including Graduate Students)	29%
Part-time/Benefits Eligible	39.60%
Part-time/Non-benefits Eligible	5.80%

For fiscal year 2019/2020, beginning September 1, 2019, the federally negotiated fringe benefit rates will be:

All Benefits Eligible (including Graduate Students and Part-Time employees)	29.8%
Part-time/Non-benefits Eligible	5.10%

Table 1: Administration Budgets

Administration Budget (includes Council Expenses)
FY 2016/2017

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

Administration Budget (includes Council Expenses)
FY 2018/2019

Budget Category		FY18 Budget	FY19 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$53,800.00	$53,700.00	$107,500.00	$67,076.88	$40,423.12
Fringe Benefits		$14,320.00	$12,930.00	$27,250.00	$16,740.86	$10,509.14
Travel		$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$1,500.00	$3,000.00	$4,500.00	$1,284.51	$3,215.49
Equipment						
Total Direct Costs		$69,620.00	$69,630.00	$139,250.00	$85,102.25	$54,147.75
Authorized Indirect Costs		$5,380.00	$5,370.00	$10,750.00	$6,707.70	$4,042.30
10% of Salaries and Wages						
Total Costs		**$75,000.00**	**$75,000.00**	**$150,000.00**	**$91,809.95**	**$58,190.05**

ITAC

Table 2: ITAC Budgets

ITAC Budget
FY 2016/2017

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

ITAC Budget
FY 2018/2019

Budget Category		FY18 Budget	FY19 Budget	Total	Expenses	Remaining Balance
Personnel/Salary						
Fringe Benefits						
Travel		$7,500.00	$7,500.00	$15,000.00	$4,384.23	$10,615.77
Supplies		$1,500.00	$1,500.00	$3,000.00	$284.86	$2,715.14
Total Direct Costs		$9,000.00	$9,000.00	$18,000.00	$4,669.09	$13,330.91
Authorized Indirect Costs						
10% of Salaries and Wages						
Total Costs		**$9,000.00**	**$9,000.00**	**$18,000.00**	**$4,669.09**	**$13,330.91**

Project Management

Table 3: Project Management Budgets

Project Management Budget
FY 2016/2017

Budget Category		FY16 Budget	FY17 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$53,470.31	$51,727.58	$105,197.89	$105,197.89	$0.00
Fringe Benefits		$11,337.19	$12,236.62	$23,573.81	$23,573.81	$0.00
Travel		$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$0.00	$0.00	$176.36	$176.36	$0.00
Other		$0.00	$0.00	$0.00	$0.00	$0.00
Total Direct Costs		$64,938.86	$63,964.20	$128,948.06	$128,948.06	$0.00
Authorized Indirect Costs		$5,347.03	$5,172.76	$10,519.79	$10,519.79	$0.00
10% of Salaries and Wages						
Total Costs		**$70,330.89**	**$69,136.96**	**$139,467.85**	**$139,467.85**	**$0.00**

Project Management Budget
FY 2018/2019

Budget Category		FY18 Budget	FY19 Budget	Total	Expenses	Remaining Balance
Personnel/Salary		$38,060.00	$38,060.00	$76,120.00	$39,949.35	$36,170.65
Fringe Benefits		$9,134.00	$9,134.00	$18,268.00	$11,055.89	$7,212.11
Travel		$0.00	$0.00	$0.00	$0.00	$0.00
Supplies		$1000.00	$1,000.00	$2,000.00	$0.00	$2,000.00
Other		$2,500.00	$1,718.00	$4,218.00	$0.00	$4,218.00
Total Direct Costs		$50,694.00	$49,912.00	$100,606.00	$51,005.24	$49,600.76
Authorized Indirect Costs		$3,806.00	$3,806.00	$7,612.00	$3,994.94	$3,617.06
10% of Salaries and Wages						
Total Costs		**$54,500.00**	**$53,718.00**	**$108,218.00**	**$55,000.18**	**$53,217.82**

Research Projects

A total of eight (8) projects requesting $1,231,101 in funding, were selected out of forty (40) proposals submitted to the AQRP RFP for the 2018-2019 biennium. Table 4 on the following page shows the distribution of the projects across the fiscal years for both FY 16-17 and FY 18-19.

The 2018 – 2019 budget allocates $1,223,000.00 for research projects ($611,500 per fiscal year). After all FY 2016 – 2017 research projects and program activities were complete, $7,559.39 in FY 2017 funds remained ($1,558,35 in Research/Contractual and $6,001.04 in Project Management). These funds were all transferred to the Research/Contractual category, and then assigned to partially fund project 19-023. That left a shortage of $541.61 in Research/Contractual funding. In order to fully fund all research projects, $782 was transferred from the FY 2019 ITAC funds to the FY 2019 Research/Contractual category. (Even though the total shortfall is $542, the FY 2018 projects do not use all of the funds allocated to them, and we cannot move funds between fiscal years, so the FY 2019 shortfall is actually $782.)

The portion of project 19-023 that was funded with FY 2017 was expended in February of 2019. This fully disburses all FY 2016 and 2017 funding.

Table 4: Contractual/Research Project Budget

FY 16-17

Contractual Expenses				
FY 16 Contractual Funding		**$815,000**		
FY 16 Contractual Funding Transfers		**$9,513**		
FY 16 Total Contractual Funding		**$824,513**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
16-008	University of Houston	$191,366	$189,684.87	$1,681.13
16-010	Sonoma Technology, Inc.	$69,075	$69,075.00	$0.00
16-011	Ramboll Environ	$158,134	$158,127.36	$6.64
16-019	Univ. of Texas - Austin	$118,019	$117,551.39	$467.61
16-019	Ramboll Environ	$62,622	$62,618.81	$3.19
16-031	UNC - Chapel Hill	$225,000	$223,820.08	$1,179.92
FY 16 Total Contractual Funding Awarded		$824,216		
FY 16 Contractual Funds Expended (Init. Projects)			$820,877.51	
FY 16 Contractual Funds Remaining to be Spent				$3,635.83
FY 16 Additional Expenditures				
	State of the Science	$3,788.49	$3,635.83	$152.66
			$824,513.34	
FY 16 Contractual Funds Remaining to be Spent				$0.00

Table 4: Contractual/Research Project Budget (continued)

FY 16-17 (continued)

FY 17 Contractual Funding		**$815,000**		
FY 17 Contractual Funding Transfers		**$15,863**		
FY 17 Total Contractual Funding		**$830,863**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
17-007	Univ. of Texas - Austin	$205,500	$202,348.20	$3,151.80
17-024	Atmospheric and Environmental Research, Inc.	$170,039	$170,039.00	$0.00
17-032	Drexel University	$59,000	$58,958.17	$41.83
17-039	Univ. of Alabama - Huntsville	$149,227	$149,226.81	$0.19
17-053	Aerodyne Research, Inc.	$185,193	$185,193.00	$0.00
17-SAFS	Univ. of Texas - Austin	$46,000	$35,999.96	$10,000.04
FY 17 Total Contractual Funding Awarded		$814,959		
FY 17 Contractual Funding Expended (Init. Projects)			$801,765.14	
FY 17 Contractual Funds Remaining to be Spent				$29,097.90
FY 17 Additional Expenditures				
	State of the Science	$22,211.51	$21,538.51	$673.00
19-023	UT Austin	$7,559.39	$7,559.39	$0.00
FY 17 Contractual Funds Expended			$830,863.04	
FY 17 Contractual Funds Remaining to be Spent				$0.00
Total Contractual Funding		$1,655,376		
Total Contractual Funding Awarded		$1,655,376		
Total Contractual Funding Remaining to be Awarded		$0		
Total Contractual Funds Expended to Date			$1,655,376	
Total Contractual Funds Remaining to be Spent				$0

Table 4: Contractual/Research Project Budget (continued)

FY 18-19

Contractual Expenses				
FY 18 Contractual Funding		**$611,500**		
FY 18 Contractual Funding Transfers		**$0**		
FY 18 Total Contractual Funding		**$611,500**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
18-005	UC - Irvine	$139,193	$6,445.87	$132,747.13
18-005	Ramboll	$28,953	$871.75	$28,081.25
18-007	Ramboll	$150,000	$23,233.06	$126,766.94
18-010	TAMU	$121,000	$13,982.88	$107,017.12
18-022	UT Austin	$85,768	$58,670.46	$27,097.54
18-022	Sonoma Tech, Inc.	$86,346	$9,487.75	$76,858.25
FY 18 Total Contractual Funding Awarded		$611,260		
FY 18 Contractual Funds Expended (Init. Projects)			$112,691.77	
FY 18 Contractual Funds Remaining to be Spent				$498,808.23
FY 19 Contractual Funding		**$611,500**		
FY 19 Contractual Funding Transfers		**$782**		
FY 19 Total Contractual Funding		**$612,282**		
Project Number		Amount Awarded (Budget)	Cumulative Expenditures	Remaining Balance
19-023	UT Austin	$85,736.61	$50,954.45	$34,782.16
19-023	Ramboll	$65,013	$43,635.82	$21,377.18
19-025	Aerodyne Research, Inc.	$199,974	$77,938.12	$122,035.88
19-031	Baylor University	$98,087	$4,310.89	$93,776.11
19-031	University of Houston	$33,207	$5,069.76	$28,137.24
19-040	Drexel University	$130,264	$53,710.76	$76,553.24
FY 19 Total Contractual Funding Awarded		$612,282		
FY 19 Contractual Funding Expended (Init. Projects)			$235,619.80	
FY 19 Contractual Funds Remaining to be Spent				$376,662.20
Total Contractual Funding		$1,223,782		
Total Contractual Funding Awarded		$1,223,542		
Total Contractual Funding Remaining to be Awarded		$240		
Total Contractual Funds Expended to Date			$348,311.57	
Total Contractual Funds Remaining to be Spent				$875,470