Work Plan for

ANALYSIS OF OZONE PRODUCTION AND ITS SENSITIVITY IN HOUSTON USING THE DATA COLLECTED DURING DISCOVER-AQ

AQRP Project 14-020

Prepared for

Air Quality Research Program (AQRP)
University of Texas at Austin

Prepared by

Xinrong Ren
Department of Atmospheric and Oceanic Science
University of Maryland
5830 University Research Court
NCWCP Room 4259
College Park, Maryland 20740
xinrong@atmos.umd.edu
301-683-1391

Revision #: R5

January 26, 2014

BACKGROUND

Despite great efforts undertaken in the past decades to address the problem of high ozone concentrations, our understanding of the key precursors that control tropospheric ozone production remains incomplete and uncertain [Molina and Molina, 2004; Xue et al., 2013]. The ozone problem is a complex coupling of emissions, chemical transformation, and dynamic transport at different scales [Jacob, 1999]. A major challenge in regulating ozone pollution lies in comprehending its complex and non-linear chemistry with respect to ozone precursors, i.e., nitrogen oxides (NO_x) and volatile organic compounds (VOCs) that varies with time and location. Understanding of the non-linear relationship between ozone production and its precursors is critical for the development of an effective ozone control strategy.

Sensitivity of ozone production to NO_x and VOCs represents a major uncertainty for oxidant photochemistry in urban areas [Sillman et al., 1995; 2003]. In urban environments, ozone is formed through photochemical processes when its precursors NO_x and VOCs are emitted into the atmosphere from many sources. Depending on physical and chemical conditions, the production of ozone can be either NO_x-sensitive or VOC-sensitive due to the complexity of these photochemical processes. Therefore effective ozone control strategies heavily rely on the accurate understanding of how ozone responds to the reduction of NO_x or VOC emissions, which is usually simulated by photochemical air quality models [e.g., Sillman et al., 2003; Lei et al., 2004; Mallet and Sportisse, 2005; Li et al, 2007; Tang et al., 2010; Xue et al., 2013]. However, those model-based studies have inputs or parameters subject to large uncertainties, which can affect not only the simulated levels of ozone but also the ozone dependence on its precursors.

There are very limited observation-based studies on ozone production and its sensitivity to NO_x and VOCs. Using in-situ aircraft observations, Kleinman et al. [2005a] studied ozone production in five U.S. cities and found that ozone production rates vary from nearly zero to 155 ppb h^{-1} with differences in ozone production depending on precursor concentrations, such as radical sources, NO_x, and VOCs. They also found that in Houston, NO_x and light olefins are co-emitted from petrochemical facilities leading to the highest ozone production of the five cities [Kleinman et al., 2005a]. Using the data collected at a single location during the Study of Houston Atmospheric Radical Precursors (SHARP) in spring 2009, a temporal variation of O_3 production was observed: VOC-sensitive in the early morning and NO_x-sensitive for most of afternoon [Ren et al., 2013]. This is similar to the behavior observed in two previous summertime studies in Houston: the Texas Air Quality Study in 2000 (TexAQS 2000) and the TexAQS II Radical and Aerosol Measurement Project in 2006 (TRAMP 2006) [Mao et al., 2010]. In a recent study using measurements in four cities in China, the ozone production was found to be in a VOC-sensitive regime in both Shanghai and Guangzhou, but in a mixed regime in Lanzhou [Xue et al., 2013]. These studies have limited spatial and/or temporal coverage in the data collected during the field campaigns. An intensive study of spatial and temporal variations of ozone production and it sensitivity to NO_x and VOCs is thus needed in order to provide a scientific basis to develop a non-uniform emission reduction strategy for O_3 pollution control in urban areas like Houston.

During the Deriving Information on Surface Conditions from COlumn and VERtically Resolved Observations Relevant to Air Quality (DISCOVER-AQ) campaign in Houston in August/September 2013 [DISCOVER-AQ whitepaper], a comprehensive suite of measurements were collected from various platforms including the National Aeronautics and Space Administration (NASA) P-3B and B-200 aircraft, ground surface sites, and mobile laboratories. The rich data sets produced during these campaigns provide a great opportunity to examine and improve our understanding of atmospheric photochemical oxidation processes related to the formation of secondary air pollutants like ozone and particulate matter (PM). Here we propose an analysis of ozone production and its sensitivity to NO_x and VOCs using an observation-constrained box model. Spatially and temporally resolved ozone production and its sensitivity will be investigated. Based on the results from this project, a non-uniform emission reduction strategy, i.e., where/when to control what, for an O_3 pollution control plan will be proposed to provide scientific information for policy decisions.

STATEMENT OF WORK

GOALS AND OBJECTIVES

The purpose of this work is to provide scientific information for policy decisions related to ozone control strategies for the State Implementation Plan (SIP) in Texas, particularly those that heavily rely on the use of appropriately represented chemical models. This project specifically addresses one of the AQRP priority research areas: Improving the understanding of ozone and particulate matter (PM) formation, and quantifying the characteristics of emissions in Texas through analysis of data collected during the DISCOVER-AQ campaign [Texas Air Quality Research Program, 2013].

2.1.1 Tasks

The following tasks will be performed in this project. The deliverable in each task and its estimated completion date are listed.

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

   - We will conduct both Weather Research and Forecasting-Community Multiscale Air Quality (WRF-CMAQ) and box model runs to calculate ozone production and its sensitivity to NOx and VOCs. Using the CMAQ and box model results, we will address the following questions. Is ozone production in downtown Houston more likely to be sensitive to VOCs or to NO_x? Is ozone production in the Houston Ship Channel more likely to be sensitive to NO_x or to VOCs? What is the relationship between ozone production sensitivity and the chemical aging of air plumes as defined by the ratio of NO_x to NO_y?

   Deliverable: A series of maps for ozone production and its sensitivity to NOx and VOCs in Houston will be produced and archived at different times of day.

   Expected completion date: June 2015

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

   - Using the CMAQ and box model results, we will examine the differences in the diurnal profiles of ozone production among the eight surface sites where the P-3B conducted spiral profiles and look into possible reasons behind these differences (e.g., different NOx and VOCs levels and their diurnal variations at the eight surface sites).

   Deliverable: A series of plots for diurnal variations of ozone production and its sensitivity to NOx and VOCs at eight spiral sites in Houston will be created and archived.

   Expected completion date: June 2015

3) To provide scientific information for a non-uniform emission reduction strategy to control O_3 pollution in Houston using spatial and temporal variations of ozone production and its sensitivity to NO_x and VOCs.
   - Using the spatial and temporal variations of ozone production and its sensitivity to NOx and VOCs, we will address the question: at a specific location and at a specific time, which one should be controlled in order to reduce ozone, NOx or VOCs, based on ozone production is sensitive to NOx or VOCs?

   Deliverable: Pollution control strategy, i.e., when, where to control what in order to control ozone pollution in Houston will be proposed based on the analysis of spatial and temporal variations of ozone production and its sensitivity to NOx and VOCs.
   Expected completion date: July 2015

4) To calculate ozone production efficiency (OPE), defined as the ratio of the ozone production rate to the NOx oxidation rate, at different locations using the ratio of ozone production rate to the NO_x oxidation rate calculated in the box model.
   - Using the CMAQ and box model results, we will calculate OPE and address these questions: what are the major factors influencing different OPEs at different locations? What are the relationships between OPE and NO_x/VOCs/radical sources?

   Deliverable: Ozone production efficiency (OPE) will be calculated and archived at the eight spiral locations.

   Expected completion date: August 2015

2.1.2 Data Analysis

We will use a chemical transport model (WRF-CMAQ) and a box model (based on the Carbon Bond mechanism Version 5 (CB05)) to analyze the data collected during DISCOVER-AQ 2013 in Houston.

(1) WRF-CMAQ Model Simulations

This project will utilize the WRF and CMAQ models run down to a horizontal resolution of 4 km that will cover the entire DISCOVER-AQ field campaign. WRF and CMAQ model descriptions can be found on their respective webpages: www.wrf-model.org and www.cmaq-model.org. The WRF model will be driven by the 12 km North American Mesoscale (NAM) model and the Multi-scale Ultra-high Resolution (MUR) sea surface temperature analysis (http://podaac.jpl.nasa.gov/Multi-scale_Ultra-high_Resolution_MUR-SST). The CMAQ model will utilize chemical initial and boundary conditions from the Model for Ozone And Related Chemical Tracers (MOZART) Chemical Transport Model (CTM) (https://www2.acd.ucar.edu/gcm/mozart) and the CB05 chemical mechanism. The 2012 baseline anthropogenic emissions from the Texas Commission on Environmental Quality (TCEQ) will be used as input to CMAQ. These emissions contain the most-up-to-date Texas anthropogenic emissions inventory and a compilation of emissions estimates from Regional Planning Offices throughout the US. Biogenic emissions will be calculated online within CMAQ with Biogenic Emission Inventory System (BEIS). Biomass burning emissions will come from the Fire Inventory from the National Center for Atmospheric Research (NCAR) Version 1 (FINNv1), and lightning emissions will be calculated online within CMAQ.

The CMAQ model will be run with process analysis to obtain ozone production ($P(O_3)$), higher oxides of nitrogen gases production (P(NOz), hydrogen peroxide production ($P(H_2O_2)$), nitric acid production ($P(HNO_3)$, and ozone production efficiency (OPE). The ratio of $P(H_2O_2)$ and $P(HNO_3)$ will be used to determine which regions are NOx and VOC limited. The 36, 12, and 4 km modeling domains that will be utilized in this study are shown in Figure 1. The CMAQ modeling domains will be slightly smaller than the WRF modeling domains (grid cells close to the horizontal edge of the WRF domains will not be included in the CMAQ domains). WRF and CMAQ will be evaluated with National Weather Service observations (meteorology), EPA's Air Quality System (AQS) observations (O_3 and particulate matter with particle diameters less than 2.5 micrometers ($PM_{2.5}$)), and final quality assured DISCOVER-AQ ground-, and aircraft-based observations of O_3, carbon monoxide (CO), oxides of nitrogen compounds (nitric oxide + nitrogen dioxide, NO_x) and NO_x plus all other higher oxides of nitrogen gases (NO_y), and ammonia (NH_3) as well as a suite of VOC species, and a suite of aerosols). DISCOVER-AQ data and descriptions of the data are available at http://www-air.larc.nasa.gov/missions/discover-aq/discover-aq.html. Curtain figures along the flight track of the P3 will be created to compare model predictions with observations. The following statistics will be calculated between the model results and observations to evaluate the model predictions and are shown in Table 1: mean bias, normalized mean bias, normalized mean error, and root mean square error. Model-observation comparisons with the figures and statistics will be analyzed to ascertain why model errors and uncertainties exist (i.e., errors in the emissions, chemistry, and/or transport processes). CMAQ model output will be analyzed to map the OPE, NO_X limited areas, and VOC limited areas throughout the Houston metropolitan area. CMAQ model output will be extracted for use in the box model.

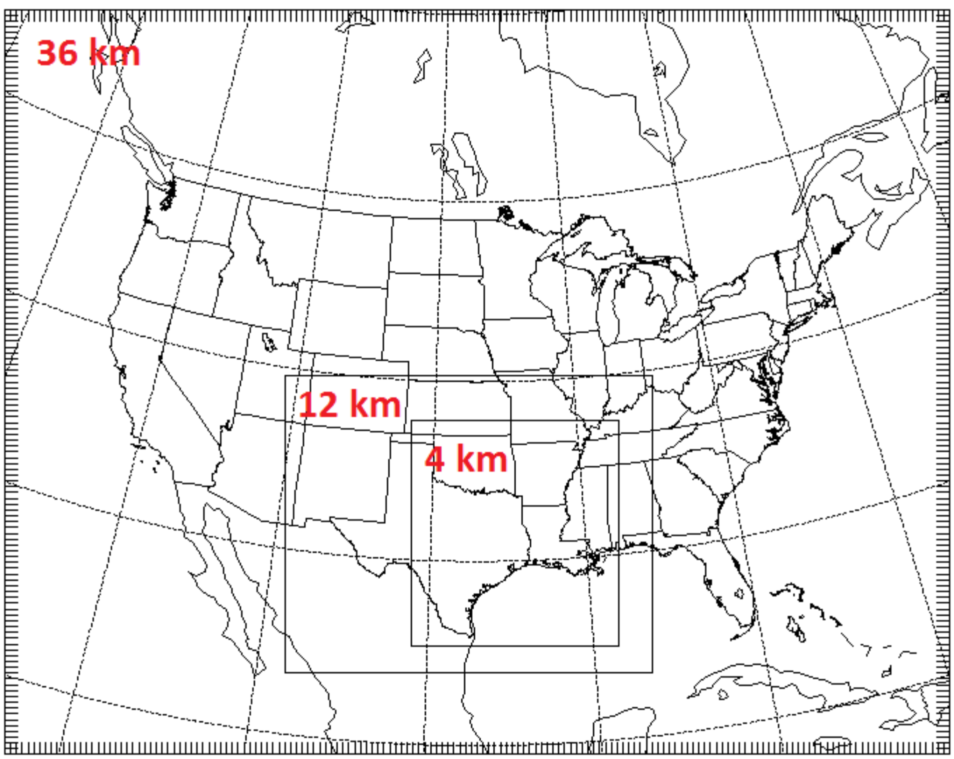

Figure 1: Location of the 36 km , 12 km, and 4 km domains that will be used in the WRF and CMAQ modeling. Results from the 4 km domain will be utilized in this project.

Table 1: Statistics that will be calculated for performing the model evaluation.

Statistic	Equation
Mean Bias	$MB = \frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)$
Normalized Mean Bias	$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i} \times 100\%$
Normalized Mean Error	$NME = \frac{\sum_{i=1}^{N}\lvert M_i - O_i\rvert}{\sum_{i=1}^{N} O_i} \times 100\%$
Root Mean-Square Error	$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$

*M: model results; O: observations

(2) Box Model Simulations

We will use an observation-constrained box model with Carbon Bond Mechanism Version 2005 (CB05) to simulate the oxidation processes in Houston during DISCOVER-AQ. Use of a box model is essential because it can quickly, in a matter of minutes, simulate environmental conditions. Measurements made on the P-3B and at the eight science sites will be used as input to constrain the box model. Using the model results, we will calculate the ozone production rate and its sensitivity to NO_x and VOCs. The model results will also allow us to calculate ozone production efficiency at different locations and at different times of a day.
The Carbon Bond Mechanism Version 2005 (CB05) will be used in box modeling for the data analysis in this project. These mechanisms are well known and have been actively in use in research and regulatory applications [Yarwood et al., 2005; Goliff et al., 2013]. The original mechanisms will be used while kinetic data will be updated based on the most recent chemical kinetic data evaluations [e.g., Sander et al, 2011; Atkinson et al., 2004; 2006; 2007; 2008]. The box model will be constructed and run on the platform of FACSIMILE for Windows software (MCPA Software, Ltd), which has been successfully used in the modeling effort for previous research projects [e.g., Chen et al., 2010; Ren et al., 2013].

The Carbon Bond Mechanism (CB05) [Yarwood et al., 2005] is an updated version of CB4. In contrast to the previous version, (1) inorganic reactions are extended to simulate remote to polluted urban conditions; and (2) two extensions are available to be added to the core mechanism for modeling explicit species and reactive chlorine chemistry. Organic species are lumped according to the carbon bond approach, that is, bond type, e.g., carbon single bond and double bond. Reactions are aggregated based on the similarity of carbon bond structure so that fewer surrogate species are needed in the model. For instance, the single-bonded one-carbon-atom surrogate photosynthetically active radiation (PAR) represents alkanes and most of the alkyl groups. Some organics (e.g., organic nitrates and aromatics) are lumped in a similar manner as done in Regional Atmospheric Chemical Mechanism, Version 2 (RACM2).

In order to run the box model, measurements, including long-lived inorganic and organic compounds and meteorological parameters (temperature, pressure, humidity, and photolysis frequencies) measured on the NASA P-3B will be averaged into 1-minute values that became the model input. For each data point, the model will run for 24 hours, long enough to allow most calculated reactive intermediates to reach steady state but short enough to prevent the buildup of secondary products. A deposition lifetime of two days will be assumed for all calculated species to avoid unexpected accumulation of these species in the model. At the end of 24 hours, the model generated time series of OH, HO_2, RO_2, and other reactive intermediates with an interval of 1 minute. The box model will cover the entire P-3B flight track during DISCOVER-AQ, including the eight science sites where the P-3B conducted spirals.

It is worth noting that unlike a three-dimensional chemical transport model, the zero-dimensional (box) model simulations will not include advection and emissions, although advection and emissions are certainly important factors for the air pollution formation. Because all of the long-lived radical precursors and O_3 precursors were measured and used to constrain the box model calculations, the advection and emissions can be neglected for this project of radicals and their production and loss rates.

During the day, the photochemical O_3 production rate is essentially the production rate of NO_2 molecules from HO_2 + NO and RO_2 + NO reactions [*Finlayson-Pitts and Pitts*, 2000]. The net instantaneous O_3 production rate, $P(O_3)$, can be written approximately as the following equation:

$$P(O_3) = k_{HO_2+NO}[HO_2][NO] + \sum k_{RO_{2i}+NO}[RO_{2i}][NO] - k_{OH+NO_2+M}[OH][NO_2][M] - P(RONO_2)$$
$$-k_{HO_2+O_3}[HO_2][O_3] - k_{OH+O_3}[OH][O_3] - k_{O(^1D)+H_2O}[O(^1D)][H_2O] - L(O_3+alkenes) \quad (1)$$

where, *k term*s are the reaction rate coefficients. The negative terms in Eq. (1) correspond to the reaction of OH and NO_2 to form nitric acid, the formation of organic nitrates, $P(RONO_2)$, the reactions of OH and HO_2 with O_3, the photolysis of O_3 followed by the reaction of $O(^1D)$ with H_2O, and O_3 reactions with alkenes.

The dependence of O_3 production on NOx and VOCs can be categorized into two typical scenarios: NO_x sensitive and VOC sensitive. We use the method proposed by *Kleinman* [2005b] to evaluate the O_3 production sensitivity using the ratio of L_N/Q, where L_N is the radical loss via the reactions with NO_x and Q is the total primary radical production. Because the radical production rate is approximately equal to the radical loss rate, this L_N/Q ratio represents the fraction of radical loss due to NO_x. It was found that when L_N/Q is significantly less than 0.5, the atmosphere is in a NO_x-sensitive regime, and when L_N/Q is significantly greater than 0.5, the atmosphere is in a VOC-sensitive regime [*Kleinman et al.*, 2001; *Kleinman*, 2005b]. Note that the contribution of organic nitrates impacts the cut-off value for L_N/Q to determine the ozone production sensitivity to NO_x or VOCs and this value may vary slightly around 0.5 in different environments.

Using the box model simulation results, we will calculate ozone production rates based on Eq. (1) and investigate the ozone production sensitivity to NO_x and VOCs along the NASA P-3B flight tracks during DISCOVER-AQ as well as at eight surface sites where the P-3B conducted spiral profiles (Figure 1). Spatial and temporal variations of ozone production and its sensitivity along the P-3B flight tracks and at the spiral sites will be investigated in detail. Science questions listed in the Objectives Section above can then be answered.

The eight spiral sites are located in Conroe, West Houston, Channelview, Moody Tower, Deer Park, Manvel Croix, Smith Point, and Galveston, respectively. At the Smith Point and Galveston sites, additional measurements were made besides the existing TCEQ measurements. The Penn State NATIVE trailer was deployed at the Smith Point site to collect data for ozone, sulfur dioxide (SO_2), nitric oxide (NO), total reactive nitrogen (NOy), carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4) and meteorological parameters (temperature, pressure, relative humidity, wind speed, wind direction, and solar radiation). At the Galveston site, research grade instrumentation was deployed at the Galveston site to measure ozone, SO_2, and $NO/NO_2/NO_y$. These additional measurements will be used to constrain the box model. Measurements were typically limited to ozone and meteorological parameters at most other sites while a few sites were equipped with the commercial NO/NO_x instrument. For those sites with limited observations, we will use the three-dimensional chemical transport model, CMAQ, to generate critical parameters such as photolysis frequencies (J values) and speciated VOCs to constrain the box model.

KEY PERSONNEL

Dr. Xinrong Ren

Dr. Xinrong Ren is a Senior Research Scientist at University of Maryland's Department of Atmospheric and Oceanic Science. He is an established atmospheric chemist with extensive experience in atmospheric chemistry through participation in a variety of ground-based and aircraft air quality studies. Dr. Ren will be the PI on this project and will oversee the project progress and be responsible for the project reporting. A few recent air quality field projects Dr. Ren and his group were involved in include the Study of Houston Atmospheric Radical Precursors (SHARP, 2009), the CalNex study (2010), the NSF/NASA Deep Convective Clouds and Chemistry (DC3) project (2012), and the DISCOVER-AQ 2013 campaign in Houston. In these studies, Dr. Ren and his group deployed highly sensitive instruments to measure important photochemical species like OH, HO_2, and HONO. During the DISCOVER-AQ study in Houston, Dr. Ren and his colleagues made some trace gas measurements at two ground sites.

Dr. Christopher Loughner

Dr. Christopher Loughner is an Assistant Research Scientist at University of Maryland's Earth System Science Interdisciplinary Center (ESSIC) and will serve as a co-I on this project. Dr. Loughner has expertise in developing, updating, and modifying regional three-dimensional meteorological and air quality models [Loughner et al., 2011, 2012], running these models at high resolutions [Loughner et al., 2011, 2013a; Goldberg et al., 2013; He et al., 2013; Tzortziou et al., 2013], and analyzing model output alongside aircraft-, ground-, ship-, and space-based observations [Loughner et al., 2011, 2013a, 2013b, Goldberg et al., 2013; He et al., 2013; Tzortziou et al., 2013; Flynn et al., 2013]. He has used a combination of models and observations to investigate the impacts of the Chesapeake Bay breeze circulation, boundary layer mixing and venting, local and regional transport processes, aqueous chemistry inside fair-weather cumulus clouds, air pollution deposition processes, and urban heat island effects on air quality. Dr. Loughner will be responsible for performing and evaluating WRF meteorological and CMAQ air quality model simulations for all of the DISCOVER-AQ deployments, including Houston. Under the proposed project, Dr. Loughner will also be responsible for revising the WRF-CMAQ with process analysis to output $P(O_3)$ and ozone production efficiency (OPE). He will help Co-I Gina Mazzuca to run the box model by providing chemical initial and boundary conditions, meteorological, and emissions input files for the box model. Dr. Loughner will re-run CMAQ using a similar model set-up as being performed for another Texas AQRP Project, Project # 14-004, with the difference being the inclusion of process analysis to output P(O3), P(NOz), ozone production efficiency (OPE), and the sensitivity of ozone production to NOx and VOCs. Dr. Loughner will analyze the CMAQ results and assist in extracting CMAQ model output for input to the box model.

Ms. Gina Mazzuca

Mr. Gina Mazzuca is a graduate student at University of Maryland's Department of Atmospheric and Oceanic Science and will be responsible in running the box model by working with Drs. Loughner and Ren. Ms. Mazzuca has been working with the data from the DISCOVER-AQ campaigns to understand the balloon profiles and the NASA P-3B profiles. She is currently working on the Houston and Edgewood balloon and P-3B profiles as well as analyzing the influence of bay/sea breezes in the lowest part of the boundary layer (first 500m) by use of the balloon profiles from the Houston campaign (at Smith Point) and the Maryland campaign (Edgewood). Ms. Mazzuca will be responsible for the box model simulations and will assist Drs. Loughner and Ren to evaluate the model results and contribute to reports and presentations for this project.

DELIVERABLES

Executive Summary

At the beginning of the project, an Executive Summary will be submitted to the Project Manager for use on the AQRP website. The Executive Summary will provide a brief description of the planned project activities, and will be written for a non-technical audience.
Due Date: Friday, January 9, 2015

Quarterly Reports

The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	January & February 2015	Friday, February 27, 2015
Quarterly Report #2	March, April, May 2015	Friday, May 29, 2015
Quarterly Report #3	June, July, August 2015	Monday, August 31, 2015
Quarterly Report #4	September, October, November 2015	Monday, November 30, 2015

Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY14-15 MTR Template found on the AQRP website.
Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start - February 28, 2015	Monday, March 9, 2015
Technical Report #2	March 1 - 31, 2015	Wednesday, April 8, 2015
Technical Report #3	April 1 - 28, 2015	Friday, May 8, 2015
Technical Report #4	May 1 - 31, 2015	Monday, June 8, 2015
Technical Report #5	June 1 - 30, 2015	Wednesday, July 8, 2015
Technical Report #6	July 1 - 31, 2015	Monday, August 10, 2015
Technical Report #7	August 1 - 31, 2015	Tuesday, September 8, 2015

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY14-15 FSR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start – February 28, 2015	Monday, March 16, 2015
FSR #2	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #3	April 1 - 28, 2015	Friday, May 15, 2015
FSR #4	May 1 - 31, 2015	Monday, June 15, 2015
FSR #5	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #6	July 1 - 31, 2015	Monday, August 17, 2015
FSR #7	August 1 - 31, 2015	Tuesday, September 15, 2015
FSR #8	September 1 - 30, 2015	Thursday, October 15, 2015
FSR #9	Final FSR	Monday, November 16, 2015

Draft Final Report

A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.
Due Date: Tuesday, August 18, 2015

Final Report

A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.
Due Date: Wednesday, September 30, 2015

Project Data

All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information.

AQRP Workshop

A representative from the project will present at the AQRP Workshop in June 2015.

SCHEDULE
The schedule for this project and key milestones are listed in Table 2-2 below.

	2014		2015								
Deliverable	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
Task 1 - Project Work Plan											
Task 2 - Monthly Reports											
Task 3 - Final Data Merge											
Task 4a - AQRP Presentations											
Task 4b - Draft Final Report											
Task 4c - Final Report											

Table 2-2. Project timeline

REFERENCES

Atkinson, R., et al., Evaluated kinetic and photochemical data for atmospheric chemistry: Volume I - gas phase reactions of Ox, HOx, NOx and SOx species, *Atmos. Chem. Phys.*, 4, 1461-1738, 2004.

Atkinson, R., et al., Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II - gas phase reactions of organic species, *Atmos. Chem. Phys.*, 6, 3625-4055, 2006

Atkinson, R., et al., Evaluated kinetic and photochemical data for atmospheric chemistry: Volume III - gas phase reactions of inorganic halogens, *Atmos. Chem. Phys.*, 7, 981-1191, 2007.

Atkinson, R., et al., Evaluated kinetic and photochemical data for atmospheric chemistry: Volume IV - gas phase reactions of organic halogen species, *Atmos. Chem. Phys.*, 8, 4141-4496, 2008.

Banta, R., C. J. Senff, J. Nielsen-Gammon, L. Darby, T. Ryerson, R. Alvarez, P. Sandberg, E. Williams, and M. Trainer, A bad air day in Houston, Bullet. Am. Meteorol. Soc., 86, 657-669, doi: 10.1175/BAMS-86-5-657, 2005.

Chen, S., X. Ren, J. Mao, Z. Chen, W. H. Brune, , B. Lefer, B. Rappenglück, J. Flynn, J. Olson, J. H. Crawford, A comparison of chemical mechanisms based on TRAMP–2006 field data, Atmos. Environ., 44(33), 4116-4125, 2010.

Chen, F., S. Miao, M. Tewari, J.-W. Bao, and H. Kusaka, A numerical study of interactions between surface forcing and sea breeze circulations and their effects on stagnation in the greater Houston area, J. Geophys. Res., 116, D12105, doi:10.1029/2010JD015533, 2011.

Darby, L. S., Cluster analysis of surface winds in Houston, Texas, and the impact of wind patterns on ozone, J. Appl. Meteorol., 44, 1788-1806, doi:10.1175/JAM2320.1, 2005.

DISCOVER-AQ whitepaper, http://discover-aq.larc.nasa.gov/pdf/DISCOVER-AQ_science.pdf.

Emmons, L.K., S. Walters, P.G. Hess, J-F Lamarque, G.G. Pfister, D. Fillmore, C. Granier, A. Guenther, D. Kinnison, and T. Laepple. “Description and Evaluation of the Model for Ozone and Related Chemical Tracers, Version 4 (mozart-4), Geoscientific Model Development, 3, 43–67, 2010.

Flynn, C. M., K. E. Pickering, J. H. Crawford, L. Lamsal, N. Krotkov, J. Herman, A. Weinheimer, G. Chen, X. Liu, J. Szykman, S.-C. Tsay, C. P. Loughner, J. Hains, P. Lee, R. R. Dickerson, J. W. Stehr, L. Brent, The Relationship between Column-density and Surface Mixing Ratio: Statistical Analysis of O_3 and NO_2 Data from the July 2011 Maryland DISCOVER-AQ Mission, Submitted to Atmos. Environ, 2013.

Finlayson-Pitts, B. J., and J. Pitts, Chemistry of the upper and lower atmosphere: Theory, experiments and applications, p.264-276, Academic Press, San Diego, California, 2000.

Goliff, W. S., W. R. Stockwell, and C. V. Lawson, The Regional Atmospheric Chemistry Mechanism, Version 2, Atmos. Environ., 68, 174–185, doi:10.1016/j.atmosenv.2012.11.038, 2013

Goldberg, D. L., C. P. Loughner, M. Tzortziou, J. W. Stehr, K.E. Pickering, L. T. Marufu, J. H. Crawford, A. Mannino, and R. R. Dickerson, Surface ozone concentrations over the Chesapeake Bay during DISCOVER-AQ, Atmos. Environ., in press, 2013.

He, H., C. P. Loughner, J. W. Stehr, H. L. Arkinson, L. C. Brent, M. B. Follette-Cook, M. A. Tzortziou, K. E. Pickering, A. M. Thompson, D. K. Martins, G. S. Diskin, B. E. Anderson, J. H. Crawford, A. J. Weinheimer, P. Lee, J. C. Hains, and R. R. Dickerson, An elevated reservoir of air pollutants over the Mid-Atlantic States during the 2011 DISCOVER-AQ campaign: Airborne measurements and numerical simulations, Atmos. Environ., in press, 2013.

Houyoux, M. R. and J. M. Vukovich, Updates to the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System and Integration with Models-3, presented at The Emission Inventory: Regional Strategies for the Future, Air and Waste Management Association, Raleigh, NC, 1999.

Jacob, D. J., Introduction to Atmospheric Chemistry, Princeton University Press, New Jersey, 1999.

Kleinman, L. I., P. H. Daum, Y.-N Lee, L. J. Nunnermacker, S. R. Springston, J. Weinstein-Lloyd, and J. Rudolph, Sensitivity of ozone production rate to ozone precursors. Geophys. Res. Lett., 28, 2903–2906 , doi: 10.1029/2000GL012597, 2001.

Kleinman, L. I., P. H. Daum, Y.-N. Lee, L. J. Nunnermacker, S. R. Springston, J. Weinstein-Lloyd, and J. Rudolph, A comparative study of ozone production in five U.S. metropolitan areas, J. Geophys. Res., 110, D02301, doi:10.1029/2004JD005096, 2005a.
Kleinman, L. I., The dependence of tropospheric ozone production rate on ozone precursors, Atmos. Environ., 39(3), 575–586, doi:10.1016/j.atmosenv.2004.08.047, 2005b.
Lei, W., R. Zhang, X. Tie, and P. Hess, Chemical characterization of ozone formation in the Houston-Galveston area: A chemical transport model study, J. Geophys. Res., 109, D12301, doi:10.1029/2003JD004219, 2004.
Li, G., R. Zhang, J. Fan, and X. Tie, Impacts of biogenic emissions on photochemical ozone production in Houston, Texas, J. Geophys. Res., 112, D10309, doi:10.1029/2006JD007924, 2007.
Loughner, C. P., D. J. Allen, K. E. Pickering, R. R. Dickerson, D. -L. Zhang , Roles of urban tree canopy and buildings in urban heat island effects: parameterization and preliminary results, Journal of Applied Meteorology and Climatology, 51, 1775-1793, 2012.
Loughner, C. P., D. J. Allen, K. E. Pickering, R. R. Dickerson, D. -L. Zhang, Y. -X. Shou, Impact of fair-weather cumulus clouds and the Chesapeake Bay breeze on pollutant transport and transformation, Atmos. Environ., 45, 4060-4072, 2011.
Loughner, C.P., B. Duncan, M. Follette-Cook, J. Hains, K.E. Pickering, M. Tzortziou, Y. Yoshida, Impact of historical air pollution emissions reductions on surface ozone during record breaking heat, presented at 12th Annual CMAS Conference, Chapel Hill, NC., 2013.
Loughner, C. P., M. Tzortziou, M. Follette-Cook, K.E. Pickering, D. Goldberg, C. Satam, A. Weinheimer, J.H. Crawford, D.K. Knapp, D.D. Montzka, G.B. Diskin, L.T. Marufu, and R.R. Dickerson, Impact of bay breeze circulations on surface air quality and boundary layer export, submitted to Journal of Applied Meteorology and Climatology, 2013a.
Mallet, V. and B. Sportisse, B., A comprehensive study of ozone sensitivity with respect to emissions over Europe with a chemistry-transport model, J. Geophys. Res., 110, D22302, doi:10.1029/2005JD006234, 2005.
Mao, J., X. Ren, S. Chen, W. H. Brune, Z. Chen, M. Martinez, H., Harder, B. Lefer, B. Rappenglück, J. Flynn, and M. Leuchner, Atmospheric oxidation capacity in the summer of Houston 2006: Comparison with summer measurements in other metropolitan studies, *Atmos. Environ.*, 44(33), 4107-4115, 2010
Molina, M. J., and L. T. Molina, Megacities and atmospheric pollution, J. Air Waste Manage., 54, 644–680, 2004.
Morris, R. E., Yarwood, G., Emery, C. A., and B. Koo, Development and Application of the CAMx Regional One-atmospheric Model to Treat Ozone, Particulate Matter, Visibility, Air Toxics and Mercury." Air & Waste Management Association's 97th Annual Conference and Exhibition, 2004
Parrish, D.D., D.T. Allen, T.S. Bates, M. Estes, F.C. Fehsenfeld, G. Feingold, R. Ferrare, R.M. Hardesty, J.F. Meagher, J.W. Nielsen-Gammon, R.B. Pierce, T.B. Ryerson, J.H. Seinfeld, and E.J. Williams, 2009. Overview of the Second Texas Air Quality Study (TexAQS II) and the Gulf of Mexico Atmospheric Composition and Climate Study (GoMACCS), Journal of Geophysical Research, 114, D00F13, doi:10.1029/2009JD001842, 2009.
Ren, X., D. van Duin, M. Cazorla, S. Chen, J. Mao, L. Zhang, W. H. Brune, J. H. Flynn, N. Grossberg, B. L. Lefer, B. Rappenglück, K. W. Wong, C. Tsai, J. Stutz, J. E. Dibb, B. T. Jobson, W. T. Luke, and P. Kelley, Atmospheric oxidation chemistry and ozone production: Results from SHARP 2009 in Houston, Texas, J. Geophys. Res., 118, 5770–5780, 2013.
Sander, S. P., J. Abbatt, J. R. Barker, J. B. Burkholder, R. R. Friedl, D. M. Golden, R. E. Huie, C. E. Kolb, M. J. Kurylo, G. K. Moortgat, V. L. Orkin and P. H. Wine, Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation No. 17, JPL Publication 10-6, Jet Propulsion Laboratory, Pasadena, 2011 (http://jpldataeval.jpl.nasa.gov).
Sillman, S., The use of NO_y, H_2O_2, and HNO_3 as indicators for O_3-NO_x-hydrocarbon sensitivity in urban locations, J. Geophys. Res., 100, 14,175–14,188, 1995.

Sillman, S., R. Vautard, L. Menut, and D. Kley, O_3-NO_x-VOC sensitivity and NO_x-VOC indicators in Paris: Results from models and Atmospheric Pollution Over the Paris Area (ESQUIF) measurements, J. Geophys. Res., 108(D17), 8563, doi:10.1029/2002JD001561, 2003.
Skamarock, W.C., J.B. Klemp, J. Dudhia, D.O. Gill, D.M. Barker, W. Wang, and J.G. Powers, A Description of the Advanced Wrf Version 3." NCAR technical note NCAR/TN/u2013475+ STR, 2008
Stauffer, R. M., A. M. Thompson, D. K. Martins, R. D. Clark, D. L. Goldberg, C. P. Loughner, R. Delgado, R. R. Dickerson, J. W. Stehr, and M. A. Tzortziou , Bay breeze influence on surface ozone at Edgewood, MD during July 2011, J. Atmos. Chem., doi: 10.1007/s10874-012-9241-6, 2013.
Tang, X., Wang, Z., Zhu, J., Gbaguidi, A. E., Wu, Q., Li, J., and Zhu, T., Sensitivity of ozone to precursor emissions in urban Beijing with a Monte Carlo scheme. Atmos. Environ., 44, 3833-3842, 2010.
Texas Air Quality Research Program, TCEQ Priority Research Areas, 2013 (available at http://aqrp.ceer.utexas.edu/docs/FY14-15/FINAL_AQRP%20Priorities%20Research%20Areas%202014-15%20(2).pdf)
Tzortziou, M., J. R. Herman, A. Cede, C. P. Loughner, N. Abuhassan, and S. Naik, Spatial and temporal variability of ozone and nitrogen dioxide over a major urban estuarine ecosystem, Journal of Atmospheric Chemistry, doi:10.1007/s10874-013-9255-8, 2013.
Vukovich, J. and T. Pierce. The Implementation of BEIS-3 within the SMOKE modeling framework, presented at Emissions Inventories – Partnering for the Future, paper presented at the 11th Emissions Inventory Conference of the U.S. Environmental Protection Agency, Research Triangle Park, NC, 2002.
Wiedinmyer, C., S. K. Akagi, R. J. Yokelson, L. K. Emmons, J. A. Al-Saadi, J. J. Orlando, and A. J. Soja, The Fire INventory from NCAR (FINN): A high resolution global model to estimate the emissions from open burning, Geosci. Model Develop., 4, 625-641, doi:10.5194/gmd-4-625-2011, 2011.
Xue, L. K., T. Wang, J. Gao, A. J. Ding, X. H. Zhou, D. R. Blake, X. F. Wang, S. M. Saunders, S. J. Fan, H. C. Zuo, Q. Z. Zhang, and W. X. Wang, Ozone production in four major cities of China: sensitivity to ozone precursors and heterogeneous processes, Atmos. Chem. Phys. Discuss., 13, 27,243–27,285, doi:10.5194/acpd-13-27243-2013, 2013.
Yarwood, G., S. Rao, M. Yocke, M., and G. Z. Whitten, Updates to the Carbon Bond Mechanism: CB05, Final Report to the US EPA (RT-0400675), 2005 (http://www.camx.com/publ/pdfs/CB05_Final_Report_120805.pdf).