Quality Assurance Project Plan

AQRP Project 14-020

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

Prepared for

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

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GENERAL REQUIREMENTS

0.1 TITLE AND APPROVAL SHEET

This document is a Level III Quality Assurance Project Plan (QAPP) for Project 14-020: Analysis of Ozone Production and Its Sensitivity in Houston Using the Data Collected During DISCOVER-AQ. This project is managed by the staff at the University of Maryland (UMD) College Park.

This QAPP was approved electronically on January 26, 2015 by Vincent M. Torres, The University of Texas at Austin

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This QAPP was approved electronically on January 26, 2015 by Cyril Durrenberger, The University of Texas at Austin

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Doug Boyer, Project Liaison
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0.2 DISTRIBUTION LIST

Below is a list of individuals and their organizations that need copies of the approved Quality Assurance Project Plan and any subsequent revisions, including all persons responsible for implementation (e.g., project managers), the QA managers, and representatives of all groups involved. Paper copies need not be provided to individuals if equivalent electronic information systems can be used.

Air Quality Research Program (AQRP), University of Texas

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PROJECT DESCRIPTION AND OBJECTIVES

ENVIRONMENTAL SYSTEM TO BE EVALUATED

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 will conduct an analysis of ozone production and its sensitivity to NO_x and VOCs using a chemical transport model and 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 in Houston will be proposed to provide scientific information for policy decisions.

PURPOSE & 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]. The following tasks have been described in the Statement of Work and will be performed in this project:

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 the sensitivity of ozone production 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

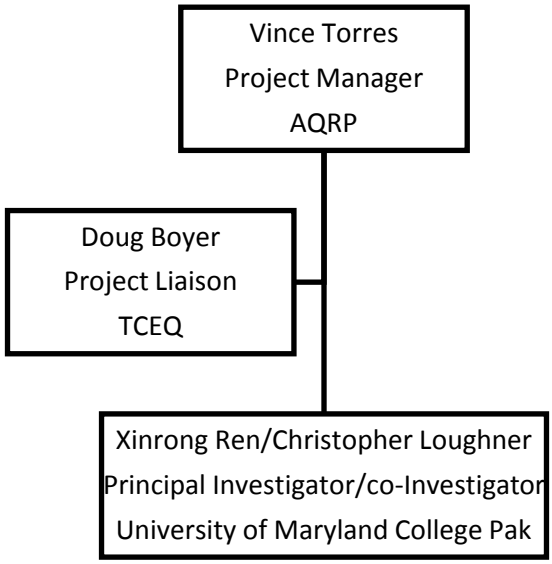
ORGANIZATION AND RESPONSIBILITIES

The organizations participating in this project are

- Air Quality Research Program (AQRP), University of Texas
- Texas Commission on Environmental Quality (TCEQ)
- University of Maryland College Park

KEY PERSONNEL

The following flow chart identifies the key personnel at each organization that are responsible for the QA and deliverables listed in this document.



PROJECT SCHEDULE

The schedule for this project and key milestones are listed in Table 1 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 1. Project timeline.

SCIENTIFIC APPROACH

The NASA DISCOVER-AQ study conducted aircraft observations over the Houston Metropolitan Area in summer 2013. The mission focused on NASA's goals to study the Earth from space to increase fundamental understanding and to enable the application of satellite data for societal benefit [DISCOVER-AQ whitepaper]. The overarching objective of DISCOVER-AQ was to improve the interpretation of satellite observations to understand near-surface conditions relating to air quality. The outcomes of DISCOVER-AQ include improved forecasting ability for current air quality conditions; assessment of air quality for purposes of attribution to specific causes; and improved estimation of emissions which undergo constant change.

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 nitrogen oxides (NO_x) and volatile organic compounds (VOCs) is expected to vary from location to location and from time to time. Few studies have been conducted to extensively examine this sensitivity in urban areas like Houston, with many based on model analyses only. In this project, we will investigate the spatial and temporal variations of ozone production and its sensitivity to NO_x and VOCs in Houston using the data collected during the DISCOVER-AQ campaign. An observation-constrained box model based on Carbon Bond mechanism Version 5 (CB05) will be used to study the photochemical processes along the NASA P-3B flight tracks as well as at eight surface sites where the P-3B conducted spiral profiles. Ozone production rates will be calculated at different locations and at different times of day and its sensitivity to NO_x and VOCs will be investigated. When measurements are available, ozone production efficiency (OPE), defined as the ratio of the ozone production rate to the NO_x oxidation rate, will be also calculated and its correlation with other parameters such as radical sources and NO_x/NO_y ratios will be evaluated. The results from this study, i.e., the spatial and temporal variations of O_3 production sensitivity, will provide scientific information for policy-makers to develop a non-uniform emission reduction strategy for O_3 pollution control in urban areas like Houston. These activities will strengthen our understanding of O_3 production and development of the State Implementation Plan (SIP), which is essential to meet the primary and secondary National Ambient Air Quality Standards (NAAQS) for ozone.

SAMPLING APPROACH

DISCOVER-AQ 2013 in Houston conducted systematic and concurrent observation of column-integrated, surface, and vertically-resolved distributions of aerosols and trace gases relevant to air quality as they evolved throughout the day. This was accomplished with a combination of two airborne platforms sampling in coordination with re-locatable and fixed surface networks. One aircraft (the P-3B) was used for extensive in situ profiling of the atmosphere while the other (the B200) conducted both passive and active remote sensing of the atmospheric column extending below the aircraft to the surface. These aircraft repeatedly overflew instrumented surface locations continuously monitoring both column and surface conditions for select variables throughout the day.

PROCESS MEASUREMENTS AND SPECIFIC TARGET ANALYTES

Airborne in situ profiling

The NASA P-3B was deployed in the DISCOVER-AQ 2013 in Houston. Measurements directly related to satellite observations of air quality include ozone (O_3), nitrogen dioxide (NO_2), formaldehyde (HCHO), and aerosol optical and microphysical properties. Additional critical variables needed for retrievals and data interpretation include atmospheric state (temperature, pressure, wind speed and wind

direction), water vapor (H_2O), carbon monoxide (CO), methane (CH_4), carbon dioxide (CO_2), nitric oxide (NO), the components of reactive nitrogen, and aerosol inorganic and organic composition. The P-3B instruments were well characterized having been deployed previously on multiple airborne campaigns and used in published research findings.

Surface observations

Eight surface monitoring stations were selected where the P-3B conducted vertical spirals. These monitoring stations provided in situ observations of trace gases (O_3, CO, NO, NOy, SO_2), aerosol lidar observations, and balloon soundings of ozone and water vapor. These eight surface monitoring stations include Smith Point, Galveston, Manvel Croix, Deer Park, Channelview, Conroe, West Houston, and Moody Tower.

Additionally, the primary component of the surface network was the Pandora instrument, a sun-tracking UV-visible spectrometer capable of continuous monitoring of trace gas columns for O_3, NO_2, and HCHO throughout the day. Pandora has demonstrated capability, is relatively low-cost, and can be left unattended making it ideal for use in a distributed network.

GENERAL APPROACH AND TEST CONDITIONS FOR THE FIELD CAMPAIGN

The general approach and test conditions for the field campaign examined the processes involved in the summertime ozone peak observed in southeast Texas. The test conditions for the continuous measurements include all cloud conditions, varying temperatures, frontal passages, dry periods, and periods of intense rain.

SAMPLING PROCEDURES

KNOWN SITE SPECIFIC FACTORS AND SITE PREPARATION

For the Houston area, ground level ozone concentrations tend to maximize in fall with September as the optimal month. Transportation emissions were important. However it was the complex, highly reactive chemical mixtures associated with petrochemical emissions that distinguish this location from others. The dominance of land-sea breeze dynamics was another important driver for air quality in this region. For this deployment, flights were conducted from Ellington Field at NASA Johnson Space Center [DISCOVER-AQ whitepaper].

The measurements during the DISCOVER-AQ 2013 in Houston were mainly made from the NASA P-3B aircraft and eight surface monitoring stations, including Smith Point, Galveston, Manvel Croix, Deer Park, Channelview, Conroe, West Houston, and Moody Tower. The major airborne platform selected for the DISCOVER-AQ mission was the P-3B. The P-3B is an ideal choice for a profiling aircraft for several reasons: 1) it is capable of hosting a comprehensive atmospheric chemistry and aerosol payload, 2) it is ideal for profiling the lower atmosphere, and 3) it has sufficient flight duration (eight hours) for sampling throughout the day [DISCOVER-AQ whitepaper].

The eight surface sites chosen for the deployment were evaluated prior to DISCOVER-AQ with regard to the presence or absence of complementary chemical and meteorological measurements which enhanced the utility of aircraft measurement suite; the nature, strength, and likely impact of nearby point and mobile emission sources; the nature, height, and extent of nearby structures and vegetation, and their likely influence on local meteorology and wind flow patterns; and any other characteristic which might render the site physically or chemically unrepresentative of the surrounding area [DISCOVER-AQ whitepaper].

SAMPLING PROCEDURES

This section describes or references each sampling procedure used and includes procedures for homogenizing, compositing, or splitting of samples, as applicable.

Sampling procedures used in this project are consistent with U.S. Environmental Protection Agency (EPA) 40 *CFR* Part 58, Appendices A through G, the *Quality Assurance Handbooks for Air Pollution Measurement Systems, Volumes I and II*, and the reference and equivalent methods designation criteria outlined in 40 *CFR* Part 53. The criteria pollutant sampling probes are sited in accordance with the EPA *Quality Assurance Handbook, Volume II*, Section 2.0.11 and EPA *Ambient Monitoring Guidelines for the Prevention of Significant Deterioration*. All materials are constructed of Teflon®, glass, or stainless steel. Ambient air was supplied to the continuous analyzers through Teflon®, stainless steel, or glass tubing. Pollutant concentrations were automatically measured and reported by the analyzers, which output data either as ASCII text via RS-232 serial connections or analog voltage signals. The instrument outputs were sampled by data acquisitions software such as LabView® at individual update rates (usually 1 Hz) and the reduced data were averaged to 1-minute intervals in the final merge file.

SAMPLE CONTAINERS AND QUANTITIES

This section lists the sample containers, sample quantities collected, and the sample amount required for each analysis, including QC sample analysis.

Ozone, NO, NO_2, and NOy

There were no discrete samples handled by individuals for this method.

NO_2, Total Peroxyl Nitrates, and Total Alkyl Nitrates

There were no discrete samples handled by individuals for this method.

Formaldehyde (HCHO)

There were no discrete samples handled by individuals for this method.

Carbon Dioxide (CO_2)

There were no discrete samples handled by individuals for this method.

Carbon monoxide (CO), Methane (CH_4) and Water Vapor (H_2O)

There were no discrete samples handled by individuals for this method.

Volatile Organic Compounds (VOCs)

There were no discrete samples handled by individuals for this method.

SAMPLE PRESERVATION

This section describes the sample preservation requirements (e.g., refrigeration, acidification, etc.) and holding times.

Ozone, NO, NO_2, and NOy

There were no discrete samples handled by individuals for this method.

NO_2, Total Peroxyl Nitrates, and Total Alkyl Nitrates

There were no discrete samples handled by individuals for this method.

Formaldehyde (HCHO)

There were no discrete samples handled by individuals for this method.

Carbon Dioxide (CO_2)

There were no discrete samples handled by individuals for this method.

Carbon monoxide (CO), Methane (CH_4) and Water Vapor (H_2O)

There were no discrete samples handled by individuals for this method.

Volatile Organic Compounds (VOCs)

There were no discrete samples handled by individuals for this method.

SAMPLE IDENTIFICATION

This section describes the methods for uniquely numbering each sample.

Ozone, NO, NO_2, and NOy

There were no discrete samples handled by individuals for this method. Data collected was stored in the PC with a unique time stamp.

NO_2, Total Peroxyl Nitrates, and Total Alkyl nitrates

There were no discrete samples handled by individuals for this method. Data collected was stored in the PC with a unique time stamp.

Formaldehyde (HCHO)

There were no discrete samples handled by individuals for this method. Data collected was stored in the PC with a unique time stamp.

Carbon Dioxide (CO_2)

There were no discrete samples handled by individuals for this method. Data collected was stored in the PC with a unique time stamp.

Carbon monoxide (CO), Methane (CH_4) and Water Vapor (H_2O)

There were no discrete samples handled by individuals for this method. Data collected was stored in a personal computer with a unique time stamp.

Volatile Organic Compounds (VOCs)

There were no discrete samples handled by individuals for this method. Data collected was stored in the PC with a unique time stamp.

SAMPLE HANDLING

This section describes the procedures for packing and shipping samples, including procedures to avoid cross-contamination, and provisions for maintaining chain-of-custody (e.g., custody seals and records), as applicable.

Ozone, NO, NO_2, and NOy

There were no discrete samples handled by individuals for this method.

SO_2 NO_2, Total Peroxyl Nitrates, and Total Alkyl Nitrates

There were no discrete samples handled by individuals for this method.

Formaldehyde (HCHO)

There were no discrete samples handled by individuals for this method.

Carbon Dioxide (CO_2)

There were no discrete samples handled by individuals for this method.

Carbon monoxide (CO), Methane (CH_4) and Water Vapor (H_2O)

There were no discrete samples handled by individuals for this method.

Volatile Organic Compounds (VOCs)

There were no discrete samples handled by individuals for this method.

MEASUREMENT PROCEDURES

ANALYTICAL METHODS

Table 2 lists specifications for the P-3B in situ trace gas measurements. All of these investigators fielded their instruments onboard the NASA DC-8 during the recent ARCTAS field campaign in 2008 [Jacob et al., 2009], and all have experience on other airborne platforms (e.g., NASA P-3B, NSF C-130, and NSF HIAPER).

Table 2. P-3B in situ trace gas measurements1

Co-I	Technique or Instrument	Species	Precision	Uncertainty
Cohen	Thermal-Dissociation, Laser-Induced Fluorescence	NO_2	10 pptv	5%
		Total Peroxy Nitrates	40 pptv	10%
		Total Alkyl Nitrates	50 pptv	15%
		HNO_3	50 pptv	20%
Weinheimer	Chemiluminescence	O_3	0.1 ppbv	5%
		NO and NO_y	20 pptv	10%
		NO_2	20 pptv	10-20%
Fried	IR Absorption Spectrometer	CH_2O	60-80 pptv	12%
Vay	modified LI-COR 6252	CO_2	0.1 ppmv	0.25 ppm
Diskin	Diode Laser Spectrometer	CO	1 ppbv	1.5%
		CH_4	2 ppbv	0.2%
	Diode Laser Hygrometer	H_2O	0.1%	5%
Wisthaler	Proton Transfer Reaction-Mass Spectrometer	methanol	100 pptv	20%
		acetaldehyde	100 pptv	15%
		acetone	50 pptv	10%
		isoprene, MVK/MACR	20 pptv	10%
		acetonitrile	10 pptv	10%
		benzene, toluene, C8-aromatics, C9-aromatics	10 pptv	10%

1-response time for all instruments is 1 s with exception of Wisthaler which has 10 s response.

Table 3 lists specifications for the P-3B in situ aerosol measurements fielded by Dr. Bruce Anderson. With the exception of the last three instruments in the table, Dr. Anderson has fielded this measurement suite many times, most recently during ARCTAS. The final three instruments were fielded during ARCTAS by other investigators, thus their airborne implementation and integration is well demonstrated.

Table 3. P-3B in situ aerosol measurements

Technique/Instrument	Response	Parameter	Precision	Size Range
Condensation Particle Counters (TSI 3025, TSI 3010)	1 s	Ultrafine, Nonvolatile CN	10%	>0.003
TSI Scanning Mobility Particle Sizer	60 s	Aerosol Particle Size	20%	0.01 – 0.3
DMT Ultra-High Sensitivity Aerosol Spectrometer	1 s		20%	0.08 – 1.0
MetOne Optical Particle Counter	1 s		40%	0.3 – 10
Aerodynamic Particle Sizer (TSI 3321)	1 s		20%	0.5 – 20
DMT Cloud Condensation Nuclei counter	1 s	Cloud Condensation Nuclei Spectra	NA	<10
Nephelometer (TSI 3563)	1 s	Scattering at 450, 550, and 700 nm	5e-7 mM or 5%	<10
Particle Soot Absorption Photometer	5-60 s	Absorption at 467, 530, and 660 nm	5e-7 mM or 5%	<10
RR Nephelometers	20 s	Humidity Dependence of Scattering	NA	<10
DMT Single Particle Soot Photometer	1 s	Black Carbon	20%	0.1 – 1.0
Particle into Liquid Sampler/Ion Chromatograph	300 s	Soluble Ion Composition	NA	0.01 – 1.0
Particle into Liquid Sampler/Total Organic Carbon	30 s	Water Soluble Organic Carbon	NA	0.01 – 1.0

Table 4 lists specifications for the P-3B navigational and meteorological observations. While these observations are often considered to be turn-key, experience has shown that loss of data or lack of adequate QC for these data can be detrimental to mission success. Mr. John Barrick has more than a decade of experience in providing these observations on the P-3B and will be responsible for collecting and reporting these data during DISCOVER-AQ.

Table 4. P-3B navigational and meteorological measurements

Parameter	Response	Technique/Instrument	Precision
GPS Location	1 s	GPS/Trimble TNL-3000	15 m
GPS Altitude	1 s		50 m
Pressure	1 s	MEMS/Rosemount MADT 2014	0.3 mb
Pressure Altitude	1 s	Calculated/Rosemount MADT 2014	5 m
Radar Altitude	1 s	Radar Altimeter/ Honeywell AA-300	3 m
Pitch, Roll, and Heading	1 s	INS/Honeywell Laseref	0.2 °
Wind Speed and Direction	1 s		3 m/s; ± 10 °
Ground Speed and Track	1 s		1 m/s; 0.5 °
True Air Speed	1s		2 m/s
Temperature	1 s	PRT/Rosemount E102 Non-Deiced	0.2 °C
Dew/Frost point	2 - 30 s	Edgetech Vigilant 137 3-Stage Chilled Mirror Hygrometer	0.5 - 1.0 °C
NO_2 Photolysis Frequency	1 s	Metcon jNO_2 Filter Radiometers	8%

QUALITY METRICS (QA/QC CHECKS)

QC CHECKS

This section identifies the QC checks (e.g., blanks, control samples, duplicates, matrix spikes, surrogates), the frequencies for performing these checks, associated acceptance criteria, and corrective actions to be performed if acceptance criteria are not met for each process measurement and analytical method.

The general QA/QC checks for the O_3, NO, NO_2, NO_Y, total peroxyl nitrates, total alkyl nitrates, HCHO, CO_2, CO, CH_4, H_2O, and VOCs measurements on the P-3B are described in the table below, along with acceptance criteria.

Assessment Parameter	Quality Control Procedure	Minimum Frequency	Acceptance Criteria	Corrective Action
Measurement system contribution - Calibration	Precision/Linearity test – Multipoint calibration	Once per flight, and prior to and following installation, repair, or adjustment of equipment	Linear fit of 0.995 or better	Check calibrator settings. Recalibrate or repair.
Measurement system contribution – Span Check	Span checks	Each flight, and prior to and following installation, repair, or adjustment of equipment	Relative Standard Deviation < 5%	Check calibrator settings. Recalibrate or repair.
Measurement system contribution – Zero Check	Zero offset check	Several times per flights	Response below detection limit	Check zero air supply. Check for leaks. Adjust zero offset.

Table 5. QA/QC checks for the trace gas measurements on the NASA P-3B during the DISCOVER-AQ 2013 in Houston.

ACCEPTANCE CRITERIA

This section addresses any additional project-specific QA objectives (e.g., completeness, mass balance) shall be presented, including acceptance criteria.

See Table 5 above for acceptance criteria.

DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

The data analyses performed during the execution of this project will use statistical analysis techniques and numerical model approaches.

DATA REDUCTION AND CALCULATIONS

The measured data have been reduced based on the performance and calibrations of the instruments. Invalid data have been removed from the reported data set, as were data collected during multi-point calibrations, zero/span checks, baseline determinations, and zero air artifact measurements. Additional indicators of invalid data include gaps in the time stamp records of the reported measurements; excessive baseline deviation within and between sequential baseline measurements; excessive deviation within and between sequential zero/span measurements; discrepancies in instrument linearity. The raw data and all calibration were evaluated for such deviations and discrepancies and are flagged accordingly.

Calibration factors and instrument sensitivities were then applied to the valid ambient data. Raw data were reduced by first subtracting from the measured signal a value corresponding to the equivalent instrument baseline. Instrument baseline values were calculated at each time step of the measurement sequence by interpolation of the baseline signal, which was monitored periodically during normal instrument operation. The resultant net raw signal was converted to engineering units by application of instrument sensitivity values determined from zero/span checks and multipoint calibrations. Where appropriate, conversion efficiencies and zero air artifact levels were also applied to the signals.

These data analysis results may be used by decision makers at the TCEQ in order to better develop ozone control strategies for the State Implementation Plan (SIP). This project will perform data analysis, using data collected during the DISCOVER-AQ campaign in Houston during the summer of 2013. The final analysis results will be archived by submitting to the NASA DISCOVER-AQ central data archive (ftp-air.larc.nasa.gov) and archived by NOAA Air Resources Laboratory on a password protected SFTP/Web server at ftp.arl.noaa.gov for a minimum of three years and will be presented at the AQRP workshop.

VALIDATION PROCESSES

The measured data have been validated based on the performance of the instruments and invalid data have been removed when the instruments malfunctioned. If concurrent, co-located measurements of a given species are available, comparison of the two measurements were made and periods with significant disagreement (i.e., larger than the stated uncertainty) were identified and validated. Possible reasons for the discrepancies were then investigated. If the results of the two measurements could not be reconciled, the measurements during these periods were considered invalid. Whenever possible, calibration standards were shared with other research groups in “round robin” evaluations to assess the validity of the certified calibration standards.

DATA ANALYSIS AND STATISTICS

We will use a chemical transport model (WRF-CMAQ) and a box model (based on 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 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(HNO3), 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.

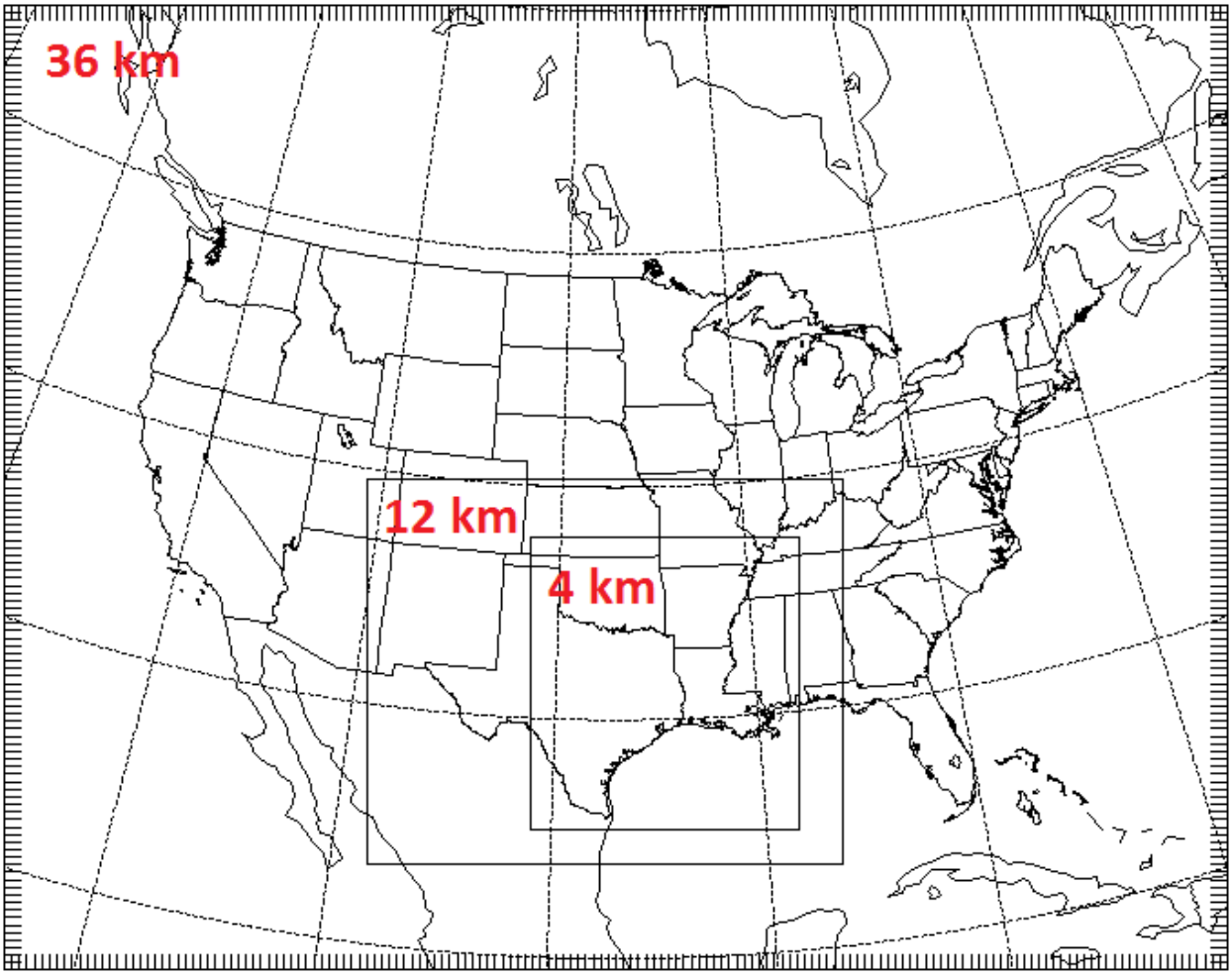


Figure 1: Location of the 36 km , 12 km, and 4 km domains that will be used in the WRF and CMAQ modeling. Results from the 4 km domain will be utilized in this project.

Table 6: 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; RO_{2i} is the individual organic peroxy radicals; and $P(RONO_2)$ is the production rate of organic nitrates ($RONO_2$). 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.

DATA STORAGE

Final data will be submitted to the NASA DISCOVER-AQ central data archive (ftp-air.larc.nasa.gov) and archived by NOAA Air Resources Laboratory on a password protected SFTP/Web server at ftp.arl.noaa.gov for a minimum of three years. The final analysis results will be delivered to the AQRP in a format conducive to import into a database at the conclusion of the project.

AUDITS OF DATA QUALITY

This section is for audits of the observation data and models used in this project. The audits will be not only for the accuracy of the inputs to the models, but also for the scripts used to run the models.

The PI (Dr. Ren), with the assistance from the co-I (Dr. Loughner) and the graduate student (Gina Mazzuca), will audit acquired at least 10% of the measurement data collected on the NASA P-3B aircraft. He will trace the data from initial versions of submitted data, through reduction and statistical comparisons, to final versions of submitted data. In this audit, the duplicate measurements of chemical species (e.g., nitrogen dioxide (NO_2) and water vapor) will be particularly focused. Time series of the duplicate measurements will be plotted in the same time stamp and scatter plots will be generated to assess the agreement between the duplicate measurements.

The PI (Dr. Ren), with the assistance from the graduate student (Gina Mazzuca), will perform the audit for the scripts used for the box model simulations. The co-I (Dr. Loughner) will perform the audit for the WRF-CMAQ model simulations, including model input and output files, scripts, and analysis products (i.e., trajectories, maps of satellite observations, maps of maximum eight-hour average ozone concentrations corresponding to anthropogenic emissions contributions in various emission source regions).

The results of data quality audits will be included in the final report.

REPORTING

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.

FINAL REPORT

The final report will include summaries of the activities conducted under this project and the results which are produced. The following table lists some of the key results expected to be addressed in the report, and how they can be used by decision makers to better develop ozone control strategies for the State Implementation Plans (SIP). These results are expected to improve our understanding of the ozone production and its sensitivity to NOx and VOCs in Houston Metropolitan.

Goals and Objectives	Benefit to SIP
Investigate spatial variations of ozone production and its sensitivity to NO_x and VOCs in Houston during DISCOVER-AQ. 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?	SIP modelers will be able to compare the spatial variations of ozone production and its sensitivity to NOx and VOCs in the SIP model to the results from this project based on in situ measurements made on the NASA P-3B to determine if the SIP model realistically represents important processes that involve in ozone chemistry.
Investigate temporal variations of ozone production and its sensitivity to NO_x and VOCs in Houston during DISCOVER-AQ to 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.	SIP modelers will be able to compare the temporal variations of ozone production and its sensitivity to NOx and VOCs in the SIP model to the results from this project based on in situ measurements made on the NASA P-3B to determine if the SIP model realistically represents important processes that involve in ozone chemistry.
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. At a specific location and at a specific time, which one should be controlled in order to reduce ozone, NOx or VOCs	This analysis will generate critical information that will help TCEQ SIP planners to implement pollution control strategies i.e., when, where to control what in order to control ozone pollution in Houston.
Calculate ozone production efficiency (OPE) at different locations using the ratio of ozone production rate to the NO_x oxidation rate calculated in the box model.	This will allow the SIP planners to better understand what are the major factors influencing different OPEs at different locations and what are the relationships between OPE and NO_x/VOCs/radical sources

Table 7. Key results to be addressed in the final report

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).