Quality Assurance Project Plan

Project 14-026
Quantifying Ozone Production from Light Alkenes Using Novel Measurements of Hydroxynitrate Reaction Products in Houston during the NASA SEAC4RS Project

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Summary of Project

QAPP Category Number: III
Type of Project: Secondary Data Project and Research or Development (Modeling)

QAPP Requirements: This QAPP includes descriptions of the project and objectives; organization and responsibilities; scientific approach; modeling procedures; quality metrics; data analysis, interpretation, and management; reporting; and references.

QAPP Requirements:
Audits of Data Quality: 10% Required
Report of QA Findings: Required in final report

May 29, 2014

DISTRIBUTION LIST

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APPROVALS

QAPP was approved electronically on April 25, 2014 by Gary McGaughey, The University of Texas at Austin

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Gary McGaughey
Project Manager, Texas Air Quality Research Program

QAPP was approved electronically on April 24, 2014 by Cyril Durrenberger, The University of Texas at Austin

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1.0 PROJECT DESCRIPTION AND OBJECTIVES

1.1 Problem Statement

Industrial emissions of highly reactive volatile organic compounds (HRVOCs) can contribute to localized ozone (O_3) production in Houston, TX (Ryerson et al., 2003). Flights during the 2013 National Aeronautics and Space Administration (NASA) Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC^{4}RS) project encountered plumes with enhanced O_3 downwind of petrochemical facilities in Houston, such as on 25 September 2013, when ground monitoring downwind of the Ship Channel showed 5-minute average O_3 values peaking at 165 ppb. Historically, direct emissions of HRVOCs (specifically ethene, propene, butenes, and 1,3-butadiene) and formaldehyde (HCHO) have been implicated in these types of high ozone events, but quantifying the relative contribution of different precursors to O_3 formation has been difficult.

1.2 Project Objectives

The objective of this project is to improve and quantify our understanding of O_3 and HCHO production from industrial HRVOC emissions in the Houston area. This objective will be accomplished by a combination of data analysis and reactive plume modeling of data taken aboard the NASA DC-8 research aircraft during the 2013 SEAC^{4}RS project in Houston. Concentrations were measured for β-hydroxynitrates produced in the gas-phase oxidation of alkenes, including those produced from the oxidation of ethene, propene, butenes, and 1,3-butadiene. These measurements of C_2-C_4 hydroxynitrates provide a novel means to link observed O_3 and HCHO enhancements to emissions of specific alkenes.

The specific objectives of the study are:

- Analysis of the highly spatially resolved airborne data, combined with known hydroxynitrate yields and in conjunction with O_3, nitrogen oxides (NOx), HCHO, and other chemical tracers measured aboard the DC-8, to determine a robust first-order attribution of observed O_3 and HCHO enhancements to the oxidation of individual alkene precursors emitted from the Houston Ship Channel
- Reactive plume modeling with SCICHEM using Revision 2 of the Carbon Bond 6 (CB6r2) chemical mechanism, with reactions added for individual HRVOCs, to evaluate current chemical mechanisms against in-situ data and test how plume dilution influences chemical processing and therefore how grid model resolution can influence modeled impacts of HRVOC sources
- Developing recommendations for grid model resolution and chemistry mechanisms for future Texas Commission on Environmental Quality (TCEQ) modeling

2.0 ORGANIZATION AND RESPONSIBILITIES

2.1 Personnel and Responsibilities

This project is being conducted by ENVIRON, National Oceanic and Atmospheric Administration (NOAA) and Caltech under a grant from the Texas Air Quality Research Program (AQRP). The project Co-Principal Investigators (PIs) are Dr. Greg Yarwood of ENVIRON, Dr. Thomas Ryerson of NOAA, and Dr. Paul Wennberg of Caltech. The Co-PIs will assume overall responsibility for the research and associated quality assurance.

ENVIRON will be responsible for updates to the CB6r2 mechanism and reactive plume modeling, as well as for overall project management and submitting periodic technical reports and the Final Report. Dr. Ryerson will lead the scientific analysis of DC-8 measurements in collaboration with Caltech scientists. Dr. Wennberg will lead the analysis and QA/QC of the raw field data.

The project will be overseen by the AQRP Project Manager, Mr. Gary McGaughey, and the TCEQ Project Liaison, Mr. Chris Kite. The scientists working on this project and their specific responsibilities are listed in Table 2-1 below.

Table 2-1. Project participants and their affiliations and key responsibilities.

Participant	Project Responsibility
Dr. Greg Yarwood (ENVIRON)	Co-Principal Investigator: Project oversight; responsible for updates to CB6r2 mechanism
Dr. Thomas Ryerson (NOAA)	Co-Principal Investigator: Responsible for scientific analysis of DC-8 measurements and contributions to periodic and final reports
Dr. Paul Wennberg (Caltech)	Co-Principal Investigator: Responsible for analysis and QA/QC of raw field data
Dr. Prakash Karamchandani (ENVIRON)	Project Manager: Responsible for day-to-day management of project and for implementing the chemistry updates in SCICHEM, setting up and supervising the SCICHEM simulations, and analyzing the results
Dr. Ilana Pollack (NOAA)	Assist Dr. Ryerson
Mr. Jeff Peischl (NOAA)	Assist Dr. Ryerson
Mr. Alex Teng (Caltech)	Assist Dr. Wennberg
Dr. John Crounse (Caltech)	Assist Dr. Wennberg and Mr. Teng
Ms. Lynsey Parker (ENVIRON)	Assist Dr. Karamchandani

2.2 Project Schedule

The schedule for specific tasks is provided in Table 2-2.

Table 2-2. Schedule of project activities.

Task	2014									2015					
	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun
Task 1: QA/QC Alkene Hydroxynitrate Measurements		━	━	━	━▶										
WP/QAPP	●														
Final Nitrate Data Publicly Released Via Submission to the SEAC^{4}RS Data Archive					●										
Task 2: Analysis of DC-8 airborne data					━	━	━	━	━▶						
Submit Results from Task 2 for peer-reviewed publication									●						
Task 3: CB6r2 mechanism and SCICHEM updates and photochemical plume modeling								━	━	━	━	━	━▶		
Reporting															
Draft Final Report														●	
Final Report															●
Project Presentation															●
Periodic Progress Reports		■	▲	▲	▲ ■	▲	▲	▲ ■	▲	▲	▲ ■	▲	▲	▲ ■	▲

Project Report Material ●

Monthly Progress Report ▲

Quarterly Progress Report ■

3.0 SCIENTIFIC APPROACH

3.1 QA/QC and Processing of Airborne Data

Airborne data, taken aboard the NASA DC-8 research aircraft during the 2013 $SEAC^4RS$ project in Houston, will be used in the study. The data includes Chemical Ionization Mass Spectrometer (CIMS) measurements of C_2-C_4 hydroxynitrates that will provide a novel means to link observed O_3 and HCHO enhancements to emissions of specific alkenes. Caltech scientists will conduct a QA/QC of the hydroxynitrate measurements and prepare a final dataset for data analysis and modeling, described below.

3.2 Data Analysis

NOAA and Caltech scientist will conduct this analysis. The final calibrated 1-Hz hydroxynitrate data will be used in conjunction with 1-Hz observations of NOx, nitric oxide (NO), peroxyacetyl nitrate (PAN), nitric acid (HNO_3), total reactive nitrogen oxides (NOy), O_3, HCHO, acetaldehyde (CH_3CHO), and other chemical and meteorological parameters measured aboard the NASA DC-8 to determine net O_3 production rates and yields for the airborne Houston study of 18 September 2013. A simple analysis based on known hydroxynitrates yields following OH-initiated reactions of their parent alkenes (Teng, Crounse, Lee, St. Clair, Cohen, Wennberg, submitted, 2014) will permit a first-order attribution of the O_3 and HCHO formed as a result of earlier emissions of each specific alkene. Alkene emissions inferred from hydroxynitrate observations will be compared to the DC-8 whole-air-sample (WAS) data on ethene, propene, butenes, and 1,3-butadiene in these plumes, and linked to the original emission ratio for individual plumes by the observed NOx/ethene ratio, which is preserved during transport from the source (Ryerson et al., 2003).

Overall plume O_3 production rates and yields deduced from airborne measurements during $SEAC^4RS$ in 2013 will be compared to rates and yields deduced from airborne measurements in Ship Channel plumes under similar flow patterns, ambient temperatures, and solar insolation during the 2000 Texas Air Quality Field Study (TexAQS) (Ryerson et al., 2003; Wert et al., 2003) and the Second Texas Air Quality Study (TexAQS II) (Washenfelder et al., 2010). Changes in plume reaction rates between these earlier studies were noted and ascribed, in part, to the decrease in HRVOCs as a result of mandated control strategies to control ozone formation in Houston (Washenfelder et al., 2010). Analysis of the 2013 NASA airborne data will highlight the effects of over a decade of control strategies focusing on mitigating ozone formation in industrial plumes in the Houston area. The fractional contribution of PAN and HNO_3 to the plume NOy budget, among other chemical diagnostics, will be examined to evaluate changes in OH reactivity and plume chemistry between these studies.

The data analysis results will also be used to constrain the reactive plume modeling, described below, by defining measurement-based estimates of plume initial conditions, background concentrations, and dispersion.

3.3 Reactive Plume Modeling

ENVIRON will conduct reactive plume modeling for selected days of the SEAC^{4}RS measurement period using the SCICHEM Lagrangian puff model with explicit photochemistry. SCICHEM is a state-of-the science puff model that uses second-order closure for puff dispersion and includes advanced chemistry modules that represent chemical interactions between plume pollutants and the surrounding atmosphere. SCICHEM has previously been successfully evaluated using helicopter measurements of power plant plumes, including plume widths and plume chemistry (Karamchandani et al., 2000). The model currently uses the CB05 gas-phase chemistry mechanism and will be updated to use the CB6r2 mechanism with additional explicit reactions to represent hydroxynitrate production from individual HRVOCs. The results from the data analysis described in Section 3.2 above will provide information on emission rates (based on initial plume concentrations), background concentrations for the plume chemistry calculations, and the plume spread or width at various downwind distances from the Houston Ship Channel. This information will be used to constrain the SCICHEM modeling. The hydroxynitrate and ozone concentrations predicted using SCICHEM will be compared with data from the DC-8 flight transects to evaluate whether the model chemistry is consistent with SEAC^{4}RS observations. In addition, the results from the plume modeling will be analyzed to compare modeled yields of O_3 and HCHO from the parent alkenes for comparison with the yields obtained from the analysis of the DC-8 measurements.

Sensitivity studies will be conducted with different initial plume dimensions to evaluate how the rate of plume dilution influences chemical processing in order to assess how grid model resolution (e.g., 4 km^2 vs. 1.3 km^2) is likely to influence modeled impacts of HRVOC sources on downwind concentrations of O_3 and HCHO. The results from this sensitivity analysis will help in understanding the effect of grid resolution on Eulerian model results and will benefit future grid modeling conducted for the region.

4.0 TASK DESCRIPTIONS

4.1 Task 1: QA/QC Alkene Hydroxynitrate Measurements by the Caltech TOF-CIMS aboard the DC-8 during SEAC4RS and Generate Final Data

This task will be conducted by Caltech. Caltech has developed the ability to detect multifunctional organic compounds using chemical ionization mass spectrometry. The Caltech CIMS method employs the clustering chemistry of the CF_3O^- reagent ion (Crounse et al., 2006; Paulot et al., 2009) to detect multifunctional OVOC:

$$[Z] + CF_3O^- \rightarrow Z \bullet CF_3O^- \quad \text{where [Z] is a target analyte.}$$

For the NASA SEAC^{4}RS campaign, the Caltech mass analyzer was upgraded from a quadrupole to a time-of-flight (ToF) analyzer (Figure 4-1). The ToF admits the sample ion beam to the ion extractor, where a pulse of high voltage orthogonally deflects and accelerates the ions into the reflectron, which in turn redirects the ions toward the multichannel plate detector. Ions in the ToF follow a V-shaped path from extractor to detector, separating by mass as the smaller ions are accelerated to greater velocities by the high voltage pulse. The detector collects the ions as a function of time following each extractor pulse. Critically for this study, the rapid-scan collection of the ToF guarantees a high temporal resolution (speeds of 10 Hz or faster) and simultaneous data products from the instrument for all masses (Drewnick et al., 2005).

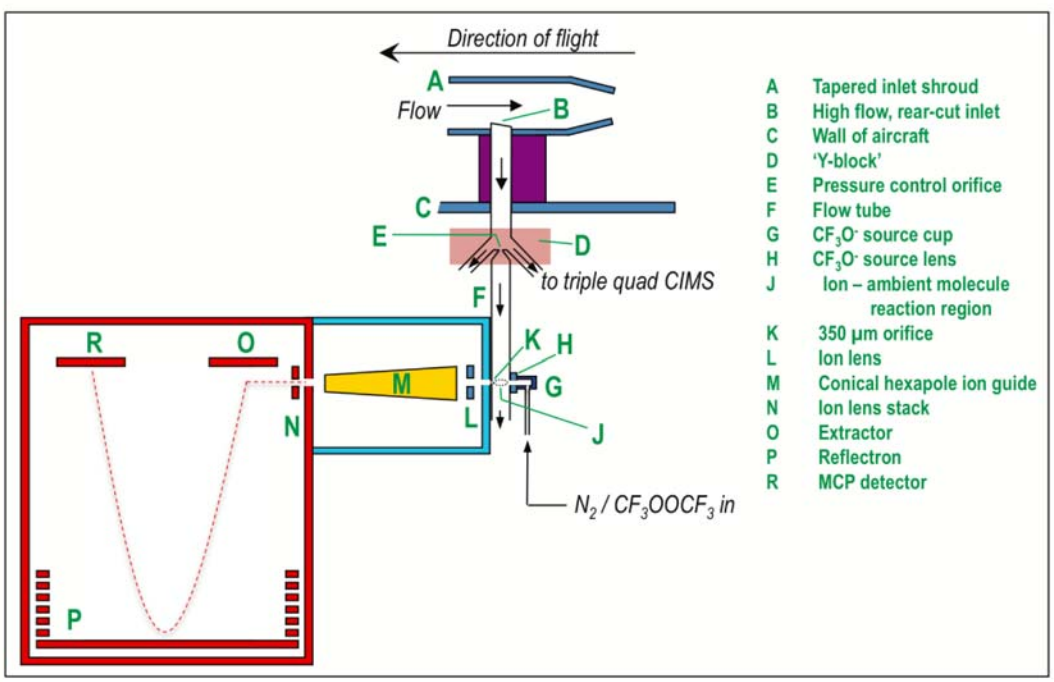

Figure 4-1. Airborne measurements of C_2-C_4 hydroxynitrates by the Caltech chemical ionization time-of-flight mass spectrometer in SEAC^{4}RS in 2013 permit a new and quantitative attribution of O_3 and HCHO produced from HRVOCs in Houston, TX.

During the SEAC⁴RS flights over Houston, the Caltech instrument detected the presence of β-hydroxynitrates produced in the gas-phase oxidation of alkenes, including those produced from the oxidation of ethene, propene, butenes, and 1,3-butadiene. While these small β-hydroxy nitrates have been previously observed in the laboratory, this is the first systematic detection of their presence in ambient air. An example is shown in Figure 4-2 where the DC-8 sampled air across the city. β-hydroxy nitrates produced from ethene, propene, butenes, and butadiene were all present and detected with excellent signal-to-noise ratios.

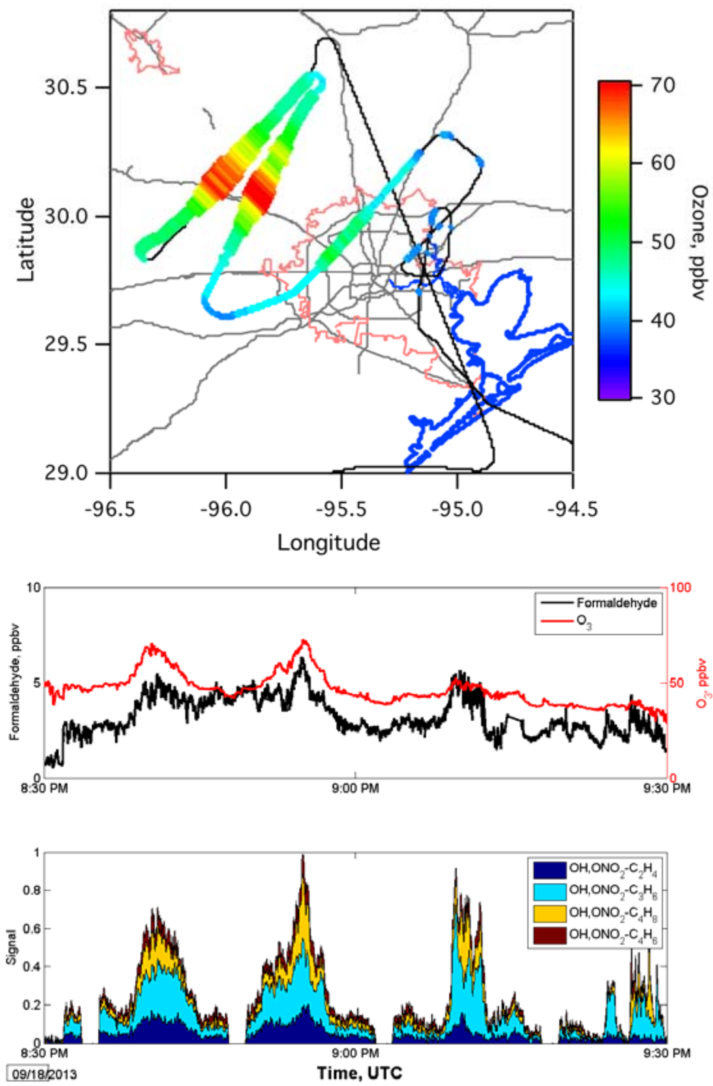

Figure 4-2. **(*Upper panel*) NASA DC-8 flight track (black line) on 18 September 2013 colored by O_3 measured in the boundary layer. (*Lower panels*) Time series data showing that observed enhancements in hydroxynitrates are correlated with O_3 and HCHO. Plume analysis and modeling will use these newly-measured products to better quantify emissions of specific HRVOCs.**

In Task 1, Caltech will undertake QA/QC of the β-hydroxy nitrates produced from ethene, propene, butenes, and butadiene, producing calibrated measurements for all SEAC^{4}RS flights over Texas. These data will enable in Tasks 2 and 3 the quantification of the role of HRVOCs in forming HCHO and O_3.

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

This task will be conducted jointly by NOAA, under a Purchase Order (PO) from ENVIRON, and Caltech. The calibrated 1-Hz hydroxynitrate data produced in Task 1 will be used in conjunction with 1-Hz observations of NOx, NO, PAN, HNO_3, NOy, O_3, HCHO, CH_3CHO, and other chemical and meteorological parameters measured aboard the NASA DC-8 to determine net O_3 production rates and yields for the airborne Houston study of 18 September 2013 (Figure 4-2). A simple analysis based on known hydroxynitrates yields following OH-initiated reactions of their parent alkenes (Teng, Crounse, Lee, St. Clair, Cohen, Wennberg, submitted, 2014) will permit a first-order attribution of the O_3 and HCHO formed as a result of earlier emissions of each specific alkene. This simple measurement-based analysis will be augmented by the modeling efforts that explicitly treat hydroxynitrate losses and 2nd-generation reaction products, described in Task 3, below.

Alkene emissions inferred from hydroxynitrate observations will be compared to the DC-8 whole-air-sample (WAS) data on ethene, propene, butenes, and butadiene in these plumes, and linked to the original emission ratio for individual plumes by the observed NOx/ethene ratio, which is preserved during transport from the source (Ryerson et al., 2003).

Overall plume O_3 production rates and yields deduced from airborne measurements during SEAC^{4}RS in 2013 will be compared to rates and yields deduced from airborne measurements in Ship Channel plumes under similar flow patterns, ambient temperatures, and solar insolation during TexAQS (Ryerson et al., 2003; Wert et al., 2003) and TexAQS II (Washenfelder et al., 2010). Changes in plume reaction rates between these earlier studies were noted and ascribed, in part, to the decrease in HRVOCs as a result of mandated control strategies to control ozone formation in Houston (Washenfelder et al., 2010). Analysis of the 2013 NASA airborne data will highlight the effects of over a decade of control strategies focusing on mitigating ozone formation in industrial plumes in the Houston area. The fractional contribution of PAN and HNO_3 to the plume NOy budget, among other chemical diagnostics, will be examined to evaluate changes in OH reactivity and plume chemistry between these studies.

The work in Task 2 will define measurement-based estimates of plume initial conditions, background concentrations, and dispersion as constraints for the Task 3 modeling, discussed below.

4.3 Task 3: Analysis of DC-8 airborne data to quantify plume initial conditions, production rates, and yields of O_3 and HCHO from parent alkenes

This task will be conducted by ENVIRON. Reactive plume modeling will be performed for selected days of the SEAC^{4}RS measurement period using the SCICHEM Lagrangian puff model with explicit photochemistry. SCICHEM is a state-of-the science puff model using second-order closure with an advanced chemistry module that represents chemical interactions between plume pollutants and the surrounding atmosphere. SCICHEM has previously been successfully evaluated using helicopter measurements of power plant plumes, including plume widths and plume chemistry (Karamchandani et al., 2000). SCICHEM was also applied in AQRP Project 10-020 conducted by NOAA and ENVIRON to study NOx reactions and transport in nighttime plumes and their impacts on next-day ozone. The model currently uses the CB05 gas-phase chemistry mechanism and will be updated to the CB6r2 mechanism (developed in AQRP Project 12-012) with additional explicit reactions to represent hydroxynitrate production from individual HRVOCs, leveraging the work done for AQRP Project 12-006.

Task 1 will identify flight dates and plume transects of interest during the SEAC^{4}RS measurement period. Task 2 will provide information on emission rates (based on initial plume concentrations), background concentrations for the plume chemistry calculations, and the plume spread or width at various downwind distances from the Houston Ship Channel. This information will serve as input for Task 3 plume modeling with SCICHEM. A similar approach was adopted in AQRP Project 10-020 to constrain the dispersion of the plume, resulting in much better agreement between predicted plume concentrations and observations made by the NOAA WP-3D aircraft in the TexAQS II study.

The hydroxynitrate and ozone concentrations predicted using SCICHEM will be compared with data from the DC-8 flight transects to evaluate whether the model chemistry is consistent with SEAC^{4}RS observations. In addition, the results from the plume modeling will be analyzed to compare modeled yields of O_3 and HCHO from the parent alkenes for comparison with the yields obtained in Task 2 from the analysis of the DC-8 measurements. The model will be used to explore the effects of hydroxynitrate deposition, HCHO losses, and constrain the impact of product reactions on the conclusions of the Task 2 analysis, which implicitly assumes negligible product losses over the 2-3 hour plume reaction and transport time scales sampled by the DC-8.

Model sensitivity tests with different initial plume dimensions will evaluate how the rate of plume dilution influences chemical processing in order to assess how grid model resolution (e.g., 4 km^2 vs. 1.3 km^2) is likely to influence modeled impacts of HRVOC sources on downwind concentrations of O_3 and HCHO. The results from this sensitivity analysis will help in understanding the effect of grid resolution on Eulerian model results and will benefit future grid modeling conducted for the region.

5.0 QUALITY METRICS

5.1 Quality Metrics for Data QA/QC and Analysis

Calibration procedures for the hydroxynitrates will be documented and the uncertainties quantified. The sensitivity of the CIMS instrument for these nitrates has been quantified and described in a recently submitted document (Teng, Crounse, Lee, St. Clair, Cohen, Wennberg, submitted, 2014). For this work, we will first remove the instrumental backgrounds which are measured every fifteen minutes during flight. The nitrate signals are converted to absolute mixing ratio using the laboratory-measured sensitivities. As part of this effort, we will carefully evaluate the uncertainty in the measured concentrations.

The measurements of other parameters that are needed to estimate chemical production rates and product yields along flight tracks include ozone, formaldehyde, acetaldehyde, nitric oxide, nitrogen dioxide, peroxyacetyl nitrate, nitric acid, and various hydrocarbons. While these are measured by a suite of different instruments aboard the NASA DC-8, the data reduction procedures are similar to that described above for the hydroxynitrates. Instrument backgrounds, where measured during flight, will be removed, and instrument sensitivities will be applied based on laboratory- or flight-measured values. The resulting atmospheric mixing ratios will be documented and the uncertainties quantified.

The hydroxynitrate data and a description of their uncertainty will be delivered in ICARTT format (http://www.esrl.noaa.gov/csd/groups/csd7/measurements/icartt_format_stds.pdf). The ancillary data (including but not limited to ozone, HCHO, CH_3CHO, NO, NO_2, PAN, HNO_3, and hydrocarbons) and a description of their uncertainties will be archived in final form on the public NASA site (http://www-air.larc.nasa.gov/cgi-bin/ArcView/seac4rs). The data and data analysis will also be presented in a manuscript submitted for publication to a peer-reviewed journal.

5.2 Quality Metrics for Modeling

The reactive puff model, SCICHEM, will be used in this project to simulate the transport and chemistry of industrial plumes from the Houston Ship Channel. SCICHEM is a state-of-the-science model that includes advanced treatments for puff dispersion and chemistry. The model has been evaluated against tracer studies (Chowdhury et al., 2013), helicopter measurements of daytime power plant plumes (Karamchandani et al., 2000), and aircraft measurements of nighttime power plant plumes (Karamchandani et al., 2011).

The data analysis results will provide information on emission rates, background chemistry, and the plume dispersion at various downwind distances, as well as meteorological parameters, such as wind vectors, temperature and pressure. This information will be used to constrain the reactive plume modeling. This approach is similar to that used in a previous AQRP study (Project 10-020) of nighttime power plant plumes (Karamchandani et al., 2011; Yarwood et al., 2012).

ENVIRON will evaluate the performance of SCICHEM in reproducing the observed hydroxynitrate and ozone measurements from the DC-8 flight transects. In addition, the results from the SCICHEM modeling will be analyzed to compare modeled yields of O_3 and HCHO from the parent alkenes for comparison with the yields obtained in Task 2 from the analysis of the DC-8 measurements.

The modeling results will be presented through the use of graphical displays, such as crosswind plume profiles and scatter plots, as well as tables showing model performance statistics (see Section 6.2).

6.0 DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

6.1 Aircraft Data Management

The aircraft data used in this project is or will be archived in data repositories at NASA. https://espo.nasa.gov/seac4rs/data_archive.php. The data manager for the NASA DC-8 data is Gao Chen (gao.chen@nasa.gov). The data are currently preliminary and are password protected. Final data, including the hydroxynitrate data produced in this project, will be publicly available beginning in October, 2014.

A member of the research team who did not conduct the measured data processing will review at least 10% of the input data for quality assurance purposes.

6.2 Analysis of SCICHEM Results

Model results will be evaluated using both graphical and statistical measures. Transect (crosswind profile) plots of observed and predicted plume concentrations of ozone and hydroxynitrates at various downwind distances will be generated for the days selected for plume modeling. Statistical measures, listed in Table 6-1 below, will be used to evaluate SCICHEM predictions of peak plume concentrations, average plume concentrations, and plume widths against observed values. In addition to these comparisons, the modeled yields of O_3 and HCHO from the parent alkenes calculated by SCICHEM will be compared with the corresponding yields from the analysis of the DC-8 measurements.

Table 6-1. Definition of performance metrics for reactive plume modeling.

Metric	Definition[1]
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$
Mean Normalized Bias (MNB) (-100% to +∞)	$\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{O_i}\right)$
Mean Normalized Error (MNE) (0% to +∞)	$\frac{1}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{O_i}\right\rvert$
Normalized Mean Bias (NMB) (-100% to +∞)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$
Normalized Mean Error (NME) (0% to +∞)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$

Metric	Definition[1]
Fractional Bias (FB) (-200% to +200%)	$\frac{2}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{P_i + O_i}\right)$
Fractional Error (FE) (0% to +200%)	$\frac{2}{N}\sum_{i=1}^{N}\left\lvert\frac{P_i - O_i}{P_i + O_i}\right\rvert$
Coefficient of Determination (r^2) (0 to 1)	$\left(\frac{\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}}\right)^2$

[1]P_i and O_i are prediction and observation at the i-th downwind distance, respectively; $\overline{P}$ and $\overline{O}$ are mean prediction and observation, respectively.

A member of the research team who did not conduct the modeling or air quality model input data processing and model simulations will review at least 10% of the input data and model output for quality assurance purposes.

6.3 Data Management

Data generated for this project, including the aircraft database, model inputs, final model outputs, and the reactive plume model, will be securely archived during the project on portable hard drives and stored for a period of at least three years following the completion of the project. All data obtained for this project will be stored in electronic format. Our teams' experience has been that 100+ GB hard drives provide an accessible and portable system for storing data files of the size routinely encountered in the type of modeling activities for this effort. If data are provided on paper, the paper documents will be scanned to electronic PDF files for storage. The University of Texas will receive an electronic copy of all data sets.

7.0 REPORTING AND DELIVERABLES

ENVIRON will prepare monthly financial and technical reports that will document the status of monthly project progress. These reports will include contributions from all the organizations participating in the study. Additionally, a quarterly report will be submitted at the end of each quarter. Interim reports/presentations may be provided upon request. A draft final report summarizing the QA findings, results of analyses, study findings, and recommendations will be prepared by May 18, 2015. Following receipt of comments from AQRP and TCEQ, a final report will be produced at the end of the project. The final report will meet State of Texas Accessibility requirements in 1 TAC 213. Electronic copies of all text, graphic, spreadsheet files and models used in the preparation of any documents related to the project reports, to document results and conclusions (e.g. sampling data, work files, etc.) or developed as work products under this Contract, will be supplied the conclusion of the project. All copies of deliverable documents and other work products will be provided in Microsoft Word and PDF format. Dr. Yarwood will supervise the completion of all reports and other deliverables.

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports 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. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

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, May 30, 2014

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	March, April, May 2014	Friday, May 30, 2014

Quarterly Report #2	June, July, August 2014	Friday, August 30, 2014
Quarterly Report #3	September, October, November 2014	Monday, December 1, 2014
Quarterly Report #4	December 2015, January & February 2015	Friday, February 27, 2015
Quarterly Report #5	March, April, May 2015	Friday, May 29, 2015
Quarterly Report #6	June, July, August 2015	Monday, August 31, 2015
Quarterly Report #7	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 - May 31	Monday, June 9, 2014
Technical Report #2	June 1 - 30, 2014	Tuesday, July 8, 2014
Technical Report #3	July 1 - 31, 2014	Friday, August 8, 2014
Technical Report #4	August 1 - 31, 2014	Monday, September 8, 2014
Technical Report #5	September 1 - 30, 2014	Wednesday, October 8, 2014
Technical Report #6	October 1 - 31, 2014	Monday, November 10, 2014
Technical Report #7	November 1 - 30 2014	Monday, December 8, 2014
Technical Report #8	December 1 - 31, 2014	Thursday, January 8, 2015
Technical Report #9	January 1 - 31, 2015	Monday, February 9, 2015
Technical Report #10	February 1 - 28, 2015	Monday, March 9, 2015
Technical Report #11	March 1 - 31, 2015	Wednesday, April 8, 2015
Technical Report #12	April 1 - 28, 2015	Friday, May 8, 2015
Technical Report #13	May 1 - 31, 2015	Monday, June 8, 2015

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by ENVIRON and Caltech using the AQRP FY14-15 FSR Template found on the AQRP website. NOAA’s invoices will be included in ENVIRON’s FSRs.

Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start - May 31	Monday, June 16, 2014
FSR #2	June 1 - 30, 2014	Tuesday, July 15, 2014
FSR #3	July 1 - 31, 2014	Friday, August 15, 2014
FSR #4	August 1 - 31, 2014	Monday, September 15, 2014
FSR #5	September 1 - 30, 2014	Wednesday, October 15, 2014

FSR #6	October 1 - 31, 2014	Monday, November 17, 2014
FSR #7	November 1 - 30 2014	Monday, December 15, 2014
FSR #8	December 1 - 31, 2014	Thursday, January 15, 2015
FSR #9	January 1 - 31, 2015	Monday, February 16, 2015
FSR #10	February 1 - 28, 2015	Monday, March 16, 2015
FSR #11	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #12	April 1 - 28, 2015	Friday, May 15, 2015
FSR #13	May 1 - 31, 2015	Monday, June 15, 2015
FSR #14	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #15	Final FSR	Wednesday, August 15, 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: Monday, May 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: Tuesday, June 30, 2015

Project Data

The project data, including the QA/QC measurement data, databases, plume model, and modeling inputs and outputs, 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. The data deliverables include the following:

- QA/QC final nitrate and ancillary data
- Data analysis spreadsheets
- SCICHEM modeling data:
    - SCICHEM source code with updated CB6r2 mechanism
    - SCICHEM run control file and run script
    - SCICHEM inputs
        - Emissions inputs
        - Meteorological inputs

    - Background chemistry inputs
- SCICHEM outputs
    - Instantaneous puff concentrations
    - Time-averaged concentrations for plume transects
- Excel spreadsheets for comparison of model outputs with aircraft observations

AQRP Workshop

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

8.0 REFERENCES

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