

## Quality Assurance Project Plan

### Project 19-040

#### Analysis of Ozone Production Data from the San Antonio Field Study

Prepared for

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

By

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Version #3

Drexel University has prepared this QAPP following a composite of the EPA guidelines for a Quality Assurance (QA) Category II Project: *Research Model Development or Application* and a category IV project: *Secondary Data Projects*. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: The QAPP describes the project description and objectives, project organization and responsibilities, model selection, model calibration, model verification, model evaluation, model documentation, and reporting procedures, as prescribed in the applicable NMRL QAPP Requirements template

(<https://www.tceq.texas.gov/airquality/airmod/project/quality-assurance>).

QA Requirements:      Technical Systems Audits - Not Required for the Project  
                                 Audits of Data Quality – 10% Required  
                                 Report of Findings – Required in Final Report

## Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the following project: *Analysis of Ozone Production Data from the San Antonio Field Study*. The Principal Investigator for the project is Ezra Wood and the Co-Principal Investigator is Shannon Capps.

Electronic Approvals:

**This QAPP was approved electronically on September 12, 2018 by Elena McDonald-Buller, The University of Texas at Austin.**

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Elena McDonald-Buller  
Project Manager, Texas Air Quality Research Program

**This QAPP was approved electronically on September 12, 2018 by Vincent M. Torres, The University of Texas at Austin.**

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Quality Assurance Project Plan Manager, Texas Air Quality Research Program

**This QAPP was approved electronically on September 12, 2018 by Ezra Wood, Drexel University.**

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Ezra Wood  
Principal Investigator, Drexel University

## **QAPP Distribution List**

Texas Air Quality Research Program  
David Allen, Director  
Elena McDonald-Buller, Project Manager

Texas Commission on Environmental Quality  
Mark Estes, Project Liaison

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Ezra Wood, Principal Investigator

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### *1.1 Description of Environmental system to be evaluated.*

Ozone is the main component of smog and has adverse effects on human health and vegetation. Unlike primary pollutants like carbon monoxide or black carbon, ozone is a secondary pollutant, formed by photochemical reactions involving volatile organic compound (VOCs) and nitrogen oxides (NO<sub>x</sub>).

The rate at which ozone is formed is effectively equal to the rate at which NO is converted to NO<sub>2</sub> by reaction with peroxy radicals (HO<sub>2</sub> and "RO<sub>2</sub>", where R represents CH<sub>3</sub>, C<sub>2</sub>H<sub>5</sub>, etc.):

$$P(O_3) = k_{HO_2+NO}[HO_2][NO] + k_{RO_2+NO}[RO_2][NO] \quad \text{Eq. 1}$$

There has been little prior research on ozone formation in San Antonio. During the 2017 San Antonio Field Study, a team of researchers from Drexel University, Aerodyne Research, Inc., University of Houston, and Rice University collaborated and collected a large dataset of measurements of gas-phase and condensed-phase (particulate matter) chemical compounds in the air. For this project we will be analyzing that data, including use of zero-dimensional and three-dimensional models. For the 0-D modeling activities, the Framework for 0-D Atmospheric Modeling (FOAM) model will be used. For the 3-D photochemical air quality modeling we will use the EPA's Community Multiscale Air Quality Modeling System (CMAQ).

### *1.2 Purpose of the project and specific project objectives*

The purpose of the project is to analyze the data collected during the 2017 San Antonio Field Study (SAFS) to characterize the rates at which ozone is formed in the greater San Antonio area, to test if current chemical mechanisms used in modeling are accurate, and to conduct 3-D air quality modeling to identify which emission sources are most important for forming ozone in San Antonio. Detailed objectives are to answer the following science questions:

- What are the rates of instantaneous ozone production (P(O<sub>3</sub>)) upwind, within the urban core, and downwind of San Antonio? Do these measured ozone production values agree with those modeled based on measured concentrations of nitrogen oxides and volatile organic compounds?
- Which emission sources are most important for ozone formation in San Antonio? (Both by type of compound emitted, e.g., NO<sub>x</sub> vs. biogenic VOCs, and by location – upwind vs. urban emissions).

## **2.0 Organization and Responsibilities**

### *2.1 Project Personnel*

The Principle Investigator of this project is Ezra Wood, Associate Professor of Chemistry at Drexel University. Dr. Wood will direct all aspects of the project,

mentor the postdoctoral researcher, be responsible for all reporting, and be responsible for the overall QA responsibilities. Shannon Capps, Assistant Professor of Civil, Architectural and Environmental Engineering at Drexel University, will be the co-Investigator, and will initiate the 3-D modeling work, train the postdoctoral fellow to use the 3-D photochemical model CMAQ, and advise on the interpretation. Daniel Anderson, postdoctoral fellow in the Department of Chemistry at Drexel University, will conduct most of the day-to-day analysis, including analysis of 2017 field data, the 0-D modeling using both the Drexel/Aerodyne and UH/Rice data, and the 3-D photochemical air quality modeling using CMAQ.

#### *2.2 Project schedule and key milestones.*

The project is divided into four Tasks as described in the Scope of Work. The timing of these tasks along with key outcomes or milestones are described below. Further information on these tasks is described in the Scope of Work and elsewhere in this document.

*Task 1: Quantify the dependence of ozone production on compounds measured during SAFS (September 2018 – December 2018)*

The primary milestone from this task is the successful analysis with documentation to be included in reports.

*Task 2: Conduct 0-D photochemical modeling using data from four SAFS measurement sites (September 2018 – March 2018).*

The outcome of this task will be analysis and associated documentation of the comparison of the measured radical concentrations and ozone production rates with those produced from the 0-D model.

*Task 3. Apportion ozone concentrations to location-specific emission sources using 3-D air quality modeling with the instrumented Community Multiscale Air Quality model (CMAQ) (November 2018 – July 2019)*

The outcome of this task will be output files from the 3-D model along w/ analysis of which emission sources contribute to ozone formation in San Antonio.

*Task 4. Project Reporting and Presentation (September 2018 – August 2019)*

This ongoing task will generate the following Deliverables: Abstract, monthly technical reports, monthly financial status reports, quarterly reports, draft final report, final report, attendance and presentation at AQRP data workshop, submissions of presentations and manuscripts, project data and associated metadata.

### **3. Scientific Approach**

Data collected by the Drexel, U. Houston, Aerodyne, and Rice University teams during the 2017 San Antonio Field Study will be the main data used for this analysis. These data were collected by a wide range of research-grade analytical instrumentation aboard mobile and stationary measurement sites. Additional sources of data will be from the monitoring sites operated by TCEQ in the greater San Antonio area, and the relevant

input files needed for CMAQ, in particular the location-specific emissions and meteorological data which we will obtain from Kirk Baker, US Environmental Protection Agency.

The model used for 0-D modeling is the “Framework for 0-D Atmospheric Modeling (F0AM)” model. For the 3-D photochemical air quality modeling we will use the EPA’s Community Multiscale Air Quality Modeling System (CMAQ); further described in section 6 “Modeling” below. Both models have been used extensively for similar type studies (Appel et al. 2007; Wolfe et al. 2016)

For Task 1, “Quantify the dependence of ozone production on compounds measured during SAFS”, the primary analysis method will be to generate graphs of the ozone production rate  $P(O_3)$  plotted vs. various other chemical measurements, including concentrations of NO, NO<sub>x</sub>, VOCs, and HO<sub>x</sub> radical precursors like ozone and formaldehyde. The ozone production rates are calculated using the measured concentrations of nitric oxide and total peroxy radicals  $[HO_2 + \Sigma RO_2]$  and a modified form of equation 1 below.

$$P(O_3) = k_{\text{eff}}([HO_2] + \Sigma[RO_2])[NO]$$

Where  $P(O_3)$  is the production rate of ozone in ppb/hr,  $k_{\text{eff}}$  is the average rate constant for the reaction of HO<sub>2</sub> and individual RO<sub>2</sub> species with NO ( $8.1 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ ), and  $([HO_2] + \Sigma[RO_2])$  is the concentration of total peroxy radicals measured by the Drexel ECHAMP instrument.

#### 4. Quality Metrics

4.1 Total peroxy radicals  $([HO_2] + \Sigma[RO_2])$  were measured by the Ethane CHEMical AMPlifier (ECHAMP) method (Wood, Deming, and Kundu 2017) on board the Aerodyne Mobile Laboratory. The measurements have a  $2\sigma$  analytical uncertainty of 20%, based on underlying uncertainty and reproducibility of the calibrations, the accuracy of the underlying NO<sub>2</sub> measurements by cavity attenuated phase shift spectroscopy, and variation in the response of the instrument to different types of peroxy radicals. The  $1\sigma$  precision of 15 min averaged measurements was usually better than (i.e., less than) 1 ppt, leading to signal-to-noise ratios of greater than 10 for most daytime measurements. Further details are described in Wood et al. (2017).

The following key species were measured aboard both the Aerodyne Mobile laboratory and the University of Houston mobile laboratory and will be used for all three tasks: nitric oxide (NO), nitrogen dioxide (NO<sub>2</sub>), ozone (O<sub>3</sub>), and speciated volatile organic compounds (VOCs) measured with a proton-transfer reaction mass spectrometer, including acetaldehyde and acetone. Additionally, formaldehyde was measured on the ARI mobile laboratory by Tunable Infrared Laser Direct Absorption Spectrometry (TILDAS). The analytical accuracy of these measurements was better than 10% ( $2\sigma$ ), largely based on the uncertainty of the calibration standards used for calibrations. After averaging the “raw” one-second data to one-minute or 15 minute averages, the  $1\sigma$

precision was almost always less than 5% of the measured concentrations (i.e., the signal-to-noise ratios were greater than 20).

The Aerodyne mobile laboratory data was recorded at three locations:

1. The University of Texas at San Antonio (UTSA), which under prevailing Southeasterly winds is downwind of central San Antonio,
2. Floresville, which is Southeast of San Antonio, and
3. Lake Corpus Christi, further Southeast of San Antonio.

The U. of Houston / Rice University mobile laboratory measured at the Traveler's World RV Resort which is situated in the urban core of San Antonio, and experienced higher NO<sub>x</sub> concentrations than measured at the three Aerodyne sites listed above. The data collected during the San Antonio Field Study by Drexel, U. of Houston, Rice University, and Aerodyne Research, Inc. have been quality assured (QA'd) by the respective principle investigators.

Neither dataset (ARI/Drexel or U. Houston/Rice) alone can be considered complete or fully representative of the range of air masses experienced by San Antonio, but combined they do constitute a decent geographic range. During the SAFS, overall air movement frequently followed the common southeasterly flows which can result in elevated ozone concentrations northwest of San Antonio, though no air quality exceedances for ozone occurred during SAFS.

## **5. Data Analysis, Interpretation, and Management**

### *5.1 Data Reduction Procedures*

Data from SAFS, including the ECHAMP peroxy radical measurements and the other measurements from the Aerodyne Mobile Laboratory and the University of Houston/Rice mobile laboratory, have already been quality assured (QA'd) and finalized. The only further data reduction that will likely be required is further averaging depending on the particular analyses.

### *5.2 Data validation procedures.*

To ensure the reporting of accurate project data we will maintain analysis code (in Matlab software) that can be re-run to ensure the correct data is used.

### *5.3 Data Analysis*

The data will be quantitatively analyzed for tasks 1, 2, and 3. Where appropriate, linear regressions will be used to compare modeled to measured concentrations. Mean and median concentrations and standard deviations in measured and modeled concentrations will be presented as appropriate.

### *5.4 Data Storage*

Data from SAFS is currently stored on two personal computers, two external hard drives, and on a cloud-based storage method (Microsoft OneDrive) that maintains compliance with the ISO 27001 standard for Information Security Management and ISO 27018 standard for Cloud Privacy and Data Protection.



## 6. Modeling

### 6.1 Modeling description and objectives

To complement the investigation with observed data, an Eulerian chemical transport modeling framework will be used to inform the impact of NO<sub>x</sub> and VOC sources on downwind ozone concentrations. Evaluation of the modeled concentrations of relevant species, including O<sub>3</sub> and NO<sub>2</sub>, against observations will constitute a key part in the analysis. Scaling individual species emissions rates from select sectors or streams over a bounded geographical area may be employed to better represent observed concentrations. Instrumented modeling with source tracking will provide insight about the contributions of emissions to ozone formation locally and downwind.

In addition, a zero-dimensional (0-D) chemical box model, constrained to observations made during SAFS, will be used to model total peroxy radical abundance and P(O<sub>3</sub>). The same modeling framework will be used with four, separate chemical mechanisms, three of which are used in air quality models. Modeled P(O<sub>3</sub>) and total peroxy radicals will be compared to the observations to determine how well each mechanism reproduces observations and to determine the speciation of peroxy radicals. This box modeling setup allows for direct comparison of the different mechanisms to help determine any deficiencies in an individual mechanism.

### 6.2 Modeling responsibilities

The co-I, Shannon Capps, will be responsible for initiating the modeling effort. She will train and guide the post-doc, Daniel Anderson, in the use of the Eulerian model. The continuing analysis including the scaling of emissions and the source apportionment technique will be conducted primarily by the post-doc with mentoring and input from the PI and co-I. Since the post-doc will be executing the model, the co-I will be responsible for quality assurance of 10% of the modeled output as described below. In addition, the post-doc will be responsible for all aspects - including model setup, evaluation, and interpretation of results - of the 0-dimensional modeling.

### 6.3 Model selection

The Eulerian chemical transport model to be used for this project is the Community Multiscale Air Quality (CMAQ) model (Byun and Schere 2006), which is developed and maintained by the U.S. Environmental Protection Agency (EPA). CMAQ calculates the concentration of chemicals, including ozone, in a three-dimensional grid. The estimated emissions of precursor gases evolve with chemical reactions and physical process in the presence of weather patterns. Specifically, CMAQ v.5.2.1, which was released in March 2018, will be used with the fourth version of Carbon Bond 6 (CMAQ option: CB6r3) (Emery et al. 2015) for treatment of gas phase reactions. The aqueous chemistry mechanism as well as aerosol dynamics and thermodynamics will be represented with the most recent treatment (CMAQ option: aero6). Additionally, primary organic aerosol will be treated with the potential to be semivolatile and age in the gas phase (Murphy 2018) (CMAQ option: nvPOA).

The model inputs will be provided by Kirk Baker of the EPA Office of Air Quality Planning and Standards. The meteorology will be driven by results from the Weather Research and Forecasting (WRF) model. Emissions will include a recent version of the National Emissions Inventory projected to 2017 as well as biogenic emissions as modeled by BEIS v.3.6.1. These will be preprocessed with the Sparse Matrix Operator Kernel Emissions (SMOKE) model for use in CMAQ. These will be provided for April-June 2017 for the continental U.S. at 12-km horizontal resolution

Similar models such as the Comprehensive Air Quality Model with Extensions (CAMx) and GEOS-Chem are alternatives to CMAQ, but this choice provides the opportunity to scale emissions locally with according to observations without rerunning SMOKE and to conduct ozone source apportionment using CMAQ's Integrated Source Apportionment Method (ISAM) (Cohan and Napelenok 2011; Kwok et al. 2015). The availability of a very recent modeling platform for CMAQ from EPA also made it a reasonable choice.

The 0-D model to be used for this project is the "Framework for 0-D Atmospheric Modeling" (F0AM) version 3.1, which is a Matlab-based tool for simulation of photochemical atmospheric processes (Wolfe et al. 2016). Observations of chemical concentrations, meteorological variables, and photolysis frequencies are used to constrain and run the model, which then calculates concentrations of unconstrained species. This model is both a tool that can further understanding of the chemistry controlling the atmospheric abundance of a given species, such as peroxy radicals, and that allows for the evaluation of the accuracy of the chemical mechanisms running in the model. Observations of relevant species and meteorological variables made during the SAFS campaign will be used to constrain the model.

There are multiple 0-dimensional box models capable of modeling  $P(O_3)$ , such as the Dynamically Simple Model of Atmospheric Chemical Complexity (DSMACC) and Module Efficiently Calculating the Chemistry of the Atmosphere (MECCA) models. These models are essentially limited to a single chemical mechanism, however. In contrast, F0AM can be run with a variety of mechanisms, including the explicit Master Chemical Mechanism (MCM) and various lumped mechanisms (e.g. CB05, CB6r3, and GEOS-Chem) traditionally used in 3-dimensional modeling, providing a common platform to evaluate their performance. F0AM has been successfully used to evaluate, among others, the chemistry of HCHO (Anderson et al. 2017; Marvin et al. 2017), peroxy radicals (Wolfe et al. 2014), OH (Kaiser et al. 2016), and HONO (Kim et al. 2015) across a wide range of VOC and NO<sub>x</sub> regimes. Good agreement was found for ozone production rates calculated by F0AM and DSMACC when constrained with the same set of observations (Anderson et al. 2016), showing that F0AM is an appropriate tool for the research proposed here.

#### 6.4 Model calibration

The modeled surface concentrations will be compared with observations of key species from the San Antonio Field Study (SAFS) sites. Additionally, the emissions ratio of CO to NO<sub>x</sub> at these urban monitoring sites will be determined through regression of CO and NO<sub>y</sub> observations as described in (Anderson et al. 2014), with a particular focus on morning observations when *in situ* CO production from isoprene oxidation is at a minimum. These emissions ratios will then be compared to the NEI inputs to CMAQ. Finally, to evaluate model NO<sub>2</sub> in the upwind region, where *in situ* observations are

sparse, the modeled concentrations of NO<sub>2</sub> will be compared to satellite retrievals of tropospheric NO<sub>2</sub> columns from the OMI and GOME2 instruments as described in (Canty et al. 2015) and (Ring et al. 2018).

These model comparisons will be used to inform sensitivity analysis runs in which a new framework for scaling emissions within the CMAQ model, which allows individual species from select sectors or streams for which an input file exists over a bounded geographical area to be adjusted by a scaling factor, will be employed. Based on the evaluation of emissions against *in situ* and satellite-based observations, select sectors and species (e.g., on-road NO<sub>x</sub> emissions) in the region around San Antonio will be scaled; then, the revised modeled concentrations will be compared against observations.

Before and after an emissions rate adjustment, the postdoc (Daniel Anderson) will compare the modeled concentrations against the observations of the scaled species from the SAFS sites to evaluate the degree of improvement or disimprovement with mean normalized bias, mean normalized error, and correlation coefficients.

#### *6.5 Model verification*

The mean normalized bias and mean normalized error of O<sub>3</sub> and NO<sub>2</sub> as compared to observations from the SAFS sites will be calculated and compared against the EPA's suggested bounds for O<sub>3</sub> of ±15% and ±35%, respectively, for the base run and for the adjusted emissions run(s). The model uncertainty will be characterized by these metrics for O<sub>3</sub> and NO<sub>2</sub> in the San Antonio region. The sensitivity of the model will be characterized by the degree of change of the O<sub>3</sub> and NO<sub>2</sub> fields with respect to the adjustments in emissions.

Similar statistical analysis will be performed for the box model output. The model will not be constrained to observed NO and H<sub>2</sub>O<sub>2</sub>, two species key to peroxy radical chemistry and ozone production. Instead, the model will be allowed to calculate the concentrations of these species as it will for total peroxy radicals. The mean normalized bias of the modeled concentrations of NO and H<sub>2</sub>O<sub>2</sub> with respect to the observations will then be used to verify that the model is able to reproduce these species within acceptable bounds.

Both of these model verification activities will be performed by the post-doc Daniel Anderson.

#### *6.6 Model evaluation*

For the base run, the inputs developed at the EPA Office of Air Quality Planning and Standards will be used. The EPA will conduct the model evaluation for the continental U.S.. As a contingency plan in the case that a substantial change is made between the platform EPA provides and the platform they evaluate, a basic evaluation of the model against AQS ozone observations nationwide will be included in this work. The plan is for the scope of this work to include only an evaluation of O<sub>3</sub> in the San Antonio region. The model will be considered sufficiently informative for the source apportionment exercise if it meets the criteria specified for the mean normalized bias and mean normalized error at the SAFS sites.

In addition to the mean normalized bias metric described above, the box model will be evaluated by determining the sensitivity of modeled P(O<sub>3</sub>) and total peroxy radicals to model inputs. This will be explored by individually perturbing the model constraints by

the measurement uncertainty and determining the resultant change in P(O<sub>3</sub>) and relevant chemical species. This process will allow researchers to determine whether measurement uncertainties for any species could potentially significantly impact the modeling results.

#### *6.7 Source apportionment*

CMAQ-ISAM allows the user to apportion O<sub>3</sub> concentrations to region- and sector-specific emissions. ISAM is projected to be available for CMAQ v.5.2.1 in early 2019, which will make it possible to use the evaluated modeling platform with this instrumented version of the model. The ISAM evaluation will be conducted entirely by EPA.

Using the base model run, the San Antonio O<sub>3</sub> contributions from emissions of NO<sub>x</sub> and VOC from the biogenic, on road, and off road sectors will be assessed for each of the following regions: upwind of San Antonio (assuming prevailing southeasterlies), urban San Antonio, surrounding region, and boundary conditions.

#### *6.8 Model documentation*

The final report will include descriptions of the CMAQ modeling platform, the method for scaling emissions, the application of ISAM, and hardware and software requirements. Additionally, the model execution will be described including settings selected in scripts to run the models, output of model runs, and results of model evaluation. The range of scaling factors applied to each sector, species, and geographic extent will be documented along with the impacts of each scaling of emissions in a summary metric. The full output files will only be maintained for select emissions scaling based on the model calibration exercise. The source apportionment results will be documented for each of the sectors, species, and geographic ranges selected in the final analysis. Similarly, the final report will also include a thorough description of the box model setup and the process used to create model inputs. All box model input and output files will be saved.

#### *6.9 Model QA/QC*

At minimum, 10% of the model input provided by EPA will be audited through visualization for quality assurance purposes. At minimum, 10% of the model output from the CMAQ base scenario, the CMAQ sensitivity scenario, and the CMAQ-ISAM application will be reviewed in detail by a team member who did not conduct the modeling activities for quality assurance purposes. Since Daniel Anderson will conduct the modeling activities under the supervision of co-PI Shannon Capps, the PI (Ezra Wood) will perform these model QA activities. These reviews are intended to satisfy the QA requirements required by this category level QAPP.

#### *6.10 Data storage*

The model inputs and scripts as well as pertinent model output will be stored for a minimum of three years with Dropbox or a similar cloud backup solution that maintains compliance with the ISO 27001 standard for Information Security Management and ISO 27018 standard for Cloud Privacy and Data Protection.

### 6.11 Reporting

The team will produce a final report that includes the content described in the model documentation. Additionally, the team will produce a journal article in which the results of the modeling, sensitivity analysis, and source apportionment efforts are used to contextualize the impact of emissions of species observed in SAFS on the San Antonio region.

## 7.0 Reporting

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.

**Abstract:** At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

**Abstract Due Date:** Friday, August 31, 2018

**Quarterly Reports:** Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Microsoft Word 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.

### Quarterly Report Due Dates:

Report	Period Covered	Due Date
Aug2018 Quarterly Report	June, July, August 2018	Friday, August 31, 2018
Nov2018 Quarterly Report	September, October, November 2018	Friday, November 30, 2018
Feb2019 Quarterly Report	December 2018, January & February 2019	Thursday, February 28, 2019
May2019 Quarterly Report	March, April, May 2019	Friday, May 31, 2019
Aug2019 Quarterly Report	June, July, August 2019	Friday, August 30, 2019
Nov2019	September, October, November 2019	Friday, November 29, 2019

**Monthly Technical Reports (MTRs):** Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY16-17 MTR Template found on the AQRP website.

**MTR Due Dates:**

Report	Period Covered	Due Date
Aug2018 MTR	Project Start - August 31, 2018	Monday, September 10, 2018
Sep2018 MTR	September 1 - 30, 2018	Monday, October 8, 2018
Oct2018 MTR	October 1 - 31, 2018	Thursday, November 8, 2018
Nov2018 MTR	November 1 - 30 2018	Monday, December 10, 2018
Dec2018 MTR	December 1 - 31, 2018	Tuesday, January 8, 2019
Jan2019 MTR	January 1 - 31, 2019	Friday, February 8, 2019
Feb2019 MTR	February 1 - 28, 2019	Friday, March 8, 2019
Mar2019 MTR	March 1 - 31, 2019	Monday, April 8, 2019
Apr2019 MTR	April 1 - 28, 2019	Wednesday, May 8, 2019
May2019 MTR	May 1 - 31, 2019	Monday, June 10, 2019
Jun2019 MTR	June 1 - 30, 2019	Monday, July 8, 2019
Jul2019 MTR	July 1 - 31, 2019	Thursday, August 8, 2019

**Financial Status Reports (FSRs):** Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY16-17 FSR Template found on the AQRP website.

**FSR Due Dates:**

Report	Period Covered	Due Date
Aug2018 FSR	Project Start - August 31	Monday, September 17, 2018
Sep2018 FSR	September 1 - 30, 2018	Monday, October 15, 2018
Oct2018 FSR	October 1 - 31, 2018	Thursday, November 15, 2018
Nov2018 FSR	November 1 - 30 2018	Monday, December 17, 2018
Dec2018 FSR	December 1 - 31, 2018	Tuesday, January 18, 2019
Jan2019 FSR	January 1 - 31, 2019	Friday, February 15, 2019
Feb2019 FSR	February 1 - 28, 2019	Friday, March 15, 2019
Mar2019 FSR	March 1 - 31, 2019	Monday, April 15, 2019
Apr2019 FSR	April 1 - 28, 2019	Wednesday, May 15, 2019
May2019 FSR	May 1 - 31, 2019	Monday, June 17, 2019
Jun2019 FSR	June 1 - 30, 2019	Monday, July 15, 2019
Jul2019 FSR	July 1 - 31, 2019	Thursday, August 15, 2019
Aug2019 FSR	August 1 - 31, 2019	Monday, September 16, 2019
FINAL FSR	Final FSR	Tuesday, October 15, 2019

**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. It will also include a report of the QA findings.

**Draft Final Report Due Date:** Thursday, August 1, 2019

**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.

**Final Report Due Date:** Tuesday, September 3, 2019

**Project Data:** All project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (September 30, 2019). The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. It will also include a report of the QA findings.

**AQRP Workshop:** A representative from the project will present at the AQRP Workshop in the first half of August 2019.

**Presentations and Publications/Posters:** All data and other information developed under this project which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

## 8.0 References

- Anderson, D. C., J. M. Nicely, R. J. Salawitch, T. P. Canty, R. R. Dickerson, T. F. Hanisco, G. M. Wolfe, E. C. Apel, E. Atlas, T. Bannan, S. Bauguitte, N. J. Blake, J. F. Bresch, T. L. Campos, L. J. Carpenter, M. D. Cohen, M. Evans, R. P. Fernandez, B. H. Kahn, D. E. Kinnison, S. R. Hall, N. R. Harris, R. S. Hornbrook, J. F. Lamarque, M. Le Breton, J. D. Lee, C. Percival, L. Pfister, R. B. Pierce, D. D. Riemer, A. Saiz-Lopez, B. J. Stunder, A. M. Thompson, K. Ullmann, A. Vaughan, and A. J. Weinheimer. 2016. 'A pervasive role for biomass burning in tropical high ozone/low water structures', *Nat Commun*, 7: 10267.
- Anderson, D. C., J. M. Nicely, G. M. Wolfe, T. F. Hanisco, R. J. Salawitch, T. P. Canty, R. R. Dickerson, E. C. Apel, S. Baidar, T. J. Bannan, N. J. Blake, D. X. Chen, B. Dix, R. P. Fernandez, S. R. Hall, R. S. Hornbrook, L. G. Huey, B. Josse, P. Jockel, D. E. Kinnison, T. K. Koenig, M. Le Breton, V. Marecal, O. Morgenstern, L. D. Oman, L. L. Pan, C. Percival, D. Plummer, L. E. Revell, E. Rozanov, A. Saiz-Lopez, A. Stenke, K. Sudo, S. Tilmes, K. Ullmann, R. Volkamer, A. J. Weinheimer, and G. Zeng. 2017. 'Formaldehyde in the Tropical Western Pacific: Chemical Sources and Sinks, Convective Transport, and Representation in CAM-Chem and the CCM1 Models', *Journal of Geophysical Research-Atmospheres*, 122: 11201-26.
- Anderson, Daniel C., Christopher P. Loughner, Glenn Diskin, Andrew Weinheimer, Timothy P. Canty, Ross J. Salawitch, Helen M. Worden, Alan Fried, Tomas Mikoviny, Armin Wisthaler, and Russell R. Dickerson. 2014. 'Measured and modeled CO and NO<sub>y</sub> in DISCOVER-AQ: An evaluation of emissions and chemistry over the eastern US', *Atmospheric Environment*, 96: 78-87.
- Appel, K Wyatt, Alice B Gilliland, Golam Sarwar, and Robert C Gilliam. 2007. 'Evaluation of the Community Multiscale Air Quality (CMAQ) model version 4.5: sensitivities impacting model performance: part I—ozone', *Atmospheric Environment*, 41: 9603-15.
- Byun, Daewon, and Kenneth L. Schere. 2006. 'Review of the governing equations, computational algorithms, and other components of the models-3 Community Multiscale Air Quality (CMAQ) modeling system', *Applied Mechanics Reviews*, 59.
- Canty, T. P., L. Hemberck, T. P. Vinciguerra, D. C. Anderson, D. L. Goldberg, S. F. Carpenter, D. J. Allen, C. P. Loughner, R. J. Salawitch, and R. R. Dickerson. 2015. 'Ozone and NO<sub>x</sub> chemistry in the eastern US: evaluation of CMAQ/CB05 with satellite (OMI) data', *Atmospheric Chemistry and Physics*, 15: 10965-82.
- Cohan, Daniel S., and Sergey L. Napelenok. 2011. 'Air Quality Response Modeling for Decision Support', *Atmosphere*, 2.
- Emery, C., J. Jung, B. Koo, and G. Yarwood. 2015. "Improvements to CAMx Snow Cover Treatments and Carbon Bond Chemical Mechanism for Winter Ozone." In. Prepared for the Utah Department of Environmental Quality, Division of Air Quality, Salt Lake City, UT. Prepared by Ramboll Environ, Novato, CA.
- Kaiser, J., K. M. Skog, K. Baumann, S. B. Bertman, S. B. Brown, W. H. Brune, J. D. Crouse, J. A. de Gouw, E. S. Edgerton, P. A. Feiner, A. H. Goldstein, A. Koss, P. K. Misztal, T. B. Nguyen, K. F. Olson, J. M. St Clair, A. P. Teng, S. Toma, P. O.



- Wennberg, R. J. Wild, L. Zhang, and F. N. Keutsch. 2016. 'Speciation of OH reactivity above the canopy of an isoprene-dominated forest', *Atmospheric Chemistry and Physics*, 16: 9349-59.
- Kim, S., S. Y. Kim, M. Lee, H. Shim, G. M. Wolfe, A. B. Guenther, A. He, Y. Hong, and J. Han. 2015. 'Impact of isoprene and HONO chemistry on ozone and OVOC formation in a semirural South Korean forest', *Atmospheric Chemistry and Physics*, 15: 4357-71.
- Kwok, R. H. F., K. R. Baker, S. L. Napelenok, and G. S. Tonnesen. 2015. 'Photochemical grid model implementation and application of VOC, NO<sub>x</sub>, and O<sub>3</sub> source apportionment', *Geo. Mod. Dev.*, 8.
- Marvin, Margaret R., Glenn M. Wolfe, Ross J. Salawitch, Timothy P. Canty, Sandra J. Roberts, Katherine R. Travis, Kenneth C. Aikin, Joost A. de Gouw, Martin Graus, Thomas F. Hanisco, John S. Holloway, Gerhard Huebler, Jennifer Kaiser, Frank N. Keutsch, Jeff Peischl, Ilana B. Pollack, James M. Roberts, Thomas B. Ryerson, Patrick R. Veres, and Carsten Warneke. 2017. 'Impact of evolving isoprene mechanisms on simulated formaldehyde: An inter-comparison supported by in situ observations from SENEX', *Atmospheric Environment*.
- Murphy. 2018. "Personal Communication." In.
- Ring, A. M., T. P. Canty, D. C. Anderson, T. P. Vinciguerra, H. He, D. L. Goldberg, S. H. Ehrman, R. R. Dickerson, and R. J. Salawitch. 2018. 'Evaluating commercial marine emissions and their role in air quality policy using observations and the CMAQ model', *Atmospheric Environment*, 173: 96-107.
- Wolfe, G. M., C. Cantrell, S. Kim, R. L. Mauldin III, T. Karl, P. Harley, A. Turnipseed, W. Zheng, F. Flocke, E. C. Apel, R. S. Hornbrook, S. R. Hall, K. Ullmann, S. B. Henry, J. P. DiGangi, E. S. Boyle, L. Kaser, R. Schnitzhofer, A. Hansel, M. Graus, Y. Nakashima, Y. Kajii, A. Guenther, and F. N. Keutsch. 2014. 'Missing peroxy radical sources within a summertime ponderosa pine forest', *Atmospheric Chemistry and Physics*, 14: 4715-32.
- Wolfe, G. M., M. R. Marvin, S. J. Roberts, K. R. Travis, and J. Liao. 2016. 'The Framework for 0-D Atmospheric Modeling (FOAM) v3.1', *Geosci. Model Dev.*, 9: 3309-19.
- Wood, Ezra C., Benjamin L. Deming, and Shuvashish Kundu. 2017. 'Ethane-Based Chemical Amplification Measurement Technique for Atmospheric Peroxy Radicals', *Environmental Science & Technology Letters*, 4: 15-19.