Quality Assurance Project Plan

Project 16 – 019
The Influence of Alkyl Nitrates from Anthropogenic and Biogenic Precursors on Regional Air Quality in Eastern Texas

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

Prepared by

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The University of Texas at Austin has prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Measurement. 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: *The Influence of Alkyl Nitrates from Anthropogenic and Biogenic Precursors on Regional Air Quality in Eastern Texas*. The Principal Investigator for the project is Elena McDonald-Buller and Co-Principal Investigators are Lea Hildebrandt Ruiz and Greg Yarwood.

Electronic Approvals:

This QAPP was approved electronically on 09/08/2016 by David Sullivan, The University of Texas at Austin.

David Sullivan
Project Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 09/15/2016 by Vincent M. Torres, The University of Texas at Austin.

Vincent M. Torres
Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 09/08/2016 by Elena McDonald-Buller, The University of Texas at Austin.

Elena McDonald-Buller
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QAPP Distribution List

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1.0 Project Description and Objectives

1.1 Project Purpose and Objectives

Mono and multifunctional alkyl nitrates (ANs) are formed from the oxidation of biogenic or anthropogenic volatile organic compound (VOC) precursors and serve as a reservoir or sink of nitrogen oxides (NO_x). Alkyl nitrates have sufficiently long atmospheric chemical lifetimes (hours to days), such that they can influence tropospheric ozone and secondary organic aerosol (SOA) formation over regional to global spatial scales. Their functionalities, yields, and fates are known to depend upon the size and structure of the VOC. Depending on their structure, ANs can be transported, chemically processed, removed by deposition to vegetation and other surfaces, or undergo partitioning to and from the aerosol phase where hydrolysis is thought to be a loss mechanism. Although knowledge gaps still exist, recent laboratory and field studies have provided new insights on these processes for ANs formed from biogenic and anthropogenic hydrocarbon precursors. An ongoing need will be to incorporate these findings into the chemical mechanisms of photochemical models used to assess regional air quality.

The objectives of this work are to apply the findings of ongoing experimental studies examining alkyl nitrates formed from the OH-initiated oxidation of C8-C11 alkanes at the University of Texas at Austin in addition to those of new publications that have focused on other biogenic and anthropogenic hydrocarbon precursor classes relevant to Texas emissions inventories, including isoprene, monoterpenes, and aromatics, to guide refinements to Revision 4 of the CB6 chemical mechanism (CB6r4) in version 6.32 of the Comprehensive Air quality Model with extensions (CAMx v6.32). Sensitivity tests with CAMx will evaluate the formation and fate of ANs in central and southeastern Texas, the influence of ANs on regional ozone by recycling NO_x, and dependencies on organic aerosol concentrations. The project consists of three tasks that include refinements to the CB6r4 Mechanism in CAMx (Task 1), evaluation of CB6r4 updates in CAMx modeling for the time period of the DISCOVER-AQ 2013 campaign (Deriving Information on Surface Conditions from Column and Vertically Resolved Observations Relevant to Air Quality, http://discover-aq.larc.nasa.gov/) (Task 2), and project reporting and presentation (Task 3).

1.2 Project Model System and Data

Refinements to the CB6r4 chemical mechanism will be guided by the findings of ongoing controlled experimental studies of gas-particle partitioning and hydrolysis of ANs from the OH-initiated oxidation of C8-C11 alkanes at the University of Texas at Austin as well as the results of a literature review of recent publications describing controlled laboratory studies and ambient observations from campaigns such as SEAC^{4}RS (Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys) and SOAS (Southern Oxidants and Aerosols Study). The experimental studies of ANs formed from alkane precursors are being conducted by Dr. Hildebrandt Ruiz's research team under the sponsorship of the Texas Air Research Center (TARC;

https://engineering.lamar.edu/research/tarc/awarded-proposals-tarc.html). The instrumentation, experimental methods, calibration procedures, and data analysis techniques have been described elsewhere (e.g., Bean et al., 2016) and are available upon request.

CAMx is an open-source modeling system for multi-scale integrated assessment of gaseous and particulate air pollution (Ramboll Environ, 2016). CAMx model inputs for the Houston DISCOVER-AQ period of September 2013 and modeled organic aerosol (OA) using the 1.5-D volatility basis set (VBS) approach developed in AQRP Project 14-024 (Hildebrandt Ruiz et al., 2015) will be applied to evaluate the effects of refinements to the representation of ANs in the CB6r4 gas-phase mechanism on regional air quality. Figure 1 shows the model domain, which consists of a 36-km continental-scale grid, a nested 12-km grid covering Texas, and a 4-km nested grid covering the Houston area. Meteorological inputs were developed using version 3.6.1 of the Weather Research Forecast (WRF) model. Anthropogenic emissions were obtained from the Texas Commission on Environmental Quality (TCEQ) for the 36/12/4 km domains compatible with the CB6 mechanism and include updates for emissions of intermediate volatility organic compounds (IVOCs; volatility range 10^4 to 10^6 μg m^{-3} in saturation concentration) developed during AQRP Project 14-024. Biogenic emissions estimates were developed for the time period using version 2.1 of the Model of Emissions of Gases and Aerosols from Nature (MEGAN; Guenther et al., 2012). Fire emissions were based on the Fire Inventory from NCAR (FINN) version 1 dataset (http://bai.acd.ucar.edu/Data/fire).

Figure 1. CAMx modeling domain with outer 36 km grid and nest 12 km (blue) and 4 km (green) grids.

Model performance evaluation will make use of monitoring data for ozone and NO_x collected at TCEQ Continuous Ambient Monitoring Stations (CAMS). CAMS data will be obtained in ASCII, comma delimited format from the TCEQ. All CAMS within the 4-km grid will be used to evaluate how mechanism changes influence ozone in and around Houston. Within the 12-km grid covering Texas and neighboring states, regionally representative monitoring sites (i.e., rural and suburban locations) will be selected from the TCEQ and EPA monitoring networks to evaluate how mechanism changes influence regional ozone concentrations. The performance evaluation will also use measurements of AN concentrations in the particle phase and OA concentrations measured at an air quality monitoring ground site in Conroe, Texas (30.350278°N, 95.425000°W) during DISCOVER-AQ. Data collection and analysis at this site has been described in previous AQRP projects (http://aqrp.ceer.utexas.edu/index.cfm) from FY 2012-2013 (12-012, 12-032) and FY 2014-2015 (14-009, 14-024, 14-029).

2.0 Organization and Responsibilities

2.1 Project Personnel

The project will be directed by Dr. Elena McDonald-Buller (Principal Investigator) and Dr. Lea Hildebrandt Ruiz (Co-Principal Investigator) of the University of Texas at Austin and Dr. Greg Yarwood (Co-Principal Investigator) of Ramboll Environ. The Principal Investigator and Co-Principal Investigators will be supported by staff members from the University of Texas at Austin and Ramboll Environ. Project participants and their responsibilities are listed in Table 1.

Drs. McDonald-Buller and Hildebrandt Ruiz and Drs. Greg Yarwood and Bonyoung Koo of Ramboll Environ will collaborate to lead and accomplish the efforts for Task 1. Dr. McDonald-Buller and Dr. Yarwood will collaborate to lead the efforts for Task 2. Dr. McDonald-Buller will lead Task 3 with assistance from Dr. Yarwood.

2.2 Project Schedule

An overall schedule of project activities by task is shown in Table 2. The schedule assumes a start date of September 1, 2016 and end date of August 31, 2017.

Table 1. Project participants from the University of Texas at Austin and Ramboll Environ and their key responsibilities.

Participant	Key Responsibilities
Elena McDonald-Buller	Principal Investigator from the University of Texas at Austin with overall responsibility for the guidance, integration, and supervision of project activities, including quality assurance and quality control activities.
Lea Hildebrandt Ruiz	Co-Principal Investigator from the University of Texas at Austin who will assist in the interpretation of experimental and observational data used to guide the CB6r4 mechanism refinements.
Greg Yarwood	Co-Principal Investigator from Ramboll Environ who will update how ANs are represented in the CB6r4 gas-phase chemical mechanism. Dr. Yarwood will collaborate with Dr. McDonald-Buller to lead key project tasks, reporting, and quality assurance and quality control activities.
Bonyoung Koo	Manager at Ramboll Environ who will implement in CAMx updates to the AN chemistry in the CB6r4 mechanism and to the pseudohydrolysis of alkyl nitrates.
Ou Nopmongcol	Manager at Ramboll Environ who will transfer the CAMx modeling database and associated model post-processing software and participate in the evaluation and interpretation of CAMx simulations performed at the University of Texas at Austin. Dr. Nopmongcol also will perform CAMx simulations at Ramboll Environ to test and quality assure model updates.
Yosuke Kimura	Research Associate at the University of Texas at Austin who will work on the coordination of the transfer of the CAMx modeling database and associated model post-processing software from Ramboll Environ to the University of Texas at Austin and conduct, evaluate, and interpret the results of the CAMx simulations.
Andy Wentland	Ramboll Environ Associate who will assist with the mechanism updates and CAMx simulations.
Tasko Olevski	Ramboll Environ Associate who will assist with the mechanism updates and CAMx simulations.

Table 2. Project schedule by task.

ID	Task	Sep.-Oct. 2016	Nov.-Dec. 2016	Jan.-Feb. 2017	Mar.-Apr. 2017	May-Jun. 2017	Jul.-Aug. 2017
1	***Refinements to the CB6r4 Mechanism in CAMx***	X	X	X			
2	***Evaluating Updates to CB6r4 in CAMx Modeling for DISCOVER-AQ***		X	X	X	X	
3	***Project Reporting and Presentation***	X	X	X	X	X	X

3.0 Model Selection

CAMx is an Eulerian photochemical model that allows for integrated "one-atmosphere" assessments of tropospheric air pollution (ozone, particulate matter, air toxics) over a range of spatial scales. It is publicly available and undergoes continues review and evolution to reflect the state of the science. Although other Eulerian photochemical grid models such as the Community Multi-Scale Air Quality (CMAQ) system are available, CAMx has been used extensively for regulatory analysis to support State Implementation Plan (SIP) development and research studies of regional air quality in eastern Texas for more than a decade. Multiple gas phase chemistry mechanism options including CB6, CB05, and SAPRC07 are available within the CAMx framework. In addition, the 1.5-D volatility basis set (VBS) approach was recently implemented in CAMx for modeling of organic aerosol. CAMx was selected for this project because of its history and on-going use by the TCEQ, the desire to continue previous improvements in the representation of the formation and fate of alkyl nitrates in the CAMx CB6 mechanism, and the need to evaluate updates to the representation of alkyl nitrates in an air quality model with organic aerosol.

4.0 Model Calibration

The CAMx modeling platform that will be used in this project was adapted from a 2013 Texas ozone forecast modeling application developed by Ramboll Environ for the TCEQ (Johnson et al. 2013). It underwent revisions during the course of Project 14-024 based on comparisons with measurements of the concentrations and composition of gas and particle-phase species taken during the DISCOVER-AQ 2013 campaign. Results of the evaluation indicated that the revised model gave considerably better agreement with measured organic carbon (OC) concentrations, Positive Matrix Factorization (PMF)-based oxygenated organic aerosol (OOA) fractions, and contemporary carbon fractions by radiocarbon analysis than the original base model. The revised model with replacement of the CB6r2 with the CB6r4 mechanism will form the baseline for modifications and comparisons for the work that will be conducted under this project. The CB6r2 mechanism was developed in AQRP project 12-012 to improve the level of detail regarding the formation and fate of organic nitrates (Hildebrandt Ruiz and Yarwood, 2013). Subsequently, CB6r3 implemented temperature and pressure dependent yields of organic nitrates for alkanes larger than ethane (Emery et al., 2015). CB6r4 adds reactions of iodine species that deplete ozone (e.g., in the marine boundary layer over the Gulf of Mexico), removes oxygen-atom (O^3P) reactions with VOCs that are important in smog chambers but not in the atmosphere, and makes no changes to gas-phase reactions of organic nitrates (Emery et al., 2016).

A primary objective of this project is to produce a refined version of the CB6r4 chemical mechanism that reflects the current scientific understanding of the formation and fate of ANs and that can be applied by the TCEQ for regulatory air quality modeling efforts. Recent and on-going observational studies at the University of Texas at Austin and elsewhere will be evaluated and interpreted with attention to those that quantify hydrolysis rates of ANs from a range of precursors and/or parameterize gas-particle partitioning of organic nitrates under varying environmental conditions. A focus will be on straight-chained and branched C8-C11 alkanes that are the subject of on-going studies by Dr. Hildebrandt Ruiz and other biogenic and anthropogenic hydrocarbon precursor classes relevant to Texas emissions inventories, including isoprene, monoterpenes, and aromatics. To the extent possible, sources, versions, and completeness of all data used to guide CB6r4 refinements as well as associated measurement techniques, calibration and validation protocols, and analysis approaches will be documented.

The findings will be used to refine the representation gas-particle partitioning and hydrolysis of ANs, propose strategies for improved differentiation of ANs in CB6r4, and test potential new strategies in CAMx via sensitivity studies. In this work, modifications to CB6r4 may require changes in emitted species (e.g., differentiation of PAR), which would be made directly to the CAMx-ready emission files. CAMx-ready emission files are available for several broad categories (on-road mobile, area, biogenic, point sources) such that changes can be adapted to the source sector. This approach is efficient for sensitivity testing and will provide sufficient information to guide and evaluate mechanism changes.

Sensitivity studies will systematically examine how individual and collective modifications to the CB6r4 mechanism influence CAMx predictions of concentrations of ozone and other key species in the gas and particle phases in eastern Texas relative to the baseline configuration. Assessment of model predictions will be made using expert judgment based on the team members' extensive histories with chemical mechanism development and comparisons with observational datasets for ozone and other key species in the gas-phase and particle-phases during the DISCOVER-AQ time period as described in Section 1.2. A desired goal is to retain or improve the predictive capabilities for ozone. However changes in the CB6r4 mechanism will neither be selected nor rejected based solely on whether they improve ozone model performance, recognizing that many factors may influence model ozone predictions. Evaluation of the capability of CB6r4 mechanism modifications to accurately represent experimental findings, the responsiveness of CAMx to mechanism changes, and model performance for NO_x and other nitrogen containing species are among other considerations in recommending modifications to CB6r4.

5.0 Model Verification

Spatial mapping and descriptive summaries of the CAMx predictions will be created to facilitate the detection of anomalies and evaluations of reasonableness and expected directional consistency with the mechanism changes. Discrepancies that warrant further investigation will be identified, and reconciliation approaches will be pursued as appropriate. Maps will be created using ArcGIS, PAVE, or alternative visualization software available through the Texas Advanced Computing Center (TACC).

Assessments of model performance will be made using expert judgment and statistical evaluations with observational datasets at all CAMS and other sites within the 4-km grid and at selected sites representative of rural and suburban areas within the 12-km grid with data collection activities during the DISCOVER-AQ time period. Metrics to be used in the evaluation are described in Section 6.0 and are based on recommended metrics from the U.S. Environmental Protection Agency's *Draft Modeling Guidance for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze* (https://www3.epa.gov/ttn/scram/guidance/guide/Draft_O3-PM-RH_Modeling_Guidance-2014.pdf) and Simon et al. (2012). In its modeling guidance document, the EPA states that it is "…not appropriate to assign bright line criteria that distinguish between adequate and inadequate model performance," instead recommending a "weight of evidence" approach be applied to assess the validity of model application. In this study, the evaluation of the model will be compared to the findings of Simon et al. (2012) who assessed photochemical model performance statistics published between 2006 and 2012, as well as to earlier evaluations of the baseline model configuration in order to understand how changes in the CB6r4 mechanism influence model performance.

Within the time period of the CAMx modeling period, approximately three days will be selected for which data will be withheld from the calibration efforts and used for model verification. These days will be selected based on criteria that will be established during the project; this could include for example representative regionally high or low ozone days or days with flow patterns from source regions of interest.

6.0 Model Evaluation

Quantitative comparisons of model performance for ozone and NOx will employ both graphical and statistical methods focusing primarily on the 4-km grid with assessments for selected sites within the 12-km grid. Graphical methods will include spatial maps and time-series comparing model predictions to observations. Statistical performance metrics to be computed are shown in Table 3.

Alkyl nitrate concentrations in the particle phase and organic aerosol concentrations measured at Conroe during DISCOVER-AQ will also be used in the performance evaluation. The numerical performance evaluation will be supplemented by comparing model predictions for nitrogen-containing secondary species, including ANs and PANs, to recent measurement campaigns (e.g., Fisher et al., 2016). Campaigns such as SEAC^{4}RS and SOAS and coordinated modeling studies (e.g. Fisher et al., 2016), although focused on the southeastern United States, serve as an additional resource for comparisons of model predictions of nitrogen-containing secondary species, including ANs and peroxyacetyl nitrates (PANs).

A minimum of 10% of the data input to the models will be audited and reviewed in detail by a team member that did not perform the analyses for quality assurance purposes. A minimum of 10% of the results of all analyses performed during this project will be audited and reviewed in detail by a project team member that did not perform the analyses for quality assurance purposes. The results of these reviews and any quality assurance findings will be included in the final report.

Table 3. Statistical metrics expected to be used in the model performance evaluation

Metric	Definition[1]
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i \rvert$
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 +∞)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i \rvert}{\sum_{i=1}^{N} O_i}$
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)	$\left(\frac{\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}}\right)^2$
Root Mean Squared Error (RMSE)	$\sqrt{\frac{\sum_{i=1}^{N}(P_i - O_i)^2}{N}}$

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

7.0 Model Documentation

Descriptions of the CAMx configuration, scripts, emissions inventory and meteorological input files, CB6r4 mechanism modifications, output files, and results of the model evaluation will be provided in the project final report. The rationale for each modification to the CB6r4 mechanism and outcomes of the CAMx sensitivity studies will be documented.

8.0 Reporting

All project data, model inputs, model outputs, and reports will be maintained by the PI for a period of 5 years, minimum.

As required, monthly technical, monthly financial status, and quarterly reports as well as an abstract at project initiation and, near the end of the project, the draft final and final reports will be submitted according to the schedule below. Dr. McDonald-Buller or her designee will electronically submit each report to both the AQRP and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources (http://aqrp.ceer.utexas.edu/). Dr. McDonald-Buller and Dr. Yarwood anticipate attending and presenting at the AQRP data workshop. Draft copies of any planned presentations (such as at technical conferences) or manuscripts to be submitted for publication resulting from this project will be provided to both the AQRP and TCEQ liaisons per the Publication/Publicity Guidelines included in Attachment G of the subaward. Final project data and associated metadata will be prepared and submitted to the AQRP archive. Each deliverable and required deadline for submission are presented below.

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: Wednesday, August 31, 2016

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
Aug2016 Quarterly Report	June, July, August 2016	Wednesday, August 31, 2016
Nov2016 Quarterly Report	September, October, November 2016	Wednesday, November 30, 2016
Feb2017 Quarterly Report	December 2016, January & February 2017	Tuesday, February 28, 2017
May2017 Quarterly Report	March, April, May 2017	Friday, May 31, 2017
Aug2017 Quarterly Report	June, July, August 2017	Thursday, August 31, 2017
Nov2017 Quarterly Report	September, October, November 2017	Thursday, November 30, 2017

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**
Aug2016 MTR	Project Start - August 31, 2016	Thursday, September 8, 2016
Sep2016 MTR	September 1 - 30, 2016	Monday, October 10, 2016
Oct2016 MTR	October 1 - 31, 2016	Tuesday, November 8, 2016
Nov2016 MTR	November 1 - 30 2016	Thursday, December 8, 2016
Dec2016 MTR	December 1 - 31, 2016	Monday, January 9, 2017
Jan2017 MTR	January 1 - 31, 2017	Wednesday, February 8, 2017
Feb2017 MTR	February 1 - 28, 2017	Wednesday, March 8, 2017
Mar2017 MTR	March 1 - 31, 2017	Monday, April 10, 2017
Apr2017 MTR	April 1 - 28, 2017	Monday, May 8, 2017
May2017 MTR	May 1 - 31, 2017	Thursday, June 8, 2017
Jun2017 MTR	June 1 - 30, 2017	Monday, July 10, 2017
Jul2017 MTR	July 1 - 31, 2017	Tuesday, August 8, 2017

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**
Aug2016 FSR	Project Start - August 31	Thursday, September 15, 2016
Sep2016 FSR	September 1 - 30, 2016	Monday, October 17, 2016
Oct2016 FSR	October 1 - 31, 2016	Tuesday, November 15, 2016
Nov2016 FSR	November 1 - 30 2016	Thursday, December 15, 2016
Dec2016 FSR	December 1 - 31, 2016	Tuesday, January 17, 2017
Jan2017 FSR	January 1 - 31, 2017	Wednesday, February 15, 2017
Feb2017 FSR	February 1 - 28, 2017	Wednesday, March 15, 2017
Mar2017 FSR	March 1 - 31, 2017	Monday, April 17, 2017
Apr2017 FSR	April 1 - 28, 2017	Monday, May 15, 2017
May2017 FSR	May 1 - 31, 2017	Thursday, June 15, 2017
Jun2017 FSR	June 1 - 30, 2017	Monday, July 17, 2017
Jul2017 FSR	July 1 - 31, 2017	Tuesday, August 15, 2017
Aug2017 FSR	August 1 - 31, 2017	Friday, September 15, 2017
FINAL FSR	Final FSR	Monday, October 16, 2017

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: Tuesday, August 1, 2017

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: Thursday, August 31, 2017

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 29, 2017). 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 2017.

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.

9.0 References

Bean, J. K., Hildebrandt Ruiz, L., Gas-particle partitioning and hydrolysis of organic nitrates formed from the oxidation of α-pinene in environmental chamber experiments, Atmos. Chem. Phys., 2016, 16, 2175–2184, doi:10.5194/acp-16-2175-2016.

Emery. C., Jung, J., Koo, B., Yarwood, G., Improvements to CAMx Snow Cover Treatments and Carbon Bond Chemical Mechanism for Winter Ozone. Final Report for Utah Department of Environmental Quality, Division of Air Quality, 2015.

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Guenther, A. B., Jiang, X., Heald, C.L. Sakulyanontvittaya, T., Duhl, T., Emmons, L. K., Wang, X. The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions. , 5, 1503- 1560., Geosci. Model Dev., 2012, 5, 1471–1492.

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Johnson, J., Karamchandani, P., Wilson, G. and Yarwood, G., TCEQ Ozone Forecasting System, Prepared for Mark Estes., 2013.

Ramboll Environ. 2016. User's Guide: Comprehensive Air Quality Model with extensions, Version 6.30. Available at http://www.camx.com.

Simon, H., Baker, K., Phillips, S. Compilation and interpretation of photochemical model performance statistics published between 2006 and 2012, Atmos Environ, 2012, 61,124-139, doi: 10.1016/j.atmosenv.2012.07.012.