

Quality Assurance Project Plan (QAPP)

Project 20-003 Characterization of Corpus Christi and San Antonio Air Quality During the 2020 Ozone Season

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

Prepared by

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**July 6, 2020
Version 2**

Rice University has prepared this QAPP following Environmental Protection Agency (EPA) guidelines for a Quality Assurance Category II/III Project: Measurement & Model Application. It is submitted to the Texas Air Quality Research Program as required in the Work Plan requirements.

QAPP Requirements: Project Description and Objectives, Organization and Responsibilities, Scientific Approach, Sampling Procedures, Measurement Procedures, Quality Metrics, Model Selection, Model Calibration, Model Verification, Model Evaluation, Model Documentation, Data Analysis, Interpretation, and Management, Reporting, References

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

PROJECT TITLE AND APPROVALS SHEET

Approvals Sheet

This document is a Category II/III Quality Assurance Project Plan for the *Characterization of Corpus Christi and San Antonio Air Quality During the 2020 Ozone Season* project. The Principal Investigator for the project is Robert Griffin. Co-PIs are Rebecca Sheesley, Sascha Usenko, Yuxuan Wang, and James Flynn.

Electronic Approvals:

This QAPP was approved electronically on July 6, 2020 by

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1. PROJECT DESCRIPTION AND OBJECTIVES

1.1. PROCESS AND/OR ENVIRONMENTAL SYSTEM TO BE EVALUATED

This project focuses on field work, data analysis, and modeling of air quality in Corpus Christi, in the area downwind (that is also upwind of San Antonio), and in and downwind of San Antonio. Compared to other urban areas in Texas, these locations have received considerably less attention from the atmospheric science/air quality research community, despite issues related to their compliance with air quality regulations. Understanding air quality in these areas is specifically highlighted as a need in the document describing the Texas Air Quality Research Program Priority Research Areas for 2020-2021.

1.2. PURPOSE AND OBJECTIVES

The scientific questions to be answered by this work focus on understanding the chemical and physical processes that govern the temporal and spatial patterns of pollutant concentrations in the highlighted region. Thus, the measurements and modeling will focus on understanding:

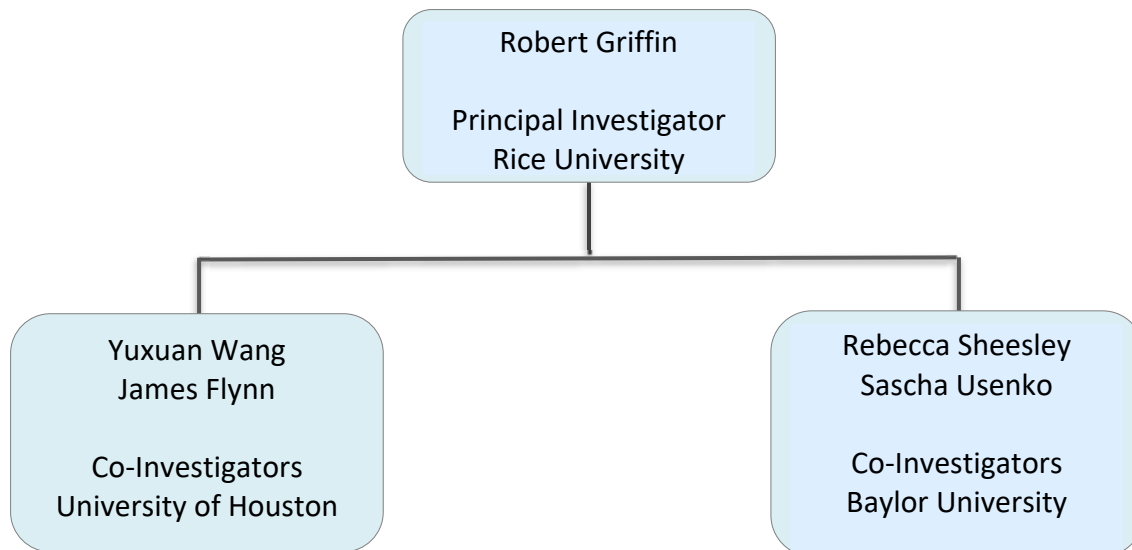
- a.) the chemistry and composition of the air transported into the Corpus Christi area from the Gulf of Mexico under the predominant ozone-season southeasterly wind;
- b.) how local emissions contribute to concentrations of both primary and secondary pollutants in Corpus Christi;
- c.) the chemical processing of air masses as they are advected out of Corpus Christi towards San Antonio; and
- d.) if ozone (O_3) and particulate matter (PM) formation dynamics in San Antonio in the latter portion of the ozone season differ from those observed in the early portion of the ozone season during the San Antonio Field Study (SAFS) conducted during May 2017.

The platform for the field measurements will be the University of Houston/Rice University/Baylor University Mobile Air Quality Laboratory (MAQL). The MAQL has been deployed successfully in both stationary and mobile modes to characterize air quality across multiple locations in Texas, including in and around Houston and in San Antonio during SAFS. The instrumentation on the MAQL will include sensors to measure meteorological parameters, inorganic trace gases that can be used as emissions tracers and that are relevant to both PM and O_3 formation (including carbon monoxide (CO), carbon dioxide (CO_2), nitrogen oxides (NO_x), total reactive nitrogen (NO_y), sulfur dioxide (SO_2), and O_3 itself), volatile organic compounds (VOCs), and PM composition. After undergoing quality assurance/quality control (QA/QC), the data generated by the MAQL instrumentation will be used in statistical analyses to determine basic parameters (mean, standard deviation, etc.) and diurnal and wind distribution patterns for stationary measurements and spatial patterns for mobile measurements. More advanced analyses using zero-dimensional photochemical modeling and positive matrix factorization on the generated data will determine values for O_3 production rate, identify the sensitivity of O_3 formation to NO_x or VOCs, and deconvolve organic particulate matter into various types. These analyses will be

supplemented by three-dimensional (3-D) air quality modeling using the Weather Research and Forecasting-GEOS Chem (WRF-GC) platform.

2. ORGANIZATION AND RESPONSIBILITIES

2.1. KEY PERSONNEL



Rice University: Robert Griffin, PI, Departments of Civil and Environmental Engineering and Chemical Biomolecular Engineering, Houston, Texas, USA, rob.griffin@rice.edu. Lead the project and focus predominantly on PM measurements, data analysis, and report/publication generation.

University of Houston: James Flynn, Co-I, Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas, USA, jhflynn@Central.uh.edu. Participate in drive planning and data analysis, coordinate field and analysis activities to ensure successful project completion, and prepare/submit reports.

Yuxuan Wang, Co-I, Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas, USA, ywang246@Central.uh.edu. Trajectory and 3-D modeling and analysis, advise and manage graduate students, assist with report preparation.

Baylor University: Rebecca Sheesley, Co-I, Department of Environmental Science, Baylor University, Waco, Texas, USA, Rebecca_Sheesley@baylor.edu. Operation of the VOC instrumentation. Assist with field campaign logistics, data analysis and interpretation, and preparation of related manuscripts and/or reports.

Sascha Usenko, Co-I, Department of Environmental Sciences, Baylor University, Houston, Texas, USA, Sascha_Usenko@baylor.edu, Operation of the VOC instrumentation. Assist with field campaign logistics, data analysis and interpretation, and preparation of related manuscripts and/or reports.

2.2. PROJECT SCHEDULE

The project timeline is given below. Note that this schedule does not include the items described in the Deliverables section below, as those Deliverables will be provided in addition to the performance of the tasks prescribed here.

- Task 1 – Field campaign preparation, AQRP issued start date – August 23, 2020
- Task 2 – Field campaign performance, August 24 – October 12, 2020
- Task 3 – Data analysis including QA/QC and 3-D modeling, October 13, 2020 – August 6, 2021 (note that preparation of 3-D modeling input can begin while the campaign is being performed)

3. SCIENTIFIC APPROACH

3.1. EXPERIMENTAL DESIGN

During the early part of the past decade, the sites that comprise the air quality monitoring network in the greater San Antonio metropolitan area exhibited at least one day per year on which the observed daily maximum eight-hour average O₃ mixing ratio exceeded 70 parts per billion by volume (ppbv), the value stipulated by the National Ambient Air Quality Standards (NAAQS), based on TCEQ data, which are publicly available online. Despite these observations, an assessment of published literature revealed very limited peer-reviewed research that elucidates the causes of enhanced O₃ mixing ratios in San Antonio. One study suggests that ~30 ppbv of O₃ in San Antonio can be attributed to anthropogenic activities (for a 2002 state-wide simulation) (Farooqui et al., 2013). In addition, Choi and Souri (2015) investigated trends of nitrogen dioxide (NO₂), formaldehyde (HCHO), and O₃ using satellite-measured columns, surface monitoring, and 3-D modeling; they observed both positive and negative trends depending on both species and the time period considered. These studies provided limited insight into the apportionment of peak O₃ mixing ratios in San Antonio. Thus, investigation of the physical and chemical processes that control O₃ formation in this region was warranted and provided the motivation for the San Antonio Field Study (SAFS), supported by TCEQ and its AQRP, that occurred in spring (May) 2017.

With respect to O₃, findings from the SAFS (documented in the project final report and in Anderson et al. (2019)) indicate that San Antonio was predominantly in a NO_x-limited regime, which led to a very high O₃ production efficiency, especially on days with relatively strong solar radiation. Compared to NO_x, O₃ formation in San Antonio was less sensitive to major VOCs such as alkanes, ethane, and acetone. Isoprene, HCHO, and alkenes exhibited high reactivity (defined as the product of the species concentration and its rate coefficient for the reaction with hydroxyl radical). Local O₃ formation at San Antonio was driven both by organic peroxy radicals and the hydroperoxy radical, with a production rate peaking at mid-day.

The SAFS also included measurement of PM because of the inextricable relationship between PM and trace gases relevant to O₃ formation (in terms of both co-emission and chemical interaction). Analyses of PM data from SAFS are ongoing but indicate that high sulfate plumes were mostly related to air masses coming from the Gulf of Mexico, which implied that the sulfate aerosol observed at San Antonio was less likely to be locally produced. Instead, the sulfate aerosols represented mostly a regional, background level which could be attributed to both biogenic marine sources and regional sulfate-related anthropogenic activities, including those in the Gulf of Mexico and potentially those in locations outside the United States. Additional PM analyses indicate the importance of secondary organic aerosol (SOA) formation over the San Antonio region and the lack of influence of wildfires and biomass burning in Central America on PM in San Antonio during SAFS.

A second urban area in Texas that suffers from relatively poor air quality (based on similar TCEQ data as those mentioned above for San Antonio) is Corpus Christi. Though smaller in population compared to San Antonio, Corpus Christi is home to much more significant infrastructure associated with the petrochemical industry; thus, the emission profiles of the two urban areas are quite different. The coastal location of Corpus Christi also causes its meteorology and the relevant atmospheric chemistry to be unlike those in San Antonio. The same modeling study referred to above indicates that on average ~9 ppbv of O₃ in Corpus Christi can be attributed to anthropogenic activity (Farooqui et al., 2013). Other previous research focused on or including Corpus Christi indicates the importance of Central American fires on average O₃ and PM levels along the coast of the Gulf of Mexico (Wang et al., 2018), how concentrations of highly reactive olefins associated with petrochemical emissions vary spatially across south Texas (Myers et al., 2015), and the contributions of secondary sulfate, SOA and marine aerosols to PM levels on an annual basis (Karnaue and John, 2011; Subramoney et al., 2013). Specific efforts have been made to understand health impacts of local emissions in Corpus Christi (e.g., Wing et al., 2017) and how regulatory efforts can improve air quality (e.g., levels of air toxics) (Capobianco et al., 2013).

It should be stressed that the data collected and the resulting conclusions made during SAFS are relevant only for the spring portion of the O₃ season, which lasts in total from April through October. Evaluation of air quality in Corpus Christi has been limited predominantly to data collected using relevant monitoring networks. Thus, the experimental design of this proposal is focused on the evaluation of air quality in Corpus Christi, San Antonio, and the region in between during the latter part of the 2020 (calendar year) O₃ season.

3.2. MEASUREMENTS PROCESS

MAQL Platform



Figure 1. Photograph of the MAQL with arm raised and an available generator.

The University of Houston/Rice/Baylor MAQL, shown in Figure 1, is comprised of a 325-ft³ fiberglass truck body in the bed of a 2013 Chevrolet Silverado 3500HD Crew Cab pickup truck. The instrumentation installation was engineered to optimize the space and allow for performance of the full suite of measurements. Integrated in the shell are three air-conditioning systems with 38,000 BTU cooling capacity, allowing for operation of instrumentation during warm weather. The truck and shell are wired to distribute power from either a generator while in motion or from a 50-A RV power outlet for stationary measurements; the power can be supplied from a towed generator when in motion. Self-sampling of generator emissions will be

avoided through appropriate inlet and exhaust line design. The ambient trace gas sample air is drawn through an inlet box that houses valves, converters, and power supplies for sampler configuration and calibration. The ambient aerosol is segregated by a 2.5- μ m cyclone inlet and transmitted to the aerosol analytical instrumentation through a 3/8-in. copper tubing inlet. The trace gas inlet box, aerosol inlet, and meteorological sensors are mounted to the end of a 4-m articulating arm that allows the MAQL to measure from approximately six meters above the ground while in motion and approximately eighteen feet with the arm raised for stationary measurements. Additionally, the MAQL is equipped with wired and wireless network, dual 4G cellular internet connections, four (front, rear, left, and right) high-definition cameras for identification of emission sources and characterization of local conditions, one hemispheric rooftop camera for cloud condition documentation, perimeter lighting for nighttime operations, and front and rear strobe lights for increased visibility.

The deployment will follow the protocols established during previous MAQL-based field campaigns (Leong et al., 2017; Wallace et al., 2018) and described subsequently in this QAPP. The cited publications describe calibration procedures, data analysis, etc.

3.3. GENERAL APPROACH

The scientific questions to be addressed as part of this proposal are based on the fact that air quality in a given time and location is controlled by a combination of the composition of the air transported into the location, the local emissions, and the in situ chemistry, all of which are influenced by meteorology. These questions will guide the approach to sampling and analysis. In the context of south Texas, the relevant scientific questions (and related hypotheses) are:

Question A: What is the nature of the air being transported into Corpus Christi from the Gulf of Mexico, and how does it compare to air being transported into Galveston/Houston (as described in Schulze et al. (2018))? *Related Hypothesis:* Because of the anthropogenic activities occurring in the Gulf of Mexico and areas outside the United States, the air coming into Corpus Christi from the ocean (a predominant wind direction during O₃ season) will be polluted (in terms of sulfate aerosol, organic PM, and NO_x) compared to other coastal locations. However, because of the smaller port in Corpus Christi, the air transported into Corpus Christi will be less polluted than that transported into Galveston, except when Corpus Christi is influenced directly by fire emissions from Central America.

Question B: What is the impact of local emissions on air quality as air is advected through Corpus Christi? *Related Hypothesis:* Within Corpus Christi itself, due to limited large tree vegetation, it will be anthropogenic activities, predominantly those associated with vehicular traffic, the port, and the petrochemical processing, that primarily drive emissions and influence chemistry. As with many urban areas, it is expected that the region will be NO_x-limited with respect to O₃ formation and that organic PM will be dominated by SOA.

Question C: What is the nature of the air being transported into San Antonio along the I-37 corridor, including potential contributions from Corpus Christi, the Gulf of Mexico, and locations outside the United States? *Related Hypothesis:* The change in air quality between Corpus Christi and San Antonio will be driven by phenomena including deposition, dispersion, emissions from local sources, and chemical processing. The emissions and chemistry associated with Corpus Christi will impact the regional background measured downwind.

Question D: How does the air quality in San Antonio in the latter part of the O₃ season differ from that in the early part of the O₃ season (i.e., May 2017 versus September/October 2020)? *Related Hypothesis:* It is expected that biogenic emission rates will be different between the two parts of the O₃ season, based on differences in meteorology between the two time periods. Given this and little expected changes in traffic patterns or anthropogenic emissions over the three-year period between the campaigns, it is hypothesized that the chemistry will remain NO_x-limited and that biogenic species will still dominate in situ reactivity despite changes in emissions. It is further hypothesized that any changes in O₃ between the two campaigns may be attributed to changes in regional background.

In order to address these scientific questions and test the related hypotheses, the general approach to the planned sampling campaign follows. Three-dimensional modeling will be utilized to test, for example, predicted pollutant sensitivity to model inputs.

- Weeks 1 and 2 (August 24 – September 6, 2020): Set up and perform stationary measurements in a coastal Corpus Christi location. Potential recreational vehicle (RV) parks have been identified on the upwind side of Corpus Christi. This period will address Questions A and B.
- Week 3 (September 7 – 13, 2020): Perform daily mobile measurements downwind (to the northwest) of Corpus Christi. Based on the safety of the research team, we estimate that we will be able to cover a linear distance out from Corpus Christi of approximately 100 miles each day. This period will address Questions B and C.

- Week 4 (September 14 – 20, 2020): Perform mobile measurements upwind (to the southeast) of San Antonio. Similarly, we predict that we will be able to cover a linear distance of 100 miles upwind each day. This period will address Questions C and D.
- Weeks 5 and 6 (September 21 – October 4, 2020): Perform stationary measurements in a location upwind of the core San Antonio area. For comparative purposes, a likely location is the Traveler's World RV Park that was used as a site during SAFS. This period will address Question D.
- Week 7 (October 5 – 11, 2020): Perform mobile measurements downwind (to the northwest) of San Antonio or to sample downwind of any identified 'hot spots' from the SAFS results. Similarly, we predict that we will be able to cover a linear distance of 100 miles downwind each day. This period will address Question D.

4. SAMPLING PROCEDURES

All techniques used by the project team members for this project utilize online measurements only. No discrete samples will be collected.

5. MEASUREMENT PROCEDURES

5.1. MEASUREMENT METHODS

All instrumentation described subsequently will be housed on the MAQL for the duration of the field campaign.

University of Houston Trace Gas Suite

In situ O₃ measurements will be performed with a 2B Technology (Boulder, CO) model 205 dual beam O₃ ultraviolet photometric gas analyzer and/or a modified Thermo Scientific (Franklin, MA) Model 42C chemiluminescent analyzer (reagent nitric oxide (NO) + ambient O₃). The NO and nitrogen dioxide (NO₂) measurements will be made with an Air Quality Design (Golden, CO) custom chemiluminescent analyzer, and NO_y measurements will be made with a modified Thermo Scientific Model 42C chemiluminescence analyzer. The NO_x channel utilizes a blue light converter (BLC) from Air Quality Design (Wheat Ridge, CO, USA) for photolysis conversion of NO₂ to NO. The BLC is more specific in that it essentially converts only NO₂ to NO, compared to the standard molybdenum (Mo)-based NO₂-to-NO converter used in most EPA and TCEQ air monitoring sites that also converts nitric acid and peroxy acyl nitrates to NO and as a consequence tends to overestimate NO₂. Measurements of NO_y are achieved by placing a Thermo Mo converter heated to 300°C for conversion of odd nitrogen species to NO at the sample inlet.

Ambient levels of CO will be measured with a Los Gatos Research (San Jose, CA) CO Analyzer, model F-CO-23r using laser-based off-axis integrated cavity output spectroscopy, while CO₂ will be measured with a Licor (Lincoln, Nebraska) LI-7000 non-dispersive infrared differential gas analyzer. Ambient levels of SO₂ will be monitored using the pulsed ultraviolet fluorescence technique employed in the Thermo Scientific Model 43c-TLE instrument, which takes advantage of the characteristic that SO₂ molecules absorb ultraviolet radiation and then fluoresce in the range of 220 to 240 nm. These basic ambient trace level chemical instruments

stream data or are queried every second with DAQFactory data acquisition software (Azeotech, Ashland, OR). The trace gas data will be post-processed and averaged into a format suitable for storage and use in a database with software such as Igor Pro and MATLAB.

University of Houston Meteorological Suite

Measurements of meteorological parameters (temperature, relative humidity, wind speed and direction, and pressure) and NO₂ photolysis rate (j_{NO_2}) will be performed at the trace gas inlet at the end of the arm. Wind speed and direction will be measured with an RM Young 86000 ultrasonic anemometer. An RM Young 41382 temperature and relative humidity probe and a 61302V barometric pressure sensor will be used. A Meteorologie Consult, GmbH filter radiometer will measure j_{NO_2} . In addition, a Vaisala CL-31 will determine planetary boundary layer height.

Rice University High-Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-ToF-AMS)

The HR-ToF-AMS to be used in this study is described in detail in DeCarlo et al. (2006). Sample at atmospheric pressure enters the HR-ToF-AMS via an aerodynamic focusing lens. At the end of the lens, the collimated particle beam enters a vacuum chamber of known dimension. Within this chamber, particles achieve a terminal velocity that determines how quickly they will traverse the chamber. From this time, it is possible to calculate the particle size. At the end of the chamber, non-refractory material is vaporized and ionized by electron impact. Material is quantified using a time-of-flight mass spectrometer. The HR-ToF-AMS provides size-resolved chemical composition data at a resolution of approximately one minute. The HR-ToF-AMS operation by the Rice group is described in detail in Leong et al. (2017) and Wallace et al. (2018). Similar sampling procedures will be followed here, including the frequency of blanks and calibrations (as described subsequently in this QAPP). The main manifold will have a cyclone on the inlet to prevent larger material from entering the HR-ToF-AMS (which is a sub-micron instrument) and clogging the inlet pinhole. The HR-ToF-AMS will subsample isokinetically at a rate of approximately 150 mL per minute.

Baylor University Proton-Transfer-Reaction mass Spectrometer (PTR-MS)

The PTR-MS operated by Baylor in this study was manufactured by IONICON Analytik, Austria (www.ionicon.com). The PTR-MS has widely served as a fast frequency atmospheric VOC analyzer for the past two decades (de Gouw and Warneke, 2007). The method applies ionization of atmospheric VOCs that have higher proton affinity than that of the water molecule (This applies for most atmospheric VOCs, except alkanes.) through the proton transfer reaction. Protonated VOCs are analyzed by a quadrupole mass spectrometer. The accuracy and precision of the measurement system has been proven to guarantee very low detection limits of most VOCs in the atmosphere (e.g. ~ few parts per trillion by volume (pptv); de Gouw and Warneke, 2007). The PTR-MS and other gas-phase measurements (excluding NO_y) will sample from a filtered Teflon® sampling line. In order to minimize inlet losses, the manifold flowrate will be supplemented by a manifold pump, and all gas-phase instruments will subsample from this manifold.

As in the SAFS deployment, a sample conditioner will be used to reduce the water content of the sample. This will allow the operation of the PTR-MS at a lower Townsend number and result in increased sensitivity and less fragmentation. It will also increase the instrument sensitivity to HCHO. In this case, the effects of instrumental drift will be eliminated by measuring the ratio between product and primary ion, which assures linearity (de Gouw et al., 2003). Instrumental background will be assessed by periodically passing air over a heated catalyst for 40-60 minutes. The frequency of the background determination and calibration frequency will be determined in the field based on instrument performance and stability. As an *in situ* method, work with the PTR-MS does not require taking any special sampling/handling precautions. We anticipate operating the instrument with a nominal cycle time of 60 seconds. A logbook will be kept for instrument operators to log information on the instrument on an as needed basis.

5.2. MEASUREMENT CALIBRATION

The measurement calibrations are described in Section 6.

6. QUALITY METRICS

6.1. QC CHECKS

General Information

Comparability is achieved when results are reported in standard units to facilitate comparisons between the data from this project and other similar programs. In order to accomplish this objective, the reporting units for the ambient monitoring performed here will adhere to standard units (mixing ratios or number densities for gases, per second for photolysis rates, and mass concentration for aerosol composition as a function of size).

The technician/student assigned to a specific monitoring instrument is responsible for operating samplers and providing minor corrective actions on equipment when required. Equipment problems are generally detected through a failed sample run or through performing routine QC checks on a routine basis. The QC checks that are performed on the sampling equipment vary by instrument. When a major equipment problem is involved, the manufacturer is to be contacted, and their responsibility is to follow up on restoring the equipment to its proper operating status. This may be accomplished through telephone consultation with the technician/student, which may result in the removal of the equipment from the site for repair. Any equipment problems that can result in the loss of data are addressed with a high priority. All situations requiring corrective action will be documented in activity logs. Some specific QC protocols will be discussed following definitions for quality metrics that will be used. An attempt is made to provide adequate information from which to estimate and control the uncertainty and potential limitations of measurements generated by the project. QC activities are generally applied to portions of a measurement process that are both critical to measurement quality and practically subject to evaluation and control. The portions of any given measurement process that are both critical and subject to evaluation and control vary with the measurement being made and the method used. The QC protocol used for any given measurement process may include some or all of the following:

- a.) Sampling system contribution to the measurements;
- b.) Measurement system contribution to the measurements;
- c.) Qualitative performance of the method;
- d.) Quantitative performance of the method;
- e.) Precision of the measurements; and
- f.) Accuracy (bias) of the measurements.

Prior to deployment, the equipment will be powered up, operating parameters will be checked, and the instruments will be tested against various calibration levels. The purpose is to run operational checks to catch problems prior to field deployment, repair all malfunctioning equipment, and familiarize the staff with the equipment. Routine preventive maintenance procedures also are performed continuously during deployment. Routine preventive maintenance procedures and schedules for trace gases measurements are described in individual instrument service manuals. Generally, technicians/students are responsible for all maintenance of monitoring systems. A backup may be called if the primary individual is not available. If problems are observed with particular instruments after being deployed, the manufacturer is to be contacted, and tests are performed to solve the problem. Corrective maintenance procedures also follow the manufacturer's recommendations in the instrument service manuals. To facilitate such procedures, some spare parts are maintained on hand to facilitate rapid repair of common maintenance needs, while others are acquired on an as-needed basis. Spare parts are receipted, installed according to the manufacturer's instructions, and tested to ensure correct instrument operation.

It should be stressed that data that do not meet acceptance criteria (for any of the instruments used) will have an associated flag attached in electronic files containing the data. In addition, laboratory notebooks will be used by personnel and will be used to specify data flags manually. In the interest of space, this is not included as a 'corrective action' in tables and discussions that follow.

Detection limit

Detection limits will be expressed in units of concentration and reflect the smallest concentration of a compound that can be measured with a defined degree of certainty. Criteria pollutants are measured using EPA designated reference or equivalent methods. The detection limits for many of these methods are specified in 40 CFR Part 53. Because of this, no specific measurements of detection limits are made for the criteria pollutants in this project. The analytical instrument detection limit (IDL) for other parameters will be established with the application of available standards according to 40 CFR Part 136, Part B, where applicable.

Blanks/Zeros

The system contribution to the measurement results is determined by analysis of a blank or "zero air" (filtered air) level as part of each calibration and span check. As part of the calibration, this zero level is used along with the upscale concentrations to establish the calibration curve. As part of the span check, this level is used as a QC check for monitor zero drift. If a method is found to have a system contribution for a target pollutant at a concentration greater than three times the detection limit or greater than 10 percent of the

median measured concentration for the pollutant (whichever is larger), efforts must be taken to remove the contribution. Any system contribution for a target pollutant (or for another constituent that interferes with analysis for a target pollutant) that is above the detection limit must be thoroughly characterized such that the extent of influence on the target pollutant measurement certainty is well understood. This may require an elevated frequency of blank analyses for an adequate period to characterize the contribution. A data flag will be used when concentrations in the blank sample measurements indicate a contribution to the sample measurement result that is determined to be significant relative to the quality objectives specified for the measurement.

Precision

Precision is a measure of the repeatability of the results. Estimates of precision are assessed in different ways for different measurement technologies.

- Precision for measurements from continuous monitors will be estimated by analysis of a test atmosphere containing the target compounds being monitored. Precision for trace gases is estimated from precision checks that are done as part of routine span checks of the monitors. This precision check consists of introducing a known concentration of the pollutant into the monitor in the concentration range required by 40 CFR Part 58, Appendix A. The resulting measured concentration is then compared to the known concentration.
- Analytical measurement precision for other species will be estimated by the comparison of replicate analyses of the test atmosphere containing the target compound or comparison to other data products, as appropriate.

Accuracy

Accuracy is the closeness of a measurement to a reference value and reflects elements of both bias and precision. Accuracy will be determined by evaluating measurement system responses for replicate analysis of samples containing the compounds of interest at concentrations representative of the ambient atmospheres typically being monitored during the study as outlined in 40 CFR 58, Appendix A. Note that technical system audits are not required for a Category III QAPP.

Completeness

Data completeness is calculated on the basis of the number of valid samples collected out of the total possible number of measurements. Data completeness is calculated as follows:

$$\% \text{ Completeness} = (\text{Number of valid measurements} \times 100) / \text{Total possible number of measurements}$$

Data Auditing

Audits of data quality will be performed by visual inspection of the data, comparison of the data to the QA/QC criteria described in this document, and comparison with other measurements, as applicable. Data that passes these examinations will be deemed acceptable.

Should data not pass examination on one or more of the checks, the data will be further examined by the researchers and as appropriate may be flagged as invalid, valid, or valid but having failed a check.

Instrument specifics

University of Houston Trace Gas Suite

Internally designed software will perform automated multi-point span QC checks on the trace gas monitors at the beginning and end of the sampling campaign in addition to baseline evaluations (zeros) on a weekly basis at a minimum. Single point span and zeros will also be performed at least daily at a minimum to track stability of the instruments. QC procedures, control limits, and formulas to calculate QC statistics are given in standard operating procedures specific to the monitoring. The purpose of the five-point span check is to evaluate drift in the calibration curve of a monitor between calibrations, evaluate monitor performance, and assess measurement precision. Data validity decisions are based only on whether a QC test exceeds the failure limit. Quality control tasks will consist of calibrations, maintenance, inspections, and record keeping.

Multi-point calibration checks are performed at the beginning and end of sampling at a minimum and as needed, such as because of instrument adjustment or repair. Five levels of O₃ calibration gas are introduced automatically at a programmed time into the inlet of the O₃ analyzer by a calibration system. These levels nominally correspond to 200, 100, 75, 50, 25, and 0 ppbv. The O₃ calibration gas is derived from a Thermo 49c-PS O₃ generator that has been standardized with an O₃ SRP by the EPA Region 6 lab in Houston. Single point span and zeros will also be performed at least daily at a minimum to track stability of the instrument.

A Praxair (formerly Scott-Marrin) NIST-traceable span gas cylinder that has been certified by the vendor containing 5.2 parts per million by volume (ppmv) SO₂, 5.2 ppmv NO, and 50.6 ppmv CO in dry nitrogen is used as gaseous standards for the routine calibration of the SO₂, CO, and all NO instruments (i.e., NO, NO₂, NO_y). A Praxair NIST-traceable span gas cylinder that has been certified by the vendor containing 4.73 ppmv NO₂ in dry nitrogen is used as a gaseous standard to determine the conversion efficiency of the NO₂ photocell. A cylinder of nominally 5 ppmv of n-propyl nitrate (NPN) is used as a gaseous standard to evaluate the conversion efficiency of the heated molybdenum converter used for the NO_y measurement. The CO₂ measurements will be referenced to a calibration cylinder of known concentration which will continuously flow through the reference cell of the instrument.

The calibrator systems in the continuous monitoring for O₃, SO₂, CO, and NO/NO₂/NO_y rely on the operation of flow controllers or flow restrictors to maintain a span gas flow and a dilution air flow at each of preset level. For each concentration level during a calibration or span check, the calibrator reports the mass flow rate from each controller to the data computer; these flows are recorded with the measurement data. These flows, along with the cylinder concentrations, are then used to calculate the reference values for each level and gas.

A multipoint calibration of five calibration gas mixtures of SO₂, CO, NO, and NO₂ are introduced automatically into the inlet of the analyzers by the calibrator. The nominal levels for each gas are shown in Table below. Five-point calibration checks are performed at the

beginning and end of sampling at a minimum and as needed, such as because of instrument adjustments or repair. The instrument responses along with reference values for all calibrations are recorded electronically. Single point span and zeros will also be performed at least daily at a minimum to track stability of the instruments.

Gas	Level 1	Level2	Level 3	Level 4	Level 5	Level 6
O3	200	100	75	50	25	0
CO	650	550	375	200	100	0
SO2	50	20	10	5	2	0
NO	50	20	10	5	2	0
NO2	50	20	10	5	2	0
NPN	50	20	10	5	2	0

Table 1. Nominal calibration levels typically used for trace gas measurements.

Conversion efficiencies for the BLC (NO₂) and heated Mo converter (NO_y) are determined by multipoint challenges with NO₂ from the cylinder. NPN checks are also performed on the NO_y system to check the conversion efficiency of the heated Mo converter. Test atmospheres of NPN will be used at the beginning and end of the campaign.

Baylor University PTR-MS

Background determinations will be performed by overflowing the PTR-MS inlet with zero-air generated by flowing ambient air across a heated catalyst. This zero-air will also be used to dilute metered flows from a compressed gas cylinder of span gases from Apel-Riemer (Bloomfield, CO). Table shows the species and mixing ratios of gases in the cylinder which were selected to cover both anthropogenic and biogenic compounds and generate appropriate test atmosphere concentrations. A separate gas cylinder has been acquired to enable HCHO calibration (Apel-Riemer Environmental Inc). Mass flow controller signals will be recorded in DAQFactory software as well as valve states and the associated data flags to indicate non-ambient data. These signals will be used to calculate mixing ratios of test atmospheres for instrument sensitivity calculations.

Species	m/z	ppbv
HCHO*	31	1030
Acetaldehyde	45	513
Methanol	33	514
Isoprene	69	506
Acetone	59	498
DMS	63	503
Acetonitrile	42	507
Methacrolein	71	516
MVK	71	471
MEK	73	526
Benzene	79	531
Toluene	93	515
Camphene	137	524

Table 2. PTR-MS span gas species and mixing ratios. * included in a separate calibration cylinder.

Rice University HR-ToF-AMS

The particle instruments will be monitored closely by staff to ensure continued satisfactory operation in the field. The HR-ToF-AMS will periodically (weekly) be zeroed by placing a particle filter upstream of the inlet; this will aid in the determination of minimum detection limits (two times the standard deviation of the mean zero value), which should be in the ng/m³ range. The calibration for the HR-ToF-AMS will be conducted as follows:

- Atomize a solution of ammonium nitrate and size select particles using a differential mobility analyzer set to a specific voltage (the differential mobility analyzer will be calibrated pre-campaign using NIST-traceable polystyrene latex spheres);
- Measure the total number concentration of these particles using a condensation nucleus counter; calculate the mass concentration of ammonium nitrate assuming spheres;
- Feed the same stream to the HR-ToF-AMS;
- Measure the particle size distribution using the HR-ToF-AMS (this will only be done at the start of the campaign and if the instrument needs to be repaired);
- Measure the ion response of the instrument to a known mass concentration of ammonium nitrate (from above); all other responses are derived from this value (this will be done weekly to monitor filament ionization and detection efficiency).

Calibrations will be performed at different times and on different days of the week (again approximately weekly for the HR-ToF-AMS or as needed) to avoid missing data at the same time/day. With this frequency, the completeness of the data should easily exceed 85% barring

unforeseen events such as pump or filament failure in the HR-ToF-AMS. The assumed acceptable accuracy and precision are 15% and 20%, respectively.

6.2. QUALITY ASSURANCE OBJECTIVES

There are no additional QA objectives beyond those described previously.

7. MODEL SELECTION

The key objective of the modeling aspect of this project is to evaluate predicted pollutant sensitivity to emissions input. To achieve this objective, a 3-D chemical transport model (CTM) with scales larger than the United States (US) continent is required so as to simulate the long-range transport of pollutants from foreign sources to the US. However, the model should be able to have a fine resolution of the field campaign domain to best compare with observations. To meet those requirements, a global 3-D chemical transport model with nested-grid capability is the ideal candidate.

The key attributes of the candidate model include the following:

- Its ability of simulating both long-range transport of pollutants and Texas air quality has been recognized;
- It has a deterministic structure;
- It has a coupled ozone-aerosol chemical mechanism;
- It is driven by meteorological fields that are specific to the simulation periods rather than climatological mean conditions;
- Its domain is at least hemispheric or with dynamic boundary conditions provided by a global model;
- It is 3-D and has the spatial resolution finer than 10 km over the field campaign domain;
- It can simulate the study period; and
- Its dynamic time step is less than 30 min so as to capture the dynamics of transport associated with turbulence and convection.

Based on those attributes, the GEOS-Chem 3-D global CTM and its nested-grid version over North America (NA) (www.geos-chem.org) are selected. It is coupled to the Weather Research and Forecasting model (WRF). It is termed WRF-GC (Lin et al., 2020). No other global CTM was considered for three reasons. First, the GEOS-Chem CTM has arguably the largest user base among all the global CTMs and state-of-the-art tropospheric chemistry. Second, the regulatory models of TCEQ use chemical boundary conditions from the GEOS-Chem global CTM. Third, the GEOS-Chem global CTM has the nested-grid simulation capability, which by coupling with WRF can offer a finer-resolution simulation over the field campaign domain.

The WRF-GC model includes a detailed NO_x-O_x-hydrocarbon-aerosol-bromine tropospheric chemistry mechanism and has a dynamic time step of less than 10 minutes. The model uses the FINN inventory for biomass burning emissions. The global version has a horizontal resolution of 2° latitude x 2.5° longitude to be used for boundary conditions and the nested-grid version over the field campaign domain will have a horizontal resolution of 10 km or finer.

8. MODEL CALIBRATION

The GEOS-Chem CTM has a standard benchmarking procedure for each major code release, using observations compiled from surface monitoring network, aircraft campaigns, and satellite retrievals around the globe. During the benchmarking procedure, each module of the model, including transport, emission, chemistry, dry deposition, and wet deposition, is calibrated and best parameters are chosen based on the benchmarking results. For example, observed global distribution of radon is used to calibrate the transport process. This project will use the most recent public release to date (on the date of project initiation) that has gone through the benchmarking procedure.

9. MODEL VERIFICATION

The objective of model verification is to use existing observations to verify the model's ability to simulate the overall features of O₃, its precursors, and aerosols during the study period. We will verify the model by comparing the simulation results with surface observations (e.g., TCEQ CAMS sites) and satellite products (MODIS, TROPOMI) during the study period. These data are independent from the field campaign observations to be collected and are publicly available. The model verification uses the same metrics described in the Model Evaluation (Section 10, Table 3).

We will conduct experiments with WRF-GC in which local anthropogenic emissions from Corpus Christi and San Antonio are separately perturbed. We will first carry out a $\pm 20\%$ emission perturbation of these emissions, which is a significant change in emissions but not large enough to change the chemical regime (in most cases). For Corpus Christi, we will conduct an additional perturbation experiment where emissions from the petrochemical industry are increased to reflect the planned expansion of that industry in the city (e.g., new Exxon facilities). The resulting changes in O₃, PM, and their precursors will be analyzed to quantify the influence of local emissions and inter-regional transport on air quality of both cities (Question C). Similar perturbation experiments will then be conducted for anthropogenic NO_x and VOC emissions separately in each city to investigate if O₃ production is NO_x-limited (Question B). The WRF-GC results can be compared to and corroborated with the LaRC zero-dimensional model. Finally, we will zero-out local emissions in Corpus Christi in the model and quantify the influence of regional and background at Corpus Christi and compare that with Houston. The overall modeling results for the 2020 O₃ season will be compared to our previous SAFS modeling work to investigate the seasonal differences in meteorology, chemistry, and transport.

10. MODEL EVALUATION

The model will be evaluated by comparing the model prediction of meteorology and of gaseous and aerosol species with observational data collected from the field campaign. The model evaluation will use the performance metrics listed in Table 3. These particular metrics were selected because they are among the most commonly used standard statistical metrics to evaluate the simulated variability (e.g. correlation coefficient) and magnitudes in both absolute , specifically, mean bias (MB) and mean absolute error (MAE) and relative terms, normalized

mean bias (NMB). The root mean square error (RMSE) gives more weights to model errors with larger absolute values than MAE, making it more appropriate to evaluate the model’s ability to simulate the high pollution cases.

The metrics of model evaluation will be compared with published results of GEOS-Chem ozone and PM simulations (e.g. Zhang et al., 2011). We will also invite a few members from the GEOS-Chem development team and users’ community to review at least 10% of the modeling results; potential peer reviewers are Dr. Daniel Jacob at Harvard University and Dr. Lin Zhang at Peking University.

Mean Bias (MB)	$MB = 1 / N \sum_{i=1}^N (M_i - O_i)$
Mean Absolute Error (MAE)	$MAE = 1 / N \sum_{i=1}^N M_i - O_i $
Normalized Mean Bias (NMB)	$NMB = \frac{\sum_{i=1}^N (M_i - O_i)}{\sum_{i=1}^N O_i} \times 100\%$
Correlation Coefficient (Corr. R)	$Corr.R = \frac{\sum_{i=1}^N (M_i - \bar{M})(O_i - \bar{O})}{\sqrt{\sum_{i=1}^N (M_i - \bar{M})^2} \sqrt{\sum_{i=1}^N (O_i - \bar{O})^2}}$
Root Mean Square Error (RMSE)	$RMSE = \sqrt{1 / N \sum_{i=1}^N (M_i - O_i)^2}$

Note: *M* is the model output, *O* is the observation, *N* is the number of samples, and

$$\bar{M} = 1 / N \sum_{i=1}^N M_i, \bar{O} = 1 / N \sum_{i=1}^N O_i.$$

Table 3. Performance metrics of model evaluation.

11. MODEL DOCUMENTATION

We will maintain documentation files for each model run that identifies model code versions, dates, analyses, and input and output files. Each input/output file used will be reviewed for QA purposes using various visualization methods, including software animations and graphing, as well by quantitative filtering using selected filter criteria to identify anomalous data. The model documentation will include summaries of the input file values that were changed, the boundary conditions, and why the changes were made, the analysis of the output files, and any other important instructions required to replicate each run.

12. DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

12.1. DATA REPORTING REQUIREMENTS

The data will be provided in time-stamped delimited text format, likely in 5- or 10-minute averages or other suitable formats as appropriate in order for the data to be used by

subsequent users, such as the AQRP or TCEQ. Data will include the time series (and relevant GPS information) of all parameters discussed above.

The output of much of the instrumentation to be used consists of time series of the measured parameters; these time series will undergo QA procedures that are described in this QAPP. The output from specific instrumentation, (e.g., the HR-ToF-AMS) requires significant post-processing using manufacturer-supplied software (the SQUIRREL and PIKA programs in Igor) to generate these time series. For stationary measurements, these time series will be utilized in standard statistical analyses (average, median, standard deviation, etc.) as well as in the determination of diurnal profiles, probability density as a function of wind direction, etc. In addition to wind direction probabilities, backward trajectory clustering and source contribution functions (e.g., as done in Schulze et al. (2018)) will provide a first-pass at larger scale transport pathways for the pollutants measured at a fixed location. These calculations, as well as those of O₃ production rate and organic aerosol characterization, will be included in the data set provided to the project sponsors. Modeling output and code will be provided as required.

12.2. DATA VALIDATION PROCEDURES

Ambient data that have passed the QA/QC checks described above will be considered to be validated. Additional comparisons to external measurements as appropriate will be completed and reported as part of the data analysis and subsequent reporting to the AQRP.

12.3. DATA ANALYSIS

The data will be used to attempt to identify causes of air pollution in the location(s) sampled. This will be achieved by standard techniques such as correlation/regression and more advanced techniques such as positive matrix factorization. The information provided by these data will be useful in understanding pollution dynamics in this region and therefore in developing control strategies and determining whether local or regional controls may be best suited for this area.

The general statistics to be used are considered standard so little detail is provided here. Metrics to be used include averages, medians, standard deviations, diurnal profiles, and similar values. Time series will be inspected to identify commonalities, and regression analysis will be used to determine relationships between specific variables. These will be applied to both the output data generated from the measurements as well as to parameters derived from these measurements such as photochemical age, the ratio of NO_x to NO_y, etc.

12.4. DATA STORAGE

All data collected/generated during the course of this project will be backed up on each institution's servers, or at UH and backed up at Rice University and will be maintained for a minimum of 3 years after the completion of the project.

13. 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 Rice PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the AQRP 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 AQRP 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, July 31, 2020

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the AQRP 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
Quarterly Report #1	May, June, July 2020	Friday, July 31, 2020
Quarterly Report #2	August, September, October 2020	Friday, October 30, 2020
Quarterly Report #3	November, December 2020, January 2021	Friday, January 29, 2021
Quarterly Report #4	February, March, April 2021	Friday, April 30, 2021
Quarterly Report #5	May, June, July 2021	Friday, July 30, 2021
Quarterly Report #6	August, September, October 2021	Friday, October 29, 2021

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY20-21 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start - June 30, 2020	Wednesday, June 10, 2020
Technical Report #2	July 1 - 31, 2020	Friday, July 10, 2020
Technical Report #3	August 1 - 31, 2020	Monday, August 10, 2020
Technical Report #4	September 1 - 30 2020	Thursday, September 10, 2020
Technical Report #5	October 1 - 31, 2020	Friday, October 9, 2020
Technical Report #6	November 1 - 30, 2020	Tuesday, November 10, 2020
Technical Report #7	December 1 - 31, 2020	Thursday, December 10, 2020
Technical Report #8	January 1 - 31, 2021	Friday, January 8, 2021
Technical Report #9	February 1 - 28, 2021	Wednesday, February 10, 2021
Technical Report #10	March 1 - 31, 2021	Wednesday, March 10, 2021
Technical Report #11	April 1 - 30, 2021	Friday, April 9, 2021
Technical Report #12	May 1 - 31, 2021	Monday, May 10, 2021
Technical Report #13	June 1 - 30, 2021	Thursday, June 10, 2021
Technical Report #14	July 1 - 31, 2021	Friday, July 9, 2021

DUE TO PROJECT MANAGER

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQR Grant Manager (RoseAnna Goewey) by each institution on the project using the AQR 20-21 FSR Template found on the AQR website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start - June 30	Wednesday, July 15, 2020
FSR #2	July 1 - 31, 2020	Friday, August 14, 2020
FSR #3	August 1 - 31, 2020	Tuesday, September 15, 2020
FSR #4	September 1 - 30 2020	Thursday, October 15, 2020
FSR #5	October 1 - 31, 2020	Friday, November 13, 2020
FSR #6	November 1 - 31, 2020	Tuesday, December 15, 2020
FSR #7	December 1 - 31, 2020	Friday, January 15, 2021
FSR #8	January 1 - 31, 2021	Monday, February 15, 2021
FSR #9	February 1 - 28, 2021	Monday, March 15, 2021
FSR #10	March 1 - 31, 2021	Thursday, April 15, 2021
FSR #11	April 1 - 30, 2021	Friday, May 14, 2021
FSR #12	May 1 - 31, 2021	Tuesday, June 15, 2021
FSR #13	June 1 - 30, 2021	Thursday, July 15, 2021
FSR #14	July 1 - 31, 2021	Friday, August 13, 2021
FSR #15	August 1 - 31, 2021	Wednesday, September 14, 2021
FSR #16	Final FSR	Friday, October 15, 2021

DUE TO GRANT MANAGER

Draft Final Report: A Draft Final Report will be submitted to the AQRP 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: Monday, August 2, 2021

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the AQRP 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, August 31, 2021

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 20, 2021). 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 2021.

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.

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