

Scope of Work For

Project # 18-010

A synthesis study of the role of mesoscale and synoptic-scale wind on the concentrations of ozone and its precursors in Houston

Prepared for

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

By

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QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

NOTE: The workplan package consists of three independent documents: Scope of Work, Quality Assurance Project Plan (QAPP), and budget and justification. Please deliver each document (as well as all subsequent documents submitted to AQRP) in Microsoft Word format.

Approvals

This Scope of Work was approved electronically on **October 1, 2018** by Elena McDonald-Buller, The University of Texas at Austin

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

This Scope of Work was approved electronically on **October 2, 2018** by Jonathan Steets, Texas Commission on Environmental Quality

Jonathan Steets
Project Liaison, Texas Commission on Environmental Quality

Contents

- 1.0 Abstract 4
- 2.0 Background 4
- 3.0 Objectives..... 6
- 4.0 Task Descriptions 6
- 5.0 Project Participants and Responsibilities 10
- 6.0 Timeline..... 11
- 7.0 Deliverables (Please use the materials in this section editing only as/if necessary. We have generated this section for you to include directly within your Scope of Work so that the schedule of required deliverables to AQRP is clearly communicated.) 11
- 8.0 References 14

1.0 Abstract

While it is known that low synoptic-scale winds and mesoscale recirculation contribute to high ozone formation in Houston, a comprehensive synthesis of all relevant data and analyses to elucidate the interaction between the mesoscale and synoptic-scale winds and air pollutants is not yet available. An improved understanding of the roles of mesoscale and synoptic-scale processes would allow researchers and policy makers to distinguish between days dominated by local emissions and those dominated by regional contributions. The overall objective of this research is to synthesize existing data, previous analyses, and photochemical model experiments to provide a comprehensive and reconciled description of how mesoscale and synoptic-scale winds affects dispersion and accumulation of air pollutants emitted in the Houston area and from other regions, and how they contribute to high ozone events. The relationship between surface winds and boundary-layer mesoscale transport features will be clarified, and a novel source- and age-resolved regional air quality model will be applied to investigate selected high ozone events under the influence of mesoscale circulations. The results from this study will facilitate a better understanding of the interaction between the mesoscale and synoptic-scale winds and air pollutants and how they contribute to high ozone events in Houston. Such information is extremely useful for understanding high ozone events as they occur and for developing appropriate control strategies and policy options for the unique Texas meteorological environment.

2.0 Background

Around the time of the TexAQS-2000 field program, the importance of mesoscale wind patterns in the Houston-Galveston-Brazoria (HGB) airshed had been recognized, even as understanding of those wind patterns has grown over time (Banta et al., 2005; Darby, 2005; Daum et al., 2003; Davis et al., 1998). Initially, the dominant mesoscale process was thought to be an ordinary sea breeze, modified by the complex coastline of HGB and conceptually separated into a (Galveston) Bay breeze and a Gulf (of Mexico) breeze. During the day under light synoptic-scale wind conditions, the Bay breeze is first to affect Houston, followed by the much stronger and larger Gulf breeze in the late afternoon. A land breeze develops at night (Day et al., 2010).

The next advance in meteorological understanding was the recognition that sea breeze behavior in the HGB area was unlike that observed at higher latitudes due to the inertial oscillation, which is in near-resonance with the daily surface heating cycle in HGB (Nielsen-Gammon et al., 2005; Parrish et al., 2009). The combined sea breeze-inertial oscillation dominates pollutant transport patterns during both day and night, leading to recirculation of pollutants and emission of “double doses” of pollutants into the already polluted air.

While the sea breeze-inertial oscillation seems key to understanding local pollution, low-level jet patterns have been found to play important roles in local and regional transport (Daum et al., 2004; Tucker et al., 2010). In a sense, the sea breeze itself features a low-level wind maximum and has been treated as a low-level jet by Tucker et al. (2010). Besides this, three

types of low-level jets distinct from conventional coastal sea breeze-inertial oscillation appear to be relevant in southeast Texas. First, under southwest wind conditions, a coastal low-level jet is established that can interact with the sea breeze to produce extremely large diurnal wind oscillations, such as were observed during late August 2000. Second, an inland surge of the sea breeze has been found to produce a local low-level wind maximum in the interior of eastern Texas that may be important for regional transport. Third, the Great Plains low-level jet is the dominant diurnal wind feature of western, central, and southern Texas. Recent work by Nielsen-Gammon (2016) has shown that the Great Plains low-level jet is at times more influential than the sea breeze in inducing an inertial oscillation in HGB and even over the open Gulf of Mexico. Also important in producing high ozone in HGB are cold front passages (Langford et al., 2009; Ngan and Byun, 2011; Rappengluck et al., 2008), though it is not yet clear how mesoscale circulations evolve during such events and interact with the changing larger-scale weather patterns.

Figure 1 is a composite analysis of mean air parcel trajectories under light wind conditions at 500 m above ground level, based on TexAQS-II profiler observations. The classic daytime stagnation and recirculation under light wind conditions are apparent in the HGB profiler observations from La Porte. The composites from other profilers in the region show that this phenomenon is not unique to Houston, although it is perhaps more important in HGB than elsewhere because of the concentrated VOC emissions from chemical processing facilities on or near the Houston Ship Channel. The inertial oscillation is simultaneously a mechanism for concentrating emissions and a strong modifier of regional transport patterns.

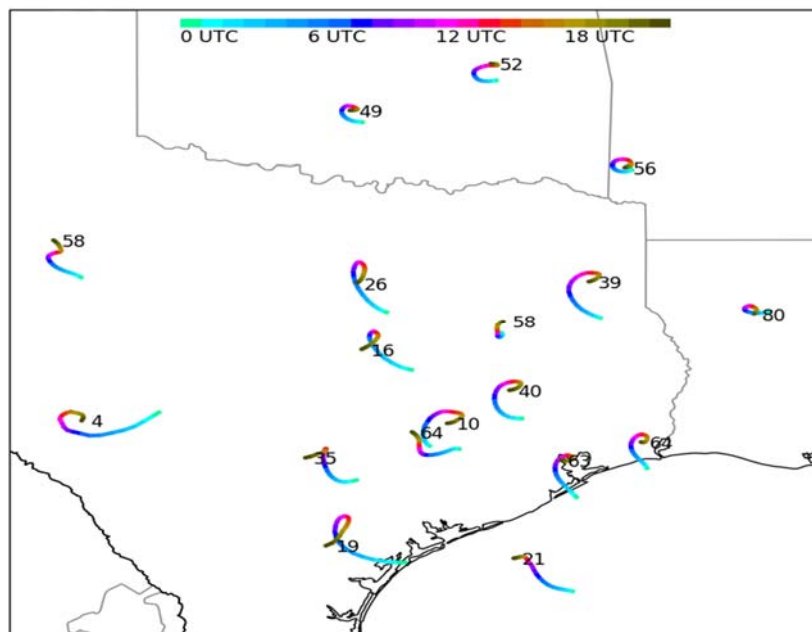


Figure 1: Composite analysis of mean air parcel trajectories under warm-season light wind conditions at 500 m above ground level, based on TexAQS-II profiler observations. Colors (bar at top) correspond to time of day (subtract six hours for LST), while numbers indicate the number of observed days meeting the low wind criterion.

Modern ozone source apportionment models such as the Ozone Source Apportionment Technique (OSAT) in CAMx (ENVIRON, 2015) and Integrated Source Apportionment Method (ISAM) in CMAQ (Kwok et al., 2015) can be used to differentiate ozone from long-range transport, local emissions, and adjacent regions. In these models, many non-reactive tracers are used to keep track of the amount of NO_x and VOCs emitted from different sources and/or source-regions. The in-situ ozone formed at each model time step is then attributed to different sources and/or source regions based on the ozone formation sensitivity regime and the NO_x and VOC source contributions. For example, Kemball-Cook et al. used CAMx-OSAT and determined that both local and regional ozone are important in Houston and Dallas. In the Houston area, however, when recirculation happens aged emissions from the Houston area can reenter the area and contribute to high ozone event (Pierce et al., 2009). Ensemble Lagrangian trajectories were used to identify potential source regions of transported background ozone. However, the computation of Lagrangian trajectories have large uncertainties and cannot fully account for entrainment. To fully understand the timescale of this recirculation that affects the Houston area and the amount of aged pollutants and O₃ re-entered through recirculation, O₃ and its precursors with different atmospheric age (i.e. time spent in the air since release) should be quantified but the models tracking ozone precursors based on their emission locations and source sectors cannot differentiate the influence of freshly-emitted and aged local emissions on ozone.

3.0 Objectives

The overall objective of this research is to synthesize existing data, previous analyses, and photo-chemical model experiments to provide a comprehensive and reconciled description of how mesoscale and synoptic-scale winds affect dispersion and accumulation of air pollutants emitted in the Houston area and from other regions, and how they contribute to high ozone events. The relationship between surface winds and boundary-layer mesoscale transport features will be clarified, and a novel source- and age-resolved regional air quality model with ozone source apportionment capability will be applied to investigate selected high ozone events.

4.0 Task Descriptions

Task 4.1. Synthesis of Mesoscale Wind Structures in Synoptic-scale Context.

To date, mesoscale wind features in HGB have been analyzed in piecemeal fashion, focused on individual phenomena, episodes, or observations. Nielsen-Gammon (2016) has recently analyzed the TexAQS-II radar wind profiler data set and used observations of synoptic-scale controls on mesoscale winds to identify the dynamical nature, spatial distribution, and physical causes of the mesoscale winds. With that comprehensive spatial analysis in hand, we will utilize the long-term radar wind profiler observations from La Porte and Cleburne to robustly determine how the amplitude and phase of these mesoscale winds are controlled by synoptic-

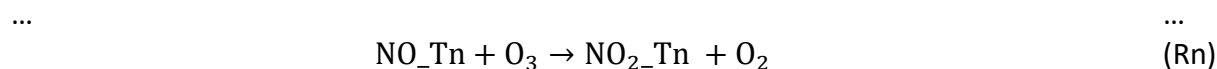
scale weather patterns. We anticipate finding strong sensitivity of mesoscale wind amplitude to synoptic-scale wind direction and wind speed. We will identify the particular synoptic-scale winds that facilitate mesoscale stagnation and recirculation. We will also investigate whether the mesoscale wind evolution can be regarded as controlled by the instantaneous synoptic-scale wind field or whether it is sensitive to the evolution of synoptic-scale winds over time. In all of these steps, we will watch for nonlinear relationships based on physical mechanisms, advancing understanding beyond what simple linear correlations can provide (e.g. Banta et al., 2011).

Since 700 m wind speeds more reliably predict ozone concentrations than do surface winds (Tucker et al., 2010), we will also seek to identify a relationship between surface winds and winds in the residual layer that will allow the winds aloft to be diagnosed from ground-level observations. We anticipate that nighttime transport winds aloft can be diagnosed from surface wind observations within the well-mixed planetary boundary layer the previous afternoon and from observations of the burst of wind the following morning when the developing daytime planetary boundary layer reaches the residual wind maximum, and that such a relationship can be derived for Houston and Dallas and applied throughout central and eastern Texas.

An important aspect of ozone evolution is the nighttime transport of the ozone plume from the Houston metropolitan area (Luria et al., 2008; Senff et al., 2010). Depending on the vertical shear in the residual layer, the plume may remain concentrated or may disperse over a broad area. We will utilize the long-term wind profiler observations to determine the circumstances in which the combined synoptic and mesoscale winds would yield a coherent ozone plume with little dispersion, and the circumstances in which synoptic and mesoscale winds would lead to a much broader dispersal of pollutants.

Task 4.2. Develop source and age-resolved CMAQ (SAR-CMAQ)

To track the atmospheric age of ozone precursors, we will develop a source- and age-resolved chemical mechanism. Conceptually, the age-resolved mechanism can be explained using the following reactions for NO and NO₂:



The NO_T[1,2...n] and NO₂_T[1,2,...,n] species are used to track NO and NO₂ with different atmospheric times from fresh to aged. In the model simulation, fresh emissions of NO and NO₂ are represented by the species with T1 tags. At the end of each model hour, a time bin advance operation is performed so that NO₂_{Ti} = NO₂_{T(i-1)} for i=1,2,...,n-1. For the last time bin, NO₂_{Tn} = NO₂_{Tn} + NO₂_{T(n-1)}. The same operations will be done for NO and other tagged reactive nitrogen species. This age-resolved concept can also be applied to primary VOCs. This scheme can be easily expanded to track age-resolved species from different sources or source regions. For O₃, it is possible to introduce non-reactive ozone tracers, O₃_{T1}, O₃_{T2}, ..., O₃_{Tn},

to represent O₃ with different atmospheric ages. At each time step, integrated process analysis (IPA) can be used to determine the ozone formation (P_{O₃}) and removal rate (D_{O₃}). O₃_T1, which represents freshly formed O₃, can be updated by equation (1) to account for ozone formation while the other O₃ tracers remain unchanged.

$$O_{3_T1}^{int} = O_{3_T1}^{t-\Delta t} + P_{O_3} \quad (1)$$

$$O_{3_Ti}^{int} = O_{3_Ti}^{t-\Delta t}, \quad i=2,3,\dots,n \quad (2)$$

The intermediate concentrations will be updated by distributing the removal of O₃ proportionally to all tagged O₃ species:

$$O_{3_Ti}^t = O_{3_Ti}^{int} - D_{O_3} \frac{O_{3_Ti}^{int}}{\sum_{j=1}^n O_{3_Tj}^{int}} \quad i=1,2,\dots,n \quad (3)$$

The above scheme shows how to resolve O₃ atmospheric ages. It is easy to expand this representation to track both O₃ age and formation regions. For example, it might be useful to track at which vertical layer the O₃ is formed because wind speed and direction changes as a function of height, leading to different transport distances. Additional ozone tracers with layer designations, such as O₃_L1_T1, O₃_L1_T2, etc., can be used for such a purpose.

The age-resolve scheme has been implemented in CMAQ to test the conceptual framework. The model is applied to study ozone formation in the Houston area during Texas Air Quality Study 2006. The predicted 8-hr ozone concentration in Galveston seems to inversely correlate with the fraction of fresh NO_x in the air (Figure 2), which supports the conclusion that high 8-hr ozone days are more influenced by aged air. Such an analysis can be repeated for different locations in Houston under different meteorological conditions to help quantitatively evaluate the role of synoptic and mesoscale recirculation on O₃ in Houston.

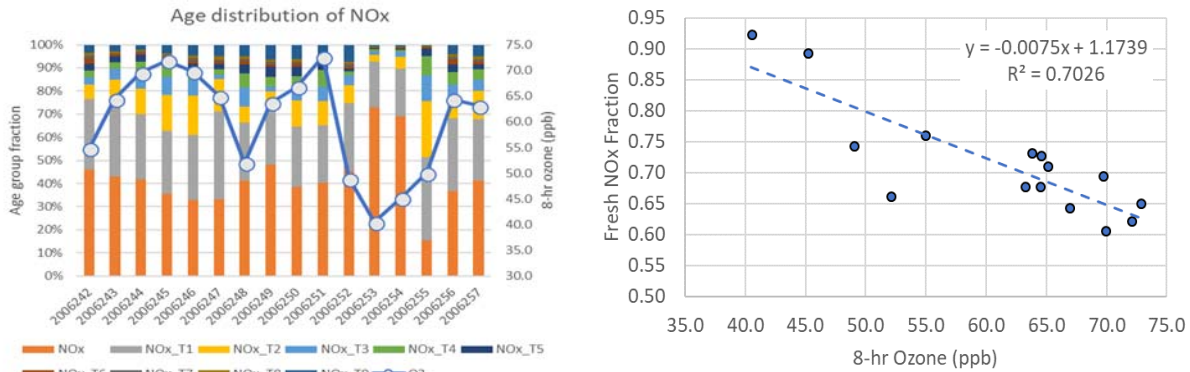


Figure 2. (left) Predicted 8-hr ozone concentrations (right y-axis) in Galveston on August 31 to September 15, 2006, and the atmospheric age distribution of NO_x (left y-axis). NO_x: NO_x 0-3 hours old. Species with X1 to X9 represents NO_x of 4-7, 8-11, 12-15, 16-19, 20-23, 24-27, 28-31, 32-35, and more than 35 hours, respectively. (right) Correlation between 8-hr ozone and fraction of “fresh” NO_x (less than 8 hours old).

Source code to implement SAR in CMAQ at the conclusion of the project. Model test/evaluation results will be provided in monthly and quarterly reports.

Task 4.3. Analysis of the interaction of mesoscale winds and ozone formation during key episodes

We will apply the source and age-resolved calculations of SAR-CMAQ to key mesoscale-dominated ozone exceedance events selected from the ozone seasons in 2000, 2006, 2009, 2013 and 2017. Meteorological inputs will be generated using a mesoscale-optimized WRF model configuration. Judicious selection of model parameterizations has been shown to lead to accurate simulations of southeast Texas mesoscale circulations (Ngan et al., 2013). In view of past issues with large-scale wind errors contaminating the mesoscale simulations (Ngan et al., 2012), we will test two reanalysis data sets (the ERA5 global reanalysis from the European Centre for Medium-Range Weather Forecasts and the FNL global reanalysis from National Center for Atmospheric Research) to drive the WRF simulations. Extensive WRF model performance analysis will be conducted and the one with the best performance for synoptic and mesoscale wind patterns will be chosen as the input data for CMAQ. High-interest air quality episodes can then be simulated by WRF and CMAQ with confidence that the synoptic and mesoscale dynamics are properly represented.

Biogenic emissions will be generated using MEGANv2.1 with emission factors based on BEIS 3.61, as a previous AQRP supported study led by Dr. Ying (AQRP 14-030) shows that this set up leads to a better estimation of biogenic emissions of isoprene (Wang et al., 2017). Nested CMAQ domains will be used in the modeling exercise with a 1×1 km² inner domain centered on the HGB region. Anthropogenic emissions will be generated using SMOKE-ready files from the Emission Modeling Platforms (EMP, available from <https://www.epa.gov/air-emissions-modeling/emissions-modeling-platforms>), which are based on the National Emission Inventory (NEI). The emissions for 2000 and 2006 ozone episodes have been previously prepared based on the 2001 and 2005 EMPs. For 2009, 2013 and 2017 ozone episodes, they will be based on the 2008, 2014 and 2016 EMPs. The Mexico and Canada emission from NEI will also be included. We will also work with TCEQ and AQRP manager to use Texas-specific emissions for the inner model domains if such data are available. Wildfire emissions will be based on the Fire INventory from NCAR (FINN) version 1.5 (<http://bai.acom.ucar.edu/Data/fire/>), which has been widely used to provide fire emission for atmospheric chemical transport models. Dust emissions from wind erosion will be calculated using an online dust module in CMAQ. SAR-CMAQ predicted concentrations will be compared with observations extensively to ensure only days with good model performance are used in the subsequent analysis.

The resulting model simulations will be diagnosed in light of the results from Task 1, both to validate the model and to determine whether simple meteorology-based inferences on the role of mesoscale circulations on ozone evolution and transport are adequate descriptions of the ozone evolution. The model simulations will also be used to fill the large unobserved gaps in vertical structure caused by the limited number of profilers and rawinsonde launches. In particular, the model simulations will allow us to determine the spatial patterns of the late afternoon and nighttime mesoscale circulations and how they are influenced by local

geographical features such as Galveston Bay. Independent verification of the model structures will be available from the surface-based wind signatures identified in Task 1.

A list of key ozone formation events under potential mesoscale influence will be compiled. The input and output data to run SAR-CMAQ will be submitted to AQRP at the end of the project. The detailed procedures to generate the model inputs and analyses of model results will be documented in monthly, quarterly and final reports.

Task 4.4. Project Reporting and Presentation

As specified in Section 7.0 “Deliverables” of this Scope of Work, AQRP requires the regular and timely submission of monthly technical, monthly financial status and quarterly reports as well as an abstract at project initiation and, near the end of the project, submission of the draft final and final reports. Additionally, at least one member of the project team will attend and present at the AQRP data workshop. For each reporting deliverable, 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 (or their 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. The report templates and accessibility guidelines found on the AQRP website at <http://aqrp.ceer.utexas.edu/> will be followed. ****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.**** Finally, our team will prepare and submit our final project data and associated metadata to the AQRP archive.

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

Schedule: The schedule for Task 4.4 Deliverables is shown in Section 7.

5.0 Project Participants and Responsibilities

Dr. Ying will be the PI of the project and will work with Dr. Nielsen-Gammon to oversee all aspects of this project. He will guide one CVEN Postdoc researcher or graduate student on Task 2 (source- and age-resolved model development) and Task 3 (CMAQ modeling of ozone exceedance events).

Dr. Nielsen-Gammon will guide ATMO Postdoc researcher on Task 1 (develop and validate quantitative relationships between surface winds and boundary-layer mesoscale transport) and Task 3 (observation data analyses of key mesoscale-dominated ozone exceedance events).

Dr Ying and Dr. Nielsen-Gammon will work together to prepare all required reporting documents.

6.0 Timeline

TASK		09/18	10/18	11/18	12/18	01/19	02/19	03/19	04/19	05/19	06/19	07/19	08/19	
	month #	1	2	3	4	5	6	7	8	9	10	11	12	
1. Synthesis of mesoscale wind structures in synoptic-scale context (N-G)		[Orange shaded]												
2. Develop source and age-resolved CMAQ (SAR-CMAQ) (Ying)		[Orange shaded]												
3. Analysis of interaction of mesoscale winds and ozone formation during key episodes (observation based) (N-G,						[Orange shaded]								
4. Draft and Final Report (Ying, N-G)											[Orange shaded]			

7.0 Deliverables (Please use the materials in this section editing only as/if necessary. We have generated this section for you to include directly within your Scope of Work so that the schedule of required deliverables to AQRP is clearly communicated.)

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 Quarterly Report	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
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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

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