Quality Assurance Project Plan (QAPP)

Project 22 – 008
Modeling analysis of TRACER-AQ and over-water measurements to improve prediction of on-land and offshore ozone

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

Prepared by

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Version 1

The University of Houston has prepared this QAPP following the Environmental Protection Agency (EPA) guidelines for a Quality Assurance (QA) Category III Project: Research Model Application Project. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: 1) Project Description and Objectives, 2) Organization and Responsibilities, 3) Scientific Approach, 4) Quality Metrics, 5) Data Analysis, Interpretation, and Management, and 6) Reporting.

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 "Modeling analysis of TRACER-AQ and over-water measurements to improve prediction of on-land and offshore ozone" project. The Principal Investigator for the project is Yuxuan Wang and Co-PIs are James Flynn and Paul Walter.

Electronic Approvals:

This QAPP was approved electronically on 08/23/2022 by Elena McDonald-Buller, The University of Texas at Austin.

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

This QAPP was approved electronically on 8/25/2022 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 09/07/2022 by Barry Exum, Texas Commission on Environmental Quality.

Barry Exum
Project Liaison, Texas Commission on Environmental Quality

QAPP Distribution List

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Paul Walter, Co-Principal Investigator

1.0 Project Description and Objectives

The Tracking Aerosol Convection interactions ExpeRimentTRACER-Air Quality (TRACER-AQ) study, including the Galveston Offshore Ozone Observations (GO3) field campaign, provided unprecedentedly rich observations of ozone air pollution covering both offshore and onshore locations that are needed to validate current air quality models. During the TRACER-AQ period (July – October 2021), there were six multi-day ozone episodes, resulting in over 20 days during which at least one land-based site or ship-based measurement with Maximum Daily 8-hour Average (MDA8) ozone concentrations exceeded the current National Ambient Air Quality Standard (NAAQS) of 70 ppbv. The proposal team's preliminary analysis of TRACER-AQ observations has revealed definitive gaps in the Weather Research and Forecasting (WRF) model and WRF-driven photochemical models in replicating the observations. This AQRP project will address these issues via continued efforts of model-observation comparisons and photochemical model intercomparisons using three models driven by the same high-resolution WRF meteorology and emissions (CAMx, WRF-GC, and WRF-Chem).

The proposed project will lead to improvements in meteorological and photochemical models to better simulate on-land and offshore ozone in the Houston-Galveston-Brazoria (HGB). The proposed model intercomparison will characterize the strengths and weaknesses of the regulatory model, CAMx, in the context of other air quality models. The modeling interpretation of TRACER-AQ observations will better understand offshore O_3 formation and transport and their effects on high ozone episodes on land that directly relate to ozone exceedances.

2.0 Organization and Responsibilities

2.1 Key Personnel

Yuxuan Wang (PI), Department of Earth and Atmospheric Sciences, University of Houston.

- Coordinates the operations of the project and is the primary contact person.
- Leads reporting requirements (GAD, QAPP, monthly reports, draft, and final reports)
- Works with UH and Saint Edward's University postdoctoral researcher and graduate students to perform the planned modeling analysis.

James Flynn (co-PI), Department of Earth and Atmospheric Sciences, University of Houston.

- Assists with reporting requirements (GAD, QAPP, draft, and final reports)
- Advises UH graduate students and postdocs to perform an observational evaluation of model outputs

Paul Walter (Co-PI), Department of Mathematics, Saint Edward's University

- Assists with reporting requirements (GAD, QAPP, draft, and final reports)
- Advises UH graduate students and postdocs to analyze ozonesonde data and other data collected in 2021

2.2 Project Schedule

The schedule for this project is listed below in Table 1.
Table 1. Schedule of Project Deliverables and Due Dates

Deliverable	**Deliverable Date**
Grant Activity Description (GAD) (Task 1) **Deliverable 1.1:** TCEQ approved GAD **Deliverable 1.2:** TCEQ approved QAPP	 **(1.1):** September 1, 2022 **(1.2):** September 1, 2022
Progress Reports (Task 2) **Deliverable 2.1:** Monthly Progress Reports	**(2.1):** Monthly by the 15th of the subsequent month
Meteorological Model Evaluation and Improvement (Task 3) **Deliverable 3.1:** Meteorological Model Evaluation and Improvement Report	**(3.1):** January 1, 2023
Photochemical Model Evaluation and Intercomparison (Task 4) **Deliverable 4.1:** Photochemical Model Evaluation and Model Inter-comparison Report	**(4.1):** May 1, 2023
Investigation of Elevated Offshore Ozone's Sources (Task 5) **Deliverable 5.1:** 2021 Elevated Offshore Ozone Sources Report **Deliverable 5.2:** Meteorological and Photochemical Modeling Files	**(5.1):** July 1, 2023 **(5.2):** July 1, 2023
Draft Final and Final Reports (Task 6) **Deliverable 6.1:** Draft Final Report **Deliverable 6.2:** Final Report	 **(6.1):** August 1, 2023 **(6.2):** August 31, 2023

3.0 Scientific Approach

3.1 Secondary Data to be Used in the Current Analysis

The primary source of secondary data to be used in the project is monitoring data from the 2021 Galveston Offshore Ozone Observations (GO3) and Tracking Aerosol Convection Interactions ExpeRiment/Air Quality (TRACER-AQ) field campaigns near Houston. Offshore monitoring data from these projects includes ship-based ozone concentrations, meteorological parameters, and ozonesondes. Additional offshore data may come from meteorological parameters measured by buoys in the Gulf of Mexico. The project will also use remote sensing data stored on the NASA Langley Data Archive for the TRACER-AQ project, including observations from the NASA G-V, Langley O_3 Lidar at the UH campus, and Goddard O_3 Lidar at the La Porte airport. Other data to be used in this project include trace gas concentrations and meteorological parameters measured at the continuous ambient monitoring stations (CAMS) in Houston and Galveston.

3.2 Modeling Approach

The project will use WRF to simulate meteorological conditions and three photochemical models (CAMx, WRF-GC, and WRF-Chem) to simulate photochemistry during periods with elevated offshore ozone concentrations.

3.2.1 WRF

WRF will be configured with the same horizontal domain (c.f. Figure 1) and vertical structure as TCEQ-funded "Analysis of 2021 Offshore Monitoring" project, to facilitate intercomparison with previous WRF simulations. The project will conduct (1) observational nudging with offshore monitoring data and vertical profiling data (i.e., ozonesondes), (2) simulation with assimilated meteorological fields (i.e. 3km High Resolution Rapid Refresh (HRRR) meteorology), and (3) re-initiation of long simulations. The results from (1) and (2) will improve WRF's representation of offshore measurements. The results from (3) will shed light on the extent of error propagation in long WRF simulations.

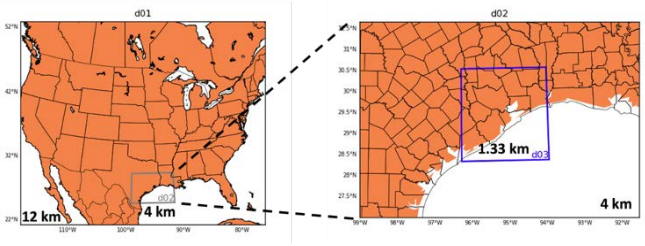

Figure 1. WRF nested model domains and horizontal resolutions.

3.2.2 Photochemical Models

The project will evaluate and compare the performance of CAMx, WRF-GC, and WRF-Chem against TRACER-AQ observations. The same meteorology and anthropogenic emissions will be used in the three models, such that the three models differ mainly in chemical processes (e.g., chemical mechanisms, deposition), natural emissions, chemistry-meteorology coupling etc. The project will probe into model processes such as chemistry mechanism and biogenic emissions, O_3 dry deposition velocity over the waters, reactive halogen chemistry and air pollution feedback on meteorology. Intercomparison among models will help identify the strengths and shortcomings of the many components in the complex meteorological-photochemical modeling system used for State Implementation Plan (SIP) and can provide "weight of evidence" information for SIP results.

The project will investigate the sources of offshore high ozone by a series of model experiments. To understand in situ ozone production, the project will carry out *soft* emission perturbation experiments in each of the three photochemical models, in which anthropogenic emissions over the land and the water are increased separately by 10% to preserve the ozone chemical regimes. By tracing the propagating effects of these added anthropogenic emissions, we will be able to identify how precursor emissions from the land affect in situ ozone formation over the waters and vice versa. To understand regional background ozone, the project will turn off anthropogenic emissions in Texas, a standard modeling approach to investigate background ozone differences during episode days and clean days. The resulting changes in vertical profiles of ozone will provide clues as to horizontal and vertical transport pathways of background ozone.

4.0 Quality Metrics

4.1 Quality of Secondary Data

The secondary data quality requirements for measurements made during the 2021 GO3 and TRACER-AQ campaigns are based on the past experience of the principal investigator who collected the data and the method used. All data used will have been determined by the individual PI responsible for the collection and QA/QC processes to be of final, publishable quality. We will follow the quality assurance and quality control protocols of these data sources and document the data versions used in this project. We will invite these measurement PIs to review the secondary data used after they are re-processed to match with the model's spatial and temporal resolutions.

4.2 Quality of Modeling Data

The project will perform an in-depth evaluation of the models' performance in simulating meteorology, ozone, and precursors from both on- and offshore monitoring,

with the specific focus on performance and differences of the innermost domain (1.33 km x 1.33 km). We will maintain documentation files for each model run that identifies model performances compared to observations using the metrics in Table 2. The impact of modeling settings on the performance will be evaluated using difference plots and the same metrics from Table 2 will be used to quantify the differences.

Table 2. Performance metrics of the WRF-CAMx model.

Performance Metrics	Formulas
Mean Bias (MB)	$MB = 1/N \sum_{i=1}^{N} (M_i - O_i)$
Mean Absolute Error (MAE)	$MAE = 1/N \sum_{i=1}^{N} \lvert M_i - O_i \rvert$
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)	$Corr.R = \frac{\sum_{i=1}^{N} (M_i - \overline{M})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N} (M_i - \overline{M})^2} \sqrt{\sum_{i=1}^{N} (O_i - \overline{O})^2}}$
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 $\overline{M} = 1/N \sum_{i=1}^{N} M_i$, $\overline{O} = 1/N \sum_{i=1}^{N} O_i$.

5.0 Data Analysis, Interpretation, and Management

The modeling performed during the execution of this project will use both statistical and process analysis techniques using the methods described in the associated GAD as in this effort.

5.1 Data Reporting Requirements

The final analysis results and associated project data will be archived by UH on a password protected server at hoth.geosc.uh.edu for a minimum of 3 years. Password protected download links will be provided to the TCEQ upon completion of the project.

5.2 Validation Process

Model outputs will be compared to the TCEQ 2019 modeling platform. The results will also be compared to modeling benchmarks from literature. Differences in modeling performance due to changes in specific modeling configurations and parameters will be quantified and documented.

5.3 Data Analysis

Descriptive (mean, median, standard error, minimum and maximum, correlation, etc.) analysis of the model-observation comparisons will be used for this project. These analyses are not expected to result in new equations or rate constants that can be used to modify model computer code.

5.4 Audits of Data Quality

To audit the quality of secondary data used in the project, a member of the research team who does not collect or compile a particular type of secondary data will review at least 10% of the data for quality assurance purposes. We will also invite colleagues and TCEQ staff who have expertise in meteorological and photochemical modeling to review the project outputs. The QA measures will include statistical analyses and graphical analyses, for example by comparing descriptive statistics and summary graphs of on- and offshore ozone from the different settings. A report on the results of the Audits of Data Quality will be included in the project Final Report.

5.5 Data Storage

The final analysis and model results will be posted to the UH server in a format conducive to import into a database at the conclusion of the project. Password protected links will be provided to the TCEQ for download access. The data will be archived by UH on a password protected server at hoth.geosc.uh.edu for a minimum of 3 years.

6. Reporting

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website 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: Ten (10) business day after notice of intent to fund

Quarterly Reports: The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 3 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	August, September, October 2022	October 31, 2022
Quarterly Report #2	November, December 2022, January 2023	January 31, 2023
Quarterly Report #3	February, March, April 2023	April 30, 2023
Quarterly Report #4	May, June, July 2023	July 31, 2023

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP Template.

Monthly Technical Report Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start - August 31, 2022	September 10, 2022
Technical Report #2	September 1 - 30, 2022	October 10, 2022
Technical Report #3	October 1 - 31, 2022	November 10, 2022
Technical Report #4	November 1 - 30, 2022	December 10, 2022
Technical Report #5	December 1 - 31, 2022	January 10, 2023
Technical Report #6	January 1 - 31, 2023	February 10, 2023
Technical Report #7	February 1 - 28, 2023	March 10, 2023
Technical Report #8	March 1 - 31, 2023	April 10, 2023
Technical Report #9	April 1 - 30, 2023	May 10, 2023
Technical Report #10	May 1 - 31, 2023	June 10, 2023
Technical Report #11	June 1 - 30, 2023	July 10, 2023
Technical Report #12	July 1 - 31, 2023	August 10, 2023

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) by each institution on the project using the AQRP FSR Template.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start - August 31, 2022	September 15, 2022
FSR #2	September 1 - 30, 2022	October 15, 2022
FSR #3	October 1 - 31, 2022	November 15, 2022
FSR #4	November 1 - 30, 2022	December 15, 2022
FSR #5	December 1 - 31, 2022	January 15, 2023
FSR #6	January 1 - 31, 2023	February 15, 2023
FSR #7	February 1 - 28, 2023	March 15, 2023
FSR #8	March 1 - 31, 2023	April 15, 2023
FSR #9	April 1 - 30, 2023	May 15, 2023
FSR #10	May 1 - 31, 2023	June 15, 2023
FSR #11	June 1 - 30, 2023	July 15, 2023
FSR #12	July 1 - 31, 2023	August 15, 2023
FSR #13	August 1 -31, 2023	September 15, 2023
FSR #14	Final FSR	October 15, 2023

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.

Draft Final Report Due Date: August 1, 2023

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: August 31, 2023

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

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2023.