Quality Assurance Project Plan (QAPP)

Project 24 – 021
Improving WRF representation of coastal, marine, and residual boundary layers and quantifying the effects on ozone prediction

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

Prepared by

Yuxuan Wang
James Flynn
University of Houston

August 21, 2024
Version 2

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

Report of Findings – Required in Final Report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the *Improving WRF representation of coastal, marine, and residual boundary layers and quantifying the effects on ozone prediction* project. The Principal Investigator for the project is Yuxuan Wang.

Electronic Approvals:

This QAPP was approved electronically on 2024-09-23 | 05:40:08 CDT
by Elena McDonald-Buller, The University of Texas at Austin.

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Project Manager, Texas Air Quality Research Program

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Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 2024-09-20 | 16:17:29 CDT
by Gabriel Lee, Texas Commission on Environmental Quality.

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TCEQ Liaison, Texas Commission on Environmental Quality

This QAPP was approved electronically on 2024-09-20 | 18:19:33 CDT
by Yuxuan Wang, University of Houston

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Principal Investigator, University of Houston

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James Flynn, Co-Principal Investigator

1.0 Project Description and Objectives

This project continues our efforts of modeling the 2021-2023 offshore field campaign data in the Houston-Galveston-Brazoria (HGB) area, with a focus on the evaluation and improvement of the meteorological model representation of coastal, marine, and residual boundary layers. The models to be investigated are the Weather Research and Forecasting (WRF) and Comprehensive Air Quality Model with Extensions (CAMx), the state's regulatory photochemical model. The field campaigns include the Tracking Aerosol Convection ExpeRiment-Air Quality (TRACER-AQ) studies during July – October 2021 (TAQ1) and April – October 2022 (TAQ2) and the 2023 Mobile and Offshore Air Quality Monitoring Project during May-Oct 2023. They collected unprecedently rich observations of meteorological factors and atmospheric composition including planetary boundary layer (PBL) and ozone (O_3) over diverse offshore locations, such as the Houston Ship Channel, Galveston Bay, and the Gulf of Mexico.

Utilizing these observations to evaluate and improve models, the project's objectives are to answer the following primary science questions:

1. How well does mesoscale meteorological and photochemical grid modeling replicate coastal/maritime boundary layers observations from the 2021-2023 offshore observations?
2. How sensitive is WRF prediction of coastal/maritime boundary layers to model parameters? To what extent do the 2021-2023 offshore observations constrain those parameters?
3. How will the simulation of residual layer ozone be improved by explicitly parameterizing the entrainment of free tropospheric ozone into the residual layer?
4. What are the effects of improved PBL and residual layer (RL) simulation on offshore ozone prediction and source attribution in CAMx?

As boundary layer dynamics are crucial for the diffusion, accumulation, and deposition of ozone and its precursors, the project will improve our predictability of ozone in the HGB and better understand the sources of high offshore O_3 that may 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 such as Grant Activity Description (GAD), QAPP, monthly reports, draft, and final reports.
- Works with UH 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 the observational evaluation of model outputs

2.2 Project Schedule

The schedule for this project is listed below in **Table 1**.

Table 1. Schedule of Project Schedule.

Deliverable	**Deliverable Date**
Grant Activity Description (GAD) (Task 1) **Deliverable 1.1**: AQRP approved Work Plan **Deliverable 1.2:** AQRP approved QAPP	 (1.1): August 23, 2024 (1.2): August 23, 2024
Progress Reports (Task 2) **Deliverable 2.1:** Monthly Progress Reports	(2.1): Monthly by the 10th of the subsequent month
Marine PBL synopsis and model evaluation (Task 3) **Deliverable 3.1:** Marine PBL synopsis and model evaluation Report	 (3.1): November 15, 2024
Improvements to marine PBL in WRF (Task 4) **Deliverable 4.1:** Report on improvements to marine PBL in WRF	 (4.1): March 15, 2025
Improvements to WRF representation of Residual Layer (Task 5) **Deliverable 5.1:** Report on improvements to residual layer in WRF	 (5.1): April 15, 2025
Effect of improved PBL on CAMx ozone prediction and source attribution (Task 6) **Deliverable 6.1:** Report on CAMx ozone prediction and source attribution **Deliverable 6.2:** Meteorological and Photochemical Modeling Files	 (6.1): June 15, 2025 (6.2): June 30, 2025
Draft Final and Final Reports (Task 7) **Deliverable 7.1:** Draft Final Report **Deliverable 7.2:** Final Report	 (7.1): August 1, 2025 (7.2): August 31, 2025

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 onshore and offshore observations from the Tracking Aerosol Convection ExpeRiment-Air Quality (TRACER-AQ) studies during July – October 2021 (TAQ1) and April – October 2022 (TAQ2) and the 2023 Mobile and Offshore Air Quality Monitoring Project during May-Oct 2023 (TAQ3). Offshore monitoring data from these projects includes ship-based ozone concentrations, PBL and other meteorological parameters, and ozonesondes. Additional offshore data may come from meteorological parameters measured by buoys in the Gulf of Mexico and the PBL measurements over the Gulf of Mexico from the Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE) 2019 (SCOAPE-19) campaign to conduct independent model evaluation. PBL measurements were collected by Vaisala CL-51 ceilometer onboard the deployed or chartered vessels. The ceilometer measured continuous atmospheric attenuated backscatter profiles. The sharp gradients in the collected backscatter were then used to detect up to three aerosol layers by the standard retrieval algorithm provided by the ceilometer manufacturer. The lowest determined aerosol layer is usually characterized as mixed layer height, defined as the volume of atmosphere in which aerosols are well mixed and dispersed. Mixed layer height does not equal PBL height by definition; it approximates the convective boundary layer (CBL) height during the daytime, which aligns with the standard model output for the PBL height during the daytime. At night, the sharp gradients in the collected backscatter can represent the height of the residual layer (RL) or the surface boundary layer (SBL) depending on retrieval algorithms.

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 the photochemical model CAMx to simulate photochemistry during periods with elevated offshore ozone concentrations.

3.2.1 WRF

The meteorological model to be improved is Weather Research and Forecasting (WRF) model, the leading mesoscale weather prediction model commonly used to drive Comprehensive Air Quality Model with Extensions (CAMx), the regulatory photochemical model. We will use WRF v4.6, the most recent release at the start of the project. The simulation will cover all the dates during 2021-2023 with available field campaign observations plus proper spinup. We set up three nested domains with different horizontal resolutions (**Figure 1**) that cover the contiguous United States, Southeast Texas, and the Houston-Galveston region, referred to as domains 1, 2, and 3, respectively, with the corresponding horizontal resolutions of 12 km × 12 km, 4 km × 4 km, and 1.33 km × 1.33 km. All domains have identical vertical resolutions with 50 hybrid sigma-eta vertical levels spanning from the surface up to 10 hPa. While WRF has different physics packages, we will use the set of configurations as in Li et al. (2023) based on the campaign-wide evaluation of the modeled meteorology during TAQ1 (Liu et al., 2023).

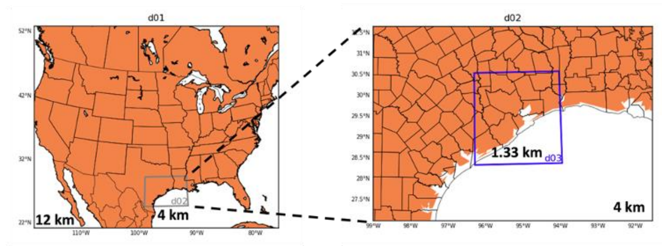

Figure 1. WRF-CAMx nested model domains and horizontal resolutions.

3.2.2 CAMx

The project uses CAMx model v7.30, the most recent release at the start time of the project. The three CAMx domains are the same as the WRF domains and grids as shown in Figure 1. The corresponding horizontal resolutions and grid numbers for domains 1–3 are 12 km × 12 km, 4 km × 4 km, and 1.33 km × 1.33 km, respectively. All domains have identical vertical resolutions with 30 vertical levels from the surface to ~100 hPa. The simulation will cover all the dates during 2021-2023 with available field campaign observations plus proper spinup. The initial conditions (IC)/boundary conditions (BC) inputs for the outmost domain are from the GEOS-Chem global simulation with NEI 2016 nitrogen oxide (NOx) emissions scaled down to 2021-2023. The Carbon Bond version 6 revision 5 (CB6r5) is used for gas-phase chemistry, including the inorganic iodine depletion of O_3 over oceanic water. Dry deposition is based on the Wesely scheme. Anthropogenic emission files with 12 km and 4 km spatial resolutions from the 2019 SIP modeling platform provided by TCEQ were used in our previous CAMx simulation with those emissions regridded to 1.33 km resolution for the HGB domain (Li et al., 2023). In the project, we will scale the 2019 SIP emissions of NOx to 2021-2023 based on scaling factors derived from TROPOspheric Monitoring Instrument (TROPOMI) -derived NOx emissions as described by Liu et al. (2022).

4.0 Quality Metrics

4.1 Quality of Secondary Data

The secondary data quality requirements for measurements made during the 2021-2023 campaigns are based on the past experience of the investigators who collected the data and the method used. All data used will have been determined by the individual PI responsible for the collection and quality assurance/quality control (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 against both on- and offshore observations, including those from the field campaigns and routine meteorology/air quality monitoring sites. The specific focus will be on performance and differences of the innermost domain (1.33 km x 1.33 km) and the 4 km-resolution domain to understand the effects on future CAMx State Implication Plan (SIP) simulations. 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 PBL improvements on the model 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 work plan.

5.1 Data Reporting Requirements

The outputs from WRF and CAMx modeling will be processed as hourly means and monthly means in netCDF format. For important case days such as high ozone periods and representative PBL case days, the modeling data will also be reported as graphs to reveal key spatial features and their temporal evolution.

5.2 Validation Process

CAMx model outputs will be compared to the TCEQ 2019 modeling platform and the upcoming TCEQ 2022 modeling platform if becoming available. WRF model outputs will be validated against reanalysis products such as High-Resolution Rapid Refresh (HRRR) outputs. Although the SIP model and project model simulations are for different years, the objectives of the validation are to compare them in terms of (1) their performances against their respective year's observations and (2) spatial and temporal features that are expected to be persistent from year to year, such as relative gradient between urban and suburban and between land and water. The results will also be compared to modeling benchmarks from literature (Simon et al., 2012; Emery et al., 2017). 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.

6.0 Reporting

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. All reports will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website 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 2024	October 31, 2024
Quarterly Report #2	November, December 2024, January 2025	January 31, 2025
Quarterly Report #3	February, March, April 2025	April 30, 2025
Quarterly Report #4	May, June, July 2025	July 31, 2025

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, 2024	September 10, 2024

Technical Report #2	September 1 - 30, 2024	October 10, 2024
Technical Report #3	October 1 - 31, 2024	November 10, 2024
Technical Report #4	November 1 - 30, 2024	December 10, 2024
Technical Report #5	December 1 - 31, 2024	January 10, 2025
Technical Report #6	January 1 - 31, 2025	February 10, 2025
Technical Report #7	February 1 - 28, 2025	March 10, 2025
Technical Report #8	March 1 - 31, 2025	April 10, 2025
Technical Report #9	April 1 - 30, 2025	May 10, 2025
Technical Report #10	May 1 - 31, 2025	June 10, 2025
Technical Report #11	June 1 - 30, 2025	July 10, 2025
Technical Report #12	July 1 - 31, 2025	August 10, 2025

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, 2024	September 15, 2024

FSR #2	September 1 - 30, 2024	October 15, 2024
FSR #3	October 1 - 31, 2024	November 15, 2024
FSR #4	November 1 - 30, 2024	December 15, 2024
FSR #5	December 1 - 31, 2024	January 15, 2025
FSR #6	January 1 - 31, 2025	February 15, 2025
FSR #7	February 1 - 28, 2025	March 15, 2025
FSR #8	March 1 - 31, 2025	April 15, 2025
FSR #9	April 1 - 30, 2025	May 15, 2025
FSR #10	May 1 - 31, 2025	June 15, 2025
FSR #11	June 1 - 30, 2025	July 15, 2025
FSR #12	July 1 - 31, 2025	August 15, 2025
FSR #13	August 1 -31, 2025	September 15, 2025
FSR #14	Final FSR	October 15, 2025

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, 2025

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, 2025

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 2025.

7.0 References

Emery, C., Liu, Z., Russell, A. G., Odman, M. T., Yarwood, G., & Kumar, N. (2017). Recommendations on statistics and benchmarks to assess photochemical model performance. Journal of the Air & Waste Management Association, 67(5), 582-598.

Li, W., Wang, Y., Liu, X., Soleimanian, E., Griggs, T., Flynn, J., and Walter, P.: Understanding offshore high-ozone events during TRACER-AQ 2021 in Houston: Insights from WRF-CAMx photochemical modeling, Atmos. Chem. Phys., 23, 13685–13699, https://doi.org/10.5194/acp-23-13685-2023, 2023

Liu, X., Wang, Y., Wasti, S., Li, W., Soleimanian, E., Flynn, J., Griggs, T., Alvarez, S., Sullivan, J. T., Roots, M., Twigg, L., Gronoff, G., Berkoff, T., Walter, P., Estes, M., Hair, J. W., Shingler, T., Scarino, A. J., Fenn, M., and Judd, L.: Evaluating WRF-GC v2.0 predictions of boundary layer height and vertical ozone profile during the 2021 TRACER-AQ campaign in Houston, Texas, Geosci. Model Dev., 16, 5493–5514, https://doi.org/10.5194/gmd-16-5493-2023, 2023

Simon, H., Baker, K. R., & Phillips, S. (2012). Compilation and interpretation of photochemical model performance statistics published between 2006 and 2012. Atmospheric Environment, 61, 124-139.

Scope of Work

Project #24-021
Improving WRF representation of coastal, marine, and residual boundary layers and quantifying the effects on ozone prediction

Prepared for

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

By

Yuxuan Wang
James Flynn
University of Houston

August 20, 2024
Version #2

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 2024-09-23 | 05:40:08 CDT
by Elena McDonald-Buller, The University of Texas at Austin

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

This Scope of Work was approved electronically on 2024-09-20 | 16:17:29 CDT
by Gabriel Lee, Texas Commission on Environmental Quality

Signed by:
Gabriel Lee
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Project Liaison, Texas Commission on Environmental Quality

Scope of Work

1. Abstract

This AQRP project continues our efforts of modeling the 2021-2023 offshore field campaign data in the Houston-Galveston-Brazoria (HGB) area, with a focus on the evaluation and improvement of the meteorological model representation of coastal, marine, and residual boundary layers. The models to be investigated are the Weather Research and Forecasting (WRF) and Comprehensive Air Quality Model with Extensions (CAMx), the state's regulatory photochemical model. The field campaigns include the Tracking Aerosol Convection ExpeRiment-Air Quality (TRACER-AQ) studies during July – October 2021 (TAQ1) and April – October 2022 (TAQ2) and the 2023 Mobile and Offshore Air Quality Monitoring Project during May-Oct 2023. They collected unprecedently rich observations of meteorological factors and atmospheric composition including planetary boundary layer (PBL) and ozone (O_3) over diverse offshore locations, such as the Houston Ship Channel, Galveston Bay, and the Gulf of Mexico. Utilizing these observations to evaluate and improve models, the project will focus on the following primary science questions:

1. How well does mesoscale meteorological and photochemical grid modeling replicate coastal/maritime boundary layers observations from the 2021-2023 offshore observations?
2. How sensitive is WRF prediction of coastal/maritime boundary layers to model parameters? To what extent do the 2021-2023 offshore observations constrain those parameters?
3. How will the simulation of residual layer ozone be improved by explicitly parameterizing the entrainment of free tropospheric ozone into the residual layer?
4. What are the effects of improved PBL and residual layer (RL) simulation on offshore ozone prediction and source attribution in CAMx?

Perturbed physics ensembles (PPEs) will be conducted to the WRF model to explore parameter uncertainties and identify parameter combinations that yield simulations most consistent with observations. As boundary layer dynamics are crucial for the diffusion, accumulation, and deposition of ozone and its precursors, the project will improve our predictability of ozone in the HGB and better understand the sources of high offshore O_3 that may relate to ozone exceedances.

The project specifically targets the AQRP Priority Research Priorities FY2024-2025: *Photochemical air quality models* concerning model improvements to WRF PBL schemes, and *TRACER-AQ and over-water measurements* concerning additional analyses of those campaign data.

2. Introduction

The Houston-Galveston-Brazoria (HGB) area has experienced nonattainment of the US National Ambient Air Quality Standards (NAAQS) for ozone over decades (TCEQ, 2022). The predictability of ozone and its precursors in the HGB is strongly dependent on complex meteorological conditions that influence ozone development (Wang et al., 2016; Bernier et al., 2019; Li et al., 2020). Among the meteorological variables affecting air quality, the planetary boundary layer (PBL) plays a vital role in atmospheric simulations through fluxes, control and dynamic processes. The PBL is the lower part (e.g., < 2 km) of the troposphere that is characterized by turbulent motions and vertical mixing of air masses.

These processes occur at various scales and respond to changes in surface forcings with a timescale of an hour or less, making it challenging to accurately represent them in numerical models. The residual layer (RL) is an important sub-structure of the PBL that influences entrainment. Entrainment through PBL growth is a key process that brings regional pollution from the free troposphere to the surface. RL is thus a crucial factor for regional background ozone estimation and diurnal evolution of surface ozone in photochemical models.

The HGB's surface is diverse, with varying land uses such as urban areas, forests, agricultural fields, and water bodies. The different surfaces absorb and release heat differently, leading to variations in PBL characteristics. PBL simulation is particularly challenging over land-water interfaces and marine areas because of persistent marine stratocumulus and a robust inversion layer where entrainment mixing plays a crucial role in influencing the mass, energy, and moisture balances of the boundary layer (Shaw et al., 2022; Vellore et al., 2007). The marine boundary layer (MBL) is also heavily influenced by large-scale subsidence because of weaker surface heating compared to the land surface (Ghonima et al., 2017), which adds another layer of complexity.

Limited observational data for the PBL, especially over coastal and marine locations, poses challenges for model validation and improvement. To address this observational deficiency, multiple field campaigns were conducted in the HGB region in 2021-2023, including the Tracking Aerosol Convection ExpeRiment-Air Quality (TRACER-AQ) studies during July – October 2021 (TAQ1) (Jensen et al., 2022) and April – October 2022 (TAQ2, TCEQ PGA# 582-22-32022-021) and the 2023 Mobile and Offshore Air Quality Monitoring Project during May-Oct 2023 (TAQ3, TCEQ PGA# 582-23-43296-028). All the campaigns augmented the extensive ground network in the HGB with additional stationary and mobile laboratories. These studies collected unprecedentedly rich observations of meteorological factors and atmospheric composition including PBL and O_3 over the waters, such as the Houston Ship Channel (HSC), Galveston Bay, and the Gulf of Mexico (**Figure 1**). These field campaigns provided, for the first time, co-located sampling of PBL and ozone at coastal and marine locations. This project aims to utilize these observations to diagnose and improve the PBL and ozone prediction in meteorological and photochemical models.

The project specifically targets the AQRP Priority Research Priorities FY2024-2025: *Photochemical air quality models* concerning model improvements to PBL schemes, and *TRACER-AQ and over-water measurements* concerning additional analyses of those campaign data.

3. Science Questions

Using 2021-2023 campaign data as constraints to improve model representation of coastal, marine, and residual boundary layers, the project is designed to focus on the following primary science questions:

1. How well does mesoscale meteorological and photochemical grid modeling replicate coastal/maritime boundary layers observations from the 2021-2023 offshore observations?
2. How sensitive is WRF prediction of coastal/maritime boundary layers to model parameters? To what extent do the 2021-2023 offshore observations constrain those parameters?

3. How will the simulation of residual layer ozone be improved by explicitly parameterizing the entrainment of free tropospheric ozone into the residual layer?
4. What are the effects of improved PBL and RL simulation on offshore ozone prediction and source attribution in CAMx?

4. Data and Models

4.1 Field campaigns and PBL observations

The project will use onshore and offshore observations from the Tracking Aerosol Convection ExpeRiment-Air Quality (TRACER-AQ) studies during July – October 2021 (TAQ1) (Jensen et al., 2022) and April – October 2022 (TAQ2, TCEQ PGA# 582-22-32022-021) and the 2023 Mobile and Offshore Air Quality Monitoring Project during May-Oct 2023 (TAQ3, TCEQ PGA# 582-23-43296-028) as model constraints. **Figure 1** displays the spatial coverage of offshore PBL measurements by year, which were collected by Vaisala CL-51 ceilometer onboard the deployed or chartered vessels. The ceilometer measured continuous atmospheric attenuated backscatter profiles. The sharp gradients in the collected backscatter were then used to detect up to three aerosol layers by the standard retrieval algorithm provided by the ceilometer manufacturer. The lowest determined aerosol layer is usually characterized as mixed layer height, defined as the volume of atmosphere in which aerosols are well mixed and dispersed. Mixed layer height does not equal PBL height by definition; it approximates the convective boundary layer (CBL) height during the daytime, which aligns with the standard model output for the PBL height during the daytime. At night, the sharp gradients in the collected backscatter can represent the height of the residual layer (RL) or the surface boundary layer (SBL) depending on retrieval algorithms. The model only provides the SBL as the standard output for nighttime PBL, lacking information on other nocturnal layers such as RL. This complication in comparing ceilometer-derived PBL and model PBL was discussed in our recent work (Liu et al., 2023). We will use the same methodology as described in Liu et al. (2023) in comparing ceilometer-derived layers with model PBL, as shown in **Figure 2**.

At all the locations of PBL measurements, meteorological factors (atmospheric pressure, wind speed, wind direction, air temperature, and relative humidity) and surface O_3 were measured. Some locations also had surface measurements of other trace gases (e.g., NO, NO_2, CO) and ozonesonde launches which will be used to evaluate model predictions of meteorological parameters and chemical composition. All data are available from the campaign website (e.g., https://www-air.larc.nasa.gov/missions/tracer-aq/) or the measurement group (PI: Flynn) after quality assurance and quality control. The project team is familiar with these datasets as demonstrated by recently published papers of the TAQ1 field campaign (e.g., Liu et al., 2023; Li et al., 2023; Soleimanian et al., 2023). Our previous AQRP (AQRP #22-008) and TCEQ projects did not cover the project synopsis analysis of PBL across the multiple campaigns (2021-2023) or model PBL improvements to be conducted in this project.

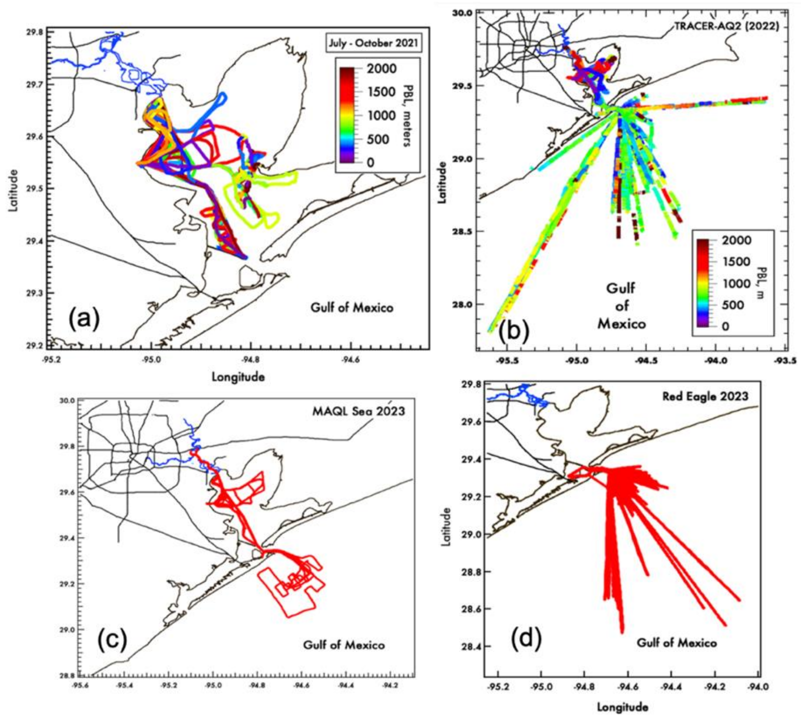

Figure 1. Offshore PBL measurements taken by the 2021-2023 field campaigns. (a) PBL heights measured by UH Pontoon boat and a shrimp boat during TAQ1 (Jul – Oct 2021); (b) PBL heights measured by the UH Pontoon boat (Galveston Bay) and Red Eagle charter boat (Gulf of Mexico) during TAQ2 (Apr – Oct 2022); (c) PBL sampling locations by the UH Osprey in Sep 2023; (d) PBL sampling locations by Red Eagle during May – Oct 2023. Red lines in (c) and (d) show the offshore sampling tracks, not PBL heights.

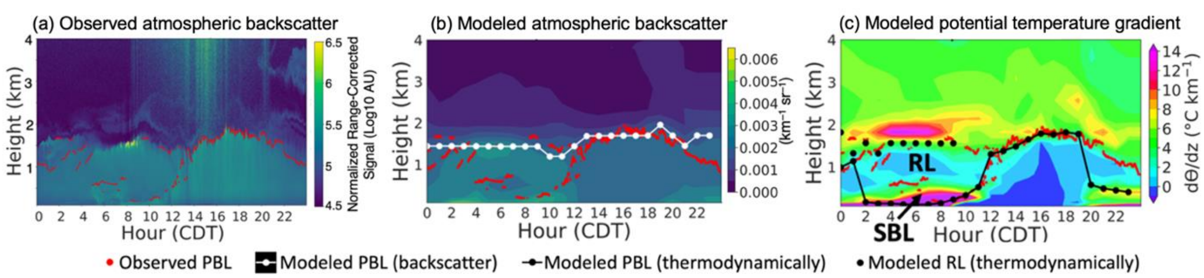

Figure 2. Comparison between ceilometer-derived (a) and modeled (b-c) heights of lower tropospheric layers at the La Porte site on September 8, 2021. The contours show (a) ceilometer-observed attenuated atmospheric backscatter by aerosols and molecules, (b) modeled unattenuated backscatter of aerosols, and (c) modeled potential temperature gradient. Red dots are ceilometer-observed mixed layers. White and black lines are backscatter-defined and thermodynamically defined mixed layers from the model. The dotted black lines show modeled RL derived from the potential temperature gradient. Adopted from Liu et al. (2023).

4.2. WRF

The meteorological model to be improved is Weather Research and Forecasting (WRF) model, the leading mesoscale weather prediction model commonly used to drive Comprehensive Air Quality Model with Extensions (CAMx), the regulatory photochemical model. We will use WRF v4.6, the most recent release at the start time of the project. We set up three nested domains with different horizontal resolutions (**Figure 3**) that cover the contiguous United States, Southeast Texas, and the Houston-

Galveston region, referred to as domains 1, 2, and 3, respectively, with the corresponding horizontal resolutions of 12 km × 12 km (373 x 311 grids), 4 km × 4 km (190 x 133 grids), and 1.33 km × 1.33 km (172 x 184 grids). All domains have identical vertical resolutions with 50 hybrid sigma-eta vertical levels spanning from the surface up to 10 hPa. While WRF has different physics packages, we will use the set of configurations as in Li et al. (2023) based on the campaign-wide evaluation of the modeled meteorology during TAQ1 (Liu et al., 2023). These configurations include the hourly High-Resolution Rapid Refresh (HRRR) meteorological data as initial condition/boundary condition (IC/BC) inputs, the local closure Mellor-Yamada-Nakanishi-Niino (MYNN) PBL option (Nakanishi and Niino, 2009), the Morrison double moment (2M) microphysics scheme (Morrison et al., 2009), the Monin-Obukhov Similarity surface layer (Foken, 2006), the Noah land surface scheme (Chen and Dudhia, 2001), the Rapid Radiative Transfer Model (RRTM) longwave and shortwave radiation schemes (Iacono et al., 2008), and the New Tiedtke cumulus parameterization (Zhang et al., 2011). The simulation will cover all the dates during 2021-2023 with available field campaign observations plus proper spinup. As described in our previous work of TAQ1 meteorological modeling (Liu et al. 2023), we will use field campaign observations when available (i.e., meteorological factors measured by boat and ozonesondes), meteorological site observations, and buoy observations to evaluate the model performance.

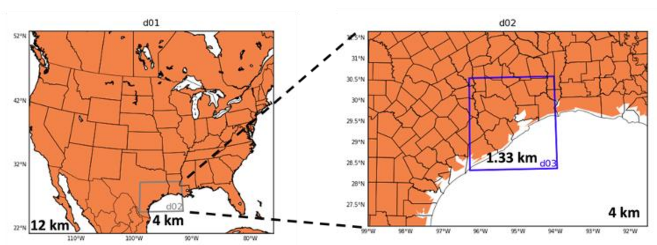

Figure 3. WRF and CAMx nested model domains and horizontal resolutions.

4.3. CAMx

The project will use CAMx model v7.30, the most recent release at the start time of the project. The three CAMx domains are the same as the WRF domains and grids as shown in **Figure 3**, with the corresponding horizontal resolutions and grid numbers for domains 1–3 are 12 km × 12 km (373 x 311 grids), 4 km × 4 km (190 x 133 grids), and 1.33 km × 1.33 km (172 x 184 grids), respectively. All domains have identical vertical resolutions with 30 vertical levels from the surface to ~100 hPa. The IC/BC inputs for the outmost domain are from the GEOS-Chem global simulation with NEI 2016 nitrogen oxide (NOx) emissions scaled down to 2021-2023. The Carbon Bond version 6 revision 5 (CB6r5) is used for gas-phase chemistry, including the inorganic iodine depletion of O_3 over oceanic water (Burkholder et al., 2019). Dry deposition is based on the Wesely scheme (Wesely, 1989). Two different vertical mixing schemes within the PBL will be tested (Section 4.3). Anthropogenic emission files with 12 km and 4 km spatial resolutions from the 2019 SIP modeling platform provided by TCEQ were used in our previous CAMx simulation with those emissions regridded to 1.33 km resolution for the HGB domain (Li et al., 2023). In the project, we will scale the 2019 SIP emissions of NOx to 2021-2023 based on scaling factors derived from TROPOspheric Monitoring Instrument (TROPOMI) -derived NOx emissions as described by Liu et al. (2022).

5. Work Plan

The project includes seven tasks, as shown in **Table 1**. Task 1 is Grant Activity Description (GAD). Task 2 covers monthly progress reports. Tasks 3 - 6 are reports on specific scientific questions shown in detail below. Task 7 is draft final and final reports.

5.1. Task 3: Marine PBL synopsis and model evaluation

Under previous TCEQ and AQRP support, the project team has identified a set of WRF model configurations on a fine resolution (1.33 km x 1.33 km) that most accurately replicates the extensive meteorological data collected during TAQ1 (Liu et al., 2023). WRF-driven CAMx was evaluated against TAQ1 observations (Li et al., 2023). WRF and CAMx modeling were further used to reveal transport and chemical factors for high ozone episodes during TAQ1 (Soleimanian et al., 2023). While the WRF-CAMx model was found to capture certain features of onshore and offshore ozone (Li et al., 2023), definitive gaps were found in the model's prediction of marine PBL (**Figure 4**).

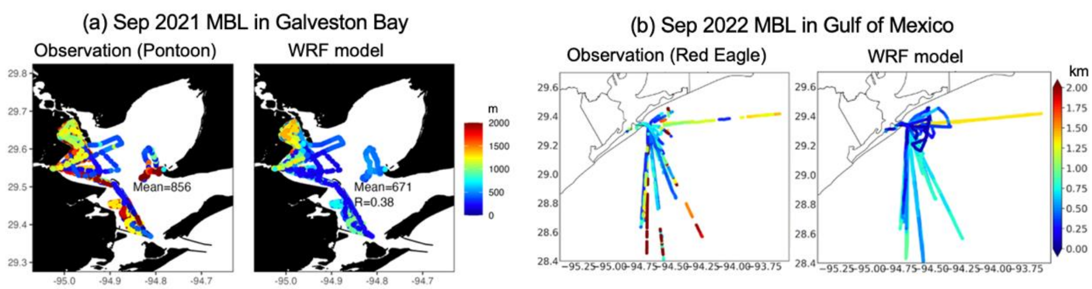

Figure 4. Comparison between observed and modeled marine boundary layer height over (a) Galveston Bay in Sep 2021 (TAQ1 campaign) and (b) the Gulf of Mexico in Sep 2022 (TAQ2 campaign). Observed MBL height is layer 1 from the ceilometer onboard the UH Pontoon boat in (a) and layer 2 from the ceilometer onboard Red Eagle in (b) as layer 1 is consistently too low than the model.

The modeling efforts conducted to date were focused on the 2021 campaign period. The 2022 and 2023 campaigns provided more spatial and temporal coverage of MBLs than in 2021, such as adding MBL observations in the Gulf of Mexico, the HSC, and the east Galveston Bay (**Figure 1**). A synopsis of these multi-year PBL measurements has not been conducted, which will be the first action item of Task 3. The synopsis analysis will reveal MBL diurnal, seasonal, and interannual variations and how such variability differs by offshore locations, such as the east vs. west Galveston Bay, Bay vs. Gulf, and the Ship Channel vs. more open waters.

The 2021-2023 field campaign data will evaluate WRF representation of coastal, marine, and residual boundary layers. This will answer Science Question #1 and provide a baseline model performance before the planned improvements (Task 4 and 5). This control simulation of WRF will use the same configurations from our TAQ1 modeling work (Liu et al., 2023). Our preliminary evaluation of WRF showed that the model deficiency in MBL differs by offshore locations (**Figure 4**). The spatial and temporal variability of the model gaps in MBL will guide model improvements to be described in the next tasks.

Deliverable 3.1: Monthly reports and a technical report describing the marine PBL synopsis and the base WRF model evaluation.

Schedule: The schedule for Task 3 Deliverables is shown in Section 6.

5.2. Task 4: Improvements to marine PBL in WRF

In our previous projects, we found that regardless of the configuration settings, WRF showed definitive gaps in simulating marine boundary layer height and its diurnal cycles (**Figure 4**). This is likely attributed to the fact that model parameterizations and assumptions over the marine environments have not been validated or tuned due to the lack of offshore observations.

As our previous work has ruled out the possibility of PBL improvements by simply changing WRF configurations, achieving further improvements to the PBL will require us to investigate individual physics parameters in the model and their assumed values. To do so, we will conduct single-model *perturbed physics ensembles* (PPEs) (Murphy et al. 2004; Parker, 2013). PPEs are a method used primarily by climate modelers to explore uncertainties and improve simulations in climate models by systematically varying model parameters or formulations within an ensemble of simulations. In the context of PBL, PPEs allow us to account for uncertainties in model physics and parameterizations, which are crucial for accurately representing the complex dynamics of the marine PBL. We will take five steps: (1) Identifying the key parameters and processes that significantly influence PBL dynamics; (2) Systematic parameter variation where a range of plausible values is assigned to selected parameters; (3) Ensemble simulation using the perturbed parameter sets where each simulation within the ensemble represents a different combination of parameter values, allowing for the exploration of a wide range of potential MBL behaviors; (4) Analysis of ensemble results to assess how variations in model physics parameters impact MBL characteristics such as boundary layer height, diurnal cycles, temperature profiles, wind patterns, and turbulence intensity; and (5) Parameter optimization and model improvement by identifying parameter combinations that yield simulations most consistent with observations. The outputs of the PPEs will answer Science Question #2.

The above steps build upon the observational synopsis and baseline model evaluation from Task 3. The candidate parameters for the first and second steps will include not only the ones used in the PBL scheme itself (i.e., turbulent length scale, factor for turbulent diffusion, diffusivity for cloud-top-driven vertical mixing by longwave radiative cooling, turbulence closure factors) but also those in other processes (e.g., convection, surface, microphysics, and radiation) that directly connect with the MBL dynamics. For the latter, example parameters will include but are not limited to surface ocean heat content, laminar boundary layer roughness in sea, entrainment rate for shallow convection, and cloud droplet concentration assumptions.

The third step, ensemble simulation, is most time-consuming. Rather than ensemble simulating the whole 2021-2023 campaign periods which is practically impossible given the project duration, we will build ensembles by the type of representative conditions from the campaigns, which comes from the synoptic analysis in Task 3. The design of ensembles will consider different seasons (e.g., late spring, summer, early fall), pollution levels (e.g., high ozone, median ozone, low ozone), offshore locations (e.g., Galveston Bay, the Gulf of Mexico, HSC transects, docking positions to represent land-water interface), and the base model's biases (e.g., most positive/negative bias days, average positive/negative, minimal bias days). We anticipate having 10-15 ensembles of 1-day simulations to cover most of the diverse conditions from the campaign (e.g., west-east Galveston Bay summer transect ensemble, south-north Gulf of Mexico fall ensemble). Each ensemble will consist of 10-20 model simulations with selected parameter perturbations. In total, we plan to conduct 100 – 300 days of WRF simulations to formulate the PPEs, which is feasible for the project length and resource.

The improved WRF parameters will be evaluated by independent PBL measurements over the Gulf of Mexico from the Satellite Coastal and Oceanic Atmospheric Pollution Experiment (SCOAPE) 2019 (SCOAPE-19) campaign (Thompson et al., 2023). The SCOAPE-19 campaign domain was over the Louisianan coast. We will conduct new WRF simulations over this domain with the tuned WRF parameters and evaluate the PBL predictions against the SCOAPE-19 data. **Figure 5** shows the planned WRF domains for the SCOAPE-19 simulation (May 10-18, 2019). The 4km-resolution model covers the Houston-Galveston while the 1.33km-resolution domain covers the Louisianan coast only.

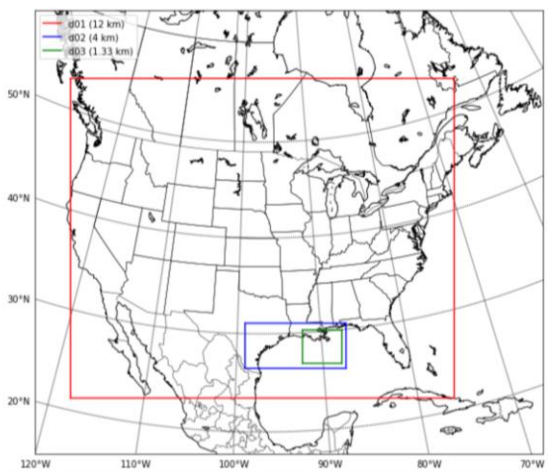

Figure 5. WRF nested model domains and horizontal resolutions for SCOAPE-19 simulation.

Deliverable 4.1: Monthly reports and a technical report describing the PPE and improvements to marine PBL in WRF.

Schedule: The schedule for Task 4 Deliverables is shown in Section 6.

5.3. Task 5: Improvements to WRF representation of Residual Layer

Ozone levels in the residual layer in Houston are significantly influenced by the entrainment process of free tropospheric air masses (Liu et al., 2023; Li et al., 2023). However, models face challenges in accurately simulating this entrainment process, resulting in poor representations of residual layer ozone. A notable discrepancy is evident on Sep 8-9, 2021 (**Figure 6**). On Sep 8, WRF-CAMx overestimated ozone levels in the residual layer compared to observations leading to less ozone subsiding to the surface from aloft. This discrepancy is attributed to the model's underestimation of the strength of a pronounced capping inversion during 0-10 CDT on that day. Consequently, the model incorrectly transports ozone-rich air from the free troposphere into the residual layer, while observations indicate that this ozone-rich air remains aloft in the free troposphere. On Sep 9, the inversion weakened, which allowed ozone-rich air in the free troposphere to reach the RL at night. As the PBL grows in the morning, the RL ozone fumigated into the surface contributing to high ozone in the afternoon. The model, however, underestimated the entrainment of free tropospheric ozone into the RL.

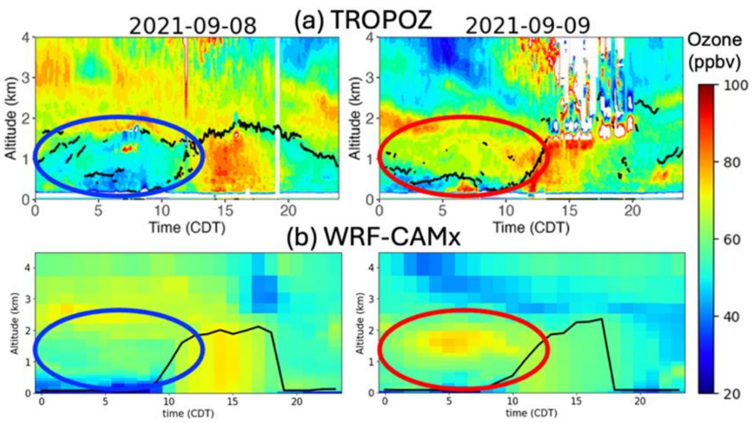

Figure 6. Vertical ozone profile from the TROPOZ ozone lidar (top row) and WRF-CAMx (bottom row) on 09/08/2021 and 09/09/2021. Observed and modeled boundary layer heights are shown as black lines in each figure. Low RL ozone is indicated by blue cycles and high RL ozone by

One key factor impacting the simulation of the entrainment process is the location of the upper boundary of the residual layer, also serving as the lower boundary of the capping inversion, where gas exchange occurs between the residual layer and the overlying free troposphere. However, we observed that the WRF model lacks the residual layer as a standard model output, capturing only the stable boundary layer in the model diagnostic outputs (**Figure 2**; Liu et al., 2023). Because the model does not identify the RL, it treats RL airmasses as part of the free troposphere and hence omits the entrainment process between the two layers.

To overcome this limitation, we examined WRF's primary outputs, specifically potential temperature and aerosol backscatter, to determine the RL height. This postprocessing analysis was tailored to suit specific days during the TAQ1 campaign and may not apply to diverse conditions in 2022-2023. To generalize our approach, we propose incorporating the calculation of the residual layer height during the model simulation and diagnosing it as a standard model output. This model development aims to identify the residual layer under broader conditions, enhancing the understanding of how free tropospheric entrainment affects residual layer ozone levels.

The new RL diagnostics will be implemented in the PPEs of Task 4 so that one can track the change in RL from the systematic perturbation of the physics parameters. We will then add an explicit entrainment parameter in the RL, with its optimized value to be derived from Task 4 PPEs. This approach will dynamically separate the RL from the free troposphere in the model, allowing for a more realistic structure of RL in the simulation. This task will answer Science Question #3.

Deliverable 5.1: Monthly reports and a technical report describing the improvements to residual layer in WRF.

Schedule: The schedule for Task 5 Deliverables is shown in Section 6.

5.4. Task 6: Effect of improved PBL on CAMx ozone prediction and source attribution

As boundary layer dynamics are crucial for the diffusion, accumulation, and deposition of ozone and its precursors, the final task examines how improved MBL and RL representation changes onshore and offshore ozone prediction in WRF-CAMx. The investigation will also address how improvements to WRF PBL schemes will influence source attribution of high ozone over Galveston Bay and the Gulf of Mexico.

The improved WRF model from Tasks 4 and 5 will serve as meteorological inputs for CAMx. The revised WRF-CAMx model will simulate ozone and its precursors in the TAQ1 campaign period and compare to WRF-CAMx outputs from the last AQRP project (22-008) for the same period. We expect to find improvements to CAMx prediction of both onshore and offshore ozone compared to the previous simulation resulting from the improved WRF PBL dynamics from Tasks 4 and 5. In particular, we will investigate if the land-water gradient in surface ozone will improve in the model, which was found to be too small compared to TAQ1 observations (**Figure 6**).

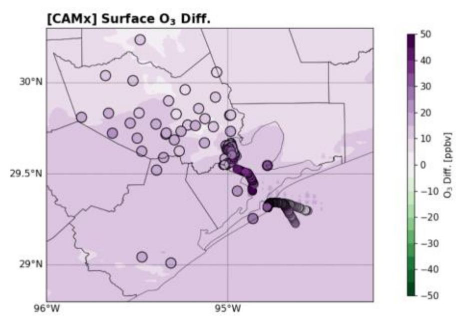

Figure 6. Comparison between observed (filled circles) and CAMx-predicted (color contours) surface ozone enhancements between episode days and clean days in Sep 2021.

In the last AQRP project (22-008), CAMx predicted that local anthropogenic emissions contribute to less than 20% of surface ozone in Houston during high-ozone periods in September 2021 because of high regional background ozone in the model. Due to the high background, offshore ozone changes by less than 0.5% in response to 10% emission reductions of land-based emissions. While the regional background ozone is sensitive to natural emissions, it also depends on how the model simulates vertical diffusion of local emissions and subsidence of regional pollution from the free troposphere to the surface, both of which are governed by the PBL dynamics. Therefore, we expect a different estimate of local vs. regional contributions to onshore and offshore ozone in the HGB from the improved WRF-CAMx model after the planned improvements to its PBL and RL representations. We will re-do the emission perturbation experiments with the revised WRF-CAMx model and investigate how the source categories of high offshore ozone and their relative contributions will change compared to our previous estimates. The revised model will also carry out source attribution experiments for the 2022-2023 campaign periods and investigate the interannual and inter-seasonal changes in source locations and source categories of offshore ozone in the HGB. This task will answer Science Question #4.

The improved model simulations will be conducted at both 4 km and 1.33 km resolutions. The resulting changes in PBL, ozone, and other trace gases at both resolutions will be quantified and documented to understand the effects on future CAMx State Implication Plan (SIP) simulations.

Deliverable 6.1: Monthly reports and a technical report describing the effects of improved PBL and RL on CAMx ozone prediction and source attribution.

Schedule: The schedule for Task 6 Deliverables is shown in Section 6.

6. Schedule

The schedule for this project is listed below in **Table 1**.

Table 1. Schedule of Project Schedule.

Deliverable	Deliverable Date
Grant Activity Description (GAD) (Task 1) **Deliverable 1.1:** AQRP approved Work Plan **Deliverable 1.2:** AQRP approved QAPP	 **(1.1):** August 23, 2024 **(1.2):** August 23, 2024
Progress Reports (Task 2) **Deliverable 2.1:** Monthly Progress Reports	**(2.1):** Monthly by the 10th of the subsequent month
Marine PBL synopsis and model evaluation (Task 3) **Deliverable 3.1:** Marine PBL synopsis and model evaluation Report	 **(3.1):** November 15, 2024
Improvements to marine PBL in WRF (Task 4) **Deliverable 4.1:** Report on improvements to marine PBL in WRF	 **(4.1):** March 15, 2025
Improvements to WRF representation of Residual Layer (Task 5) **Deliverable 5.1:** Report on improvements to residual layer in WRF	 **(5.1):** April 15, 2025
Effect of improved PBL on CAMx ozone prediction and source attribution (Task 6) **Deliverable 6.1:** Report on CAMx ozone prediction and source attribution **Deliverable 6.2**: Meteorological and Photochemical Modeling Files	 **(6.1):** June 15, 2025 **(6.2):** June 30, 2025
Draft Final and Final Reports (Task 7) **Deliverable 7.1:** Draft Final Report **Deliverable 7.2:** Final Report	 **(7.1):** August 1, 2025 **(7.2):** August 31, 2025

7. Deliverables

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 2024	**October 31, 2024**
Quarterly Report #2	November, December 2024, January 2025	**January 31, 2025**
Quarterly Report #3	February, March, April 2025	**April 30, 2025**
Quarterly Report #4	May, June, July 2025	**July 31, 2025**

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, 2024	**September 10, 2024**
Technical Report #2	September 1 - 30, 2024	**October 10, 2024**
Technical Report #3	October 1 - 31, 2024	**November 10, 2024**
Technical Report #4	November 1 - 30, 2024	**December 10, 2024**
Technical Report #5	December 1 - 31, 2024	**January 10, 2025**

Technical Report #6	January 1 - 31, 2025	**February 10, 2025**
Technical Report #7	February 1 - 28, 2025	**March 10, 2025**
Technical Report #8	March 1 - 31, 2025	**April 10, 2025**
Technical Report #9	April 1 - 30, 2025	**May 10, 2025**
Technical Report #10	May 1 - 31, 2025	**June 10, 2025**
Technical Report #11	June 1 - 30, 2025	**July 10, 2025**
Technical Report #12	July 1 - 31, 2025	**August 10, 2025**

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, 2024	September 15, 2024
FSR #2	September 1 - 30, 2024	October 15, 2024
FSR #3	October 1 - 31, 2024	November 15, 2024
FSR #4	November 1 - 30, 2024	December 15, 2024
FSR #5	December 1 - 31, 2024	January 15, 2025

FSR #6	January 1 - 31, 2025	February 15, 2025
FSR #7	February 1 - 28, 2025	March 15, 2025
FSR #8	March 1 - 31, 2025	April 15, 2025
FSR #9	April 1 - 30, 2025	May 15, 2025
FSR #10	May 1 - 31, 2025	June 15, 2025
FSR #11	June 1 - 30, 2025	July 15, 2025
FSR #12	July 1 - 31, 2025	August 15, 2025
FSR #13	August 1 -31, 2025	September 15, 2025
FSR #14	Final FSR	October 15, 2025

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, 2025

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, 2025

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 2025.

8. Project Organization and Responsibilities

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 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 the observational evaluation of model outputs

9. References

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Budget and Budget Justification

Project #24-021
Improving WRF representation of coastal, marine, and residual boundary layers and quantifying the effects on ozone prediction

Prepared for

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

By

Yuxuan Wang

James Flynn

University of Houston

August 21, 2024

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

Approvals

This Budget was approved electronically on 2024-09-20 | 16:15:51 CDT
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Program Manager, Texas Air Quality Research Program

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Project Liaison, Texas Commission on Environmental Quality

Budget and Budget Justification

Principal Investigator: Yuxuan Wang

Project Dates: 08/12/2024 - 08/31/2025

			Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
A. SENIOR PERSONNEL: PI, Co-PI						
	FirstName LastName	**Title**				
1.	Yuxuan Wang	Associate Professor	$12,551	16.2%	1.00	$12,551
2.	James Flynn	Research Associate Profes	$8,352	25.9%	1.00	$8,352
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$20,903**
B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)						
1	1	Other Professionals / Postdoctoral Researcher	$4,520	45.4%	12.00	$54,240
2	1	Other Professionals / Postdoctoral Researcher	$4,060	39.7%	1.00	$4,060
3	1	Graduate Student	$2,300	7.0%	12.00	$27,600
	TOTAL OTHER PERSONNEL					**$85,900**
	TOTAL SALARIES AND WAGES (A+B)					**$106,803**
C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)						
1.	Senior Personnel					**$4,201**
2.	Other Personnel					**$28,194**
	TOTAL FRINGE BENEFITS					**$32,395**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					**$139,198**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)						
a)	*Data storage and archive*					$20,000
b)						$0
c)						$0
	TOTAL EQUIPMENT					**$20,000**
E. TRAVEL			**Cost per Trip**	**# of Trips**		
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)		$2,000	2		$4,000
2.	Foreign					$0
	TOTAL TRAVEL					**$4,000**
F OTHER DIRECT COSTS						
1.	Materials and Supplies					$2,000
2.	Professional Services - Idependent Contractors					$0
3.	Subcontracts (contracts will be issued by UT)					
	a)					$0
	b)					$0
	c)					$0
	d)					$0
4.	Tuition and Fees					$0
5.	Other					$0
	TOTAL OTHER DIRECT COSTS					**$2,000**
G. TOTAL DIRECT COSTS (A THROUGH F)						**$165,198**
H. TOTAL INDIRECT COSTS		**(MTDC Base $145,198)**	**IDC Rate:**	**15.000%**		**$21,780**
I. TOTAL COSTS						**$186,978**

A. SALARIES

Dr. Yuxuan Wang, Principal Investigator, 8.33% effort, will be responsible for supervising all the modeling work and project reports.

Dr. James Flynn, Co-Investigator, 8.33% effort, will be responsible for supervising the quality of observational data used to compare with the model and advise on model-observation comparisons.

Dr. Travis Griggs, postdoctoral scholar, 8.33% effort, will perform the compilation and quality controls of marine PBL and trace gases measurements collected from different boat platforms.

TBD, postdoctoral scholar, 100% effort, will perform WRF model improvements and WRF-CAMx simulations.

TBD, Graduate Research Assistant (GRA), 100% effort, will perform model-observation comparisons and assist in WRF and CAMx simulations.

B. FRINGE BENEFITS

Fringe benefits rates are based on University of Houston's federally negotiated rates for the appropriate employee benefits level at the time of proposal submission. Total fringe benefits budget requested: $32,395

C. EQUIPMENT

Funds are requested for the following equipment:

1. Equipment 1: The budget of $20,000 for adding a 60-disk server that will have 1,000 TB data storage capacity to add to the PI's research cluster to store modeling outputs and data.

Total equipment budget requested: $20,000

D. OTHER DIRECT COSTS

MATERIALS AND SUPPLIES

Supplies are calculated at $1,000 per year for computational supplies needed to archive model outputs, such as external drives and storage.

PUBLICATION: $1000 is requested to cover publication fee of one journal article in AGU or EGU journal.

Total materials and supplies budgeted requested: $2,000

TRAVEL

Funds are requested for project personnel to travel to travel to two national conferences such as the AGU Fall Meeting and EPA's Conference on Air Quality Modeling. Travel costs in this budget are based on sponsored research travel for previous similar trips and are calculated for the domestic travel of two personnel to take one trip each. Total travel budget requested: $4,000

TUITION

None requested.

SUBCONTRACT(S)

None requested.

INDIRECT COSTS

The indirect cost rate of 15% of modified total direct costs (MTDC) is used as instructed by the AQRP's published proposal preparation instructions. Modified total direct costs shall exclude equipment, capital expenditures, charges for patient care, rental costs, tuition remission, scholarships and fellowships, participant support costs and the portion of each subaward in excess of $25,000. Total indirect cost budget requested: $21,780.

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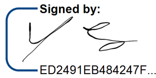
Yuxuan Wang ywang246@Central.UH.EDU Security Level: Email, Account Authentication (None)	 Signature Adoption: Drawn on Device Using IP Address: 73.166.244.221 Signed using mobile	Sent: 9/20/2024 4:15:15 PM Viewed: 9/20/2024 6:18:50 PM Signed: 9/20/2024 6:19:33 PM

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