AIR QUALITY RESEARCH PROGRAM

Texas Commission on Environmental Quality
Contract Number 582-22-20017
Awarded to The University of Texas at Austin

Quarterly Report
November 15, 2022 – February 14, 2023

Submitted to

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PREPARED IN COOPERATION WITH THE TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

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Texas Air Quality Research Program

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OVERVIEW

The goals of the State of Texas Air Quality Research Program (AQRP) are:

(i) to support scientific research related to Texas air quality, in the areas of emissions inventory development, atmospheric chemistry, meteorology, and air quality modeling,

(ii) to integrate AQRP research with the work of other organizations, and

(iii) to communicate the results of AQRP research to air quality decision-makers and stakeholders.

PROGRAM ACTIVITIES FOR THE QUARTER

Between November 15, 2022 through February 14, 2023, the AQRP efforts were focused primarily on finalizing execution of subaward agreements between The University of Texas at Austin (UT) and subaward entities not yet executed, audits of project Financial Status Reports (FSR), internal UT account audits, monthly UT FSR preparation, Project Management Monthly Technical Report (MTR) reviews and discussions, AQRP website upgrades, site access negotiation affiliated with projects 22-006 and 22-010, and other program management tasks. The Research Projects section of this report indicates project subaward status and summary details of progress made to date.

All project details are posted on the AQRP website (https://aqrp.ceer.utexas.edu/projects.cfm).

As of the February 14, 2023, all projects had fully executed subaward agreements with UT. All projects have a retroactive start-date of August 22, 2022, to allow for project initiation expenses (such as report writing, equipment purchases, personnel effort, etc.) prior to full execution. Expiration date for all projects is August 31, 2023. Summary details of awarded projects are listed in Appendix A.

Projects submitted Monthly Technical Reports (MTR) on the 10th of each month in the quarter. Due to contract negotiations extending longer than expected, some projects expressed concerns, which were noted by Project Managers and TCEQ Liaisons. Details are in the Research Projects section of this report. Project MTRs through February 2023 will be posted on the AQRP website (https://aqrp.ceer.utexas.edu/projects.cfm) by mid-March 2023.

Second quarterly reports from all projects were collected on January 31, 2023. All reports have received acceptance by AQRP Project Managers and TCEQ Project Liaisons. Project Quarterly Reports are not posted on the AQRP website, but copies can be requested by emailing aqrp@ceer.utexas.edu.

Projects 22-006 and 22-010 are currently in the process of working with The University of Texas at Austin (UT) and Fort Worth Meachum Airport legal counsel to gain site access. Due to UT's extensive history with negotiating Site Access Agreements (SAAs) with publicly and privately owned property, the AQRP Project Manager, Vincent Torres, volunteered to lead the effort to execute an Airport Use and License Agreement between UT and Forth Worth Meachum Airport. At the time of this report submission, Fort Worth Meachum Airport legal counsel are reviewing the agreement. Projects 22-006 and 22-010 do not have access to the Meachum Airport site currently. AQRP Project and Program Managers are communicating frequently with the TCEQ and Principal Investigators from projects 22-006 and 22-010 to disseminate the details and status of the agreement review.

In January 2023, the TCEQ issued an amendment to the Prime Agreement with UT to allow for the submission of the Personnel Eligibility List (PEL) in lieu of the monthly Level of Effort Certification (LEC) form, to decrease the time and effort involved in monthly reporting. The Amendment was fully executed on January 6, 2023.

The AQRP website redesign project is progressing. Data and file transfers of publicly available reports currently published on the AQRP website were migrated this quarter. Additionally, extensive research on search functionality is underway to allow for search options that pull from files, reports, as well as web pages. Current estimated time of completion of the project is August 2023.

The Financial Status Report section of this report includes accounting through January 2023 from Fiscal Year 2022-2023 (FY 22-23). The month of February 2023 expenses cannot be reported until the University accounting month closes in late March 2023.

Throughout the reporting period, the AQRP Program Manager communicated regularly with the TCEQ Project Manager regarding program deadlines, deliverables, program updates, submission of monthly FSRs, and provided any addition information as requested by the TCEQ.

The AQRP 2023 Workshop will be August 31, 2023, from 9:00 AM CT to 4:00 PM CT at the J. J. Pickle Research Campus, hosted by the Center for Energy and Environmental Resources (10100 Burnet Road, Building EME (#133), Austin, TX 78758). A hybrid option for remote attendees will be available over Microsoft Teams. Additional information regarding speakers and agenda will be updated next quarter.

Next quarter, the AQRP plans to continue audits of project FSRs, collect and publish MTRs to the AQRP website, progress on the website redesign project, communicate weekly with the TCEQ with program updates, ensure all AQRP FSRs are submitted and documented properly with the TCEQ, and perform regular financial reconciliation of the AQRP grant at UT.

BACKGROUND

Section 387.010 of House Bill (HB) 1796 (81st Legislative Session), directs the Texas Commission on Environmental Quality (TCEQ) to establish the Texas Air Quality Research Program (AQRP). The University of Texas at Austin (UT) was selected by the TCEQ to administer the program. A contract for the administration of the AQRP was established between the TCEQ and UT. Consistent with the provisions in HB 1796, up to 10% of the available funding is to be used for program administration; the remainder (90%) of the available funding is to be used for research projects, individual project management activities, and meeting expenses associated with an Independent Technical Advisory Committee (ITAC).

The current AQRP contract was executed for the 2022-2023 biennium and funding of $750,000 per year was awarded.

RESEARCH PROJECT CYCLE

The Research Program is implemented through a nine-step cycle each biennium. The steps in the cycle are described from project concept generation to final project evaluation for a single project cycle.

1) The project cycle is initiated by developing (in year 1) or updating (in subsequent years) the research priorities. The Air Quality Research Program (AQRP) Director, in consultation with the Independent Technical Advisory Committee (ITAC), the Advisory Council (the Council) and the Texas Commission on Environmental Quality (TCEQ), develop research priorities; the research priorities are released along with a Request for Proposals (RFP).
2) Project proposals relevant to the research priorities are solicited. The RFP will be found at http://aqrp.ceer.utexas.edu/ once released.
3) The ITAC performs a scientific and technical evaluation of the proposals.
4) The project proposals and ITAC recommendations are forwarded to the TCEQ. The TCEQ evaluates the project recommendations from the ITAC and comments on the relevancy of the projects to the State of Texas's air quality research needs.
5) The recommendations from the ITAC and the TCEQ are presented to the Council and the Council selects the proposals to be funded.
6) All Investigators are notified of the status of their proposals, either intent to fund, not funded, or contingent (not funded at this time, but being held for possible reconsideration if funding becomes available).
7) Intent to fund projects are assigned an AQRP Project Manager at UT Austin and a Project Liaison at TCEQ. The AQRP Project Manager is responsible for ensuring that project objectives are achieved in a timely manner and that effective communication is maintained among investigators involved in multi-institution projects. The AQRP Project Manager has responsibility for documenting progress toward project measures of success for each project. The AQRP Project Manager works with the researchers, and the TCEQ, to create an approved work plan for the project. The AQRP Project Manager also works with the researchers, TCEQ, and the Program's Quality Assurance officer to develop an approved Quality Assurance Project Plan (QAPP) and Work Plan for each project. Subaward Agreements are issued. The AQRP Project Manager reviews monthly, quarterly, annual, and final reports from the researchers and works with the researchers to address deficiencies.
8) The AQRP Director and the AQRP Project Manager for each project describe progress on the project in the ITAC and Council meetings dedicated to on-going project review.
9) The project findings are communicated through multiple mechanisms. Final reports are posted to the AQRP web site (http://aqrp.ceer.utexas.edu/); research briefings are developed for the public and air quality decision makers; and a bi-annual research conference/data workshop is held.

During this quarter, the AQRP performed step 7.

Research Projects

FY 2022-2023 Projects

Project 22-003 (Atmospheric and Environmental Research, Inc.)

Title: Evaluating the Ability of Statistical and Photochemical Models to Capture the Impacts of Biomass Burning Smoke on Urban Air Quality in Texas **PI**: Matthew Alvarado	**STATUS: ACTIVE** (08/22/2022 – 08/31/2023) **Funded Amount**: $161,388 **AQRP Project Manager**: Elena McDonald-Buller **TCEQ Project Liaison**: Chola Regmi

Abstract: Understanding the impact of domestic fire smoke on urban air quality (AQ) requires understanding (i) the chemistry of the smoke before it reaches the city and (ii) the changes in the urban production rate of ozone (O_3) and particulate matter ($PM_{2.5}$) caused by the smoke. The relative importance of these two pathways on the air quality impacts of domestic fire smoke is not well understood and it is unclear which processes should be targeted to reduce the overall uncertainty.

In addition, three-dimensional (3D) photochemical models like the Comprehensive Air Quality Model with Extensions (CAMx) can have trouble representing the near-source chemistry of the smoke plume and the impact of smoke mixing with urban pollution due to a combination of low spatial resolution near fires and incorrect representation of the chemistry of smoke-specific volatile organic compounds (VOCs). These limitations in physical approaches have led to the development of a variety of statistical approaches to estimate the impact of biomass burning on urban AQ. However, little work has been done to compare the statistical and 3D photochemical approaches or to identify priorities for further development of both approaches. Thus, the United State Environmental Protection Agency (US EPA) and United States (US) Forest Service organized assessment of smoke research needs noted this was a key priority for future smoke chemistry research. A statistical analysis of the impacts of domestic fire emission on urban air quality in Texas and a statistical evaluation of the ability of the CAMx model to simulate these impacts would greatly help TCEQ air quality managers understand the impacts of domestic fires on Texas air quality and human health.

Thus, the objectives of this project are to:

(1) Use generalized additive models (GAMs) driven with satellite and surface observations to examine the impact of fires on background and total O_3 and $PM_{2.5}$ in Texas urban areas.

(2) Examine the ability of CAMx photochemical model to simulate these fire impacts by applying similar statistical methods to the CAMx results.

(3) Use any statistically significant differences found to prioritize different approaches to improve the ability of CAMx to simulate the impacts of domestic fires on air quality.

This project will examine the impact of fires on urban AQ in Texas using statistical modeling. Two urban areas will be examined: Houston-Galveston-Brazoria (HGB) and El Paso. Background O_3 and $PM_{2.5}$ concentrations will be estimated using the lowest value observed at sites near the border of the area of interest, as TCEQ has done in the past (e.g., Berlin et al., 2013). Analyzing the impacts of fires on background and urban sites separately will allow examination of the change in O_3 and $PM_{2.5}$ due to the mixing of smoke with urban pollution separately from the impact of smoke before it mixes with urban pollution. The same statistical methods will be applied to both the real-world surface observations and CAMx-simulated surface observations to determine if the impact of fires on urban air quality as simulated in CAMx is statistically equivalent to the impacts seen in the real-world data. Statistically significant differences will be examined to determine avenues for improving the handling of smoke and urban air chemistry in the photochemical models.

Project Update: November updates included continued Stochastic Time-Inverted Lagrangian Transport (STILT) footprint modeling. Continued gathering Hazard Mapping System (HMS) smoke and fire data and translating it into Generalized Additive Mixed Model (GAMM) predictors.

In December 2022, code was written and successfully tested to determine whether smoke occurred at a monitor location on a given day from the HMS smoke polygons. A remaining challenge is that in the current configuration it will take approximately 38.9 hours to process 10 years of data. Investigations into whether breaking up the runs into multiple batch jobs and then combining the resulting comma-separated-values file format (.csv) later will give faster performance are being conducted.

In January 2023, development of python scripts to project the National Oceanic and Atmospheric Administration (NOAA) Hazard Mapping System (HMS) smoke polygons for 2012 – 2021 to the Geostationary Operational Environmental Satellites Continental United States (GOES CONUS) grid for *Task 1: Using GAMs to Quantify Urban Smoke Impacts* and *Deliverable 1 Q3 Compile meteorological and fire predictors into a single dataset (Task 1*) was completed. The scripts will produce hourly files of 2 kilometer (km) gridded smoke density data. In this initial step we used the density data to determine a binary flag indicating that smoke occurred (1) or did not occur (0) over the selected Houston and El Paso monitoring locations during a given day. The flags will be incorporated into the Generalized Additive Models (GAMs) as predictors.

Preliminary Analysis: No preliminary analysis to report this quarter.

Data Collected: No data to report this quarter.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: The HMS to GOES scripts have many python package dependencies. We discovered that it is critical to start with a "clean" conda environment and install all the necessary packages at once for the installation to work properly. It is also recommended to install all the packages from the same repository to avoid incompatibilities. We documented this process and will include this information with the code delivered to TCEQ upon completion of this project.

Goals and Anticipated Issues for the Succeeding Reporting Period: In the next reporting period, we will begin our analysis to determine the impact of smoke on O_3 and $PM_{2.5}$.

Detailed Analysis of the Progress of the Task Order to Date: Completed initial drafts of Work Plan and QAPP. Held project kickoff. Started work on analyses and gathering data. Wrote and tested code to determine whether smoke occurred at a monitor location on a given day from the HMS smoke polygons.

Project 22-006 (Aerodyne Research, Inc. (ARI) (Primary), Baylor University (Collaborator))

Title: Hydrogen Cyanide for Improved Identification of Fire Plumes in the $(BC)^2$ Network **PI**: Tara Yacovitch (ARI) **Co-PI:** Rebecca Sheesley (Baylor) **Co-PI**: Sascha Usenko (Baylor)	**STATUS: ACTIVE** (08/22/2022 – 08/31/2023) **Funded Amount**: $108,480 (ARI: $51,255; Baylor: $57,225) **AQRP Project Manager**: Vincent Torres **TCEQ Project Liaison**: Erik Gribbin

Abstract: Wildfire incidents in the US have and will continue to increase with a changing climate. Smoke can impact the local air quality in Texas from both local/in-state fires and transported emissions from other parts of the US and from Mexico. The 2020 Black and Brown Carbon $(BC)^2$ study demonstrated how wavelength-dependent aerosol optical properties could be used to track the influence of biomass burning. The $(BC)^2$ network operated in El Paso, Houston, and Galveston in 2020-21 and is being expanded to include Dallas-Fort Worth (DFW) in 2022 and 2023. Hydrogen cyanide (HCN) is a small nitrogen-containing molecule produced in significant quantities from biomass burning, and in limited quantities from vehicle combustion. The goal of this project is to improve smoke plume characterization with the addition of HCN to the $(BC)^2$ smoke monitoring network. This goal explicitly addresses the AQRP's 2022-2023 research priorities, notably "Domestic Fire Emissions" including transported emissions from wildfires (domestic, international) and their impacts on exceptional events in Texas. Performing this monitoring at a Dallas-Fort Worth site ties in with the AQRP's 2022-2023 research priority "Changing Emission Patterns in Texas", which includes additional research along the Interstate-35. This project will deploy a laser-based instrument to measure HCN at a new $(BC)^2$ network site in Dallas-Fort Worth. The work is laid out as 3 tasks: 1) Design measurement campaign; 2) Execute field campaigns; and 3) Data Analysis.

Project Update: The project team continued to hold project meetings on a weekly basis via telecon.

In mid-January, Dr. Usenko coordinated a tentative schedule (pending approval by TCEQ at the time) with electrical contractors (Prism Electric), utility representatives (Oncor), and on-site management at Mecham Airport in Fort Worth (Mr. Dakota Shaw, Airport Operations Manager). Efforts to install service at this site included digging a trench, cable and panel installation, and service switchover. During this process, inspection performed by city officials dictated the need for further work prior to service connection. Inclement weather and scheduling issues have pushed the final service hookup date to mid-February when all necessary parties can be present. If successful, the $(BC)^2$ equipment can be promptly deployed.

Aerodyne engineers replicated and documented the faulty valve behavior experienced at Baylor University. Relevant components were incrementally tested to identify the source issue. Replacement parts were installed after the issue was understood to conclusively determine that the change would bring back expected behavior and performance. Understanding this in great detail will hopefully lead to insights into the decreased detector performance as well since the issues appeared to occur concurrently and may be related.

Preliminary Analysis: No preliminary analysis to report this quarter.

Data Collected: Ambient data at Baylor University was collected. This data is not part of the project deliverables but was used to identify an instrument issue.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: Previous delays with site electrical upgrades, combined with the instrument issues identified in November have caused the measurement days from the anticipated fall campaign to be moved to the spring campaign.

The original project design included a 45-day deployment in the fall, (Sept – Oct); and a 21-day deployment in the spring (to coincide with Aerodyne mobile lab project AQRP 22-010, which is tentatively being scheduled for April). The full 66 HCN measurement days will now be allocated to this spring measurement period. We expect redeployment to occur in March when $(BC)^2$ network sites first get turned on, in advance of the April 1st $(BC)^2$ network start.

Accomplishing the science goals of this project depends on measuring biomass burning emissions in the DFW area. An extended spring campaign will give us the greatest likelihood of capturing such emissions from a variety of sources.

Goals and Anticipated Issues for the Succeeding Reporting Period: Dr. Usenko and others previously mentioned have nearly completed setting up electrical service at the Mecham Airport site. We anticipate that one of the $(BC)^2$ trailers will be deployed as soon as possible to this site. At that point, we hope to review the logistics of reintegrating the HCN instrument when ready.

Evaluation and repair the HCN instrument at Aerodyne continued this period. Assessment of the instrument has taken longer than expected due to the staffing availability (illness, personal matters). Efforts have increased in the last couple weeks and should result in forward progress soon. Once the instrument has been repaired and operates to our satisfaction (with the same precision as initially achieved prior to the original shipment), it will be monitored and operated for a short period of time (1-2 weeks) before being shipped back to collaborators at Baylor University. It is expected that Aerodyne engineers will diagnose and repair the HCN instrument in a timely manner, but new issues could be found upon close inspection.

Detailed Analysis of the Progress of the Task Order to Date: Measurement days originally assigned to the fall campaign have been added to the spring campaign.

Personnel Changes: As described in the Workplan documents, and discussed directly with AQRP project management, Dr. Yacovitch will be on family medical leave beginning mid-December for approximately 4 months, with Conner Daube handling project management and reporting during her absence.

Delays Expected: Given the ongoing delays with the electrical work at the sampling sites in the DFW, measurement days have been added to the spring campaign from the fall campaign.

Project 22-008 (University of Houston (Primary), St. Edward's University (Collaborator))

Title: Modeling analysis of TRACER-AQ and over-water Measurements to improve prediction of on-land and offshore ozone	**STATUS: ACTIVE** (08/22/2022 – 08/31/2023)
PI: Yuxuan Wang (UH)	**Funded Amount**: $181,724 (UH: $175,621; St. Ed's: $6,103)
Co-PI: James Flynn (UH)	**AQRP Project Manager**: Elena McDonald-Buller
Co-PI: Paul Walter (St. Ed's)	**TCEQ Project Liaison**: Barry Exum

Abstract: The Tracking Aerosol Convection ExpeRiment-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 had Maximum Daily 8-hour Average (MDA8) ozone concentrations exceeding the current National Ambient Air Quality Standard (NAAQS) of 70 ppbv. The project 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 activities are designed to focus on the following primary science questions:

1. Which configurations and simulation settings of WRF most accurately replicate the extensive meteorological data collected as part of TRACER-AQ?
2. How well do coupled mesoscale meteorological and photochemical grid modeling of coastal/maritime boundary layers replicate observations?
3. How well do photochemical grid models predict over-water concentrations and formation rates of ozone?
4. What are the spatial distributions of ozone and ozone precursors during TRACER-AQ on days with on-land monitors recording exceedances of the NAAQS and how well does the photochemical model predict such distributions?
5. Which emission source categories affect ozone formation over Galveston Bay and the Gulf of Mexico?

The project specifically targets the AQRP Priority Research Area FY2022-2023: *TRACER-AQ and over-water measurements*. The 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 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.

Project Update: For Task 3 (Meteorological model evaluation and improvement), temporal and spatial variabilities of all model simulations (Table 22-008-1) against the TCEQ continuous ambient monitoring stations CAMS and boat measurements were evaluated.

Table 22-008-1. List of model experiments. The first five simulations were conducted for another TCEQ-funded project. The last three are proposed in this AQRP project.

Simulations	BC Meteorology	PBL	Microphysics	Nudging	Reinitializing
[Base]	NCEP FNL	MYNN	2M	No	No
[WSM6]	NCEP FNL	MYNN	WSM6	No	No
[YSU]	NCEP FNL	YSU	2M	No	No
[ACM2]	NCEP FNL	ACM2	2M	No	No
[ERA5]	ECMWF ERA5	MYNN	2M	No	No
[HRRR]	HRRR	MYNN	2M	No	No
[Nudged]	NCEP FNL	MYNN	2M	Yes	No
[Reinit]	NCEP FNL	MYNN	2M	No	Yes

For Task 3 (Meteorological model evaluation and improvement), the WRF-modeled planetary boundary layer (PBL) height with mixed layer height from the NASA Langley Research Center (LaRC) High Spectral Resolution Lidar-2 (HSRL2) instrument was evaluated. The HSRL2 scanned Houston three times per day at approximately 8:00-10:00, 11:00-13:00, and 14:00-16:00 local time (CDT) for ten days during September 2021 and measured spatial distribution of mixed layer height.

Model simulation for Task 4 (Photochemical model evaluation and model inter-comparison) began in this period. In Task 4, best-performing [HRRR] meteorology identified in Task 3 was used to conduct photochemical modeling with three different models including the Comprehensive Air Quality Model with Extensions (CAMx), the Weather Research and Forecasting (WRF)-driven GEOS-Chem model (WRF-GC), and the WRF model coupled with Chemistry (WRF-Chem).

Preliminary Analysis: The three simulations proposed in Task 3 were combined with five simulations from another TCEQ-funded project to select the simulations with best performance on land and over water. Onshore CAMS and offshore boat meteorological measurements are used to validate WRF simulations. Figures 22-008-1 and 22-008-2 respectively show the spatial and temporal variability between CAMS-observed and WRF-modeled meteorology for five ozone episodes, which is Jul 28, Aug 25, Sep 6-11, Sep 23-26, and Oct 6-9 in 2021. Table 22-008-2 show corresponding statistics for the combined spatial and temporal variabilities. Figures 22-008-3 and 22-008-4 respectively show the spatial and temporal variability between boat-observed and WRF-modeled meteorology. Table 22-008-3 show corresponding statistics for the combined spatial and temporal variabilities. Figure 22-008-5 summarizes the assessments of simulated meteorological variables against observations in Taylor diagrams.

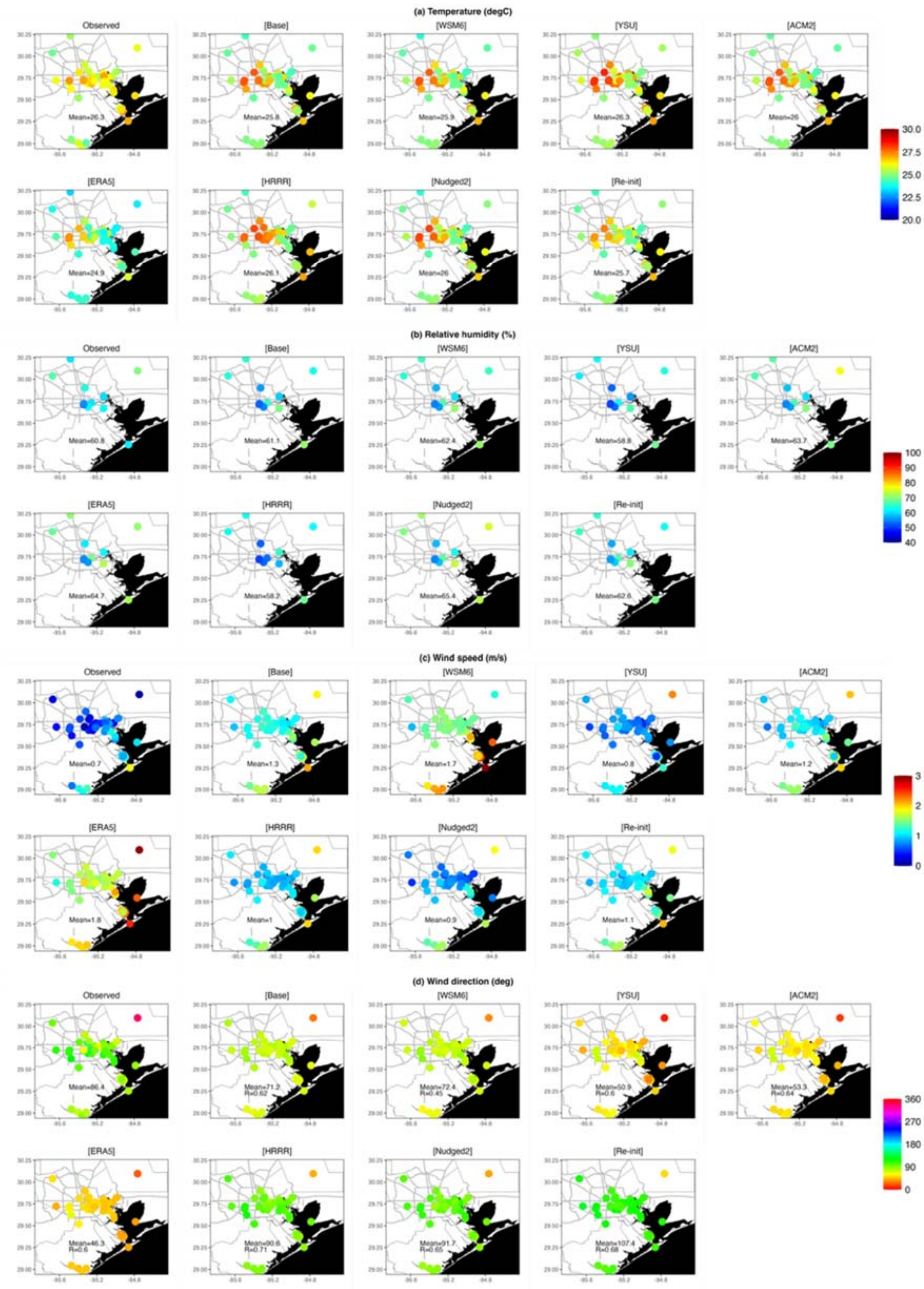

Figure 22-008-1. Spatial distribution of CAMS-observed and modeled mean meteorology during ozone episodes.

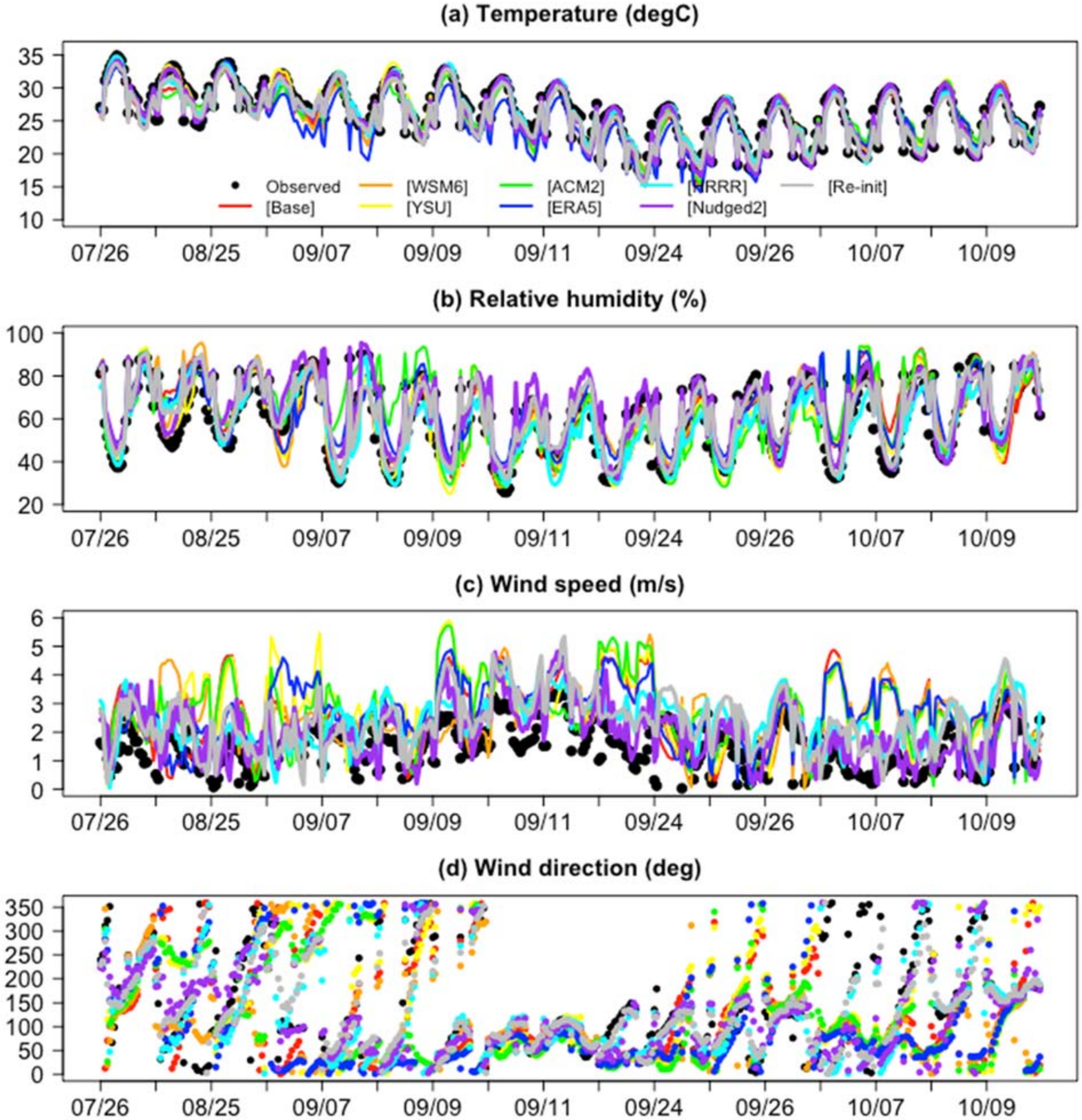

Figure 22-008-2. Time series of (a) air temperature, (b) relative humidity, (c) wind speed and (d) wind direction between CAMS observations and WRF model simulations for five ozone episodes, which is Jul 28, Aug 25, Sep 6-11, Sep 23-26, and Oct 6-9 in 2021.

Table 22-008-2. Performance metrics of spatiotemporal variability between CAMS-observed and WRF-modeled meteorology for five ozone episodes. Hourly meteorology at all stations is used for calculation of performance metrics below. All metrics have the same unit as meteorological variables, except that correlation coefficient (R) and normal mean bias (NMB) are unitless.

Variables	Simulation	OBS	MOD	R	NMB	MB	MAE	RMSE
Temperature (°C)	[Base]	26.18	25.82	0.88	-0.01	-0.36	1.69	2.15
	[WSM6]		25.84	0.89	-0.01	-0.35	1.57	1.99
	[YSU]		26.29	0.89	0.00	0.11	1.65	2.11
	[ACM2]		25.95	0.86	-0.01	-0.23	1.76	2.23
	[ERA5]		24.91	0.85	-0.05	-1.28	2.17	2.71
	[HRRR]		26.12	0.89	0.00	-0.06	1.59	2.05
	[Nudged]		25.92	0.92	-0.01	-0.26	1.43	1.84
	[Re-init]		25.69	0.92	-0.02	-0.49	1.41	1.77
Relative humidity (%)	[Base]	60.12	60.94	0.76	0.01	0.82	10.25	13.04
	[WSM6]		62.21	0.78	0.03	2.09	9.85	12.28
	[YSU]		58.45	0.80	-0.03	-1.68	9.54	12.31
	[ACM2]		62.73	0.71	0.04	2.60	11.40	14.71
	[ERA5]		64.21	0.77	0.07	4.08	10.55	12.76
	[HRRR]		57.82	0.79	-0.04	-2.30	9.13	12.13
	[Nudged]		64.63	0.82	0.08	4.51	9.54	12.05
	[Re-init]		62.57	0.84	0.04	2.45	8.37	10.66
Wind speed (m/s)	[Base]	0.67	1.29	0.35	0.59	1.01	1.40	1.70
	[WSM6]		1.67	0.37	0.61	1.04	1.39	1.72
	[YSU]		0.80	0.39	0.75	1.29	1.55	1.87
	[ACM2]		1.16	0.38	0.66	1.12	1.44	1.77
	[ERA5]		1.76	0.43	0.64	1.09	1.38	1.66
	[HRRR]		1.00	0.54	0.49	0.83	1.12	1.36
	[Nudged]		0.89	0.55	0.30	0.51	0.96	1.20
	[Re-init]		1.14	0.61	0.48	0.82	1.07	1.31
Wind direction (deg)	[Base]	87.76	72.32	0.43	-0.05	-7.67	56.5	73.36
	[WSM6]		72.56	0.38	-0.04	-5.51	56.41	72.93
	[YSU]		53.26	0.41	-0.08	-12.14	60.30	77.29
	[ACM2]		54.87	0.37	-0.07	-10.64	64.15	81.29
	[ERA5]		47.32	0.43	-0.07	-10.92	58.05	74.83
	[HRRR]		92.51	0.61	-0.02	-3.43	40.16	57.55
	[Nudged]		93.29	0.48	0.02	3.00	46.05	64.70
	[Re-init]		109.03	0.47	0.00	-0.32	39.99	57.67

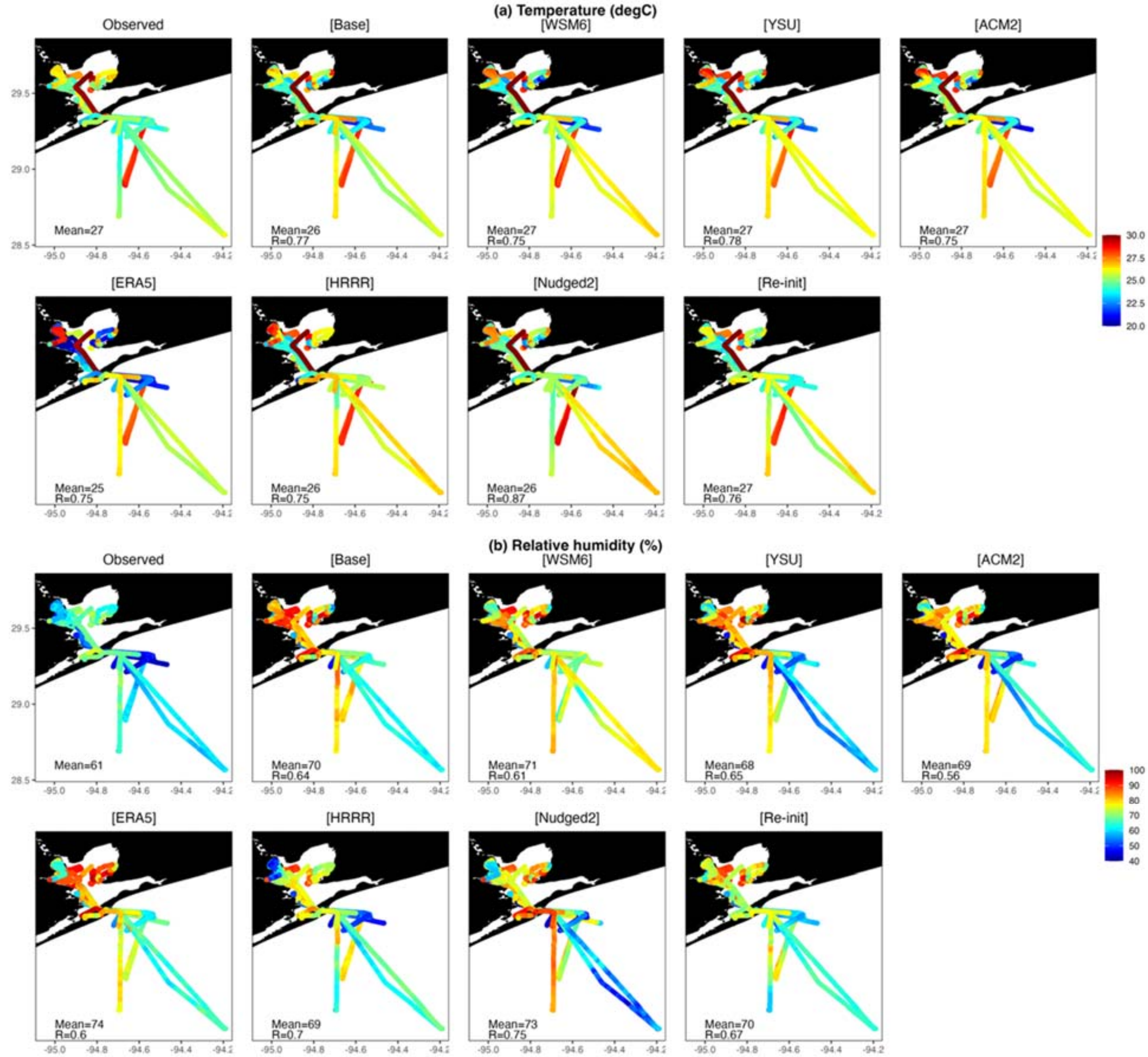

Figure 22-008-3. Spatial distribution of boat-observed and modeled meteorology during ozone episodes.

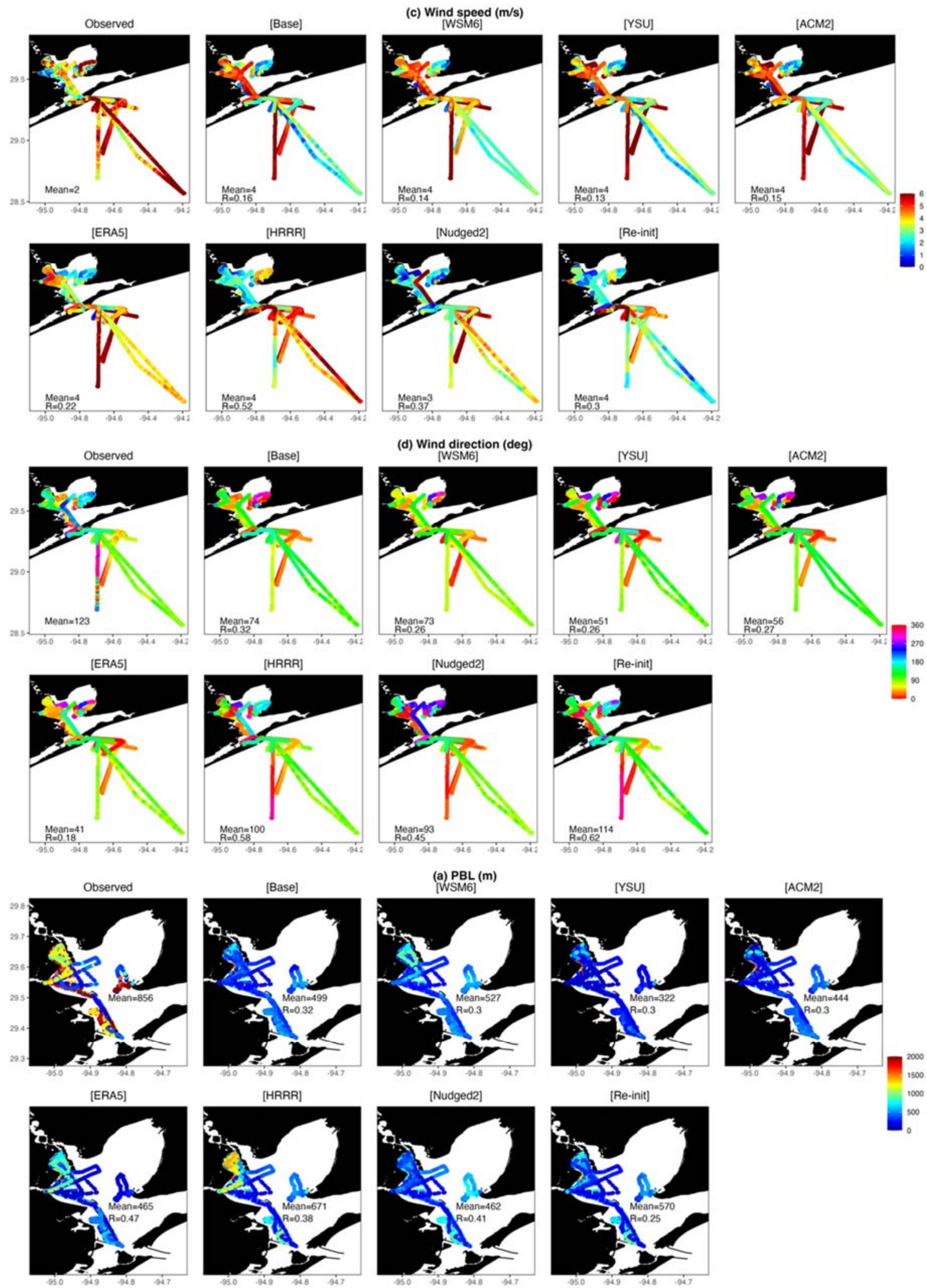
(c) Wind speed (m/s)
Observed
[Base]
[WSM6]
[YSU]
[ACM2]
Mean=2
Mean=4
R=0.16
Mean=4
R=0.14
Mean=4
R=0.13
Mean=4
R=0.15
[ERA5]
[HRRR]
[Nudged2]
[Re-init]
Mean=4
R=0.22
Mean=4
R=0.52
Mean=3
R=0.37
Mean=4
R=0.3
(d) Wind direction (deg)
Observed
[Base]
[WSM6]
[YSU]
[ACM2]
Mean=123
Mean=74
R=0.32
Mean=73
R=0.26
Mean=51
R=0.26
Mean=56
R=0.27
[ERA5]
[HRRR]
[Nudged2]
[Re-init]
Mean=41
R=0.18
Mean=100
R=0.58
Mean=93
R=0.45
Mean=114
R=0.62
(a) PBL (m)
Observed
[Base]
[WSM6]
[YSU]
[ACM2]
Mean=856
Mean=499
R=0.32
Mean=527
R=0.3
Mean=322
R=0.3
Mean=444
R=0.3
[ERA5]
[HRRR]
[Nudged2]
[Re-init]
Mean=465
R=0.47
Mean=671
R=0.38
Mean=462
R=0.41
Mean=570
R=0.25

Figure 22-008-3 (continued). Spatial distribution of boat-observed and modeled meteorology during ozone episodes.

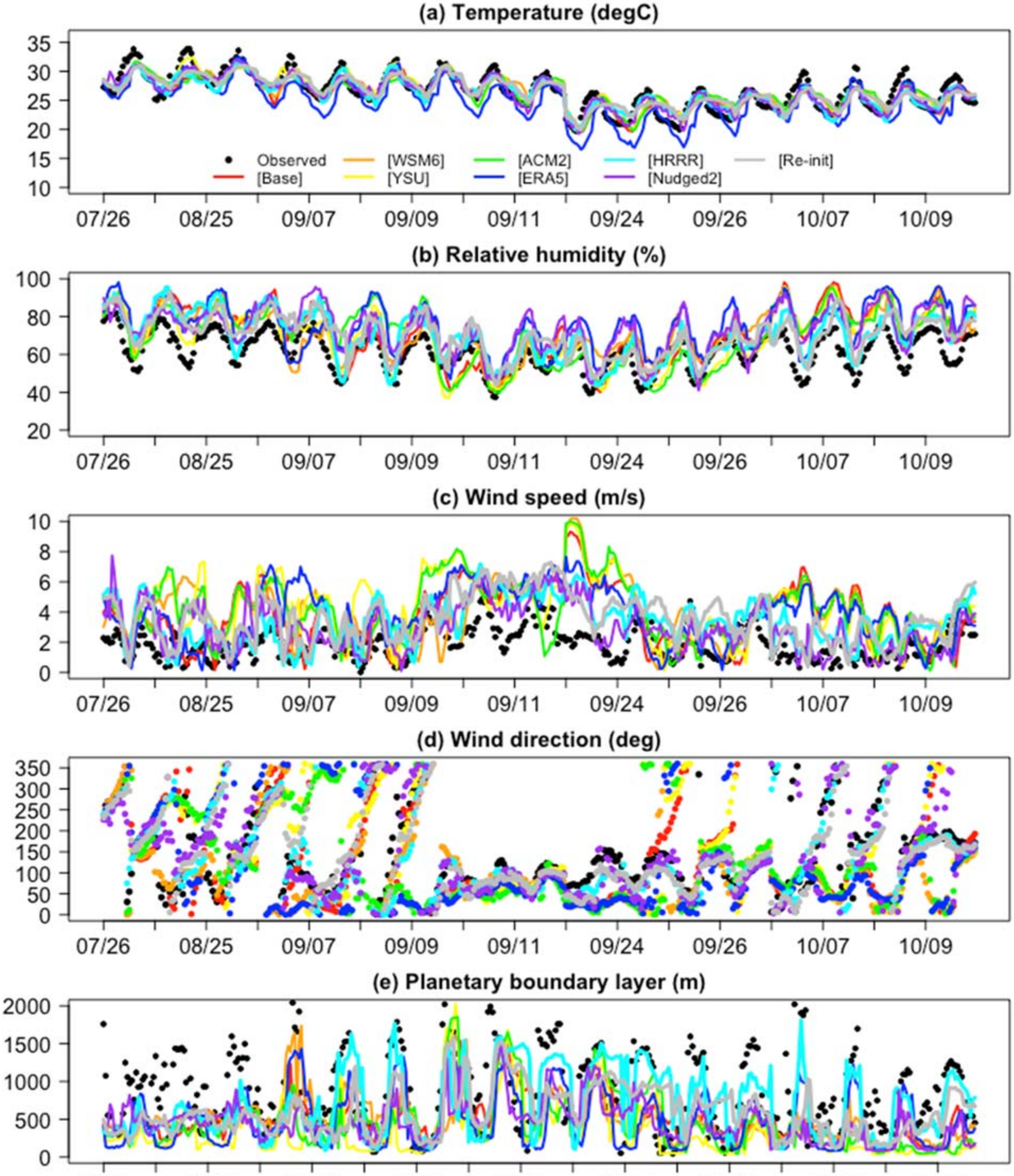

Figure 22-008-4. Time series of (a) air temperature, (b) relative humidity, (c) wind speed, (d) wind direction and (e) boundary layer height between 1-min boat observations and WRF model

simulations for five ozone episodes, which is Jul 28, Aug 25, Sep 6-11, Sep 23-26, and Oct 6-9 in 2021.

Table 22-008-3. Performance metrics of spatiotemporal variability between boat-observed and WRF-modeled meteorology for five ozone episodes. 1-minute meteorology is used for calculation of performance metrics below. All metrics have the same unit as meteorological variables, except that correlation coefficient (R) and normal mean bias (NMB) are unitless.

Variables	Simulation	OBS	MOD	R	NMB	MB	MAE	RMSE
Temperature (°C)	[Base]	26.55	26.45	0.77	0.00	-0.11	1.71	2.14
	[WSM6]		26.50	0.75	0.00	-0.05	1.77	2.20
	[YSU]		26.78	0.78	0.01	0.22	1.71	2.10
	[ACM2]		26.51	0.75	0.00	-0.04	1.78	2.21
	[ERA5]		24.85	0.75	-0.06	-1.70	2.21	3.00
	[HRRR]		26.30	0.75	-0.01	-0.25	1.89	2.29
	[Nudged]		26.30	0.87	-0.01	-0.25	1.26	1.65
	[Re-init]		26.53	0.76	0.00	-0.02	1.71	2.15
Relative humidity (%)	[Base]	60.96	70.24	0.64	0.15	9.28	11.95	14.59
	[WSM6]		71.09	0.61	0.17	10.14	11.76	14.38
	[YSU]		68.20	0.65	0.12	7.24	10.96	13.29
	[ACM2]		69.35	0.56	0.14	8.40	12.75	15.33
	[ERA5]		74.38	0.60	0.22	13.42	14.66	17.23
	[HRRR]		69.20	0.70	0.14	8.24	10.38	12.68
	[Nudged]		73.35	0.75	0.20	12.39	12.87	14.92
	[Re-init]		69.68	0.67	0.14	8.72	10.25	12.42
Wind speed (m/s)	[Base]	0.73	2.47	0.16	0.74	1.67	2.20	2.78
	[WSM6]		2.62	0.14	0.82	1.85	2.33	2.92
	[YSU]		2.17	0.13	0.99	2.22	2.63	3.19
	[ACM2]		1.99	0.15	0.92	2.07	2.49	3.09
	[ERA5]		1.89	0.22	0.78	1.74	2.21	2.72
	[HRRR]		1.68	0.52	0.59	1.32	1.69	2.05
	[Nudged]		1.75	0.37	0.41	0.92	1.57	1.96
	[Re-init]		2.02	0.30	0.69	1.55	2.00	2.41
Wind direction (deg)	[Base]	144.15	118.78	0.32	-0.08	-11.45	57.74	75.38
	[WSM6]		113.5	0.26	-0.13	-19.10	60.40	77.29
	[YSU]		135.77	0.26	-0.11	-16.44	63.52	81.13
	[ACM2]		125.25	0.27	-0.11	-17.20	68.93	85.92
	[ERA5]		96.69	0.18	-0.17	-25.20	69.00	85.30
	[HRRR]		137.93	0.58	-0.08	-12.53	41.54	58.16
	[Nudged]		146.95	0.45	-0.05	-7.68	47.87	65.51
	[Re-init]		146.96	0.62	-0.10	-14.98	42.98	59.66

Table 22-008-3 (continued). Performance metrics of spatiotemporal variability between boat-observed and WRF-modeled meteorology for five ozone episodes. 1-minute meteorology is used for calculation of performance metrics below. All metrics have the same unit as meteorological variables, except that correlation coefficient (R) and normal mean bias (NMB) are unitless.

Variables	Simulation	OBS	MOD	R	NMB	MB	MAE	RMSE
Boundary layer height (m)	[Base]	855.58	499.27	0.32	-0.42	-356.30	529.63	699.67
	[WSM6]		526.69	0.30	-0.38	-328.88	526.38	691.82
	[YSU]		322.22	0.30	-0.62	-533.36	612.29	817.16
	[ACM2]		443.60	0.30	-0.48	-411.97	562.12	747.06
	[ERA5]		464.75	0.47	-0.46	-390.83	507.51	680.30
	[HRRR]		671.27	0.38	-0.22	-184.31	461.30	637.68
	[Nudged]		462.09	0.41	-0.46	-393.48	516.18	696.37
	[Re-init]		569.57	0.25	-0.33	-286.00	518.21	689.22

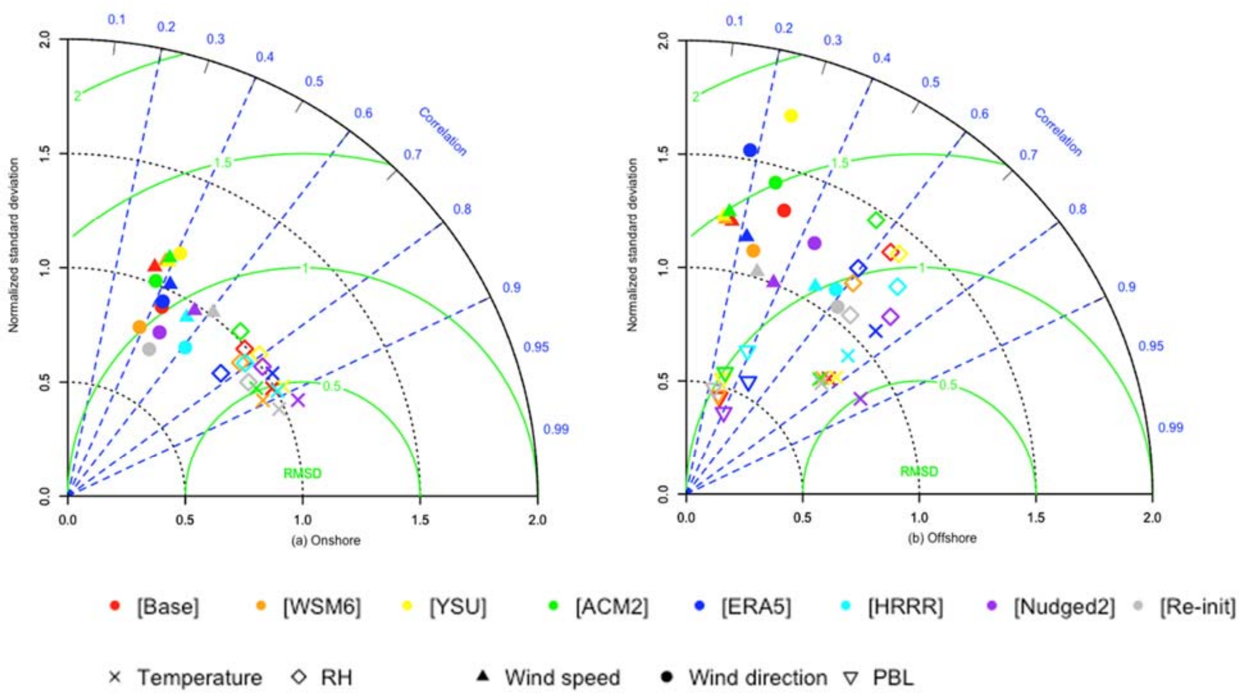

Figure 22-008-5. Assessments of meteorological variables simulated by the WRF model configurations against (a) CAMS hourly measurements and (b) boat 1-minute measurements for all sites during high ozone days. Green, black, and blue lines indicate contours of the normalized centered root-mean-square differences (RMSD), the normalized standard deviations, and the correlation coefficients, respectively. The reference point representing observed state is plotted at 1 along x axis, and the distances to reference point show model performance.

Figures below show the evaluation of spatial (**Figure 22-008-6**) and diurnal (**Figure 22-008-7**) variabilities of the PBL from the three WRF model simulations, i.e. [HRRR], [Nudged2] and [Re-init], against the HSRL2 observations. The HSRL2 scans the greater Houston regions three times a day for ten non-consecutive days in September of 2021, that is September 1, 3, 8-11 and 23-26. Among these days, one ozone exceedance day, which is September 9, is taken as an example to demonstrate the PBL spatial variabilities in **Figure 22-008-6**. The model simulations show the mean morning, noon, and afternoon PBL heights of 275-324 m, 886-1128 m, and 1408-1555 m, in comparison with the observed values of 471 m, 983 m, and 1675 m, respectively. The model simulations capture spatial variabilities at noon (R=0.62–0.77) and in the afternoon (R=0.71–0.76) but have difficulties capturing that in the morning (R=-0.1–0.14). Relatively less correlation in the morning is probably related to the presence of complex nocturnal PBL structure with both a residual layer and a stable surface layer. Despite less spatial correlation in the morning, land-water differences are well represented by the model throughout the day, with lower PBL heights over water than on land. Meanwhile, diurnal variations of PBL heights over the ten days are shown in **Figure 22-008-7**. Compared to water, land has a relatively stronger increase in PBL heights from early morning to afternoon. The model simulations capture the strong PBL variations on land with consistent minor underestimation throughout all hours, but the model has difficulty in capturing PBL variations over water particularly in the afternoon hours despite different configurations.

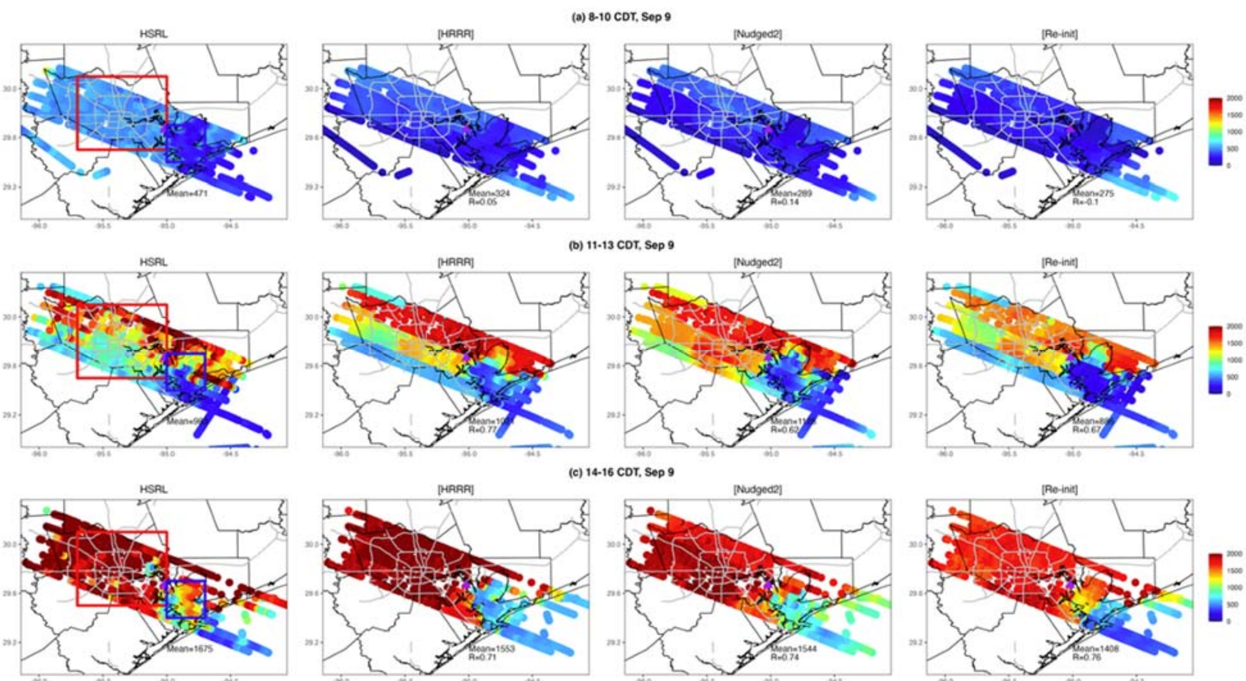

Figure 22-008-6. Spatial distribution of HSRL2-observed and modeled PBL (a) in the morning, (b) at noon, and (c) in the afternoon of September 9, 2021. Red and blue boxes denote land and water, respectively.

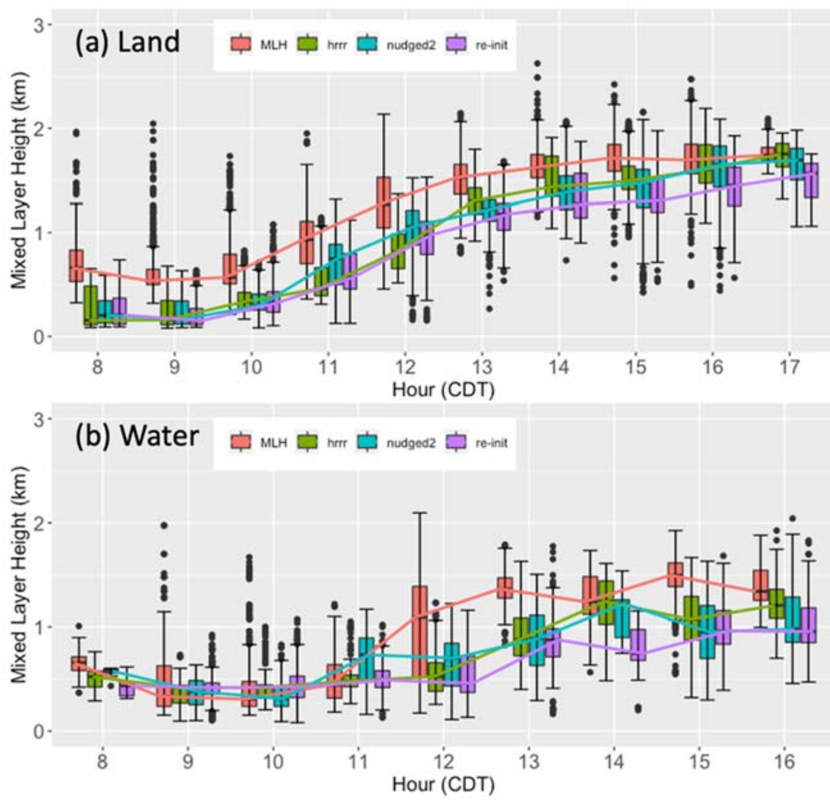

Figure 22-008-7. Diurnal variabilities of HSRL2-observed and modeled PBL (a) on land and (b) over water. Land and water are respectively defined as red and blue boxes in Figure 22-008-6.

Data Collected: No data to report this quarter.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: None.

Goals and Anticipated Issues for the Succeeding Reporting Period: We will start Task 4 of photochemical model evaluation and model inter-comparison in the succeeding report period.

Detailed Analysis of the Progress of the Task Order to Date: N/A.

Project 22-010 (Aerodyne Research, Inc.)

Title: Dallas Field Study (DFS); Ozone Precursors, Local Sources and Remote Transport Including Biomass Burning	**STATUS: ACTIVE** (08/22/2022-08/31/2023)
	Funded Amount: $228,418
PI: Edward Fortner	**AQRP Project Manager**: Vincent Torres
	TCEQ Project Liaison: David Westenbarger

Abstract: The Dallas Fort Worth (DFW) Metropolitan area is the most populous metropolitan area (MSA) in the state of Texas and the fourth most populous MSA in the country. It is also experiencing a high rate of growth and is located along the Interstate 35 (I-35) corridor an area which the AQRP 2022-2023 research priority “Changing Emission Patterns in Texas” addresses as a research focus. The Aerodyne Mobile Laboratory (AML) will conduct measurements in the Spring of 2023 in the DFW area. This project’s first objective is to conduct measurements of point sources in the DFW metropolitan area characterizing the volatile organic compounds (VOC) signature of these sources. This will lead to a better understanding of the VOC component of regional ozone production and an improved assessment of optimum strategies for ozone reduction in the DFW area.

The second goal of this project is to determine the influence of biomass burning impacted airmasses on the DFW metropolitan area. We will conduct measurements upwind and downwind of the DFW when biomass burning impacted airmasses enter the DFW area and determine the impact of these airmasses relative to typical ambient airmasses transiting the DFW area. We will also characterize any wildfires regionally by conducting measurements of the biomass burning plume, better characterizing the evolvement of the plume over time. This goal is complimentary to the AQRP 2022-2023 research priority of “Domestic Fire Emissions”.

Project Update:

Task 2: Base Site Selection: The Fort Worth Northwest Site operated by TCEQ at the Meachum field airport continues to be the primary choice for the base site location. There continue to be two issues which need to meet a positive resolution prior to the arrival of the Aerodyne Mobile Laboratory. The first issue is the execution of a legal agreement with Meachum Field for site access. Vince Torres and RoseAnna Goewey (TX AQRP) along with Ed Fortner are continuing dialogue with the airport operations manager Dakota Shaw at Fort Worth Meachum Field regarding the site access agreement and the most recent information as of Feb. 9, 2023, is that a draft of this legal agreement should be completed during the week of Feb. 13-17. The second issue of concern is the completion of electrical upgrade work at the Meachum Field site which has begun but has not been finished yet. The electrical upgrade work is nearing completion, a switchover to the new electrical lines is due to occur on 16 Feb. and the new lines performance will be inspected at that time.

Task 3: Campaign Planning: The field staffing plan has been completed, all positions are filled, and date commitments have been made. The measurement intensive dates are being planned for Apr 3 – 23. Some personnel will be on-site for the entire campaign while others will be split into first and second half crews. The AML and key instrument availability has been coordinated for the time period of mid-March - April with May considered to be an alternate measurement month if needed. A two-week integration plan of the AML at Aerodyne is scheduled to occur during the last two weeks of March. The necessary ordering of calibration equipment has occurred to ensure its availability for the measurement campaign.

Preliminary Analysis: No preliminary analysis to report this quarter.

Data Collected: No data collected to report this quarter.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: A concern is whether the site agreement and the electrical upgrade will both be completed prior to the intensive which will occur in April. As stated above, work on both matters is occurring and it is still the primary plan to have the Northwest (Meachum Airport) field site used as the base for the AML during the intensive. If this site cannot be made ready, then backup solutions being considered are a different TCEQ measurement site in the Dallas – Fort Worth (DFW) area or Recreational Vehicle (RV) parks in the DFW area. The preference for co-measuring with both TCEQ and project 22-006 has motivated the site selection to be a TCEQ measuring location, however, the AML has used RV parks in past measurement intensives, and it would be possible to do so for this campaign.

Goals and Anticipated Issues for the Succeeding Reporting Period: Executing a site agreement and completing the electrical upgrade work on the Northwest site are priorities for the month of February. These issues will be a point of focus for both the 22-006 and the 22-010 projects.

Detailed Analysis of the Progress of the Task Order to Date: Regarding progress of the tasks relative to the task execution timeline detailed in the Statement of Work Task 1 (Work Plan including QAPP) has been completed and Task 3 (Campaign Planning) has progressed smoothly with respect to staffing and instrument readiness. Task 2 (Base Site Selection) as detailed above does still need to progress with respect to the Meachum Field site and a secondary plan utilizing an RV park as a base site is being investigated currently although due to a lack of any other complementary measurements it is not the primary base site location strategy.

Project 22-019 (University of Houston)

Title: Refining Ammonia emission using inverse modeling and satellite observations over Texas and the Gulf of Mexico and investigating its effect on fine particulate matter **PI**: Yunsoo Choi	**STATUS: ACTIVE** (08/22/2022 – 08/31/2023) **Funded Amount**: $131,366 **AQRP Project Manager**: Elena McDonald-Buller **TCEQ Project Liaison**: Khalid Al-Wali

Abstract: The overall goal of this project is to conduct an inverse modeling study over the State of Texas and the Gulf of Mexico using Community Multiscale Air Quality (CMAQ) models integrated with ammonia (NH_3) remote sensing data from the Cross-track Infrared Sounder (CrIS) for 2019. Objectives of this project are 1) updating the emissions inventory over Texas and the Gulf of Mexico; 2) investigating the contribution of the updated NH_3 emissions on fine particulate matter ($PM_{2.5}$) concentrations; and 3) analyzing the effect of adjusted NH_3 emissions on atmospheric chemistry. In this inverse modeling study, we will use CrIS satellite observations to adjust National Emissions Inventory (NEI) NH_3 emissions, which are highly uncertain owing to a lack of NH_3 observations and therefore more likely to result in errors in the calculated bottom-up NH_3 emissions. To proceed with the emission adjustment approach, we will apply the iterative Finite Difference Mass Balance (iFDMB) inverse modeling technique to revise the NEI NH_3 emissions with respect to CrIS observations. Since running iFDMB is computationally expensive and requires numerous iterations, the employment of a reduced complexity CMAQ model (RCCM) for simulations can reduce the burden of computations while maintaining the accuracy of predictions. We will conduct the iFDMB by implementing a RCCM to simulate NH_3 concentrations over the regions of interest. Following this project, we will develop adjustment factors for modifying NH_3 emissions until they reach an optimum state in which NH_3 concentrations are the closest to the CrIS observations. After updating the emissions inventory, we will investigate the consequent impacts of the adjusted NH_3 emissions on the behaviors of such atmospheric constituents as the concentrations of $PM_{2.5}$ and inorganic $PM_{2.5}$ species.

Project Update: Progress updates for Tasks 1-3 are listed below:

Task 1: Preparation of comprehensive satellite, in situ, and modeling data for the iterative Finite Difference Mass Balance (iFDMB) method: The UH-AQF modeling has obtained biweekly ammonia data from Ammonia Monitoring Network (AMoN) and has prepared the data for preliminary ammonia concentration evaluation. To do so, we wrote a python code to prepare the observation data and to find the corresponding grid points in the modeling domain for all stations.

Task 2: Development of the Reduced-Complexity CMAQ Model (RCCM) for NH_3 and refinement of NH_3 emissions using iFDMB with the combination of the CMAQ model and CrIS satellite observations: The UH-AQF modeling has continued working on producing offline files over the modeling domain. Offline files contain hourly sulfate (SO_4^{-2}), nitric acid (HNO_3), nitrate (NO_3^-), chloride (Cl), sodium (Na), hydrochloric acid (HCl) concentration in all times steps required for RCCM process. To produce the offline files, we implement a CMAQ model, which can write the concentration of species of interest in all time steps in separate files based on time.

Task 3: Investigation of $PM_{2.5}$ concentrations using the updated emission inventory: No activities during the reporting period.

Preliminary Analysis: No preliminary analysis to report this quarter.

Data Collected: AQS observations data for 2019 have been collected. Biweekly ammonia data from Ammonia Monitoring Network (AMoN) for 2019 over the modeling domain.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: None.

Goals and Anticipated Issues for the Succeeding Reporting Period: UH-AQF team will continue running the iFDMB over Texas and the Gulf of Mexico.

Detailed Analysis of the Progress of the Task Order to Date: Making progress as scheduled.

Project 22-020 (Texas A&M University)

Title: Quantifying the Emissions and Spatial/Temporal Distributions of Consumer Volatile Chemical Products (VCPs) in the Greater Houston Area **PI**: Yue Zhang **Co-PI**: Qi Ying	**STATUS: ACTIVE** (08/22/2022 – 08/31/2023) **Funded Amount**: $160,182 **AQRP Project Manager**: Elena McDonald-Buller **TCEQ Project Liaison**: Bob Gifford

Abstract: Air pollution is the fifth largest cause of death in the world. Volatile organic compounds (VOCs) can also undergo chemical reactions with atmospheric oxidants to form major atmospheric pollutants, such as photochemical ozone (O_3) and particulate matter (PM). With this changing emission profile of carbonaceous compounds in urban areas, volatile chemical products (VCPs) have become one of the most significant sources of anthropogenic VOCs. VCPs typically consist of organic species from consumer products and business activities, including cleaning agents, printing inks, personal care products, pesticides, and coatings. In the populated urban regions, such as New York City, where O_3 formation is VOC-limited, VCPs account for more than half of the 20-ppb maximum daily average 8-h (MDA8) O_3 attributed to anthropogenic VOCs. As the fourth largest city in the US, with more than 7 million people in the surrounding areas, Houston has no reported ambient measurements of the VCP to our knowledge, highlighting the urgent need to update the VCP emission inventory in the Greater Houston Area validated by ambient measurements with detailed spatial and temporal resolution. Our primary hypothesis is that the VCPs in the Greater Houston Area account for a significant portion of the total VOC emission and have important implications on the regional ozone concentrations that were previously not captured by the emission inventory and models. To address this hypothesis, our primary goal is to use existing field measurement data to provide temporal, spatial, and seasonal information of the VCPs in the Greater Houston Area and use a high spatial resolution regional chemical transport model with a detailed photochemical mechanism to further improve the VCP emission inventory and understand the impacts of VCP on air quality, including ozone.

Project Update:

1. Continued deploying of our instrument (Vocus, aerosol mass spectrometer, CO monitor, NO_2 monitor, soot monitor, scanning electric mobility sizer, ozone monitor, and other supporting devices) around Houston.
2. Deployed the instrument to Rockport, Corpus Christi, San Antonio, and Austin for comparison with the VCP concentration in Houston and for background concentration calculations.
3. Analyzing data from all instruments (Vocus, aerosol mass spectrometer, CO monitor, NO_2 monitor, soot monitor, scanning electric mobility sizer, ozone monitor, and other supporting devices) deployed in the fall around Houston.
4. Designed four different routes around Houston to sample the volatile consumer products (VCP) and other species in the Greater Houston area.
5. Launching a second deployment for the mobile lab with all instruments (Vocus, aerosol mass spectrometer, CO monitor, NO_2 monitor, soot monitor, scanning electric mobility sizer, ozone monitor, and other supporting devices) in Houston.

Data Collected:

1. We have collected full suite of data of the trace gases (Vocus), particle phase chemical composition (AMS), CO, NO_2, O_3, aerosol size distribution, GPS location through our deployment around Houston, Rockport, Corpus Christi, San Antonio, and Austin.
2. We have collected the above gas and particle information both during the day and at night, during weekends and weekdays, and on sunny, cloudy, and rainy days.
3. We also have collected Vocus data both in ammonia (NH_4^+) mode and water cluster (H_3O^+) mode.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: None.

Goals and Anticipated Issues for the Succeeding Reporting Period:

1. Dr. Zhang's lab expects to complete at least 10 deployments for the AQRP project during our second deployment period.
2. Dr. Qi Ying's lab continues to work on the CAMQ model simulation to prepare to analyze the VCP data collected from this deployment.

Based on the current progress, both goals are on track. We will analyze the data after the field deployment to achieve the second goal.

Detailed Analysis of the Progress of the Task Order to Date: We successfully completed the fall field measurement and performed some of the data analysis. Figures 22-020-1 and 22-020-2 are the route maps we have conducted during this field study. We are working on analyzing the full suite of data since the deployment finished.

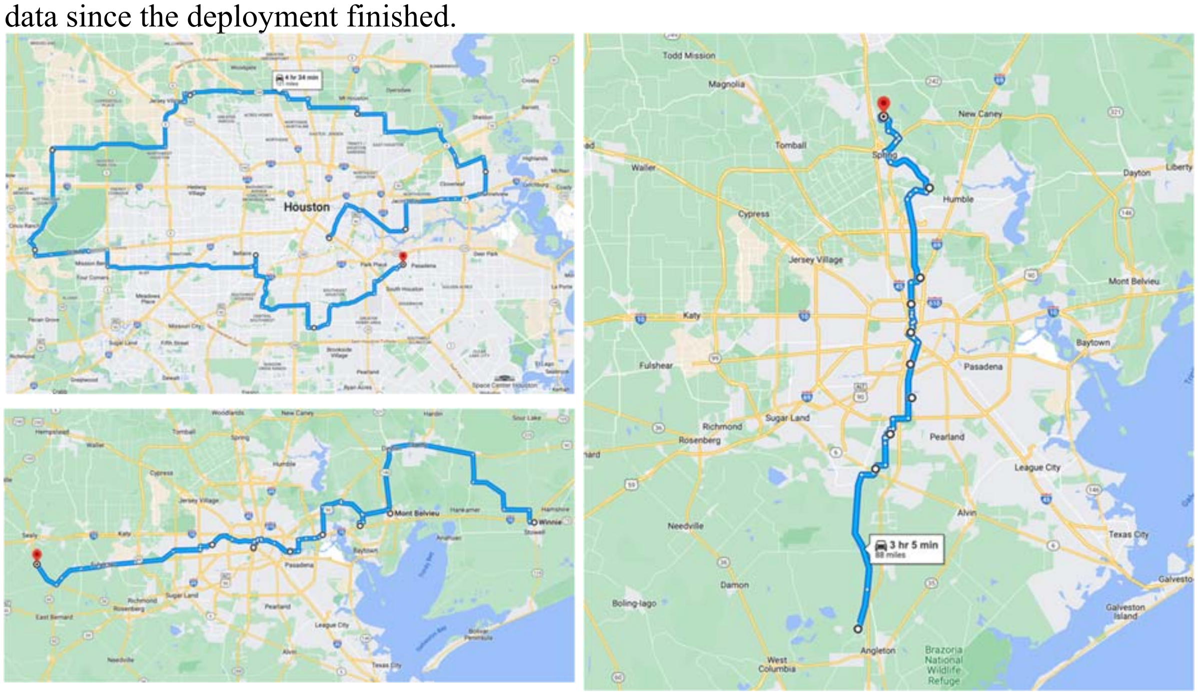

Figure 22-020-1. Deployment map during the field project in November 2022 (Houston route)

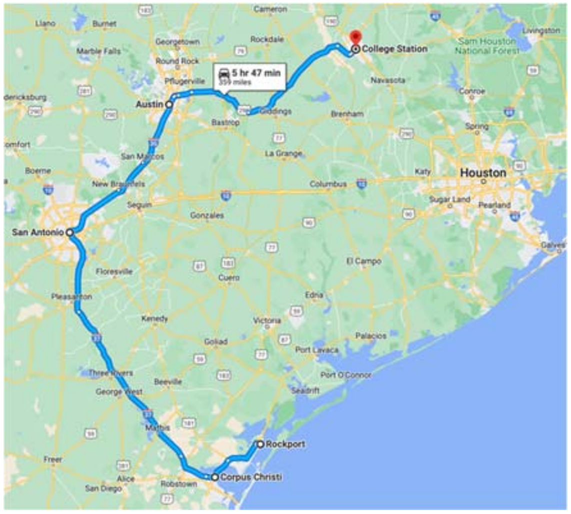

Figure 22-020-2. Deployment map during the field project in November 2022 (Rockport, Corpus Christi, San Antonio, and Austin route)

So far, we have completed all the calibration analysis of AMS and Vocus. We have identified more than 3000 peaks in the mass spectra of Vocus software and calculated the mass concentrations of the aerosol species. Below is the preliminary data of the aerosol mass concentration with other measurement performed during the whole deployment.

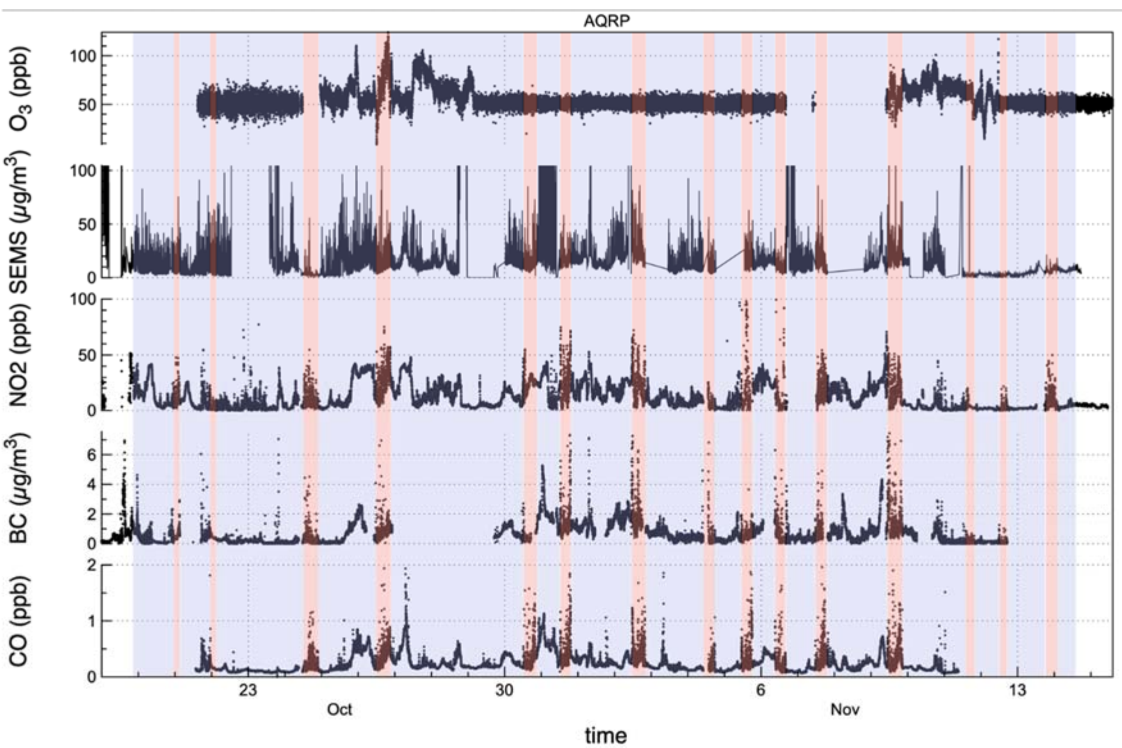

Figure 22-020-3. Aerosol Mass, Ozone, CO, NO_2, and black carbon measurement during the whole deployment. The purple shaded areas were when vehicles are parked, and the orange shaded areas were when instruments are deployed in motion.

In December 2022, we continued to analyze the data collected during the fall field measurement period. We have finished the quality control and preliminary analysis of most of the data from the instruments during our fall deployment.

Below are some of the analyzed results from the fall deployment. Figure 22-020-4 shows the time series data of all major instrument on October 30th. Figure 22-020-5 shows the mapped concentrations of various volatile consumer products for the deployment on October 30th.

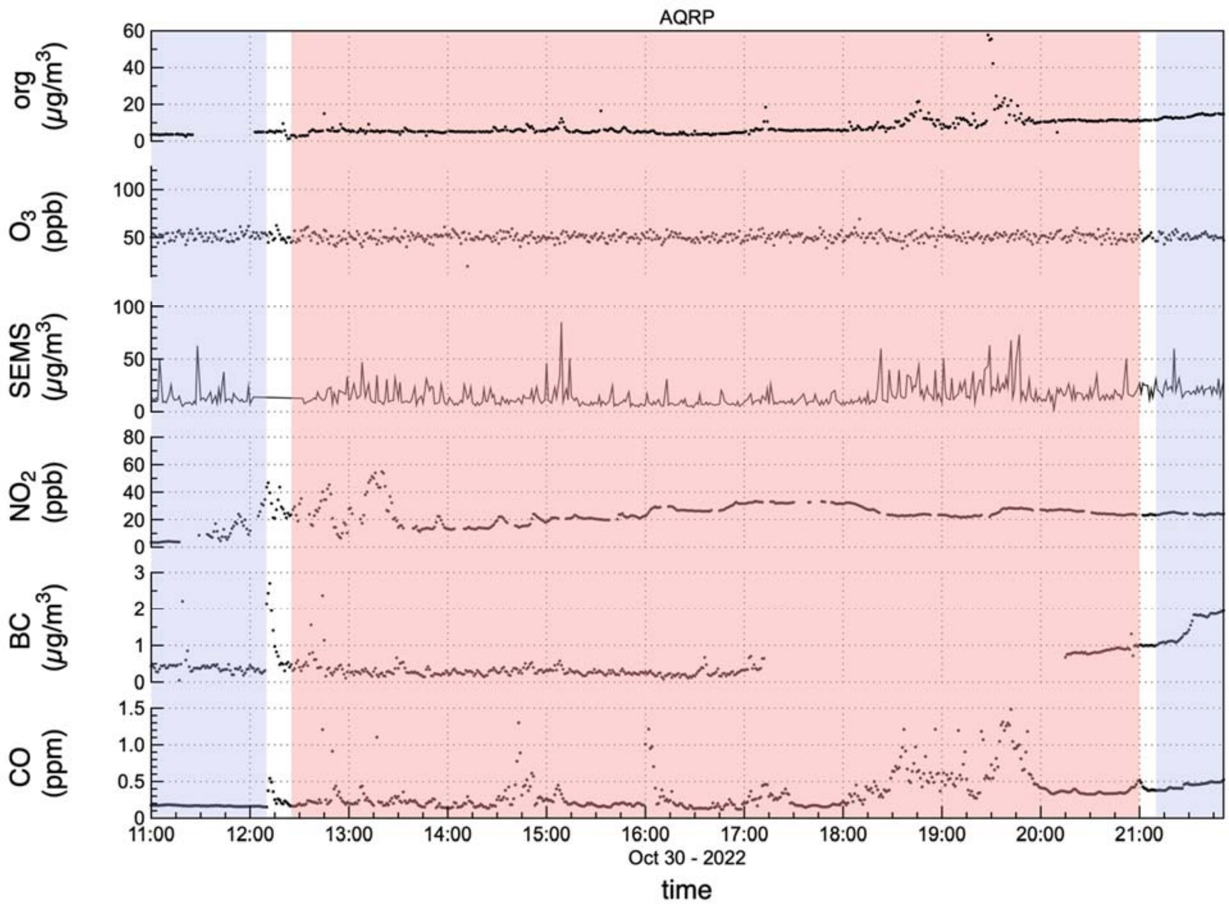

Figure 22-020-4. Time series data of major instruments during the fall deployment in Houston (October 30th as an example)

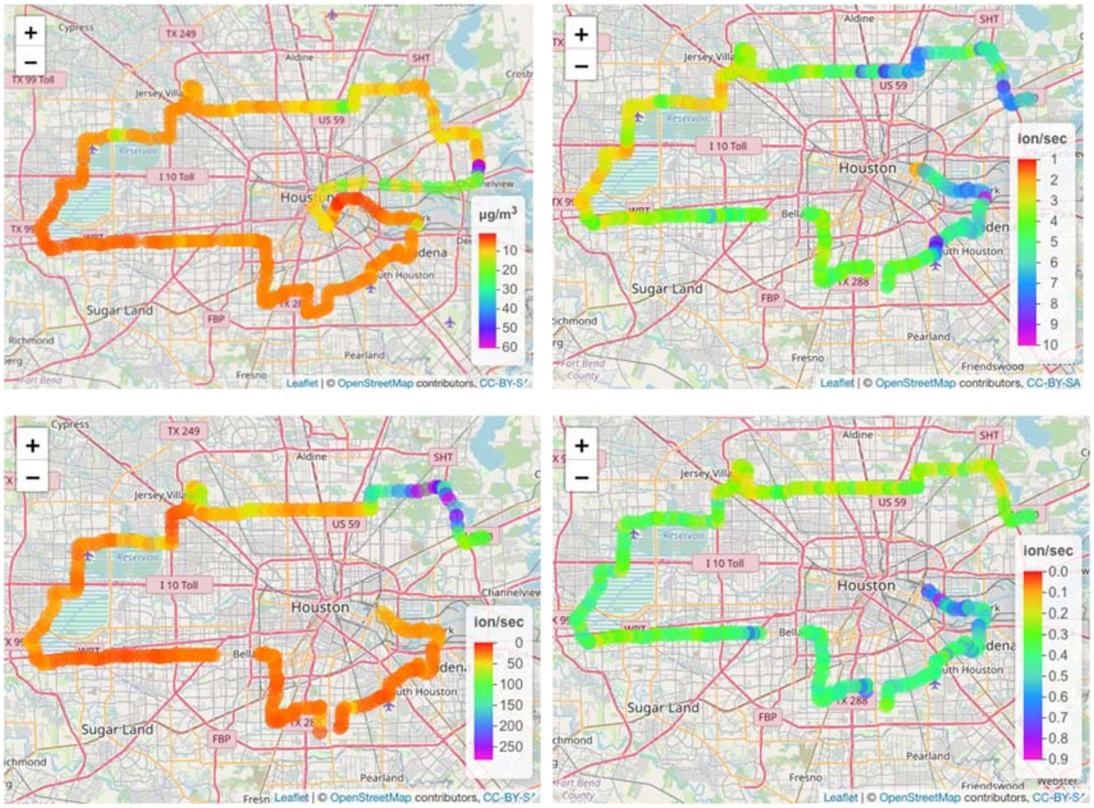

Figure 22-020-5. Concentration of aerosol mass concentration and three major VCPs sampled on October 30th in Houston. The upper left is total organic aerosol mass loading. The upper right plot is texanol. The lower left and lower right plots are monoterpenes and D4-siloxane.

Figures 22-020-4 and 22-020-5 above demonstrate the concentration of VCPs and other parameters measured during the circular mobile deployment. Figures 22-020-6 and 22-020-7 below demonstrate the east-west route of the mobile deployment data.

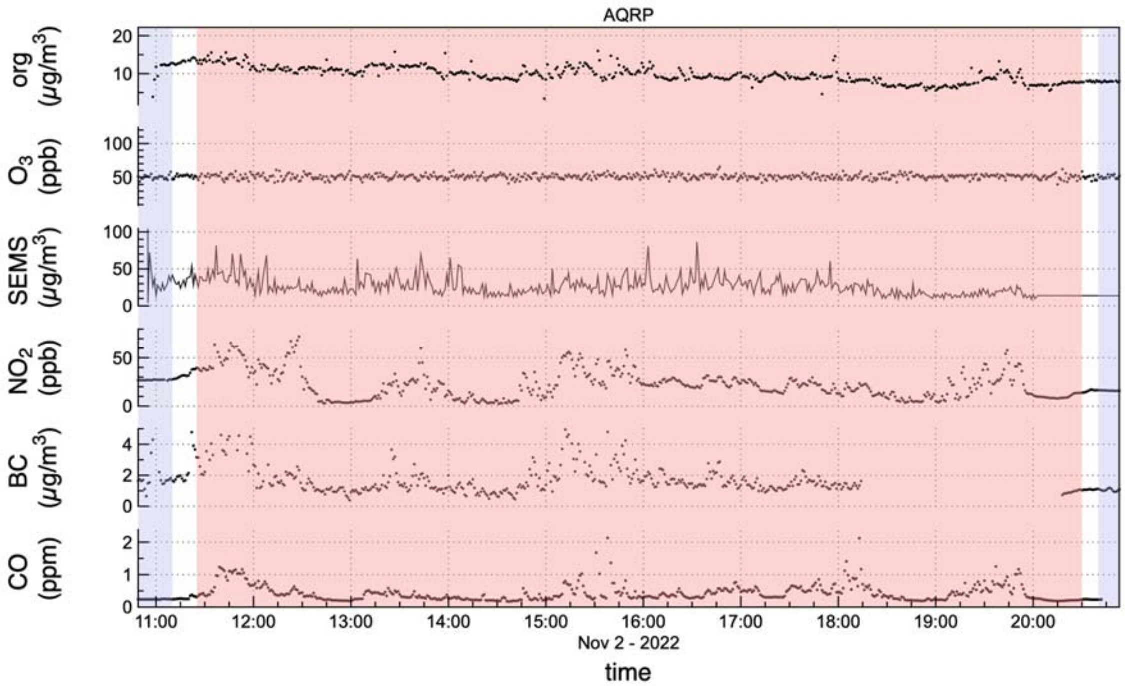

Figure 22-020-6. Time series data of major instruments during the fall deployment in Houston (Nov. 2nd as an example)

The time series data shows variations of aerosol mass concentration, ozone, particle mass, NO_2, black carbon, and CO as the mobile lab is driving through Houston.

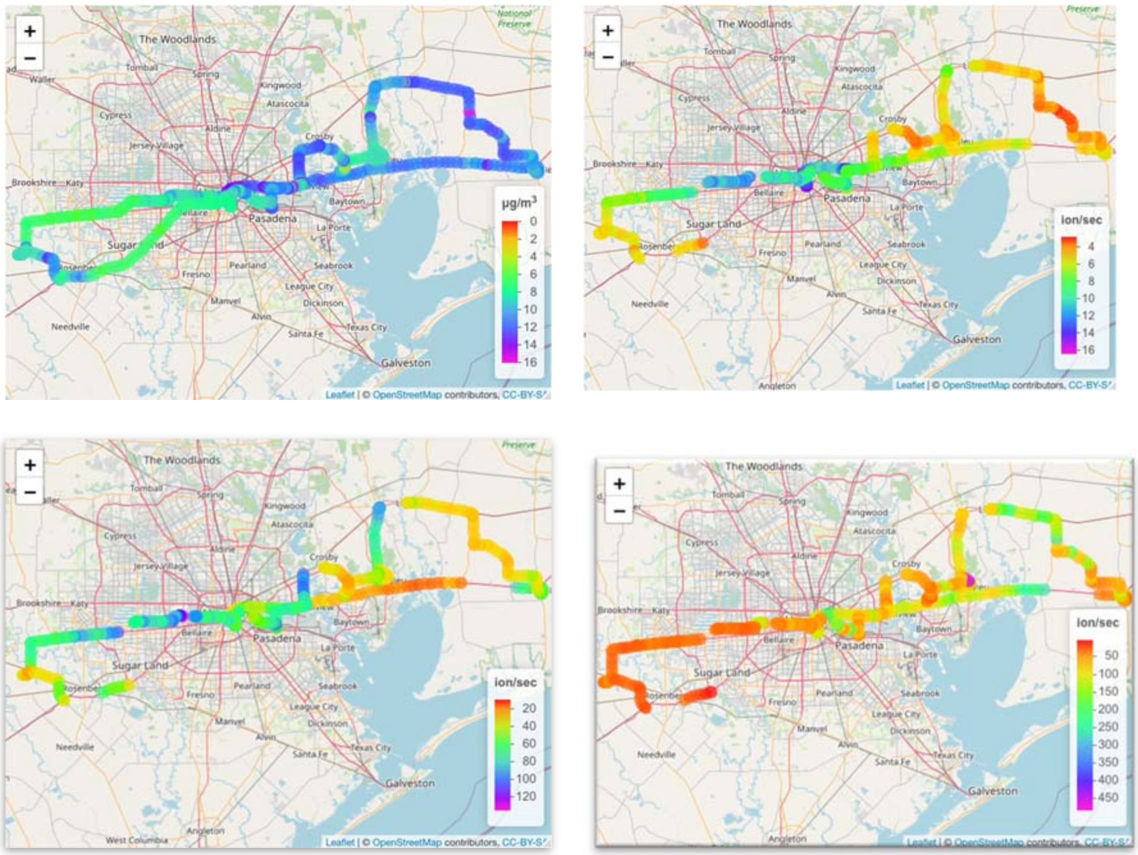

Figure 22-020-7. Concentration of aerosol mass concentration and three major VCPs sampled on November 2nd in Houston. The upper left is total organic aerosol mass loading. The upper right plot is texanol. The lower left and lower right plots are D5-siloxane and monoterpenes.

We are still working on analyzing and compiling all data from the fall campaign, and plan to write the above results into a scientific paper.

On January 4th, PI Zhang's lab started loading the instruments to the mobile lab and prepared for the second deployment. The reason for the second deployment is to understand the seasonal difference of VCP emissions and also to remove any interference from the vegetation.

We are currently conducting field measurement and performed initial data analysis. Figure 22-020-8 has the route maps we have conducted during this field study in January 2023. We plan to analyze the full suite of data after the deployment finishes.

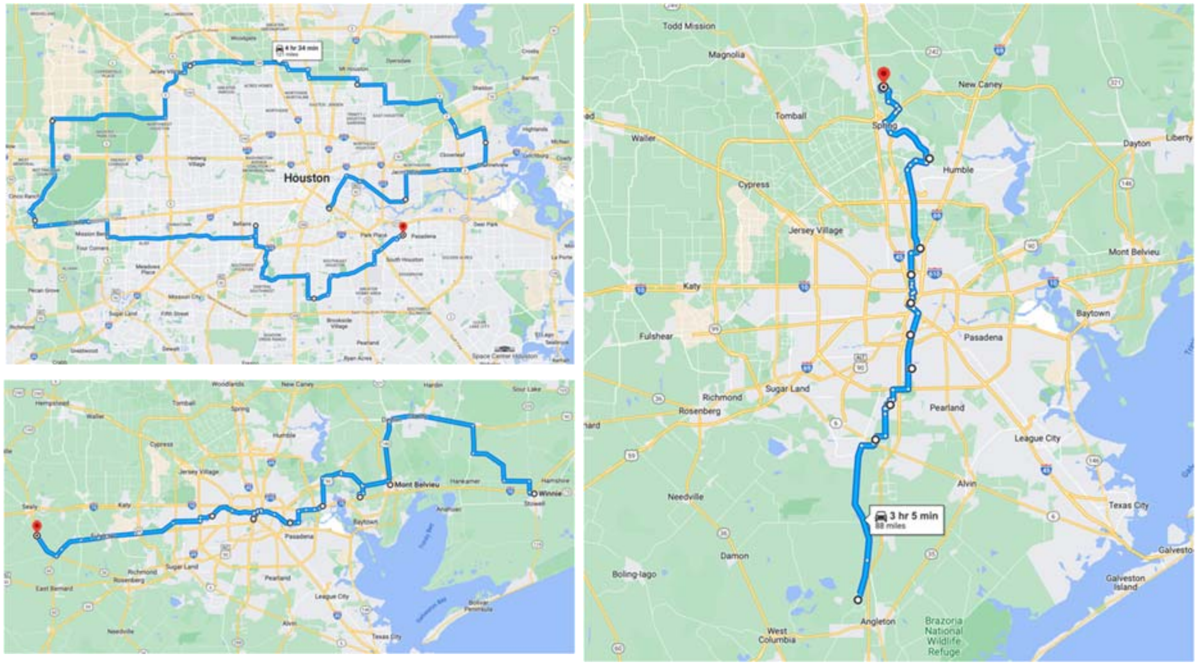

Figure 22-020-8. Deployment map during the field project in January 2023

In addition, below (Figure 22-020-9) are the exterior and the interior images of the mobile lab. We have a wireless 5G service that can connect all instruments and project the screen to the front passenger seat.

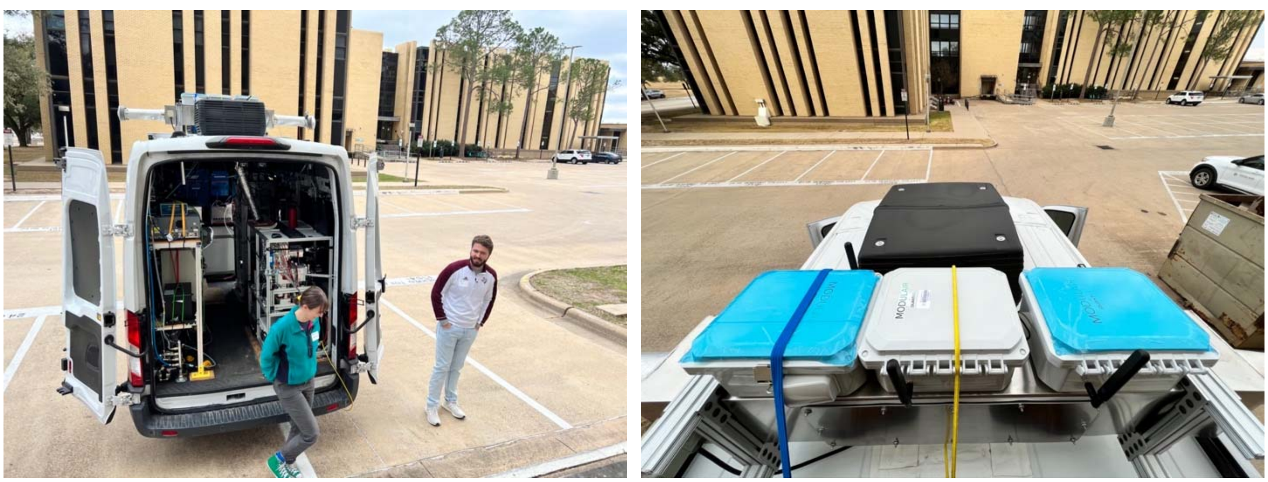

Figure 22-020-9. Exterior and roof top (with three air sensors) view of the mobile laboratory

By the end of January, we have already completed 12 deployments, fulfilling our initial goal of the second deployment.

Project 22-023 (The George Washington University (Primary), Ramboll (Collaborator))

Title: Source-sector NOx emissions analysis with sub-kilometer scale airborne observations in Houston during TRACER-AQ **PI**: Daniel Goldberg (GWU) **Co-PI**: Greg Yarwood (Ramboll)	**STATUS: ACTIVE** (08/22/2022 – 08/31/2023) **Funded Amount**: $248,146.60 (GWU: $103,425; Ramboll: $144,721.60) **AQRP Project Manager**: Elena McDonald-Buller **TCEQ Project Liaison**: Sushil Gautam

Abstract: Nitrogen oxide (NO_X) emissions are a critical participant in ozone formation. Many North American cities already have NO_X-limited ozone formation during the warm season (Jin et al., 2020; Jung et al., 2022), and the remaining cities should have primarily NO_X-limited conditions in the coming years (Koplitz et al., 2021). Further reducing ozone production rates within cities will therefore require improved quantification of NO_X emissions. One major limitation of our current observing network is the inability to accurately quantify NO_X emissions on a sector-by-sector basis in a timely fashion, with the exception of continuous emissions monitoring systems (CEMS) on electricity generating units. Many non-road sources of NO_X emissions, such as industrial or construction emissions, have large uncertainties (Zawacki et al., 2018).

In this project we will use fine spatial resolution nitrogen dioxide (NO_2) information (250 × 560 m^2) from the Geostationary Coastal and air pollution events Airborne Simulator (GCAS) instrument (Janz et al., 2019; Nowlan et al., 2018), available during the September 2021 NASA/TCEQ Tracking Aerosol Convection ExpeRiment – Air Quality (TRACER-AQ) field campaign, to better understand the fine-scale structure of NO_X emissions in the Houston metropolitan area including a sector-by-sector analysis.

Complementing the airborne observations, the Comprehensive Air Quality Model with Extensions (CAMx) will be run with a fine spatial resolution (444 × 444 m^2) using the 2019 TCEQ emissions inventory. The model output will then be compared to data from the GCAS and the Tropospheric Monitoring Instrument (TROPOMI) in order to identify gaps in our understanding of NO_X emissions. We will compare/contrast NO_2 concentrations near large CEMS and non-CEMS point sources, major highways, large population centers, airports, railyards, and commercial marine vessels to determine whether the magnitude of the NO_X emissions agree between the inventory and observations. We will also use GCAS observations to estimate NO_X emissions directly from individual point sources or quasi-points sources (e.g., airports, petrochemical complexes, etc.). To maximize the value of the airborne measurements, we will use a Generalized Additive Model (GAM) to estimate the contributions from different NO_X emission sectors that best matches the airborne retrievals.

This work maps to at least four Research Priority Areas of the Texas Air Quality Research Program (AQRP), as shown in the Table 22-023-1 below. This project will combine aircraft and satellite observations with high resolution models, to provide actionable information

about TCEQ’s 2019 Emissions Inventory for NO_X. These results will provide a new perspective for aiding in decision-making for improving ozone air quality in the region.

Project Update:

Task 1: Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx: The WRF simulation has been run for the full period (August 20, 2021 - September 27, 2021) and for all of the domains (36, 12, 4, 1.333, and 0.444 km). The emissions for the CAMx simulation are being processed. This includes downloading and processing the CEMS data, line source data, and meteorology needed for the biogenic emissions data. The emissions for the CAMx simulation continue to be processed. This includes processing the CEMS data, line source data, biogenic emissions data. The group also decided which emission source sectors will be tagged in the CAMx simulation.

In January 2023, the emissions for the CAMx simulation have been fully processed, merged, and spot checked for completeness. The group also finalized which emission source sectors will be tagged in the CAMx simulation. The CAMx simulation will begin in early February 2023.

Task 2. Process the GCAS measurements: Preliminary comparison between GCAS and Pandora NO_2 and HCHO in the TRACER-AQ domain has been completed. This is assuming the NASA GEOS-CF simulation *a priori* profiles. GCAS agrees with Pandora to within ± 21% for NO_2.

The native files of the GCAS data are being re-processed to better account for missing data. New files with very minor adjustments should be available in January 2023.

The GCAS data has been successfully re-gridded in three-dimensions (x, y, time) to the WRF-CAMx grid. Spatial plots of the full monthly and daily averages have been developed.

The native files of the GCAS data have been re-processed to better account for missing data. New files with very minor adjustments will be made available to the full team in early February 2023.

Task 3. Process the satellite NO_2 data: In November 2022, the satellite data has been processed to the WRF-CAMx grid. Code has been developed to ingest model simulation output. Waiting on model simulation in order to re-process the air mass factor.

As of December 2022, the GCAS NO_2 data has been qualitatively compared to operational TROPOMI NO_2 data now that both are on the same grid.

Code has been optimized to ingest model simulation output. Waiting on model simulation (See Task 1) to re-process the satellite air mass factor.

Task 4. Calculating NO_X from NO_2 airshed measurements: Re-gridding and processing of the GCAS data for this analysis has begun (See Task 2). As of January 2023, the team was waiting on re-formatted GCAS data (See Task 2).

Task 5. Comparison of NO_2, HCHO, O_3 between model, aircraft, and satellite: Task 5 has not yet been initiated.

Task 6. Use of machine learning to estimate emission factors for individual sectors: Task 6 has not yet been initiated.

Preliminary Analysis: No preliminary analysis to report this quarter.

Data Collected: No data collected this quarter.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: Project approvals occurred later than anticipated. Development of the WRF-CAMx simulation is delayed by approximately 6-weeks. Model simulation output now expected in mid-February 2023 instead of the end of December 2022. Effort for Tasks 3 – 6 will be back-loaded, and we do not anticipate any end-of-project delays.

Goals and Anticipated Issues for the Succeeding Reporting Period: The first simulation of WRF-CAMx model output should be complete, and relevant output variables will be made available to the rest of the team.

Re-processing of the air mass factor (within the scope of Tasks 2 & 3) will commence when the model output is available in late February or early March.

Task 4 – deriving NO_X emissions from the aircraft data – will restart now that the updated GCAS is available.

We expect to engage in Tasks 5 & 6 in earnest starting in March 2023.

Detailed Analysis of the Progress of the Task Order to Date: on schedule.

FINANCIAL STATUS REPORT

The Air Quality Research Program (AQRP) contract was awarded for FY 22-23 for $750,000 per year. Funds were distributed across several different reporting categories as required under the contract with TCEQ. The reporting categories are listed below in detail.

Program Administration: Limited to 10% of the overall funding per fiscal year. This category includes all staffing, materials and supplies, and equipment needed to administer the overall AQRP. It also includes the costs for the Council meetings.

ITAC: These funds are to cover the costs, largely travel expenses, for the Independent Technical Advisory Committee (ITAC) meetings.

Project Management: Limited to 8.5% of the funds allocated for Contractual budget category. Each research project is assigned a Project Manager to ensure that project objectives are achieved in a timely manner and that effective communication is maintained among investigators in multi-institution projects. These funds are to support the staffing and performance of project management.

Research Projects / Contractual: These are the funds available to support the research projects that are selected for funding.

Program Administration

Program Administration includes salaries and fringe benefits for those overseeing the program, as well as materials and supplies, travel, equipment, and other expenses. This category allows indirect costs in the amount of 10% of salaries and wages. Table 1 details the FY 22-23 Administration budget.

Dr. David Allen, Principal Investigator and AQRP Director, is responsible for the overall administration of the AQRP. RoseAnna Goewey, AQRP Program and Grant Manager, coordinates all aspects of program management. Randy George, AQRP Information Technology (IT) Manager, assists the Director and Program Manager with all website development updates, data storage, and handling of all other IT related issues. Nohemi Cazares, Senior Administrative Associate, performs required accounts payable services to ensure timely reimbursement payments to subaward entities.

The University of Texas at Austin's federally negotiated fringe rates for full-time/benefits eligible employees is 30% through August 31, 2023. The University of Texas at Austin's Cost Rate Agreement was finalized in June 2022 and can be viewed in detail at https://research.utexas.edu/wp-content/uploads/sites/5/2022/06/FY23_Fringe_Benefit_Rates_063022.pdf.

Table 1: Administration Budget FY 22-23 (expenses through January 2023)

Budget Category	FY22 Budget	FY23 Budget	Total Budget	Expenses*	Remaining Balance
Personnel/Salary	$44,702.77	$51,800.00	$96,502.77	$51,864.31	$44,638.46
Fringe Benefits	$13,812.96	$16,265.00	$30,077.96	$15,890.42	$14,187.54
Supplies	$12,013.99	$1,755.00	$13,768.99	$1,117.90	$12,651.09
Total Direct Costs	$70,529.72	$69,820.00	$140,349.72	$68,872.63	$71,477.09
Authorized Indirect Costs *(10% of Personnel/Salary)*	$4,470.28	$5,180.00	$9,650.28	$5,186.42	$4,463.86
Total Costs	**$75,000.00**	**$75,000.00**	**$150,000.00**	**$74,059.05**	**$75,940.95**

ITAC

There are no ITAC expenditures in this reporting quarter. Table 2 details the FY 22-23 ITAC budget.

Table 2: ITAC Budget FY 22-23 (expenses through January 2023)

Budget Category	FY22 Budget	FY23 Budget	Total Budget	Remaining Balance
Travel	$5,000.00	$5,000.00	$10,000.00	$10,000.00
Supplies	$625.00	$625.00	$1,250.00	$1,250.00
Total Direct Costs	$5,625.00	$5,625.00	$11,250.00	$11,250.00
Authorized Indirect Costs	$0.00	$0.00	$0.00	$0.00
Total Costs	**$5,625.00**	**$5,625.00**	**$11,250.00**	**$11,250.00**

Project Management

Table 3 details the FY 22-23 Project Management Budget.

Table 3: Project Management Budget FY 22-23 (expenses through January 2023)

Budget Category	FY22 Budget	FY23 Budget	Total Budget	Remaining Balance
Personnel/Salary	$38,000.00	$38,000.00	$76,000.00	$39,966.92
Fringe Benefits	$11,438.00	$11,932.00	$23,370.00	$12,523.32
Supplies	$3,012.00	$2,518.00	$5,530.00	$5,203.15
Other	$1,875.00	$1,875.00	$3,750.00	$3,750.00
Total Direct Costs	$54,325.00	$54,325.00	$108,650.00	$61,443.39
Authorized Indirect Costs *(10% of Personnel/Salary)*	$3,800.00	$3,800.00	$7,600.00	$3,996.67
Total Costs	**$58,125.00**	**$58,125.00**	**$116,250.00**	**$65,440.06**

RESEARCH PROJECTS

All research projects have Subaward Agreements fully executed as of February 14, 2023. Table 4 shows the FY 22-23 Research Project budgets. The FY 22-23 budget allocates $1,222,500.00 for research projects.

Table 4: FY 22-23 Contractual/Research Project Budget

FY 22 Contractual Funding		**$611,250.00**		
FY 22 Total Contractual Funding		**$611,250.00**		
Project Number	**Institution**	**Amount Awarded**	**Cumulative Expenditures**	**Remaining Balance**
22-003	Atmospheric and Environmental Research, Inc (AER)	$161,388.00	$0.00	$161,388.00
22-006	Aerodyne Research, Inc. (ARI)	$51,255.00	$0.00	$51,255.00
22-006	Baylor University	$57,225.00	$0.00	$57,225.00
22-008	University of Houston	$175,621.00	$0.00	$175,621.00
22-008	St. Edward's University	$6,103.00	$0.00	$6,103.00
22-010	Aerodyne Research, Inc.	$228,418.00	$0.00	$228,418.00
22-019	University of Houston	$131,366.00	$0.00	$131,366.00
22-020	Texas A&M University	$160,182.00	$0.00	$160,182.00
22-023	The George Washington University	$103,425.00	$0.00	$103,425.00
22-023	Ramboll	$144,721.60	$0.00	$144,721.60
FY 22 Total Contractual Funding Awarded		$1,219,704.60		
FY 22 Contractual Funds Expended (Init. Projects)			$0.00	
FY 22 Contractual Funds Remaining to be Spent				$611,250.00
FY 22 Contractual Funding Carry-Forward		**PENDING**		
FY 23 Contractual Funding		**$611,250.00**		
FY 23 Total Contractual Funding		**$611,250.00**		
Project Number	**Institution**	**Amount Awarded**	**Cumulative Expenditures**	**Remaining Balance**
22-003	Atmospheric and Environmental Research, Inc (AER)	$161,388.00	$0.00	$161,388.00
22-006	Aerodyne Research, Inc. (ARI)	$51,255.00	$16,784.34	$34,470.66
22-006	Baylor University	$57,225.00	$0.00	$57,225.00
22-008	University of Houston	$175,621.00	$0.00	$175,621.00
22-008	St. Edward's University	$6,103.00	$0.00	$6,103.00
22-010	Aerodyne Research, Inc.	$228,418.00	$0.00	$228,418.00
22-019	University of Houston	$131,366.00	$7,547.90	$123,818.10
22-020	Texas A&M University	$160,182.00	$0.00	$160,182.00
22-023	The George Washington University	$103,425.00	$0.00	$103,425.00
22-023	Ramboll	$144,721.60	$27,706.39	$117,015.21
FY 23 Total Contractual Funding Awarded		$1,219,704.60		
FY 23 Contractual Funds Expended (Init. Projects)			$52,038.63	
FY 23 Contractual Funds Remaining to be Spent				$559,211.37
Total Contractual Funding		**$1,222,500.00**		
Total Contractual Funding PENDING AWARD		**$2,795.40**		
Total Contractual Funding Remaining to be Awarded		**$2,795.40**		
Total Contractual Funds Expended to Date			**$52,038.63**	
Total Contractual Funds Remaining to be Spent				**$1,170,461.37**

APPENDIX A. CONTRACTUAL RESEARCH PROJECTS APPROVED FOR FUNDING (BIENNIUM 2022-2023)

Proj. Nbr.	Project Title	Research Priority Area	PI, *Collab. PI*	Co-PI, *Collab. Co-PI*	Primary Institution, *Collab. Institution*	Institution Budget	Total Project Budget	AQRP Project Manager	TCEQ Liaison, Backup Liaison
22-003	Evaluating the Ability of Statistical and Photochemical Models to Capture the Impacts of Biomass Burning Smoke on Urban Air Quality in Texas	Domestic fire emissions	Matthew Alvarado	n/a	Atmospheric and Environmental Research, Inc (AER)	$161,388.00	$161,388.00	Elena McDonald-Buller	Chola Regmi, Thuy Phi
22-006	Hydrogen Cyanide for Improved Identification of Fire Plumes in the (BC)^2 Network	Domestic fire emissions	Tara Yacovitch *Rebecca Sheesley*	n/a *Sascha Usenko*	Aerodyne Research, Inc. *Baylor University*	$51,255.00 *$57,225.00*	$108,480.00	Vincent Torres	Erik Gribbin, Alexander Adame
22-008	Modeling analysis of TRACER-AQ and over-water Measurements to improve prediction of on-land and offshore ozone	TRACER-AQ and over-water measurements	Yuxuan Wang *Paul Walter*	James Flynn *n/a*	University of Houston *St. Edward's University*	$175,621.00 *$6,103.00*	$181,724.00	Elena McDonald-Buller	Barry Exum, Miranda Kosty
22-010	Dallas Field Study (DFS); Ozone Precursors, Local Sources and Remote Transport Including Biomass Burning	Changing emission patterns in Texas	Edward Fortner	n/a	Aerodyne Research, Inc.	$228,418.00	$228,418.00	Vincent Torres	David Westenbarger, Cara Scalpone
22-019	Refining Ammonia emission using inverse modeling and satellite observations over Texas and the Gulf of Mexico and investigating its effect on fine particulate matter	Improve emission inventories	Yunsoo Choi	n/a	University of Houston	$131,366.00	$131,366.00	Elena McDonald-Buller	Khalid Al-Wali, Shay Guerin
22-020	Quantifying the Emissions and Spatial/Temporal Distributions of Consumer Volatile Chemical Products (VCPs) in the Greater Houston Area	Improve emission inventories	Yue Zhang	Qi Ying	Texas A&M University	$160,182.00	$160,182.00	Elena McDonald-Buller	Bob Gifford, Michael Ege
22-023	Source-sector NOx emissions analysis with sub-kilometer scale airborne observations in Houston during TRACER-AQ	TRACER-AQ and over-water measurements	Daniel Goldberg *Greg Yarwood*	n/a *n/a*	The George Washington University *Ramboll*	$103,425.00 *$144,721.60*	$248,146.60	Elena McDonald-Buller	Sushil Gautam, Lam Nguyen