AIR QUALITY RESEARCH PROGRAM

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

Quarterly Report
February 15, 2023 – May 14, 2023

Submitted to

Jocelyn Mellberg
Texas Commission on Environmental Quality
12100 Park 35 Circle
Austin, TX 78753

Prepared by

David T. Allen, Principal Investigator
The University of Texas at Austin
10100 Burnet Rd., MC: R7100
Austin, TX 78758

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PREPARED IN COOPERATION WITH THE TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

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Texas Air Quality Research Program

Quarterly Report

February 15, 2023 through May 14, 2023

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 February 15, 2023 through May 14, 2023, the AQRP efforts were focused primarily maintaining project management communications with subaward Principal Investigators (PI), 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 operational 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). 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. Details are in the Research Projects section of this report. Project MTRs through May 2023 will be posted on the AQRP website (https://aqrp.ceer.utexas.edu/projects.cfm) by mid-July 2023.

Third quarterly reports from all projects were collected on April 30, 2023. All reports have received acceptance by AQRP Project Managers and Texas Commission on Environmental Quality (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 worked with The University of Texas at Austin (UT) and Fort Worth Meachum Airport legal counsel to gain site access. At the time of this report submission, Fort Worth Meachum Airport legal counsel approved the agreement and field observations were completed in late April and early May 2023.

In this quarter, the TCEQ and UT coordinated the Prime Contract amendment to increase the maximum reimbursable amount by $1.5 million in preparation for the upcoming biennium, starting September 1, 2023. The amendment was fully executed in April 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, search functionality development is underway to allow for search options that pull results from file text, 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 May 2023 from Fiscal Years 2022-2023 (FY 22-23).

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 additional 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. The Program Manager will finalize the agenda in July 2023.

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. The 2023-2025 biennium amendment funding is awarded at $750,000 per year.

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: In February and March, preparation began for the smoke emission related predictors for the GAM study based on the Fire INventory from the National Center for Atmospheric Research (NCAR FINN) inventory 0.1 x 0.1 degree files. Development of Stochastic Time-Inverted Lagrangian Transport (STILT) footprints for use in the GAMS continued.

In April, fire count predictors were developed using the Fire INventory from NCAR version 2.5 (FINN v2.5) emission inventory. The number of fires each day within 0.5, 1.0, 2.5, 5, 10, and 25 degrees of El Paso and Houston was calculated and merged with the rest of the GAM training data set. Initial results suggested that the number of fires within 2.5 degrees of Houston was a significant predictor of ozone in Houston, but the effect saturated at > 100 fires ($p<0.001$, Figure 1). However, the number of fires did not appear to be a significant ozone predictor for El Paso.

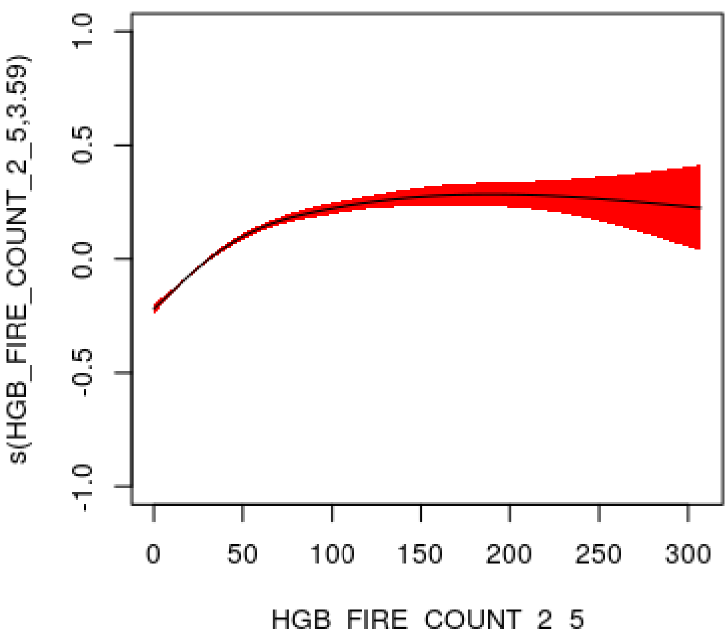


Figure 22-003-1. Log(O_3) response to changes in the number of fires reported in the FINN v2.5 inventory within 2.5 degrees of Houston.

We continued working on the smoke emission-related predictors for the GAM study based on the FINN inventory 0.1x0.1 degree files. We also continued developing Stochastic Time-Inverted Lagrangian Transport (STILT) footprints for use in the GAMS.

In May, a memo was submitted (Deliverable 2) on our initial statistical analysis using generalized additive models (GAMs) to see how fires impacted background and maximum concentrations of O_3 and PM2.5 in Houston and El Paso. Our results suggested that on days when the Hazard Mapping System (HMS) indicated smoke over Houston and El Paso, the daily average PM2.5 was elevated by 1.4-2.6 $\mu g/m^3$ on average (background and maximum), while the background Maximum Daily 8-hour Average (MDA8) O_3 was elevated by 6-8 parts per billion by volume (ppbv) on average. These impacts may have been related to long-distance transport of smoke from the Yucatan (Houston and El Paso) and California (El Paso only). In Houston, the impact on the maximum MDA8 O_3 was much higher than the background (6 ppbv on average), suggesting that urban area chemistry amplified the impact of the smoke on ozone. However, in El Paso, we instead saw a decrease of 1.5 ppbv in the average impact of smoke, suggesting that the response of the chemistry in these urban areas to smoke transport was very different.

During this reporting period, we used TCEQ CAMx data to calculate background and maximum MDA8 O_3 values for El Paso and Houston for the 2019 ozone season. This data was used in additional GAM training to determine if the relationships seen between smoke and fire predictors and O_3 in the monitoring data were the same as those seen in the CAMx data. These results were reported in Deliverable 3 planned for the end of June. We also continued developing STILT footprints for use in the GAMS.

Data Collected: None to date.

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

Goals and Anticipated Issues for the Succeeding Reporting Period: During the next reporting period we will complete work to include FINN Nitrogen Oxides (NOx), VOC, and $PM_{2.5}$ emissions multiplied by the daily surface "footprints" to the GAM input datasets. We will also submit a preliminary CAMx analysis report to TCEQ.

Due to limits on Dr. Hegarty's availability for the next few months, we are having Dr. Mike Iacono step in to complete the initial GAMM analysis. Dr. Hegarty trained Dr. Iacono on the necessary scripts and steps in this reporting period. Mr. Henderson has also been assisting Dr. Hegarty with the development of STILT footprints.

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 STILT analyses and gathering data for GAMM studies. Wrote and tested code to determine whether smoke occurred at a monitor location on a given day from the HMS smoke polygons. Performed initial GAM analysis and wrote report. Calculated minimal detectable activity (MDA) 8 O_3 values from TCEQ CAMx output.

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: In February, the project team continued to hold update meetings on a weekly basis via telecon. Dr. Usenko and the Baylor team worked with TCEQ and local officials to evaluate work performed by electrical contractors at the Mecham Airport site. After much effort and coordination, the site was successfully updated.

During troubleshooting of the HCN instrument at Aerodyne, a contact issue on a data acquisition card connector was found to be the cause of the faulty valve behavior. Valves were now responsive to being toggled in the instrument software. Upon removing the side cover of the instrument, loose hardware near the main power supply was also discovered. During turn-on at Baylor, an intermittent power cycling issue appeared to have been caused by other loose hardware found in the same area. Otherwise, all of the electrical connections were tested and physically evaluated with no notable findings. The instrument was running in the laboratory and sampling room air with a 1 Hz precision of ~60 parts per trillion (ppt). However, the team continued assessing and testing the system to fully understand the unusual behavior (i.e., high noise, voltage offset on detector) witnessed in the field. They operated with the same detector as before, though they were prepared to install a new one if necessary.

Aerodyne had an opportunity in March (3/13 – 3/17) to test this instrument in the presence of biomass burning signal as part of a laboratory-scale controlled study using the Aerodyne Mobile Laboratory

(AML) at their facility in Billerica, MA. A suite of instruments would be sampling smoke from wood samples prepared and burned by a team from Stanford University. Participating in this work offered a chance to evaluate instrument performance in the context of these real-world emissions and use the time to find any remaining hardware issues.

Looking ahead to the spring measurement period, the plan was to bring the HCN analyzer back to Texas in the AML during transit to the DFW area for a concurrent field campaign (AQRP 22-010). Several logistical and scientific benefits would arise from this arrangement. With Aerodyne managing the instrument transportation, they could ensure a careful shipping and handling process (e.g., air-ride truck, Aerodyne loading and unloading). Since the instrument would be integrated into the AML during the collaboration with Stanford, transitioning into mobile measurement use in the DFW area (first week of April) prior to off-loading and beginning the stationary sampling period would be possible without adding additional effort. Mobile surveying throughout the region would seek to provide useful context for several $(BC)^2$ sites in the area, especially in the event that airmasses impacted by biomass burning emerged during this time period.

If mobile sampling occurred during the first week of the AQRP 22-010 project, installation into the $(BC)^2$ trailer could then happen by April 8th. Stationary sampling would continue until at least June 13th to fulfill the 66-day measurement period. Discussion on acquiring consumables for the stationary work had begun (for spectral backgrounding of the analyzer).

Between March 13th and 17th, the HCN tunable infrared laser direction absorption spectroscopy (TILDAS) instrument was integrated into the AML and collected samples for a biomass burning experiment conducted by Stanford University at Aerodyne. This work provided an opportunity to assess the renewed performance of the instrument. Noise precision (~60 ppt) and valve operation were notably improved.

An HCN laser that had been ordered several months ago arrived at Aerodyne on March 24th. A second HCN instrument was built (using an existing chassis) and installed on the AML prior to departure to Texas for a concurrent field campaign (AQRP 22-010). Thus, the HCN instrument previously deployed for this project could be installed into the trailer as soon as it arrived in Texas with no need for use as a mobile instrument. A vibration-isolated rack provided a stable but absorbent platform during transport. While the travel to Texas went smoothly, it appeared that some increase in noise occurred (~150 ppt), likely due to minor movements of the optical mirrors. After the laser temperature had stabilized for some time, hands-on alignment of the mirrors should improve performance.

Installation into the $(BC)^2$ trailer happened by April 8th. Stationary sampling continued until at least June 13th to fulfill the 66-day measurement period.

In April, the HCN TILDAS was integrated into the $(BC)^2$ network trailer located at Mecham International Airport. After several days of thermal equilibration, the instrument exhibited similar noise to laboratory testing back at Aerodyne (< 70 ppt in 1 s). On April 14th, gas cylinders were delivered to enable regular background zeroing procedures. A calibration was performed on April 22nd by Aerodyne personnel using a standard previously used for calibrations at Baylor in November 2022.

On April 10th, the Aerodyne Mobile Laboratory (AML) arrived at Mecham International Airport to conduct measurements as part of a concurrent field campaign (AQRP 22-010). While parked stationary at night between April 10th and April 23rd, the AML gathered data that could help inform data analysis for this project (species such as CO, HCN, and various VOCs). A measurement of CO would be available from the trailer, but the instrument had yet to be calibrated or operated at this point.

Stationary sampling would continue until at least mid-June to fulfill the 66-day measurement period.

In May, the instrument continued to run at Meacham International Airport, collecting HCN data collocated with the BB2 trailer. Instrument zeroes stopped near the end of the month and needed to be restarted.

Stationary sampling would continue until at least mid-June to fulfill the 66-day measurement period. The exact measurement de-integration date would be determined based on whether active wildfire smoke was present at the time.

Preliminary Analysis: The in-field calibration performed in April has been worked up: Aerodyne scientists, as part of the Aerodyne Mobile Laboratory deployment in Dallas/Fort-Worth were able to conduct an HCN instrument calibration for this project on 4/22/2023. Results of HCN calibration are shown below in Table 22-006-1 and Figure 22-006-1:

4/22/23	14 UTC	*5 ppm HCN in N_2 balance*	
HCN Calibration (Field Site)			
Small HCN flow (sccm)	*Big UZA flow (SLPM)*	*HCN Standard Conc (ppb)*	*HCN Measured Conc (ppb)*
500	5.65	406.504	437.615
400	5.65	330.579	350.197
200	5.65	170.940	174.056
100	5.65	86.957	86.36
0	5.65	0	0.0327
300	5.65	252.101	251.356

Table 22-006-1. HCN Calibration (Field Site)

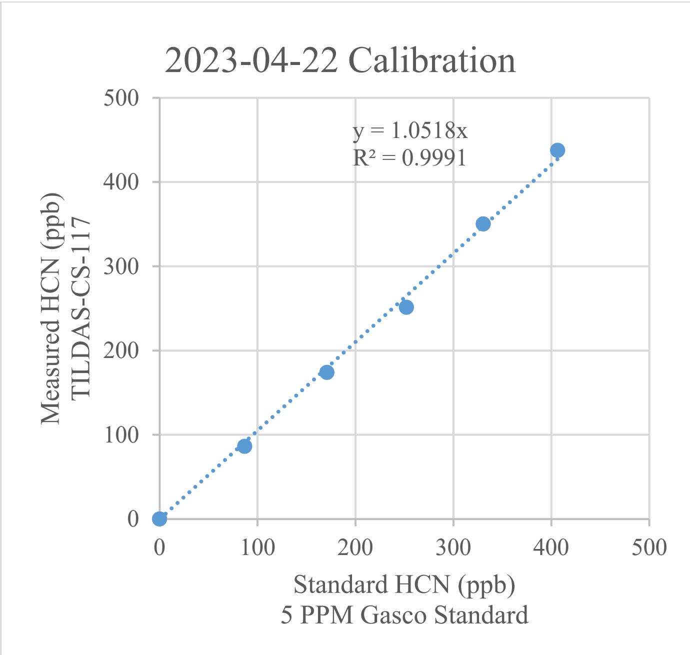


Figure 22-006-1. 2023-04-22 Calibration

A calibration factor *m* = 1.05 was determined on 4/22/2023, where HCN_meas = *m* * HCN_true. This means that raw HCN values will be divided by 1.05 in the final QA'ed dataset. The instrument was undergoing auto backgrounds, and had a cell pressure of 40 Torr during this measurement. This calibration uses a 5 ppm HCN GasCo standard purchased from Concept Controls (Quotation 11002165) in a balance of zero air.

This calibration result is more in line with expected instrument performance than a previous calibration done on 10/26/2022 at Baylor campus, which showed a calibration factor *m*=1.26. We will discard the first calibration factor since the instrument was sent back to Aerodyne for repair and assessment prior to the above campaign calibration.

A first-pass data QA has been conducted on the HCN trace to remove calibration periods, zero periods, and select glitches is in Figure 22-006-2. We have identified periods requiring offsets to be applied due to the absence of ultra-zero air (UZA) zeroes, but have not yet applied these offsets. In the graph below, we observe about a 0.8 ppb positive offset in HCN mixing ratios when the instrument is operating without UZA auto backgrounds, as it was prior to the 04/16 delivery of UZA. A similar offset is observed after 5/31 when there was an unexpected instrument restart, and zeroes stopped. Troubleshooting of these zeroes and if necessary, replacement of this tank will be done as soon as possible in the next reporting period.

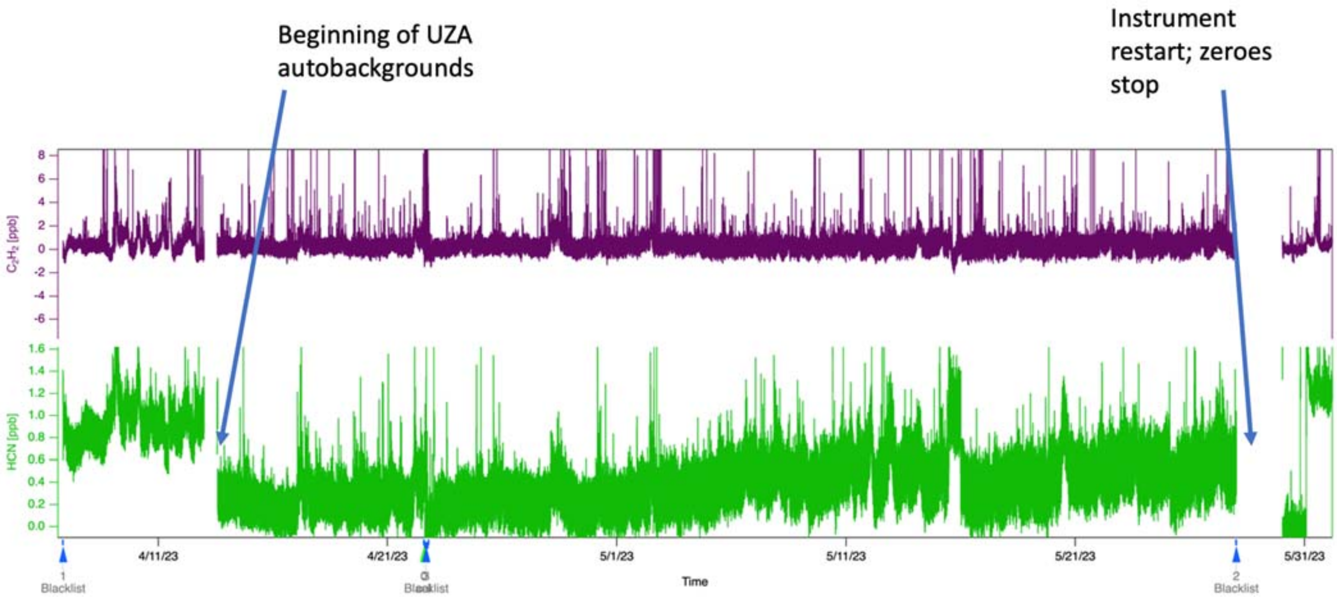


Figure 22-006-2. A first-pass data QA has been conducted on the HCN trace

In-field instrument performance has been assessed is displayed in Figure 22-006-3. We choose a period of quiet data in April, during the co-deployment of the AML, and do an Allan-Werle variance plot. This shows a 1-second 1-sigma performance of 78 ppt, averaging down to <8 ppt after 3 minutes.

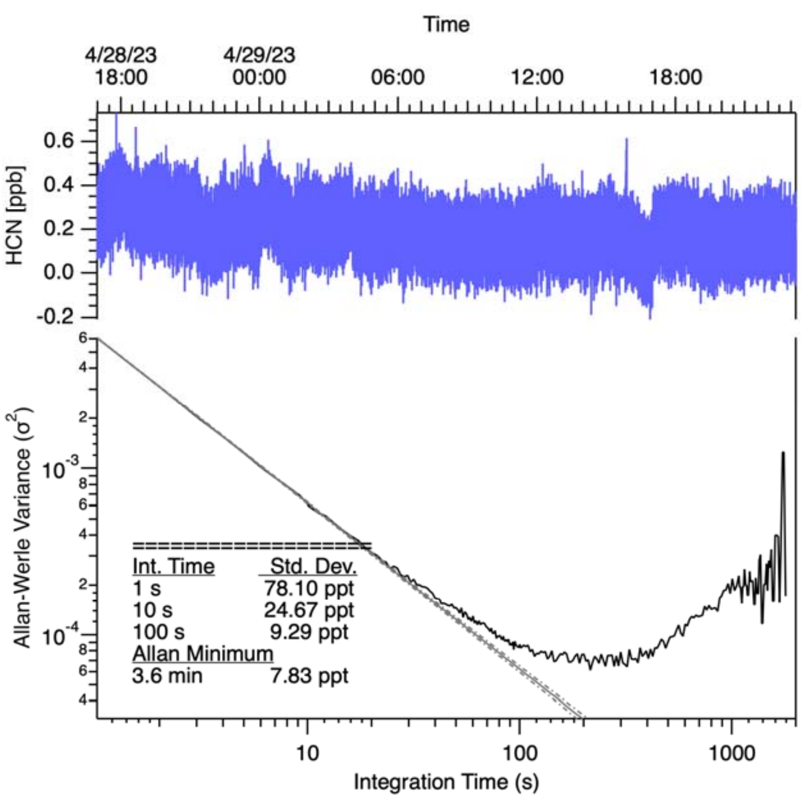


Figure 22-006-3. In-field instrument performance has been assessed

Data Collected: Ambient data was collected at Meacham International Airport in April from the sample inlet at the $(BC)^2$ network trailer. Auxiliary data collected by the AML in this area as part of a separate project (AQRP 22-010) could supplement interpretation of this dataset.

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 to deploy the instrument to the trailer in early April.

Accomplishing the science goals of this project depends on measuring biomass burning emissions in the DFW area. We still believe an extended spring campaign gives us the greatest likelihood of capturing such emissions from a variety of sources.

Goals and Anticipated Issues for the Succeeding Reporting Period: Coordination of consumables at the site (ultra zero air) might prove challenging and will depend on the support from Baylor University co-Principal Investigators (and associated colleagues). Given the slow consumption of zero air gas by the HCN instrument, this should be a rather periodic need that ought to be manageable. Additional support with respect to data backup will be required.

Recent site conditions have enabled successful measurements (stable power, reliable internet, consumable availability), but we continue to monitor the instrument via daily remote log-ins.

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. As of April 6th, measurements towards the spring campaign have commenced.

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

Delays Expected: Given the previous delays with the electrical work at the sampling sites in the DFW, measurement days were 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)
	Funded Amount: $181,724
PI: Yuxuan Wang (UH)	(UH: $175,621; St. Edward'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: In February, for Task 4 (Photochemical model evaluation and model inter-comparison), we installed and configured the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to conduct photochemical modeling, considering the best-performing meteorology identified in Task 3.

WRF-Chem simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology. It is a powerful integrated modeling system that can support a wide range of applications including air quality forecasting services, case study modeling of chemistry-meteorology feedbacks and climate change assessment studies focusing on chemistry.

We installed the latest version of the WRF-Chem (4.2.2) using Intel compilers and taking into account the characteristics of Carya Cluster. We use the model to perform meteorological and air quality modeling for a high ozone episode on September 6-11. We also considered two nested domains with horizontal resolutions of 4 km x 4 km and 1.33 km x 1.33 km (Figure 22-008-1), due to the temporal and spatial resolutions of the High-Resolution Rapid Refresh (HRRR) from National Oceanic and Atmospheric Administration (NOAA) Amazon Web Service which are hourly and 3 km (d02 and d03, shown in Figure 22-008-1).

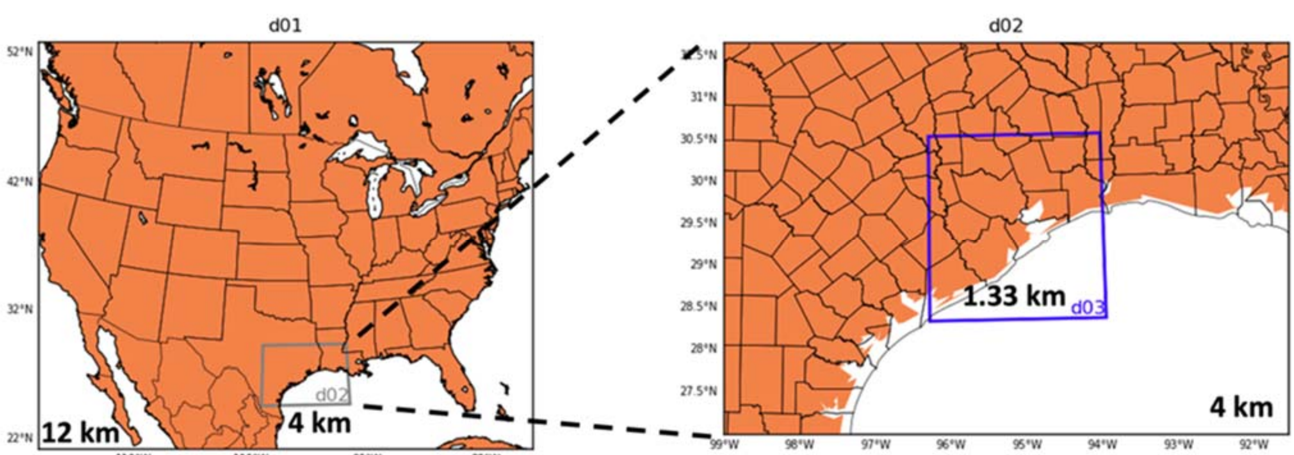


Figure 22-008-1. WRF-Chem nested modeling domains and horizontal resolutions.

The outermost domain (d01=d02 Figure 1) contains 129 x 186 grid points and covers the Southeast Texas region. The second domain (d02 = d03 Figure 22-008-1) contains 183 x 171grid points and focuses on the Houston-Galveston region. All domains have identical vertical resolutions with 50 vertical layers. The model spin-up time was 24 hours for the first forecast.

In order to have optimal representation of the meteorological and chemical fields, we are using the physics parameterization shown in Table 22-008-1.

Table 22-008-1. Physics parameterizations used in the simulations with WRF-Chem

Process	Scheme
Cloud microphysics	Morrison 2-moment scheme (mp_physics)
Longwave and shortwave radiation	RRTMG scheme (ra_lw_physics/ ra_sw_physics)
Cumulus parameterization	Grell 3D ensemble scheme (cu_physics)
Planetary boundary layer	MYNN (bl_pbl_physics)

Regarding the bl_pbl_physics option, the same configuration proposed by the best performance configuration from Task 3, was chosen. However for cu_physics, it was necessary to choose a different configuration, because for the compiled version of the model, an error is documented when it is choose the combination of that physical option with the rest physics desired for this parameterization: cu_rad_feedback= .true. We follow the recommendation of the user guide where it refers that cu_rad_feedback will only work with cu_phys=3 or 5.

To test the operation of WRF-Chem model, a total of five different configurations shown in Table 22-008-2 were assumed. At first, the best performance configuration with the new cumulus parameterization will be called best performance for WRF-Chem or Best Performance modified (BPm). BPm configuration was used together with the EDGAR-HTAP anthropogenic emission files (2010) emissions inventory for the MOZART-MOSAIC chemical mechanisms with 10 levels in the vertical (z_dim_stag) was used for case 1, while in case 2, Edgar_HTAPv5 (2015) was used. The 2017 National Emission Inventory (NEI) was taken in case 3 through anthro_emis utility; cases 4 and 5 have the same characteristics as cases 1 and 3 but with WRF-Chem version 4.0 installation. It was decided to do these tests with a different model version than the one initially installed, because this is a version that is still compatible with version 3.9.1.1 (Task 3 performed version).

The MOZART gas-phase chemistry coupled with MOSAIC aerosol chemistry was used as the chemical mechanism. Biogenic emissions are generated using the model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN 2.1) and adapted through WRF-Chem Tool Preprocessor. The Fire INventory from NCAR (FINN), a high-resolution global model, was used to estimate the emissions from open burning of biomass, which includes wildfire, agricultural fires and prescribed burning.

Table 22-008-2. WRF-Chem model experiments

	Best Performance (HRRR)	**WRF Version**	**Emission Inventory**
Case 1	BPm	v 4.4.2	EDGAR – HTAP v2 (2010)
Case 2	BPm	v 4.4.2	EDGAR – HTAP v5 (2015)
Case 3	BPm	v 4.4.2	2017 NEI (EPA)
Case 4	BPm	v 4.0	EDGAR – HTAP v5 (2015)
Case 5	BPm	v 4.0	2017 NEI (EPA)

In March, we continued with Task 4 (Photochemical model evaluation and model inter-comparison), we ran the WRF-Chem model, starting from the configuration described in the previous MTR (Monthly Technical Reports), Best Performance modified configuration (BPm). We conducted the modeling considering the 2017 National Emission Inventory (NEI) from Environmental Protection Agency (EPA) and this emissions inventory scaled with the TCEQ (Texas Commission on Environmental Quality) emissions inventory (EPAsTCEQ). In the first case, the EPA emissions were taken for all modeling domains (d01, d02). In the second case the EPA emissions inventory scaled with TCEQ inventory was used in the two modeling domains, while for the third case the EPA emissions were taken for the coarser domain d01 (4 km), while for the finer domain d02 (1.33 km), the EPA inventory scaled with TCEQ was taken (See **Table 22-008-3).**

Table 22-008-3. WRF-Chem model experiments

	Period	**Emission Inventory**
Case 1	First September episode	2017 NEI (EPA) (d01, d02)
Case 2	First September episode	2017 NEI (EPA) scaled with TCEQ (d01, d02)
Case 3	Full September, three episodes	2017 NEI (EPA) (d01), 2017 NEI (EPA) scaled with TCEQ (d02)

In April, we completed Task 4 (Photochemical Model Evaluation and Model Intercomparison). Submitted Deliverable 4.1 (Photochemical Model Evaluation and Model Intercomparison Report). Detailed analysis of Task 4 can be found from the Deliverable 4.1 Report.

In May, we conducted process analysis in the CAMx model to identify key processes which led to simulated O_3 change during high-O_3 episodes relative to clean days. The process analysis is calculated over a subregion of the Gulf of Mexico with high O_3 mixing ratios observed and integrated across the lowest five model layers comparable to the morning PBL heights over water. The diurnal average of each process on clean and O_3 episode days is shown in Figure 1. Chemistry (CHEM) is the major O_3 source during daytime and becomes the primary O_3 sink after sunset. Advection (ADV) serves as a pathway for an O_3 sink for most hours, especially during the day, while vertical diffusion (DIF) mostly contributes as an O_3 source. Deposition (DEP) constantly removes O_3 from the atmosphere at all hours, yet with a marginal value of 0.1 ppb/hr. During high-O_3 events, CHEM is the most important process causing higher O_3 levels over water relative to clean days, followed by vertical DIF (Figure 1b). We found that O_3 across the entire profile is higher on episode days than clean days, indicating an elevated O_3 background on high-O_3 days. In addition, the O_3 gradient above and below the PBL is also higher on episode days, especially during morning hours, which can induce more vertical diffusion if downmixing occurs from above the PBL when the capping inversion is weak.

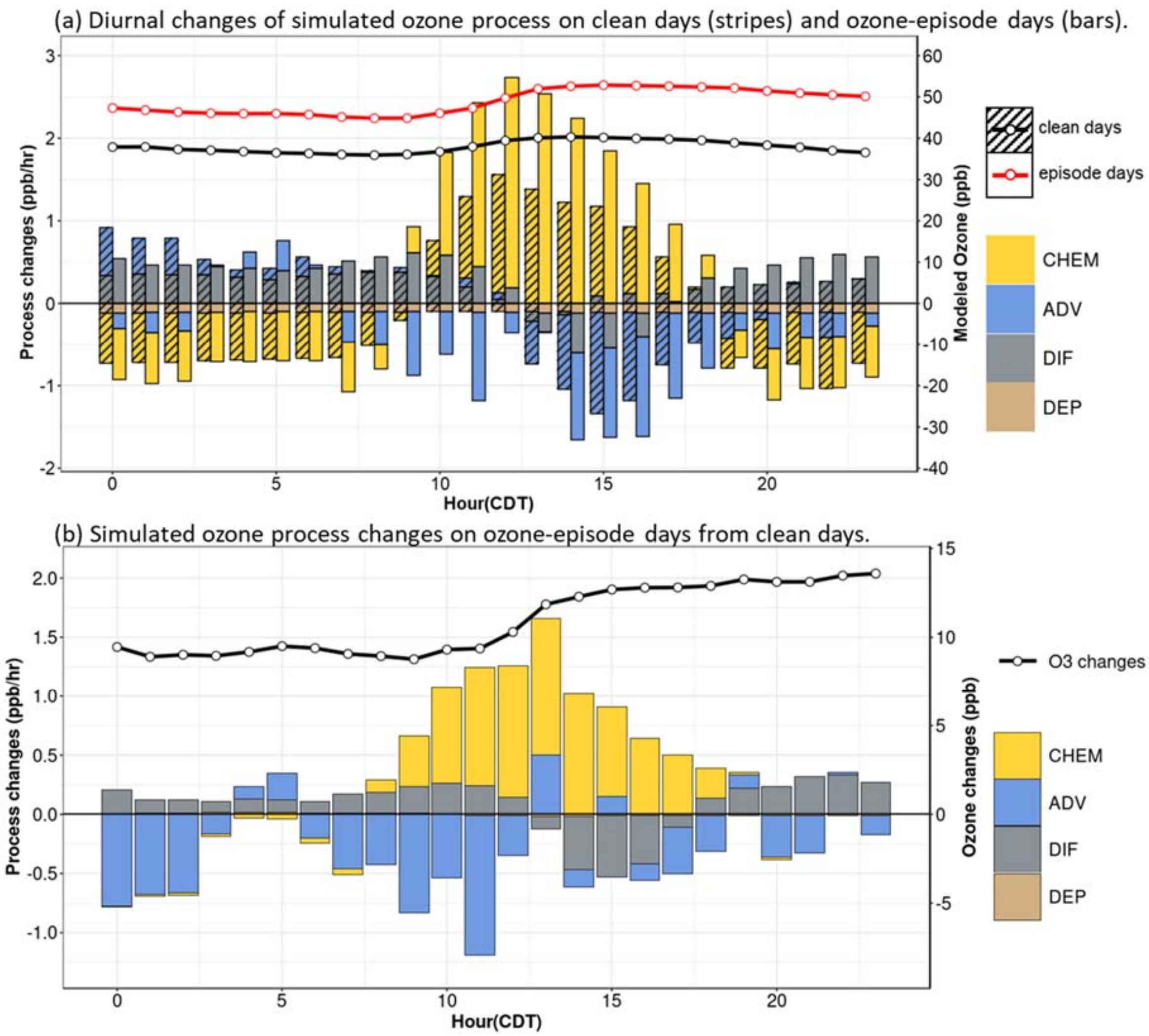


Figure 22-008-2. (a) Diurnal changes of simulated ozone processes over the Gulf of Mexico, including chemistry (CHEM), advection (ADV), vertical diffusion (DIF), and deposition (DEP) on clean days (stripes) and O_3-episode days (bars) integrated across the lowest five model layers.

Overlaid lines and points are simulated hourly ozone on clean (black) and O_3-episode (red) days. (b) Process (filled bars) and O_3 (black line) changes during high-O_3 episodes relative to clean days.

The process analysis on a case-study day (September 9, 2021) over the Gulf of Mexico shows that ADV, in addition to CHEM, contributes to the enhanced O_3 levels at 10:00 and 13:00 (Figure 22-008-3), which respectively corresponds to the two plumes under northerly and easterly winds and highlights the importance of regional transport. This demonstrates that the contributions from ADV to the increase of O_3 can be high on some specific cases, although its mean contributions over multiple days are averaged out in Figure 22-008-2.

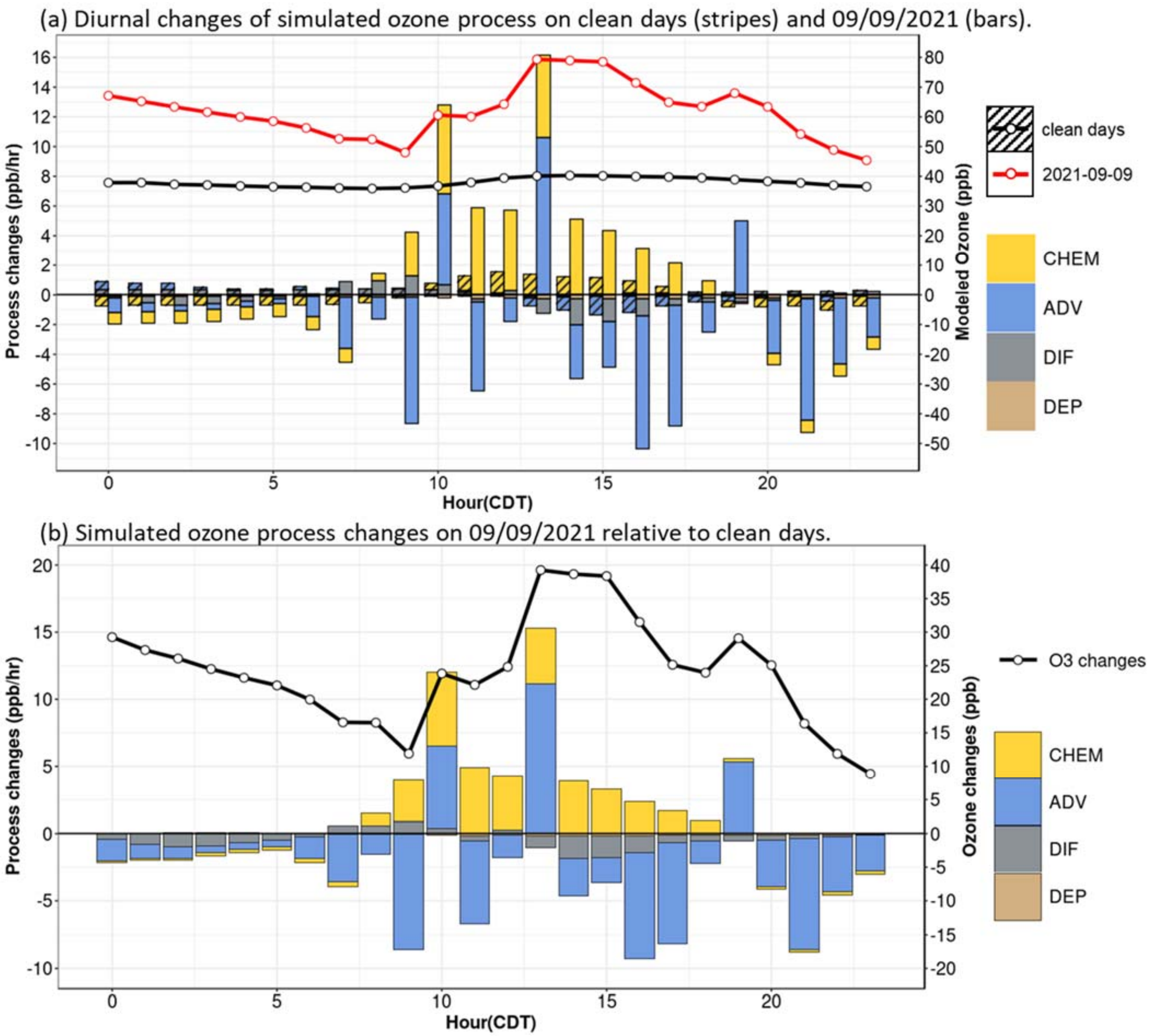


Figure 22-008-3. (a) Diurnal changes of simulated ozone processes over the Gulf of Mexico, including chemistry (CHEM), advection (ADV), vertical diffusion (DIF), and deposition (DEP) on clean days (stripes) and 09/09/2021 (bars) integrated across the lowest five model layers. Overlaid

lines and points are simulated hourly ozone on clean (black) and 09/09/2021 (red) days. (b) Process (filled bars) and O_3 (black line) changes on 09/09/2021 relative to clean days.

Preliminary Analysis: Figure 22-008-4 shows the spatial distribution of ozone at 18 h (local time) for the cases shown in Table 22-008-2 (Domain d01). The highest values of the variable and with the highest level of detail for domain 1 are observed in case 2, which uses the latest version of the WRF-Chem model and the most up-to-date EDGAR inventory (2015). Cases 1, 3 and 5 show a similar pattern to each other, although they were built through different versions of the model and the emissions inventory. Case 4 presents the lowest and smoothest O_3 values in the domain, using Edgar_HTAPv5 (2015) but an older version of the model (v 4.0).

Figure 22-008-5 shows the spatial distribution of ozone at 18 h (local time) for the cases shown in Table 2 (Domain d02). In addition, the result of another simulation for O_3 using Environmental Protection Agency (EPA) scaled with TCEQ data is shown. Taking this last simulation as a reference, we can see similar patterns for cases 1, 2, O_3 and 5, and the range of modeled values does not present great difference.

Figures 22-008-6 and 22-008-7 show emissions of Nitrogen Monoxide (E_NO) (Domain d01) and Nitrogen Dioxide (E_NO_2) (Domain d01) respectively, from the emissions inventories EDGAR-HTAPv5, NEI 2017 (EPA) and EPA scaled with TCEQ respectively, at 18 h Local time. The highest values are observed in the emissions generated through EDGAR-HTAPv5, which is in correspondence with what was described in case 2, Figure 1. The emissions generated from EPA and EPA scaled with TCEQ show a similar pattern, the first being slightly higher.

Based on what was observed in the previous Figures, cases O_3 and 5 are the most comparable with the reference case, in terms of emissions source. Therefore, the following modeling and chemical evaluation, for the six cases of high ozone, will be carried out taking the above into account.

The modeled outputs were compared spatially within the TCEQ continuous ambient monitoring stations (CAMS) across the greater Houston area. The results shown below correspond to the first (6-11) and third (23-26) ozone episodes, the most important episodes during September 2021.

Figure 22-008-4 shows the spatial distribution of CAMS-observed and modeled ozone for Cases 2-3, in the first two days of the first high ozone episode (Sept. 6, 2021 and Sept. 7, 2021) at 21 UTC (16 h local time). In the hours around the ozone maximum, the behavior is different from that observed in Figure 1, because it is Case 3 that shows a better correspondence between the observed and modeled data, mainly in the areas where the maximum values are found.

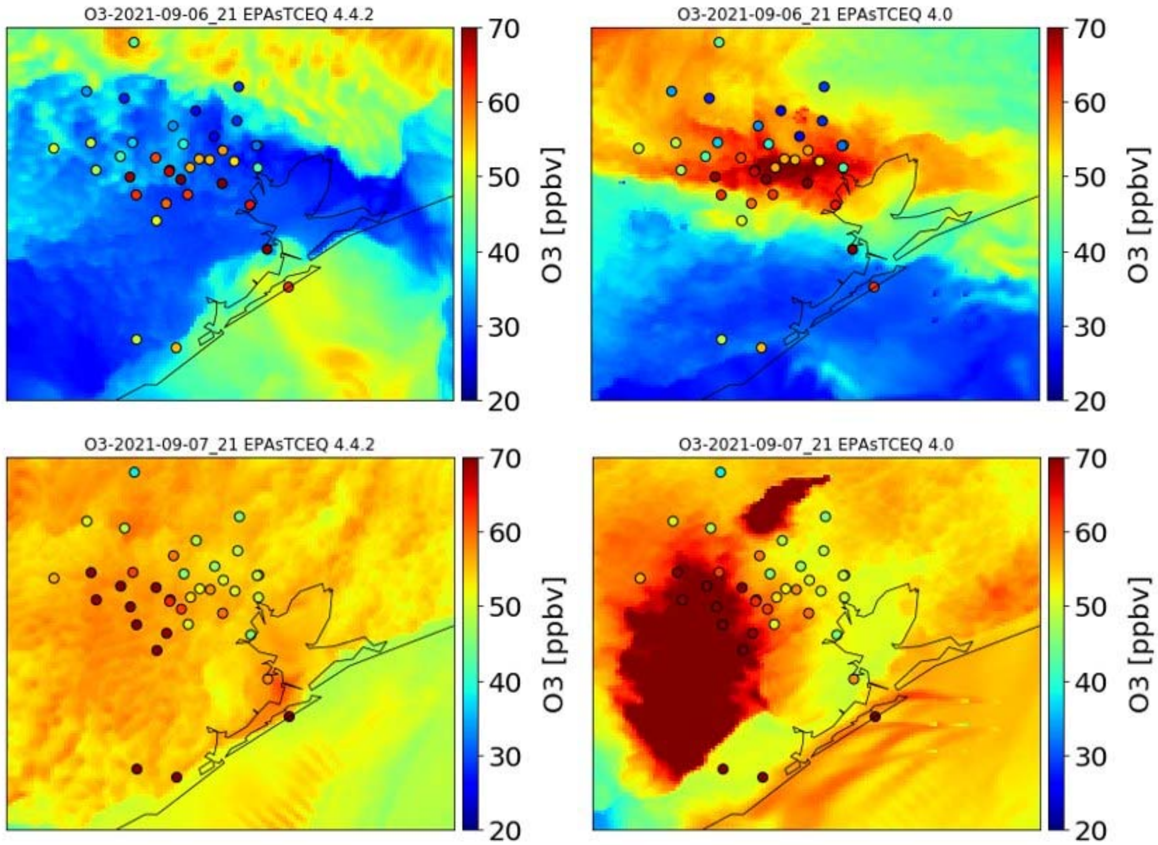
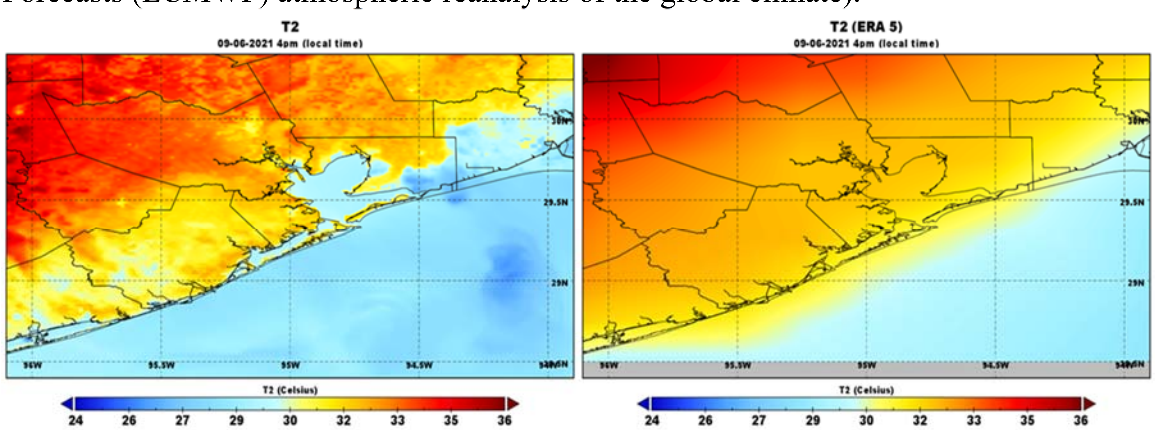


Figure 22-008-4. Spatial distribution of CAMS-observed and modeled ozone for Cases 2 (left) and Case 3 (right) at 16 h local time (Sept. 6, 2021, and Sept. 7, 2021), domain d02.

Figure 22-008-5 shows spatial distribution of modeled meteorological values (temperature T2, wind velocity and direction) and ERA 5 reanalysis output at 16 h local time, domain d02. The range of values of the model for the temperature and wind direction and speed is in accordance with the obtained by the ERA5 (Fifth generation of the European Centre for Medium-Range Weather Forecasts (ECMWF) atmospheric reanalysis of the global climate).



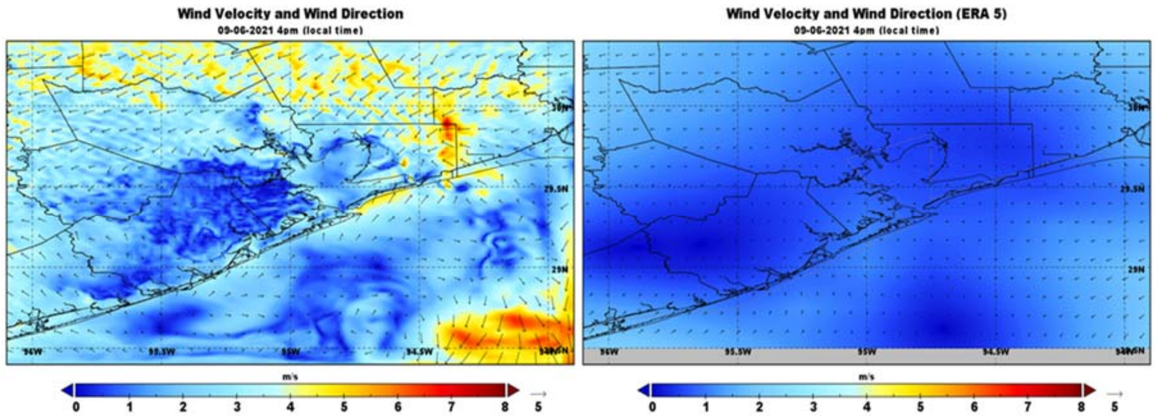
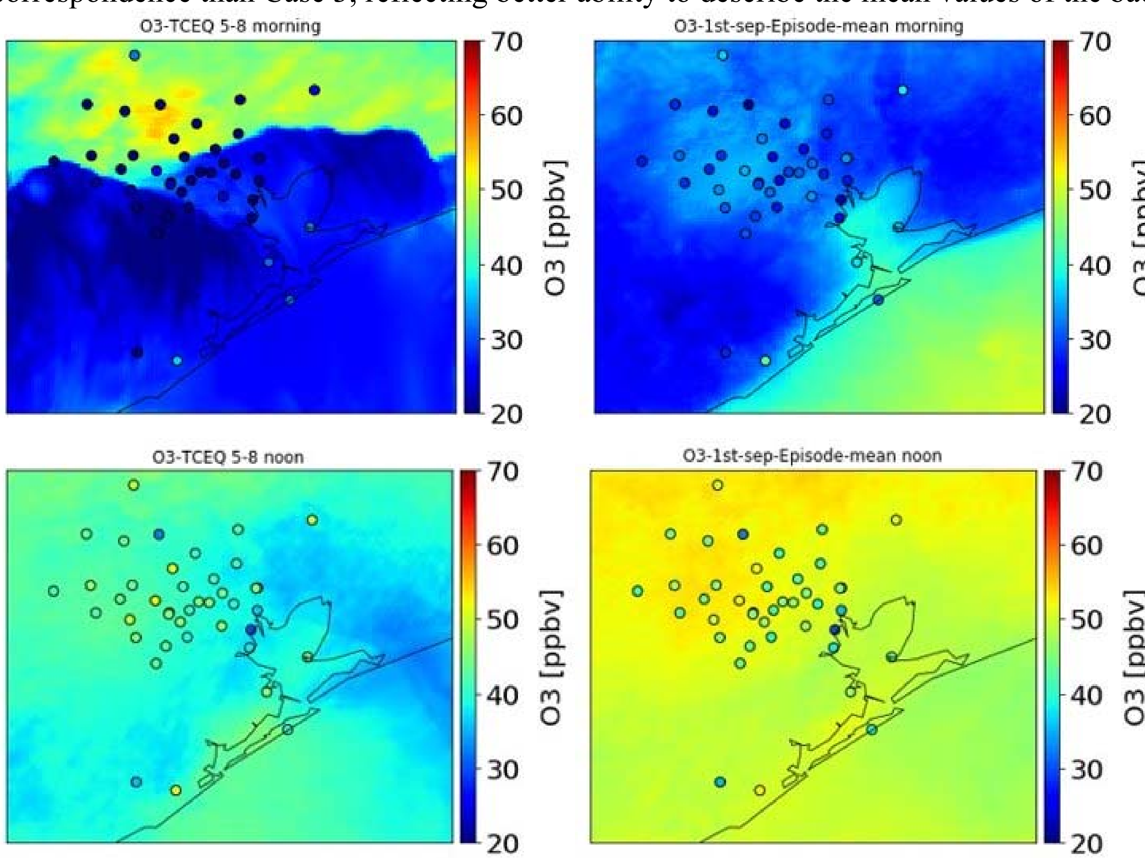


Figure 22-008-5. Spatial distribution of modeled meteorological values (temperature T2, wind velocity and direction) and ERA 5 reanalysis output at 16 h local time, domain d02.

Figure 22-008-6 shows the spatial distribution of CAMS-observed and modeled mean ozone for Cases 2 and 3 at morning, noon, night, and midnight for the first high ozone episode (Sept. 6-11, 2021). In general, the best correspondence is obtained for Case 3, when using the EPA inventory for domain one and the EPA inventory scaled with TCEQ for domain two. The best correspondence times are morning and noon, while for the case of night and midnight, the modeled values tend to overestimate the observations. For Case 2, the hours of night and midnight have a better correspondence than Case 3, reflecting better ability to describe the mean values of the background.



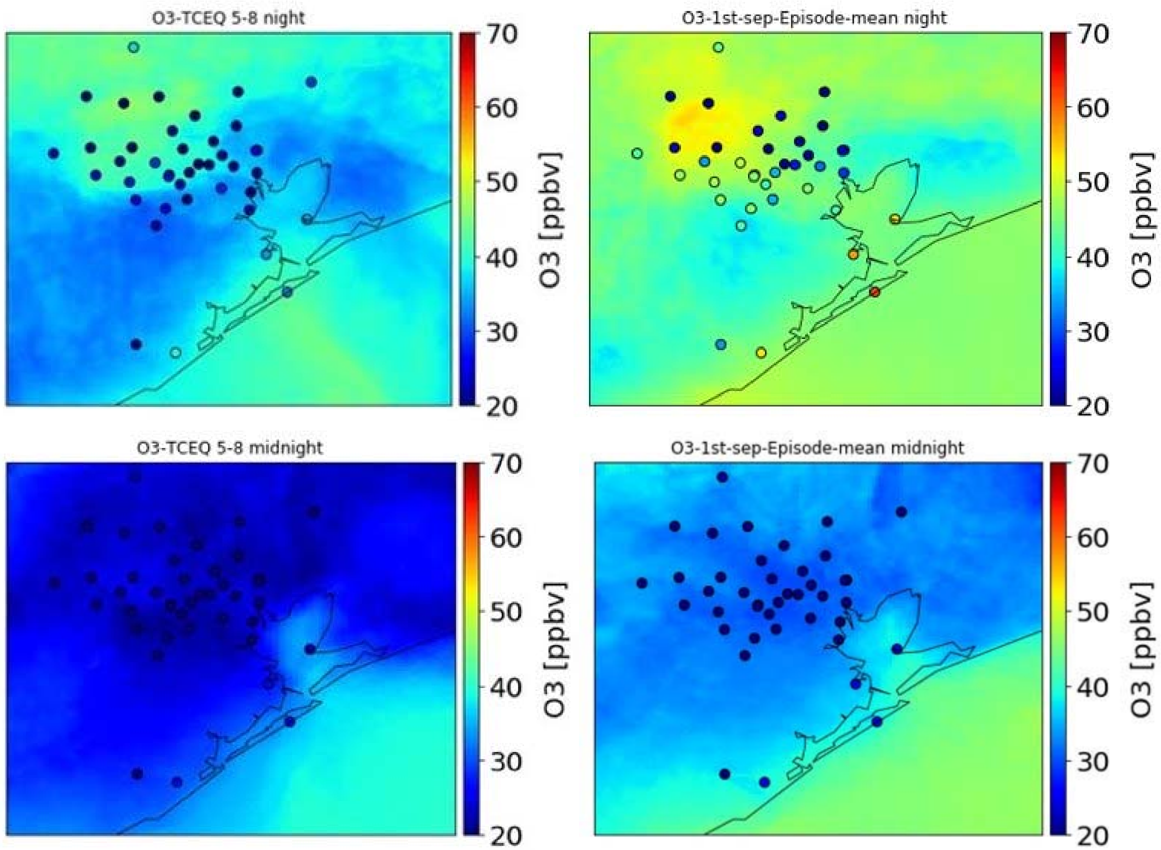
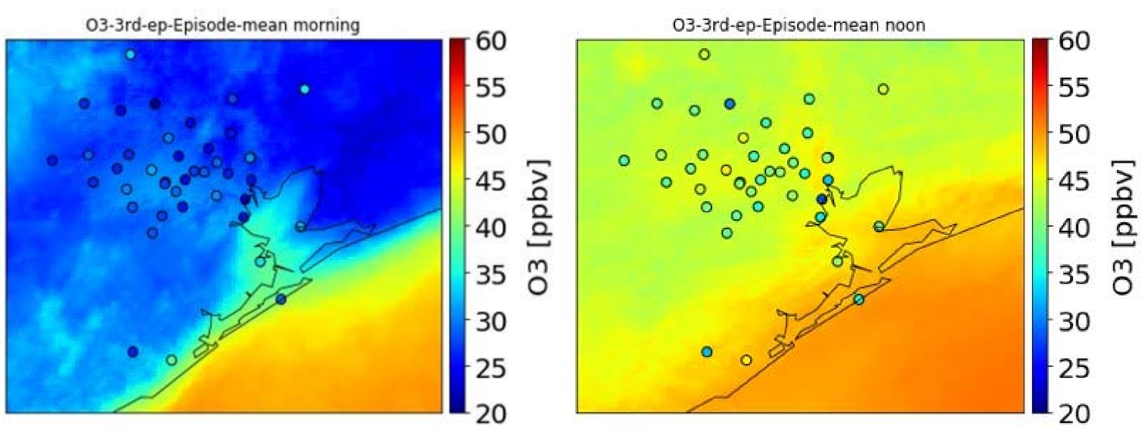


Figure 22-008-6. Spatial distribution of CAMS-observed and modeled mean ozone for Cases 2 (left) and Case 3 (right) at morning, noon, night, and midnight for the first high ozone episode (Sept. 6-11, 2021).

Figure 22-008-7 shows the spatial distribution of CAMS-observed and modeled mean ozone for Case 3 at morning, noon, night, and midnight for the third high ozone episode (Sept. 23-26, 2021). The best correspondence times are morning and noon again. At night and midnight, the modeled values overestimate the observations.



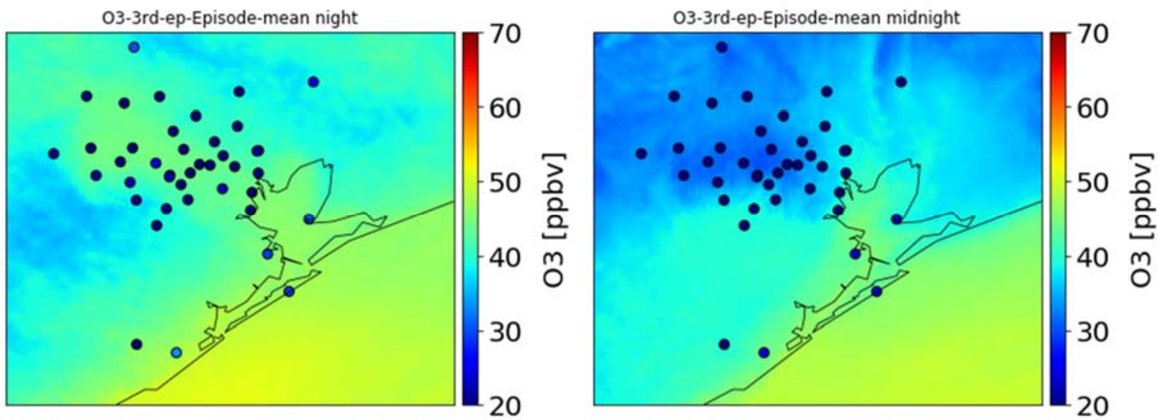
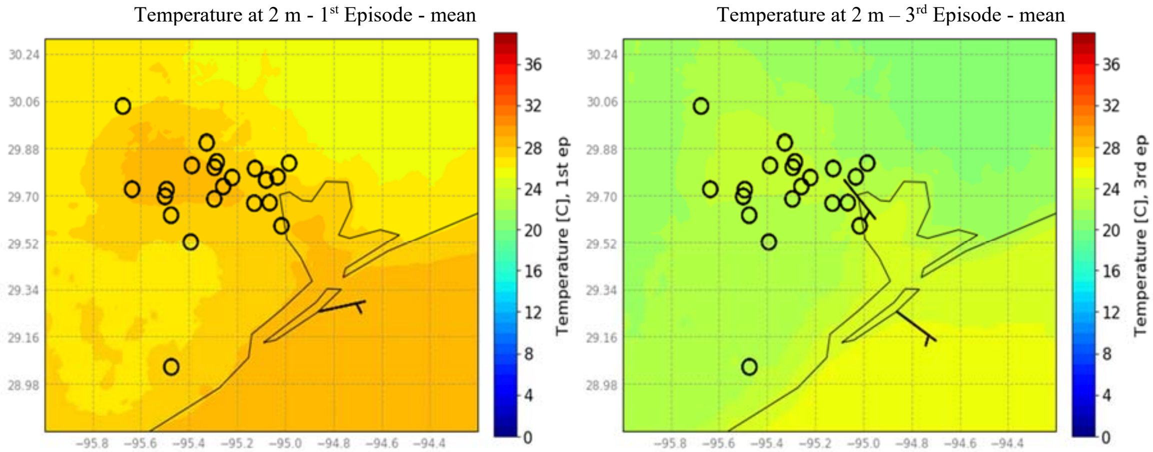


Figure 22-008-7. Spatial distribution of CAMS-observed and modeled mean ozone for Case 3 at morning, noon, night, and midnight for the third high ozone episode (Sept. 23-26, 2021).

Figure 22-008-8. shows spatial distribution of CAMS-observed and modeled mean meteorological variables (temperature, relative humidity, wind speed and direction) for the first (Sept. 6-11, 2021) and third (Sept. 23-26, 2021) high ozone episodes. For temperature, in both cases, the modeled values correspond to the observed ones adequately, the mean modeled values oscillate around 27.10 °C with 1.73 of standard deviation, and the observed values mean is 27.32 with 0.57 of standard deviation. For relative humidity, Case 1 shows better results, while in Case 2 the model underestimates the value of the variable by up to 10%. Regarding the wind, the correspondence is better in wind speed than in direction. In this variable, the model's outputs for the first episode have a better performance with respect to the observed values.

Temperature at 2 m - 1st Episode - mean　　　Temperature at 2 m – 3rd Episode - mean



Relative Humidity - 1st Episode - mean　　　Relative Humidity – 3rd Episode - mean

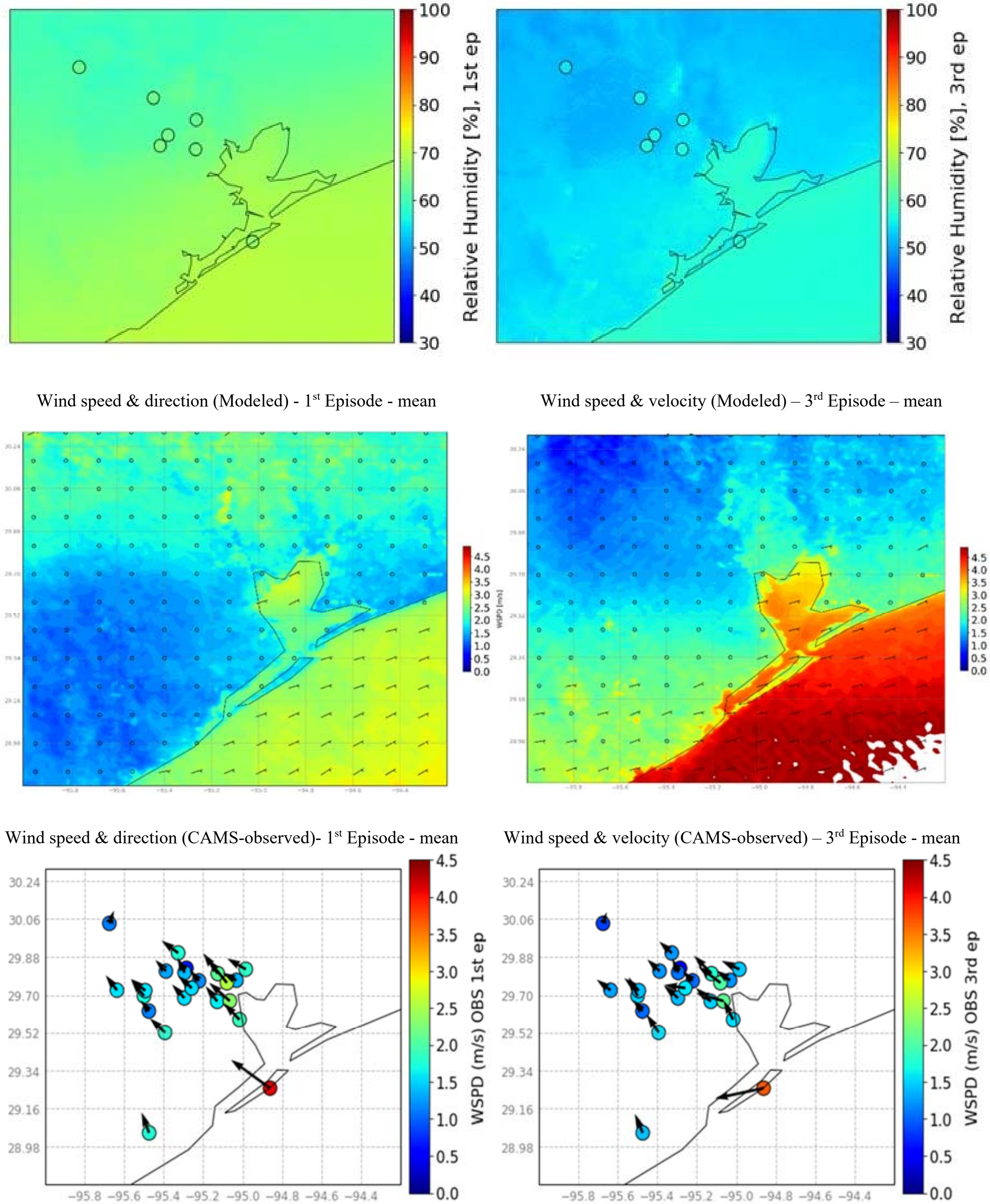


Figure 22-008-8. Spatial distribution of CAMS-observed and modeled mean meteorological variables (temperature, relative humidity, wind speed & direction) for the first (Sept. 6-11, 2021) and third (Sept. 23-26, 2021) high ozone episodes.

Figures 22-008-9 and 22-008-10 show the spatial distribution of CAMS-observed O_3 and modeled mean O_3, CO, SO_2 and NO_2 for first (Sept. 6-11, 2021) and third (Sept. 23-26, 2021) high ozone episodes. The third period shows the best results overall for O_3, since the modeled values are closest to the observations. For the other variables, the model simulates their spatial behavior according to the average normal values in the study area.

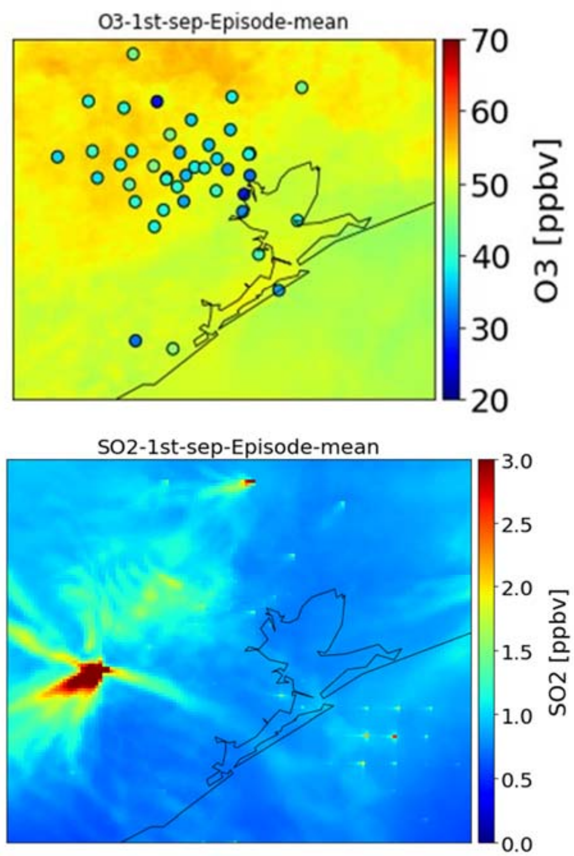


Figure 22-008-9. Spatial distribution of CAMS-observed O_3 and modeled mean O_3, CO, SO_2 and NO_2 for first (Sept. 6-11, 2021) high ozone episodes.

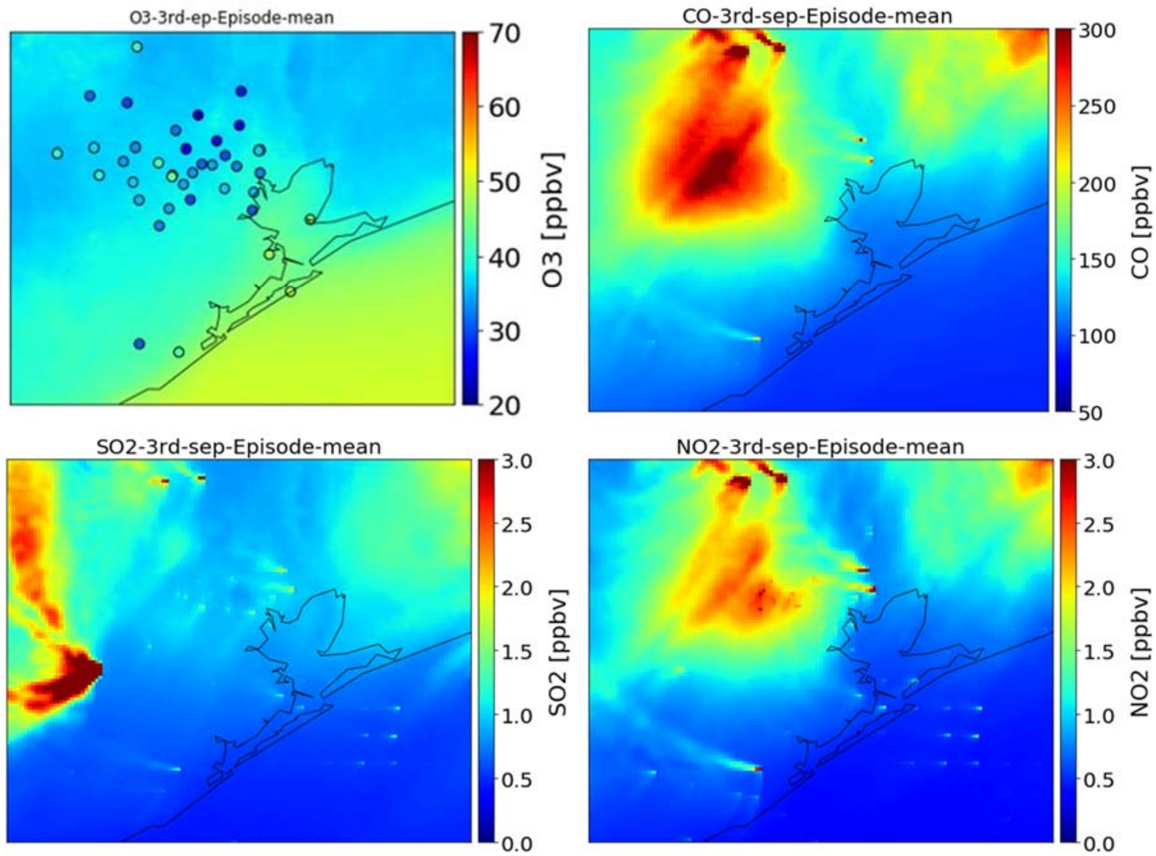


Figure 22-008-10. Spatial distribution of CAMS-observed O_3 and modeled mean O_3, CO, SO_2 and NO_2 for third (Sept. 23-26, 2021) high ozone episodes.

Data Collected: None.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: N/A

Goals and Anticipated Issues for the Succeeding Reporting Period: We will evaluate the six ozone episodes WRF-Chem simulations in the succeeding report period. Finish Task 5 (Investigation of Elevated Offshore Ozone's Sources) in the succeeding report period.

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

Publications, Presentations related to project currently under development:

Li et al., Understanding offshore high-ozone events during TRACER-AQ 2021 in Houston: Insights from WRF-CAMx photochemical modeling. Submitted to *Atmospheric Chemistry and Physics*.

Liu et al., Evaluating WRF-GC v2.0 predictions of boundary layer and vertical ozone profiles during the 2021 TRACER-AQ campaign in Houston, Texas. Submitted to *Geoscientific Model Development (GMD)*

Wang et al., Using TRACER data to Evaluate High-Resolution Air Quality Models for Houston and Understand High Ozone Episodes. Poster presentation planned for the TRACER Workshop during 16-17 May, 2023 at Texas Southern University.

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 addresses the AQRP 2022-2023 research priority of "Domestic Fire Emissions".

Project Update: In February:

Task 2: Base Site Selection: The Fort Worth Northwest Site owned by TCEQ at the Meachum field airport continued to be the primary choice for the base site location. A major accomplishment during the month of February was an upgrade to the electrical infrastructure to accommodate both the Aerodyne Mobile Laboratory (AML) and the Baylor trailer, which would be operating there as part of project 22-006. The site access agreement for this location had been drafted with the inputs of Vince Torres and RoseAnna Goewey (TX AQRP), Ed Fortner from Aerodyne Research Incorporated, and Dakota Shaw at Fort Worth Meachum Field. This document had been sent to officials in the city government of Fort Worth for their approval. Considering that this document may not have been approved by the time that measurements were scheduled to begin (Apr 2), alternative base location plans were being established. The Fort Worth RV Park at 5319 Rueben Lane, Fort Worth TX, was being discussed as a preferred RV park location if it became necessary to locate somewhere other than the Meachum Field Site. Communications with the RV park had begun, and the necessary reservations would be executed within the next week (03/13 – 03/17) unless the Meachum Field Site obtained approval by that time. Other RV parks were also being considered, as well as the possibility of shifting intensive measurement timing slightly (one to two weeks) in order to give more time for the approval of the access agreement at Meachum Field.

Task 3: Campaign Planning: The field staffing plan had been completed, all positions were filled, and date commitments had been made. The measurement intensive dates were being planned for Apr 3 – 23. Lodging (refundable) had been booked by members of the measurement intensive team, and flights would be booked within the next week. Regarding the option of slightly shifting the timing of the campaign, while this could be done if necessary, it presented some staffing issues, and so this would be the last base siting option to consider if Meachum Field and RV parks in the area were unavailable. Flights would not be booked until a base siting location for the AML at the appropriate time was established. The necessary ordering of calibration equipment had occurred to ensure its availability for the measurement campaign.

Task 4: Instrument Integration: Instruments were being integrated into the AML at Aerodyne and would continue to be optimized over the next 2 ½ weeks at Aerodyne.

In March:

Task 2: Base Site Selection: The Texan RV Ranch in Mansfield TX was chosen as the base site for the first week of the intensive campaign (Apr 2-9). The Aerodyne Mobile Laboratory (AML) based out of this RV park for the first week of the campaign, staying at that location overnight and making daily mobile measurements throughout the DFW metropolitan area. The Fort Worth Northwest Site owned by TCEQ at the Meachum field airport became available for the AML to operate out of starting on April 10th. An important development was the approval of site access for the AML beginning at that time. The site access agreement for this location had been completed due to the diligent efforts of Vince Torres and RoseAnna Goewey (TX AQRP), Dakota Shaw at Fort Worth Meachum Field, and TCEQ.

Task 3: Campaign Planning: It was ultimately determined that it would be better to keep the schedule of this campaign within the April timeframe originally planned for rather than delaying with the hope of eventual Meachum Field approval. Certain personnel constraints contributed to the decision to not delay. Intensive measurements began on April 3rd.

Task 4: Instrument Integration: This task had been completed with all instruments installed and ready for measurements.

In April:

Task 5: Campaign Execution: The campaign intensive occurred from April 2nd to 24th. The Aerodyne Mobile Laboratory (AML) was based out of RV Ranch in Mansfield TX from Apr 2nd to 9th and then moved its base to Meacham Field in Fort Worth from Apr 10th to 24th. The Mansfield site was close to many large industrial point sources in the Midlothian TX area, and the stationary data at Mansfield could serve as an upwind or downwind site when winds were out of the South or North, respectively. The Meacham Field Site provided the advantage of the AML being co-located with both a TCEQ monitoring station and the Baylor University atmospheric chemistry trailer associated with Project 22-006.

The campaign featured the measurement of many large point source emitters in the DFW region. Point source measurements were carried out on 14 days at a variety of locations within the DFW metropolitan area. Over 50 industrial facility point sources of interest were measured, with over 30 facilities preliminarily identified as emitting measurable plumes of gas-phase and particle-phase compounds above the neighborhood background levels. On four days, the AML conducted a more general upwind/downwind measurement experiment where inflow to DFW and outflow from the metropolitan area was measured on a given day by placing the AML in two different locations and conducting stationary measurements for 2 to 6 hours at both the upwind and downwind sites. This was done on both weekend days and weekdays and under both North and South winds. The AML also directly measured a wildfire on one measurement day. This fire could have potentially impacted the DFW metro air quality at some point during the campaign, so it was useful to obtain a direct measurement of it.

Task 6: Preliminary Data Analysis: At this time, data analysis conducted was for the purpose of guiding future measurements on a daily basis. Areas of signal enhancement were recognized, wind conditions were considered, and determinations were made regarding the source of the signal enhancement. A couple of examples are discussed below, primarily to give an indication of the thought process used in near real-time preliminary analysis guiding future mission planning. These examples were a very small subset of the total number of facilities looked at and plumes encountered.

Johns Manville Cleburne TX: On April 7th, while conducting measurements in Cleburn, TX, a plume of organic aerosol was encountered emanating from the Johns Manville plant (Figure 1). This was one of the more straightforward plume transects to analyze due to the ability to conduct a close upwind and a close downwind on this day, which featured a consistent East-Northeast wind. Attempts were always made to go to facilities that had the correct road structure surrounding them to enable close upwind and downwind transects given the correct wind orientation with a limited number of potential interferences. While Figure 22-010-1 only depicted one transect, there were multiple transects of this plume on this day.

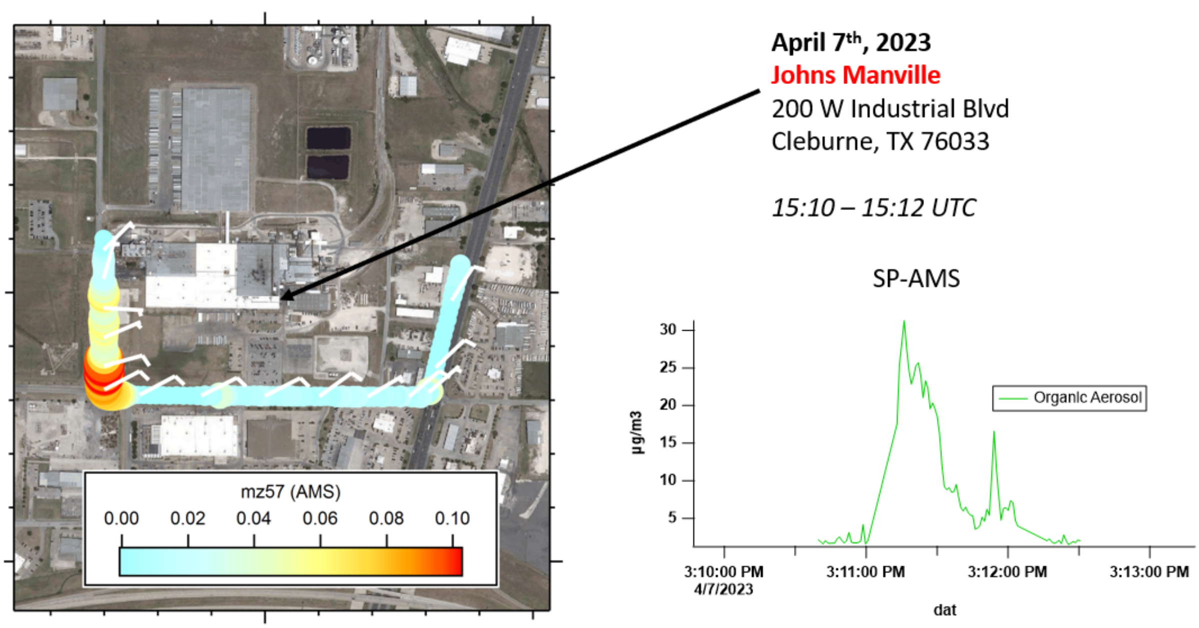


Figure 22-010-1. The map at left shows the route of the AML colored by concentration of mz57 as measured by the SP-AMS is an organic dominated mz. The matching time series for total Organic is depicted at right (preliminary data)

Dartco/Owens Corning Waxahatchie TX: A more difficult-to-interpret sequence of measurements was conducted in the Waxahatchie area, which is interesting to consider. There were multiple facilities in this area, and there were roads present to sample on; however, the road structure was not grid like, and under many different wind vectors, it was difficult to isolate just one potential source. On April 4th, while driving in the Waxahatchie area, a clear plume was encountered immediately downwind of the Owens Corning facility. Winds were strong out of the South on this day, and VOCs detected by the VOCUS instrument showed immediate enhancement (Figure 22-010-2). It should also be noted that Dartco Container Corporation is further downwind of this plume, so it was hard to rule out any impact from the Dartco facility.

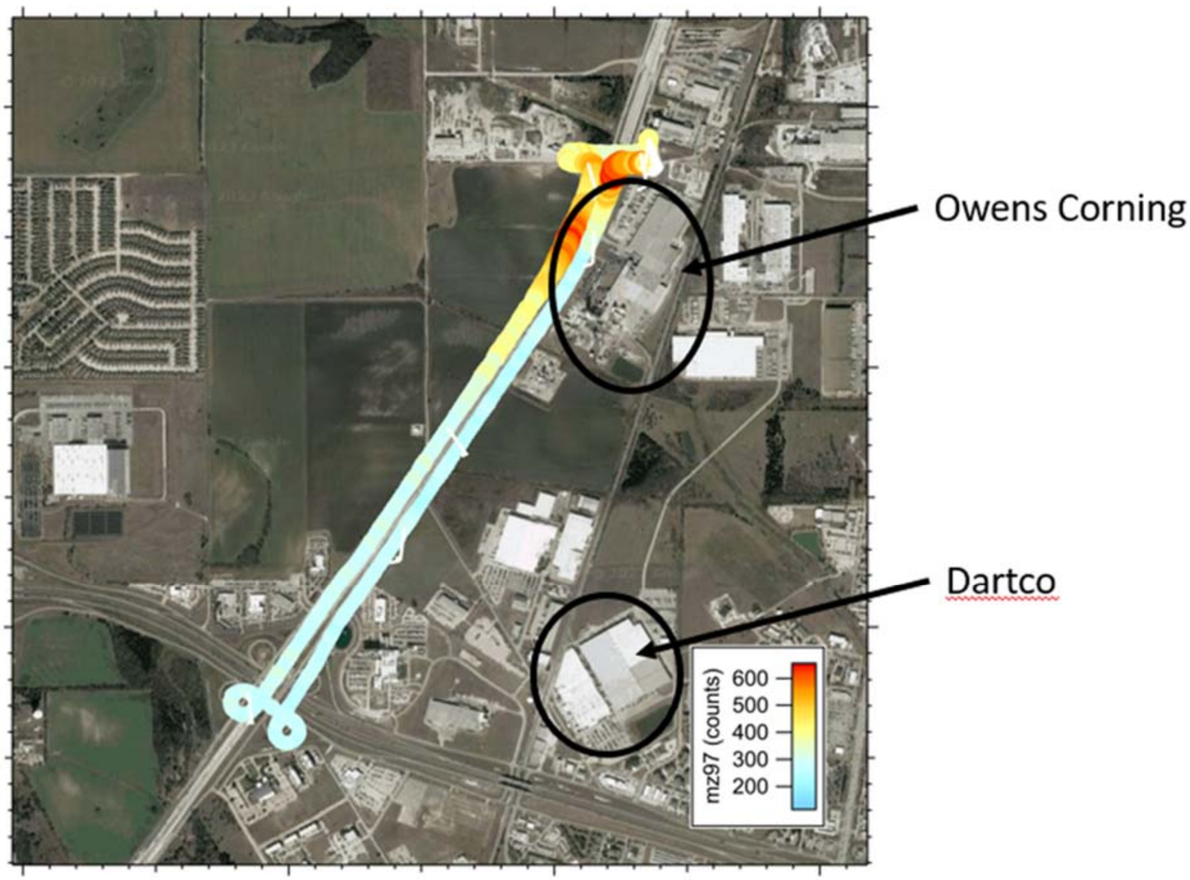


Figure 22-010-2. The route of the AML is depicted by the colored trace. The trace is colored by mz97 counts from the VOCUS typically attributed to vinyl chloride.

The next day April 5th winds shifted to being out of the Northwest and while this wind does not work well for sampling Owens Corning it is useful for sampling Dartco. Figure 22-010-3 depicts measurements of a plume immediately downwind of the Dartco facility. The AML was able to park in this plume enabling GC-EIToF measurements of this plume in addition to the typical one second measurements of gas phase and particle phase species.

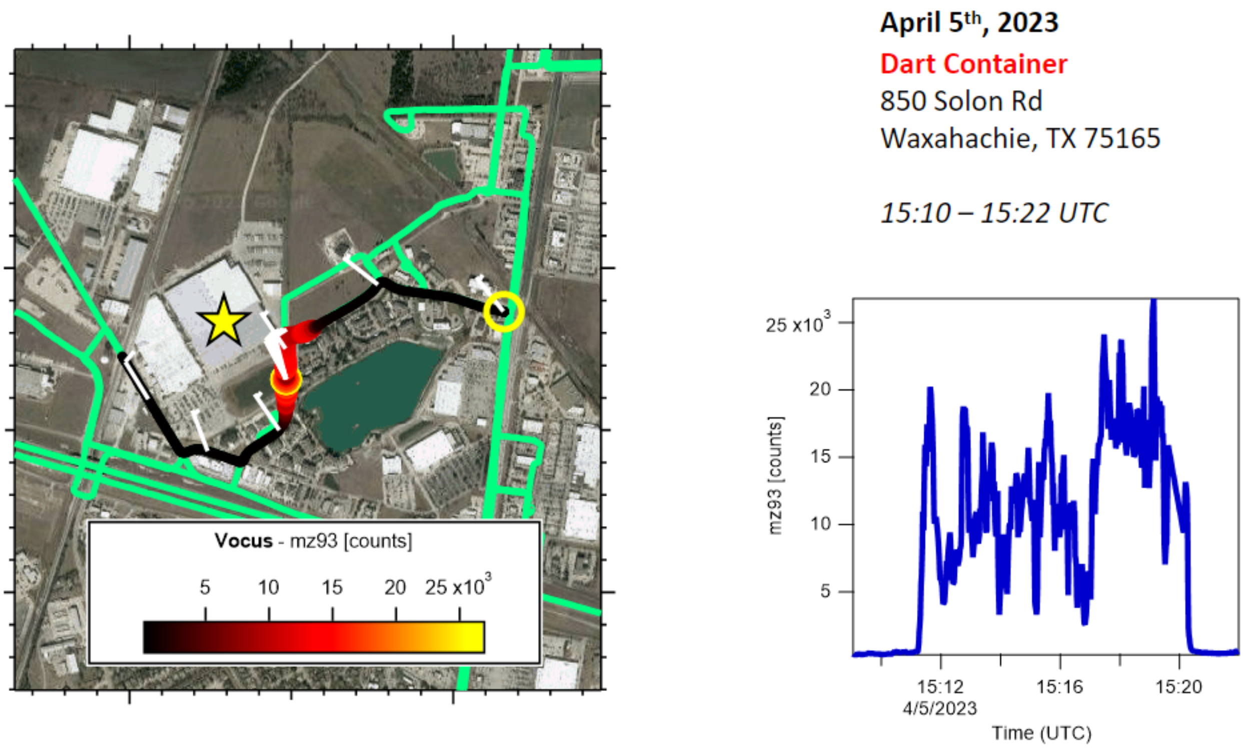


Figure 22-010-3. The route of the AML is depicted at left colored by the mz93 (toluene) intensity as measured by VOCUS and the time series of mz93 (toluene) is depicted at right.

Finally on April 10th measurements were conducted in the Waxahatchie area with an East wind. This wind worked well for measuring both Owens Corning and Dartco without their respective plumes overlapping each other (Figure 22-010-4)

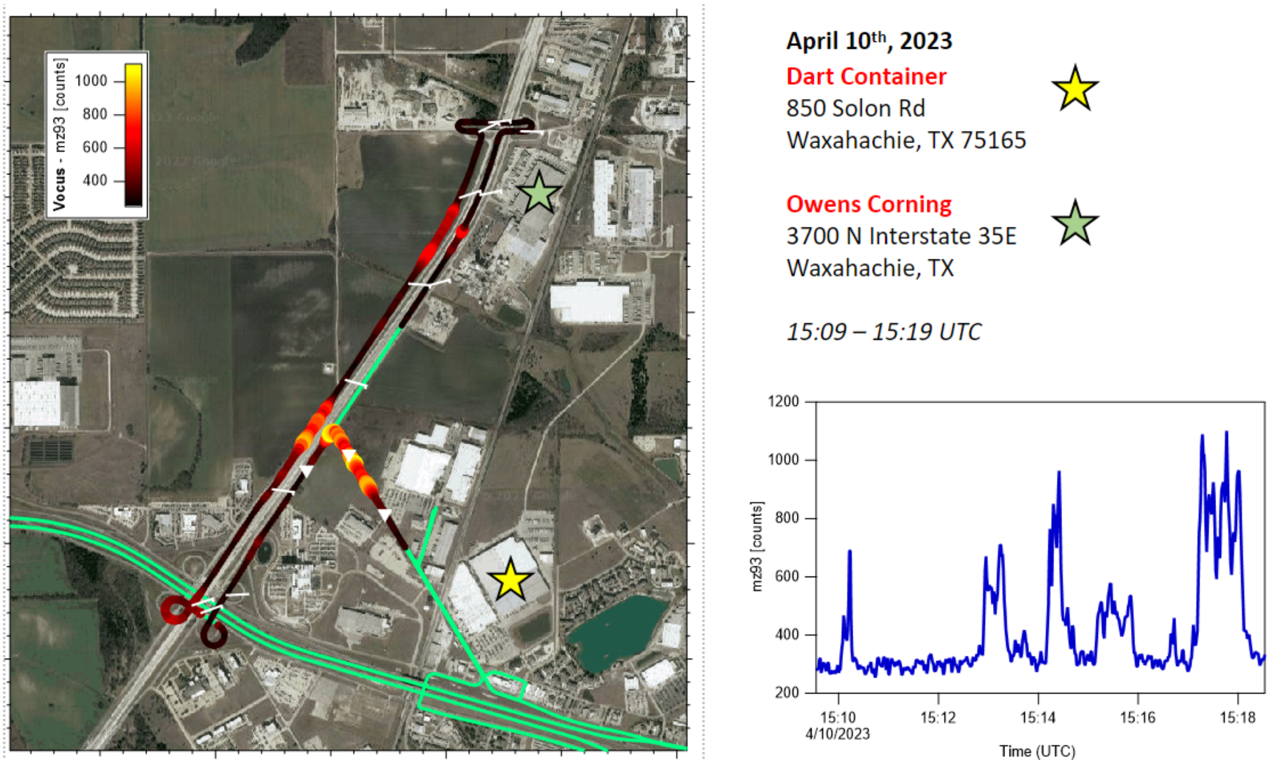


Figure 22-010-4. The route of the AML is depicted at left colored by the mz93 (toluene) intensity as measured by VOCUS and the time series of mz93 (toluene) is depicted at right.

In May:

Task 6: Data Analysis: During the month of May the focus of data analysis has been entirely on developing quality assured (QA) time series waves for the many different parameters measured during the Dallas FS field study. Currently this work is in progress with the respective personnel who have expertise in the data analysis of the various instruments including the TILDAS instruments, the SP-AMS, the VOCUS and GC-EI Tof. To date this analysis process has proceeded without any major problems but this is a very detailed and lengthy QA process. The goal that has been set internally is to have this data QA'd and available for further intercomparison work by the end of June.

Preliminary Analysis: Primary analysis is being conducted as detailed in Task 6 above.

Data Collected: All raw data from all instrumentation has been saved on respective instruments and at a central server location at Aerodyne. Analysis of this data occurred.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: As discussed above in tasks 2 and 3 the site access to Meachum Field is being worked through and this has major implications. Solutions are discussed within tasks 2 and 3 above.

Goals and Anticipated Issues for the Succeeding Reporting Period: The successful execution of a site agreement at Meachum Field was an important goal for the month of March.

The intensive measurement campaign occurs entirely within the April (1 April – 30 April). The measurement campaign is on track with base locations and particular measurement points of emphasis determined.

During this next reporting period significant efforts towards quality assuring the various gas phase particle phase and other time series measured parameters will occur.

The goal that has been set internally for this next reporting period is to have all of the Dallas FS data QA'd and available for further intercomparison work.

Detailed Analysis of the Progress of the Task Order to Date: Issues are discussed above regarding tasks 2 and 3. Task 4 is proceeding on schedule.

Task 5 was successfully executed and the assistance of the Fort Worth Meachum Field airport personnel as well as AQRP and TCEQ personnel towards making facilities available to our measurement team is greatly appreciated. Task 6 (Data Analysis) is underway and on schedule.

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: In February:

Task 2: Development of the Reduced-Complexity CMAQ Model (RCCM) for NH3 and refinement of NH3 emissions using iFDMB with the combination of CMAQ model and CrIS satellite observations: The UH-AQF modeling continued working on producing offline files over the modeling domain. An issue was faced while generating the offline files. The UH-AQF modeling resolved the issue; however, the CMAQ model had to be restarted to create the offline files. The issue was unexpected but can happen during running CMAQ. Generating offline files was an important part of running RCCM and iFDMB. As mentioned, offline files contained concentrations of sulfate (SO4-2), nitric acid (HNO3), nitrate (NO3-), chloride (Cl), sodium (NA), and hydrochloric acid (HCl) in all time steps. A CMAQ model was implemented to produce files containing the concentration of species of interest in all time steps as offline files.

Task 3: Investigation of PM2.5 concentrations using the updated emission inventory: Our team reviewed the literature to improve our understanding of underlying chemistry related to inorganic PM2.5.

In March:

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 team produced offline files over the modeling domain for 2019, and we worked on running iFDMB with the Cross-track Infrared Sounder (CrIS) over the domain. An issue arose regarding the availability of CrIS data from March 25th to August 12th, 2019.

Task 3: Investigation of PM2.5 concentrations using the updated emission inventory: The UH-AQF modeling team ran the Community Multiscale Air Quality (CMAQ) model over the modeling domain for 2019 using apriori emissions. We investigated the effect of apriori NH_3 emissions on inorganic fine particulate matter (PM2.5) over Texas and the Gulf of Mexico.

In April:

Task 2: Development of the Reduced-Complexity CMAQ Model (RCCM) for NH3 and refinement of NH3 emissions using iFDMB with the combination of CMAQ model and CrIS satellite observations: Due to the missing Cross-track Infrared Sounder (CrIS) data, the UH-AQF modeling team downloaded the remote sensing data from the Infrared Atmospheric Sounding Interferometer (IASI) NH_3 data for March through August 2019. Currently, the team is developing an observation operator to utilize the IASI data for a data assimilation application.

Task 3: Investigation of PM2.5 concentrations using the updated emission inventory: The UH-AQF modeling team has performed an extensive literature review on inorganic PM2.5 chemistry and its emission inventory over Texas.

In May:

Task 2: Development of the Reduced-Complexity CMAQ Model (RCCM) for NH_3 and refinement of NH3 emissions using iFDMB with the combination of CMAQ model and CrIS satellite observations: The UH-AQF modeling team has finished developing an observation operator to utilize the Infrared Atmospheric Sounding Interferometer (IASI) data for an inverse modeling application. The evaluation of the IASI observation operator has been performed. The framework has been updated to use the IASI observation operator. The team is running the framework to produce updated emissions.

Task 3: Investigation of PM2.5 concentrations using the updated emission inventory: The UH-AQF team is working on interpreting sulfate, nitrate, ammonium, and ammonia results based on updated and prior emissions. The team has also started preparing the final report.

Preliminary Analysis: None during the reporting period.

Data Collected: The modeling team obtained the IASI NH_3 data for March through August 2019.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: We had an issue regarding running the CMAQ model to generate offline files. The issue came from the subroutine of ZADVYPPM for failing vertical advection at 090000 with an advection step of 001200 HHMMSS. It happens because the max iterations to calculate it is more than 30. The solution to fix the issue is to reduce CTM_MAXSYNC value. We set both CTM_MAXSYNC and CTM_MINSYNC equal 300, and the issue was resolved.

In March, we had an issue regarding the availability of CrIS data from March 25 to August 12, 2019. It seems that the CrIS observations on the Suomi National Polar-Orbiting Partnership (SNPP) for the period are not available because of some issues in the sensor. For the missing data, the CrIS data provider was supposed to provide the CrIS observations from National Oceanic and Atmospheric Administration-20 (NOAA-20). But it is not uploaded yet. We are in contact with them to ensure we have the missing data.

We have two alternatives if the missing data are not provided: 1. using the Infrared Atmospheric Sounding Interferometer (IASI) satellite when the CrIS data are unavailable. 2. switching from 2019 to 2018 or 2017 when all data are available.

Goals and Anticipated Issues for the Succeeding Reporting Period: The UH-AQF team will continue to run the framework and investigate updated emissions. The team will continue working on preparing the final report.

Detailed Analysis of the Progress of the Task Order to Date: Progress being made as planned.

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: In February, the winter deployment was completed, and 14 days of data were obtained in the Houston area to sample volatile chemical products (VCP). Data was collected from four different routes around the Greater Houston area. The initial data analysis for the trace gases (Vocus) for the fall campaign and the particle phase chemical composition (AMS) for both the fall and winter campaigns was completed.

In March, the initial data analysis for the trace gases (Vocus) for the fall campaign and the particle phase chemical composition (AMS) for both the fall and winter campaigns was completed. Work continued on the analysis of trace gases (Vocus) for the winter campaign. Undergraduate students were trained to use IgorPro software to analyze trace gas concentrations.

In April, the initial data analysis for the trace gases (Vocus) and the particle phase chemical composition (AMS) for both the fall and winter campaigns was completed. Work continued on the analysis of trace gases (Vocus) to account for instrument calibration.

In May, the initial data analysis for the trace gases (Vocus) and the particle phase chemical composition (AMS) for both the fall and winter campaigns was completed. Work continued on the analysis of trace gases (Vocus) to account for instrument calibration.

Data Collected: Collected a full suite of data on trace gases (Vocus), particle phase chemical composition (AMS), CO, NO_2, O_3, aerosol size distribution, and GPS location during our deployment around Houston, Rockport, Corpus Christi, San Antonio, and Austin.

Collected the above gas and particle information during the day and at night, on both weekends and weekdays, and on sunny, cloudy, and rainy days, during the fall and winter.

Collected Vocus data in both ammonia (NH4+) mode and water cluster (H3O+) mode.

Obtained the organic concentration of particle phase compounds and identified concentrations for volatile chemical products (VCPs) for both the fall and winter campaigns.

Identified concentrations for 61 different VCP compounds for the fall and winter campaigns.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: N/A

Goals and Anticipated Issues for the Succeeding Reporting Period: Dr. Zhang's lab worked on the data analysis for all data collected from both the Fall and Winter field campaigns. The data was paired with GPS locations to identify areas of high and low VCP concentrations. The data included trace gases (Vocus), particle phase chemical composition (AMS), CO, NO_2, O_3, aerosol size distribution, and GPS location.

Dr. Qi Ying's lab worked on the CMAQ model simulation to prepare for analyzing the VCP data collected from this deployment.

Based on the progress made, both goals were on track.

Detailed Analysis of the Progress of the Task Order to Date: Beginning in February, the lab completed the second field campaign for winter. PI Zhang's lab went to Houston, Corpus Christi, San Antonio, and Austin to sample. The Corpus Christi sample is to cross compare with the data obtained in the Houston to determine a background concentration, as shown in Figure 22-020-1. Graduate students Alana Dodero, Sining Niu, and Sahir Gagan have all participated in the project.

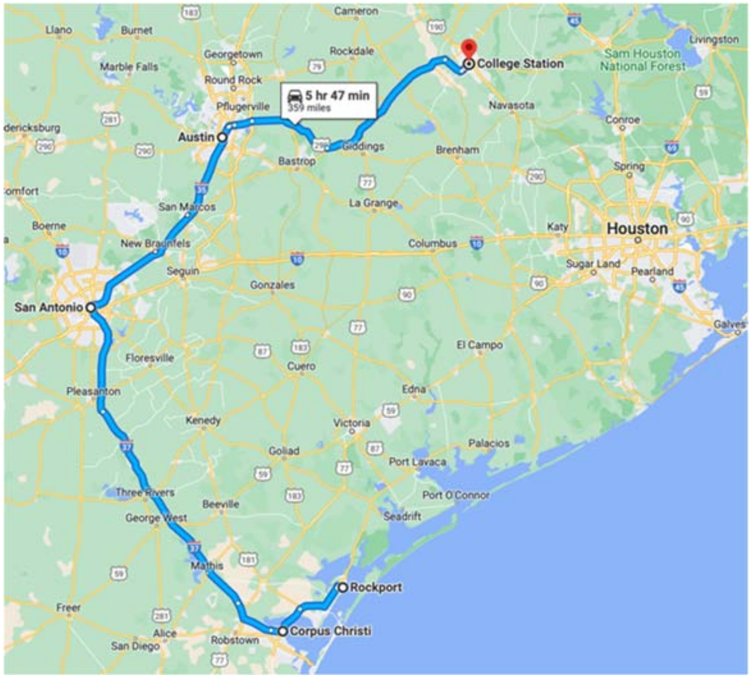


Figure 22-020-1. Deployment map during the field project in November 2022 (Rockport, Corpus Christi, San Antonio, and Austin route)

We are conducting the initial data analysis to determine spatial trends of VCPs in the Houston area. Then we will compare the fall and winter deployments to understand the seasonal variation of VCP and the impact vegetation has on VCP concentrations. We will additionally analyze the diurnal trend of VCP.

We are currently completing the initial data analysis for the gas phase compounds. Below are preliminary results of the organic concentration of particle compounds in the Houston area shown in Figure 22-020-2. Additionally, Figure 22-020-3 shows the concentration of D5 Siloxane, a compound commonly used in personal care products. The peaks in concentration are due to calibration of Vocus, which occurred every hour. Next steps will include correcting for the calibration points, and converting the ions/s data to concentration (parts per trillion).

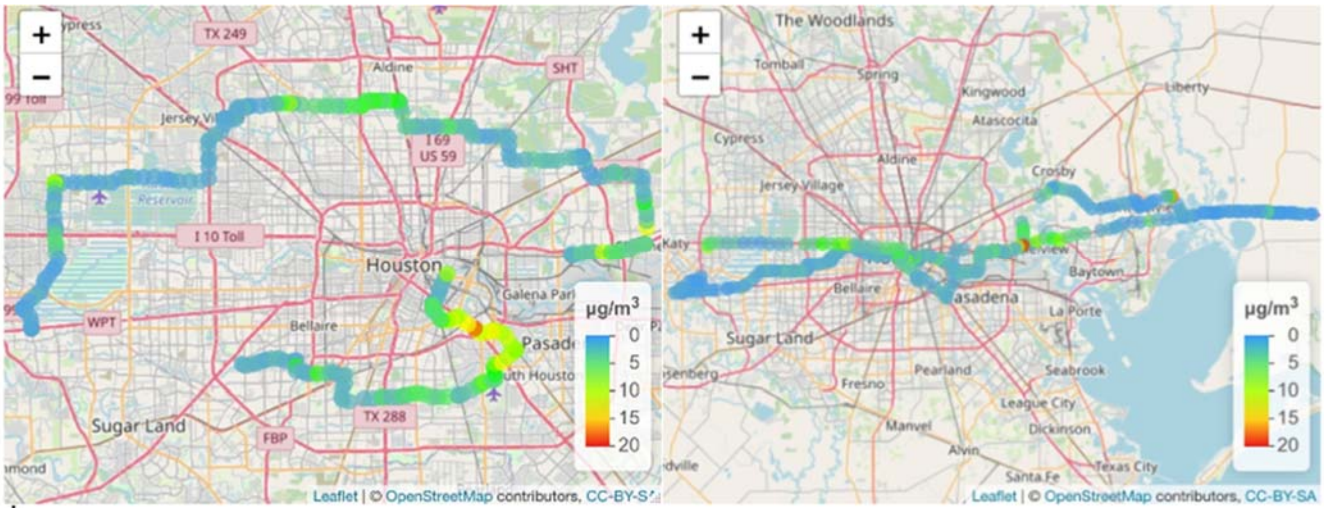


Figure 22-020-2. Organic concentration of particle compounds (AMS)

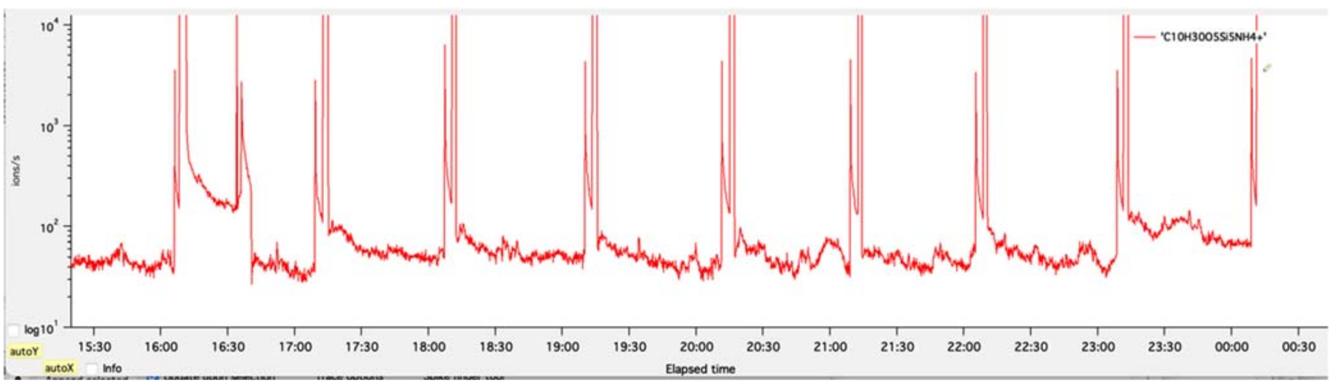


Figure 22-020-3. D5 Siloxane ambient concentration

We plan to complete the initial data analysis to determine spatial trends of VCPs in the Houston area. Then we will compare the fall and winter deployments to understand the seasonal variation of VCP and the impact vegetation has on VCP concentrations. We will additionally analyze the diurnal trend of VCP.

We are currently completing the initial data analysis for the gas phase compounds. From the initial analysis, Alana has identified more than 3000 compounds from the air in Houston. Once these compounds are identified, Alana has been working on the time series of some key VCP compounds.

Below are some of the important VCP compounds from the mobile measurements during the winter campaign. Figure 22-020-4 shows the m/Q of ~216 and the different compounds assigned to this peak. One of these compounds is Texanol ($C_{12}H_{22}O_2$), a compound found in water-based coatings and adhesives. Similarly, Figure 22-020-5 shows the peak for D4 siloxane ($C_8H_{24}O_4Si_4$), which is found in adhesives and insecticides, and Figure 22-020-6 shows the peak for D5 siloxane ($C_{10}H_{30}O_5Si_5$), which is found in personal care products. Next steps will include correcting for the calibration points, and converting the ions/s data to PPT.

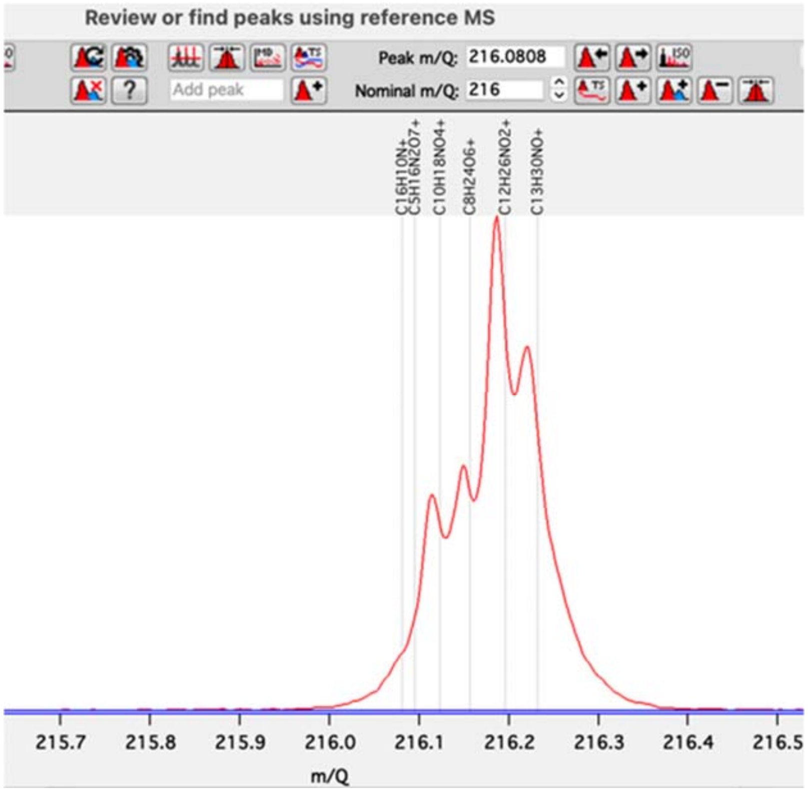


Figure 22-020-4. Peak for D5 Siloxane

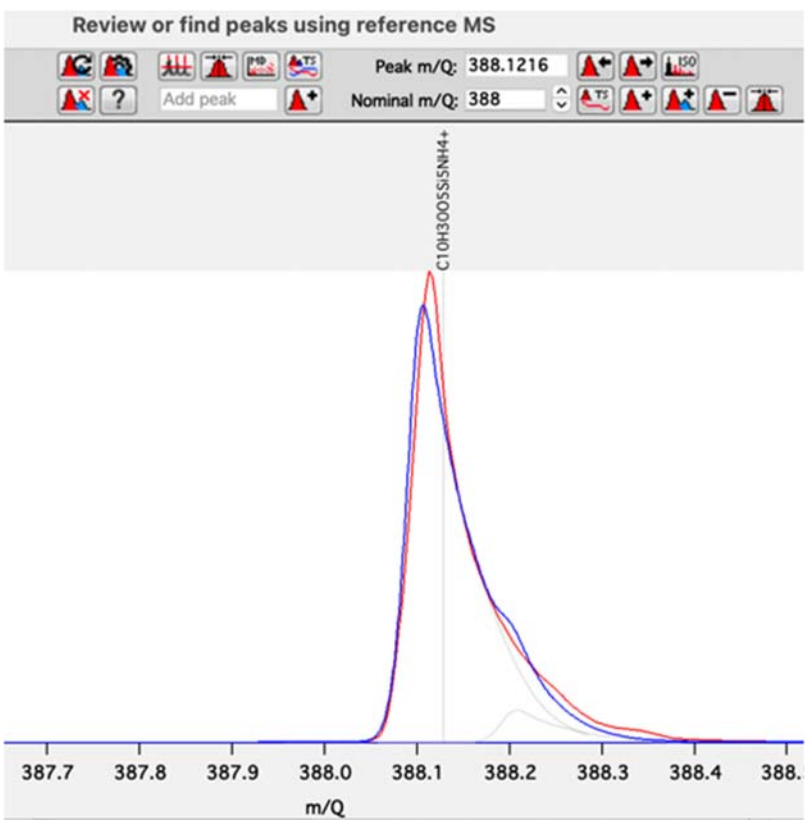


Figure 22-020-5. Peak for D4 Siloxane

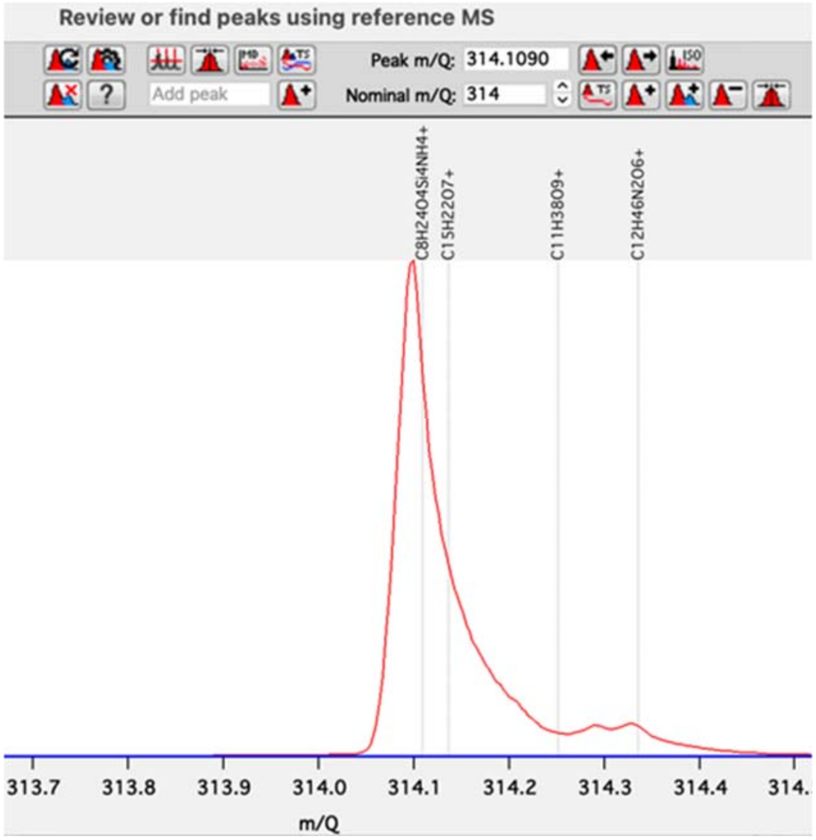


Figure 22-020-6. Peak for D5 Siloxane

We plan to complete the initial data analysis to determine spatial trends of VCPs in the Houston area. Then we will compare the fall and winter deployments to understand the seasonal variation of VCP and the impact vegetation has on VCP concentrations. We will additionally analyze the diurnal trend of VCP.

We are completing the final steps for analyzing gas phase compounds. We need to account for the calibrations that occurred ~every hour during deployments. We next need to convert the gas phase compound data from ions/second to ppb.

Dr. Qi Ying's lab has added 29 different VCP compounds to their simulations. Once we have finished the analysis of the gas phase compound data, we will work with them to compare our measurements with their simulations. Additionally, we can compare our measured ozone, CO, and NO_2 data with their simulations.

We plan to complete the initial data analysis to determine spatial trends of VCPs in the Houston area. Then we will compare the fall and winter deployments to understand the seasonal variation of VCP and the impact vegetation has on VCP concentrations. We will identify the factors impacting days of high concentrations and areas with high concentrations. We will additionally compare the field measurements with CMAQ model simulations. Figures 22-020-7 and 22-020-8 show the average model concentrations for ozone and CO from 10/16/2022-10/31/2022.

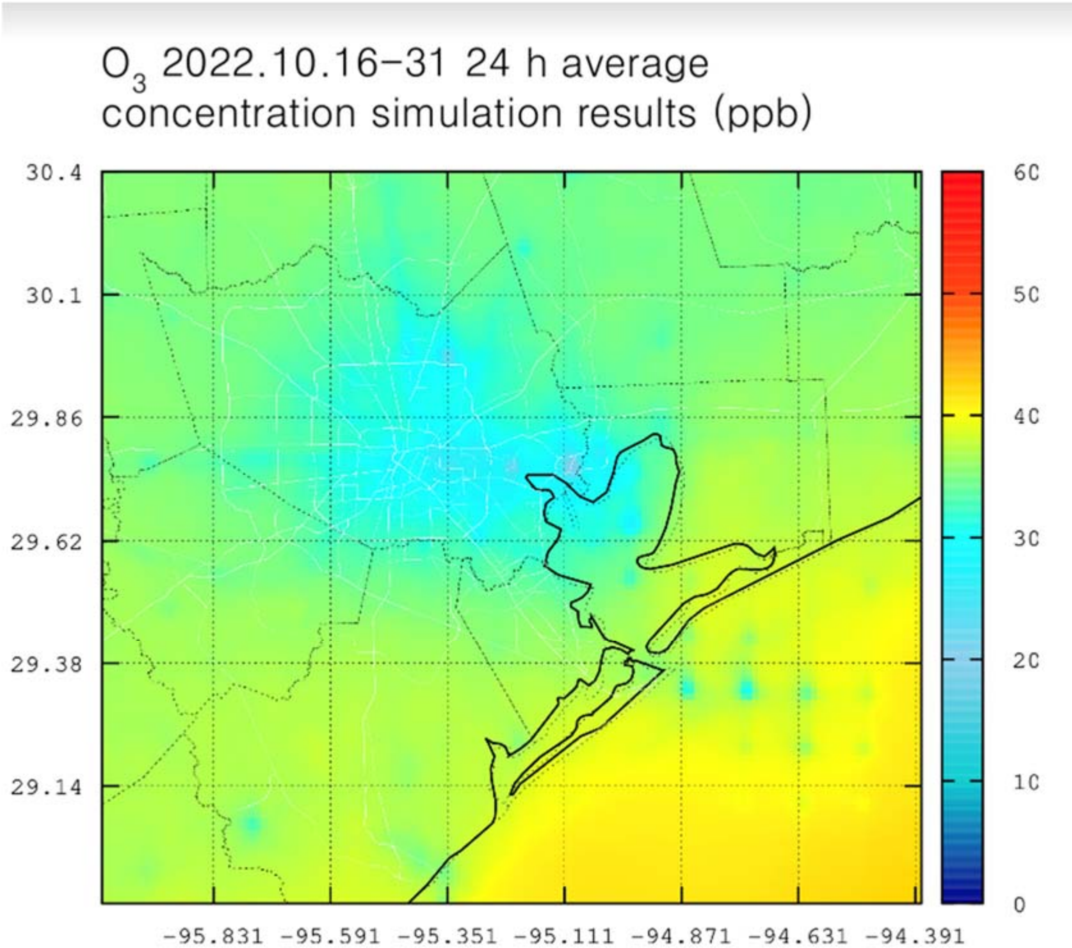


Figure 22-020-7. Average O_3 concentration 10/16-10/31

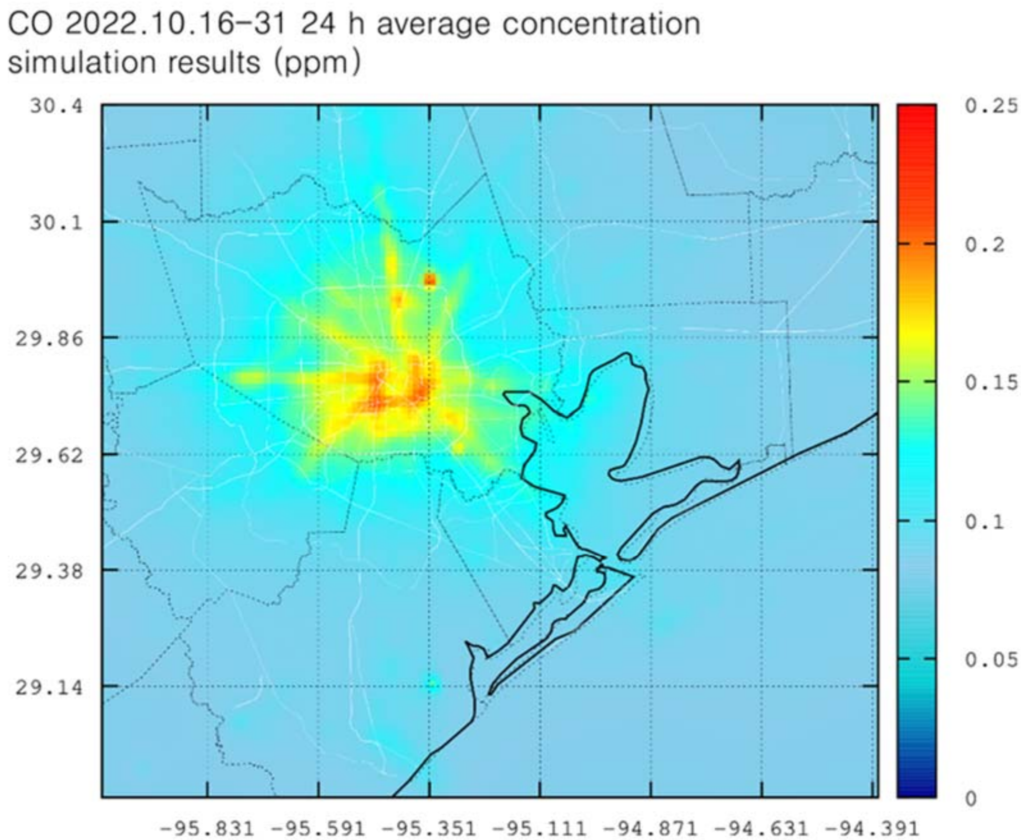


Figure 22-020-8. Average CO concentration (10/16-10/31)

We are completing the final steps for analyzing gas phase compounds. We need to account for the calibrations that occurred ~every hour during deployments. We next need to convert the gas phase compound data from ions/second to ppb. The figures below show the spatial distribution for monoterpenes (Figure 22-020-9), texanol (Figure 22-020-10), D4 siloxane (Figure 22-020-11), and D5 siloxane (Figure 22-020-12).

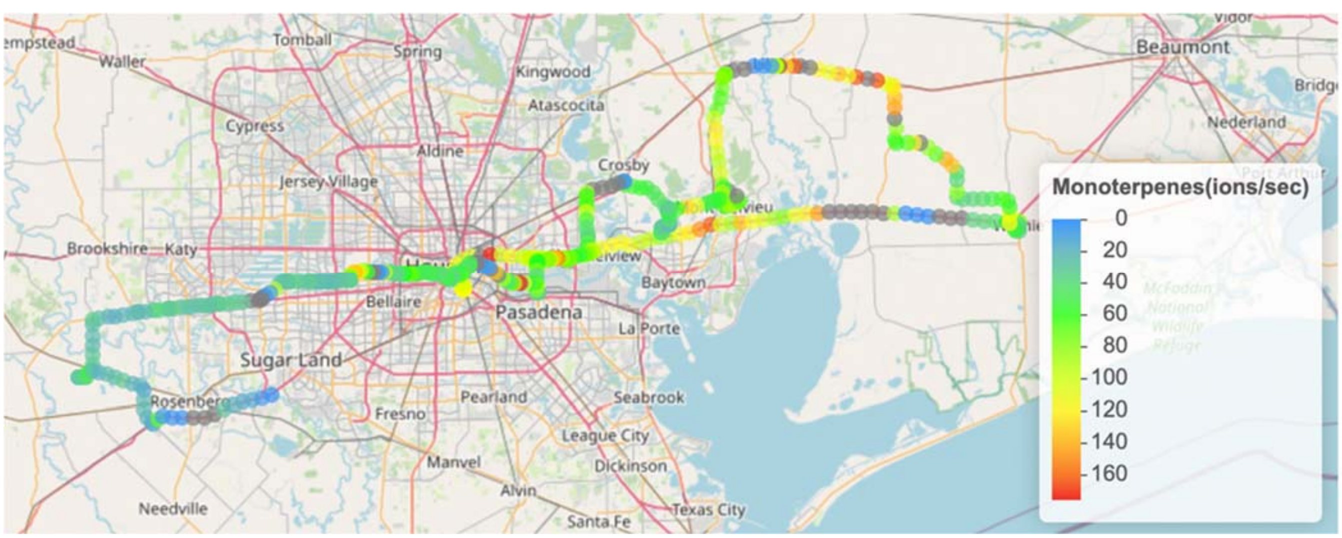


Figure 22-020-9. Monoterpenes

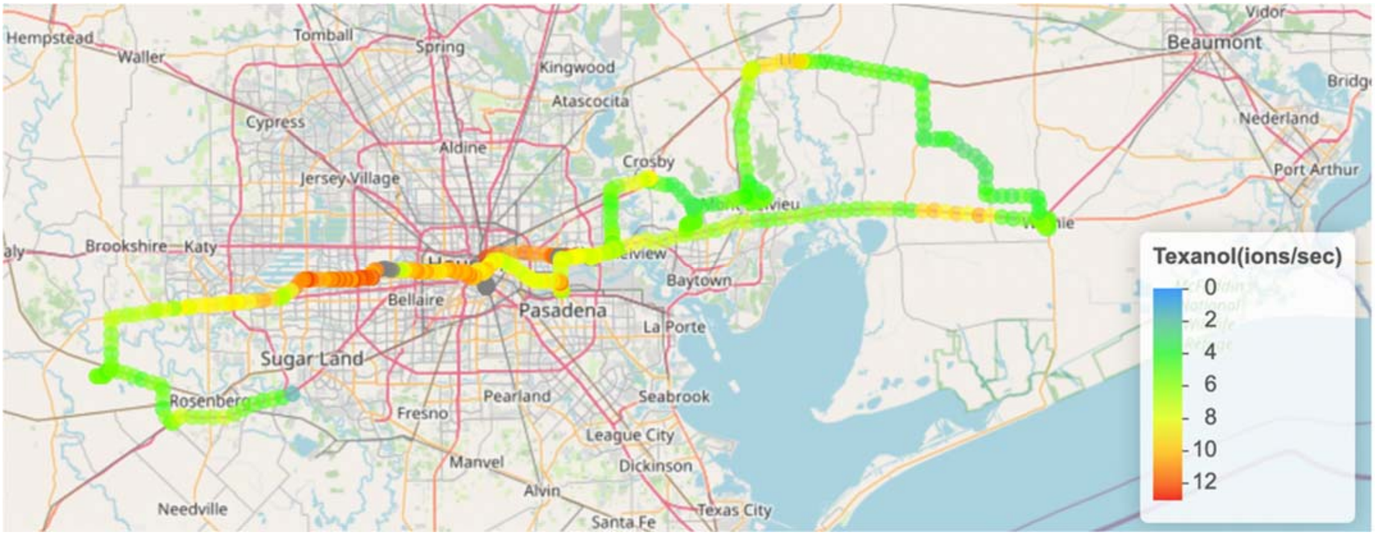


Figure 22-020-10. Texanol

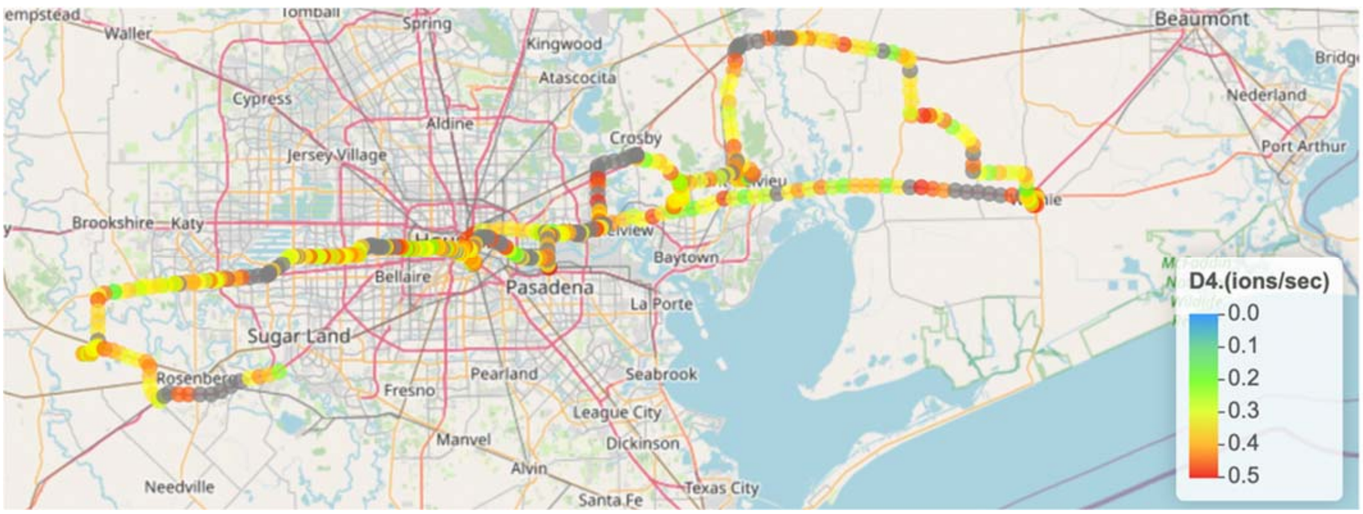


Figure 22-020-11. D4 Siloxane

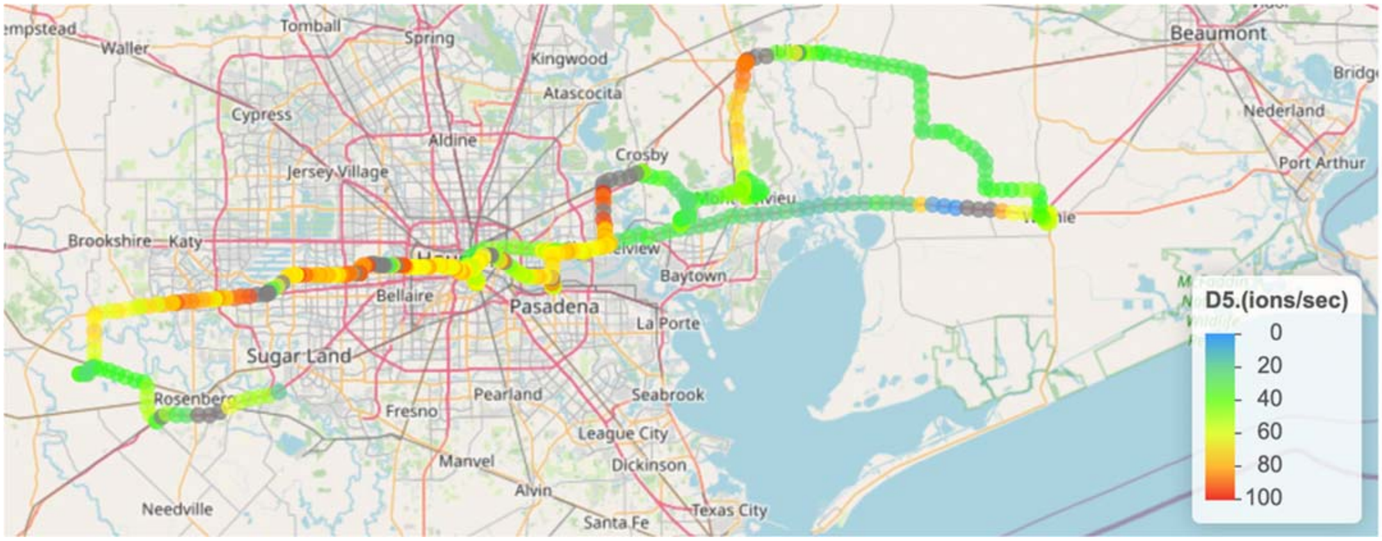


Figure 22-020-12. D5 Siloxane

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:

In February, *Task 1: Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx:* The WRF-CAMx simulation was completed in February 2023. The model output for the two GCAS measurement periods, August 30 to September 11, 2021, and September 23 to September 27, 2021, with additional days of spin-up, was provided to the full team. Model output for all days in August and September for which there was GCAS data was provided. The model was re-run in April 2023 to fix some of the model source apportionment tagging, and the updated output was provided to the team for further analysis. QA/QC of the model output was ongoing.

Task 2. Process the GCAS measurements: The reprocessing of the GCAS aircraft measurements with very minor adjustments was completed in February 2023, and all new files were made available to the full team, and posted on the TRACER-AQ data archive (https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021).

Task 3. Process the satellite NO_2 data: Waited on model simulation (See Task 1) in order to re-process the satellite air mass factor. This task was re-initiated in March 2023.

Task 4. Calculating NO_X from NO_2 airshed measurements: This task was re-initiated in February 2023. NO_X emissions from three point sources (Parish Power Plant, Texas City, and Mont Belvieu) were calculated from the new GCAS data. The team was able to generate reasonable NO_X emissions estimates from these point sources. Additional QA/QC on the methodology – comparison with the CEMS data when available – occured in March 2023.

Task 5. Comparison of NO_2, HCHO, O_3 between model, aircraft, and satellite: An in-depth comparison between the aircraft, satellite, and Pandora instruments for NO_2 was initiated, and code was prepared to handle the model simulation.

In March, *Task 1: Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx:* The first WRF-CAMx simulation was completed in February 2023. There is model output for the two GCAS measurement periods: August 30 – September 11, 2021 and September 23 – September 27, 2021 with additional days of spin-up prior to each episode that will not be utilized. The QA/QC of the simulation – comparison with ground monitor data – is currently on-going. Model output for all days in August and September for which there is GCAS data has been provided to the full team. In March 2023, the model was re-run to fix some of the model source apportionment tagging. QA/QC of the model output is on-going.

Task 2. Process the GCAS measurements: The reprocessing of the GCAS aircraft measurements with very minor adjustments was completed in February 2023, and all new files were made available to the full team, and posted on the TRACER-AQ data archive (https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021). The GCAS measurements are now being re-processed with the CAMx model output.

Task 3. Process the satellite NO_2 data: The satellite air mass factor has been processed for all days in September using the CAMx model output, and the resulting data has been provided to the team. Further minor adjustments may be made in April 2023.

Task 4. Calculating NO_X from NO_2 airshed measurements: NO_X emissions from several point sources (W.A. Parish Power Plant, Texas City, Bayview ExxonMobil, Lyondell Basell Channelview, and Mont Belvieu) were calculated from the new GCAS data. The team was able to generate reasonable NO_X emissions estimates from these point sources. Additional QA/QC on the methodology – and comparison with the CEMS data when available – will occur in April 2023.

Additionally, NO_2 divergence has been calculated for the Houston area. On-going work is determining which assumptions should be made in order to calculate NO_X emission rates.

Task 5. Comparison of NO_2, HCHO, O_3 between model, aircraft, and satellite: An in-depth comparison between the aircraft, satellite, model, and Pandora instruments for NO_2 is on-going. Additional results are expected in April 2023.

In April, *Task 1: Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx:* The first WRF-CAMx simulation was completed in February 2023. There is model output for the two GCAS measurement periods: August 30 – September 11, 2021 and September 23 – September 27, 2021 with additional days of spin-up prior to each episode that will not be utilized. Model output for all days in August and September for which there is GCAS data has been provided to the full team. See Figure 1c. In April 2023, the model was re-run to fix some of the model source apportionment tagging, and has been provided to the team for further analysis. QA/QC of the model output is on-going.

Task 2. Process the GCAS measurements: The reprocessing of the GCAS aircraft measurements with very minor adjustments was completed in February 2023, and all new files were made available to the full team, and posted on the TRACER-AQ data archive (https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021).

The GCAS measurements are now being re-processed with the CAMx model output. We expect only minor adjustments.

Task 3. Process the satellite NO_2 data: The satellite air mass factor has been processed for all days in September using the CAMx model output, and the resulting data has been provided to the team. This task is now fully completed.

Task 4. Calculating NO_X from NO_2 airshed measurements: NO_X emissions from several point sources (W.A. Parish Power Plant, Texas City, Bayview ExxonMobil, Lyondell Basell Channelview, and Mont Belvieu) were calculated from the new GCAS data. The team was able to generate reasonable NO_X emissions estimates from these point sources.

We are now completing an in-depth comparison between the GCAS data, TROPOMI satellite data, and CAMx model output at the location of the W.A. Parish plant to better understand uncertainties in the three datasets before making any firm conclusions. See Task 5.

Additionally, NO_2 divergence has been calculated for the Houston area. On-going work is determining which assumptions should be made in order to calculate NO_X emission rates. This task should be complete in May 2023.

Task 5. Comparison of NO_2, HCHO, O_3 between model, aircraft, and satellite: An in-depth comparison between the aircraft, satellite, model, and Pandora instruments for NO_2 is on-going. Please see the Preliminary Analyses section for more updates.

In May, *Task 1: Simulate NO_2, HCHO, O_3 at 444 × 444 m^2 spatial resolution using WRF-CAMx:* The final WRF-CAMx simulation was completed in May 2023. There is model output for the two GCAS measurement periods: August 30 – September 11, 2021 and September 23 – September 27, 2021 with additional days of spin-up prior to each episode that will not be utilized. This latest model run includes updated emissions based on CEM hourly data for two additional power plants. Model output for all days in August and September for which there is GCAS data has been provided to the full team. See Figure 1c. QA/QC of the model output is on-going.

Task 2. Process the GCAS measurements: The reprocessing of the GCAS aircraft measurements with very minor adjustments was completed in February 2023, and all new files were made available to the full team, and posted on the TRACER-AQ data archive (https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021).

In May, GCAS measurements were re-processed with the initial CAMx model output. The team is exploring the differences now, but the average increase in the AMF is 5% and the average difference in the vertical column density is 2.2×10^{14} molecules cm^{-2}. These files will be updated with the most up-to-date model run in June 2023 and used for the final version of the products delivered in Tasks 4, 5 and 6.

Task 3. Process the satellite NO_2 data: The satellite air mass factor has been processed for all days in September using the CAMx model output, and the resulting data has been provided to the team. This task is now fully completed.

Task 4. Calculating NO_X from NO_2 airshed measurements: NO_X emissions from several point sources (W.A. Parish Power Plant, Texas City, Bayview ExxonMobil, Lyondell Basell Channelview, and Mont Belvieu) were calculated from the new GCAS data. The team was able to generate reasonable NO_X emissions estimates from these point sources.

We are now completing an in-depth comparison between the GCAS data, TROPOMI satellite data, and CAMx model output at the location of the W.A. Parish plant to better understand uncertainties in the three datasets before making any firm conclusions. See Task 5.

Additionally, NO_2 divergence has been calculated for the Houston area. On-going work is determining which assumptions should be made in order to calculate NO_X emission rates. The flux divergence was calculated using the new GCAS retrievals that use the CAMx Air Mass Factors. This led to an improved characterization of ship emissions and reduced noise in the background. We also performed the method on the CAMx fields themselves in order to better constrain the emission estimates and identify calibration factors.

This task will be completed in June 2023.

Task 5. Comparison of NO_2, HCHO, O_3 between model, aircraft, and satellite: An in-depth comparison between the aircraft, satellite, model, and Pandora instruments for NO_2 is on-going. Please see the Preliminary Analyses section for more updates.

Task 6. Use of machine learning to estimate emission factors for individual sectors: Task 6 was initiated in May 2023. Preliminary tests have been conducted with the new CAMx simulations. A multi-linear regression model was set up to estimate scaling factors for each of 16 source sectors in order to obtain an optimal match between CAMx simulations and GCAS retrievals. We are currently testing the code and performing sensitivity tests.

Preliminary Analysis:

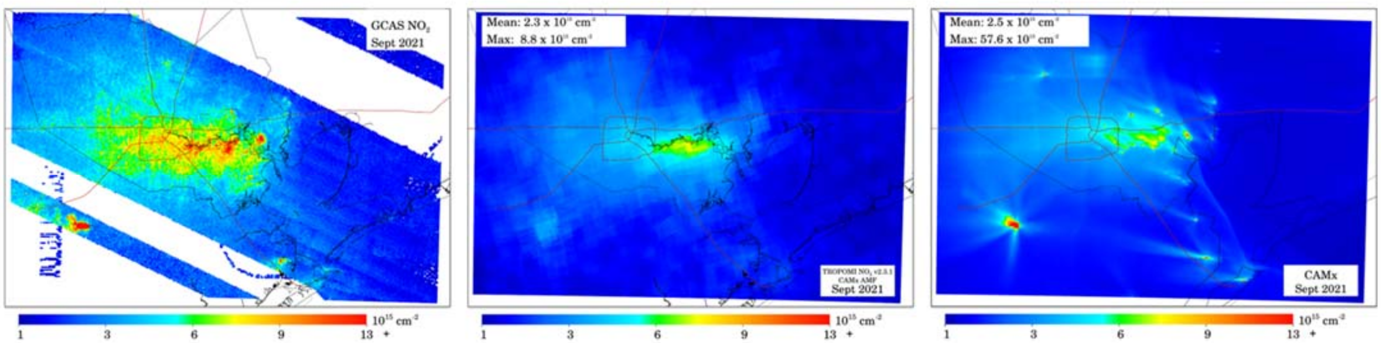


Figure 22-023-1. Vertical column NO_2 averaged during the early afternoon for September 2021. Left panel shows the monthly average from the aircraft (GCAS). Center panel shows the monthly average from the satellite (TROPOMI) with an air mass factor re-processed using the CAMx model simulation. Right panel shows the monthly average from the CAMx model simulation. All datasets are on the same grid.

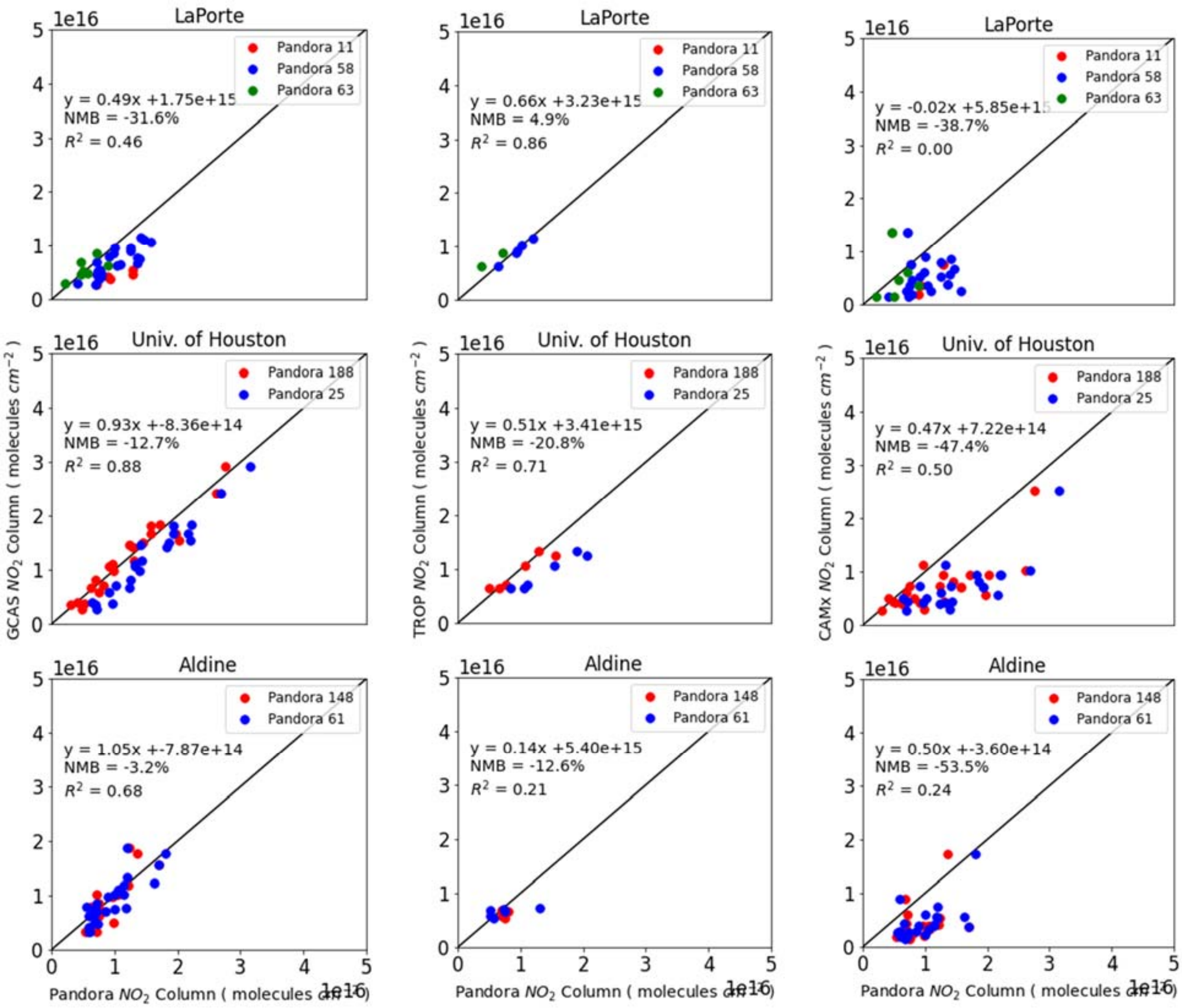


Figure 22-023-2. Comparison of the vertical column NO_2 between the Pandora instruments and the (left column) GCAS measurements, (center column) TROPOMI measurements, (right column) model output for all collocations in time and space during September 2021. Each row represents a different Pandora location: (top) LaPorte, (center) University of Houston, (bottom) Aldine.

Satellite vs GCAS **CAMx vs GCAS** **CAMx vs Satellite**

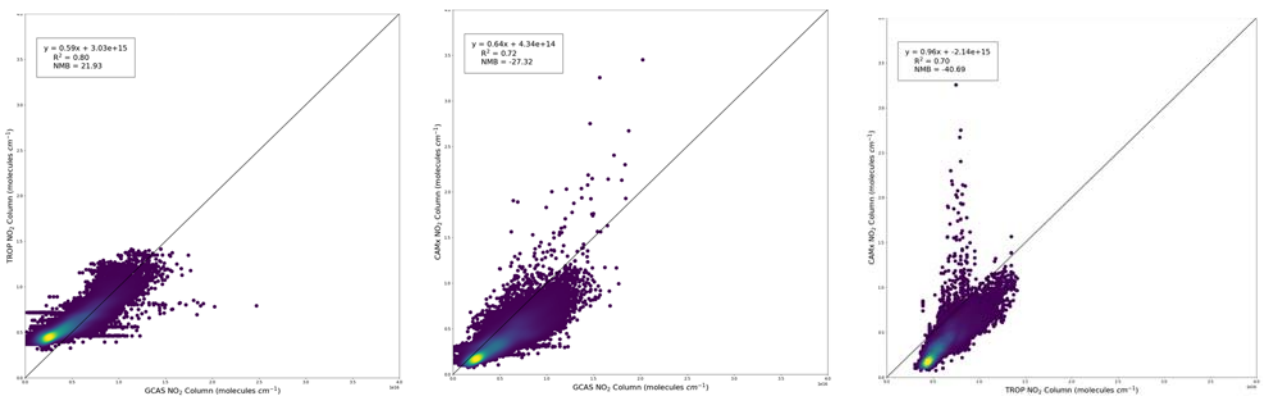


Figure 22-023-3. Comparison of the vertical column NO_2 between the (left) satellite and GCAS, (center) CAMx and GCAS, and (right) CAMx and satellite. CAMx appears to have smaller column NO_2 values than both GCAS and the satellite, except in the presence of point source plumes. The satellite has larger column NO_2 values than GCAS in rural areas, and may be related to missing column NO_2 measurements above the aircraft which was not accounted for in this analysis.

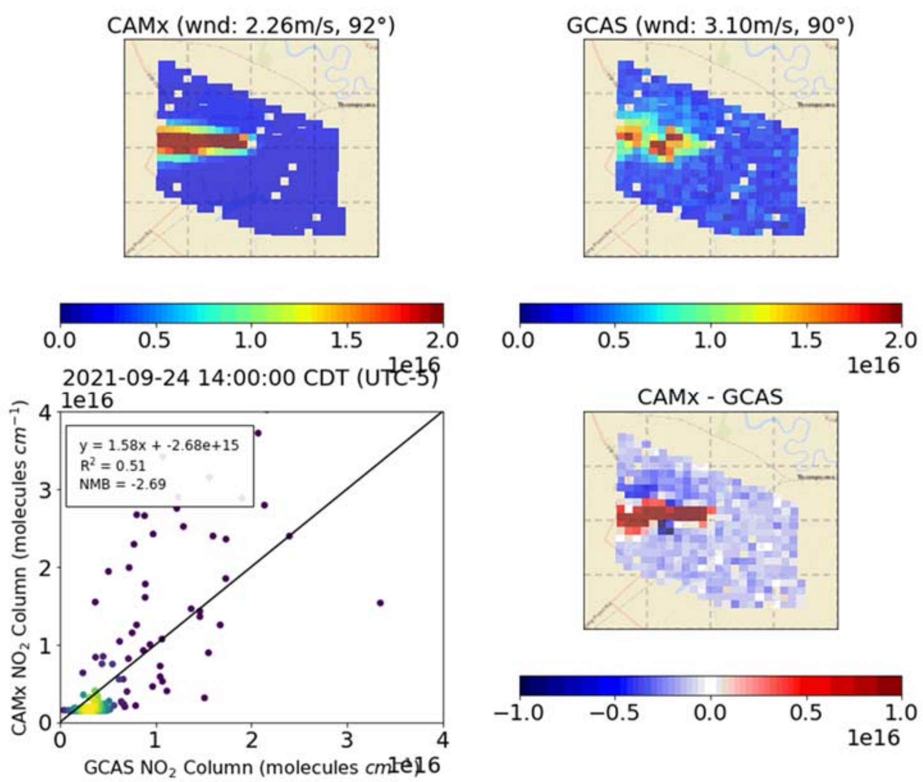


Figure 22-023-4. Comparison of the vertical column NO_2 at the location of the W.A. Parish Power Plant on September 24, 2023 between the (top left) model and (top right) GCAS. There is excellent agreement in the location of the wind plume direction. (Bottom left) Scatterplot comparison between the two plots in the top row. (Bottom right) Difference plot between the two plots in the top row.

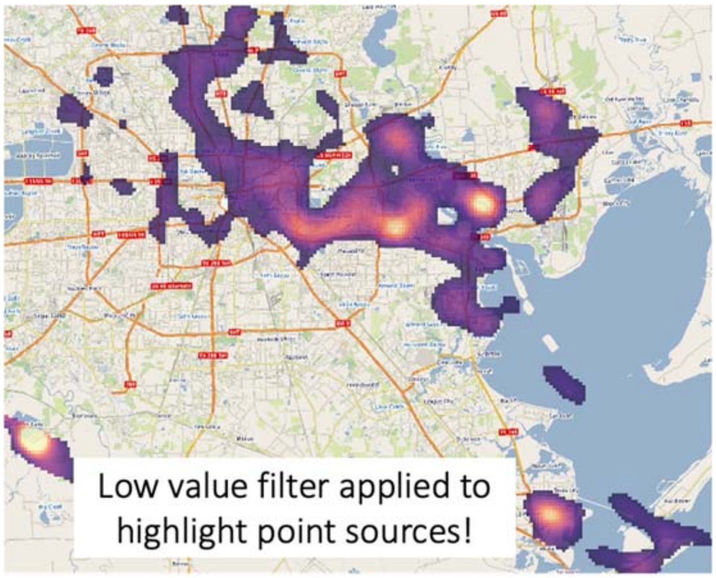


Figure 22-023-5. Smoothed NO_2 flux divergence – incremental addition of NO_2 in each grid cell – using all the measurements from the GCAS aircraft. Lighter color are larger values, darker colors are smaller values; ***a low value filter is applied to highlight point sources***. Additional assumptions will need to be made to derive NO_X emission rates.

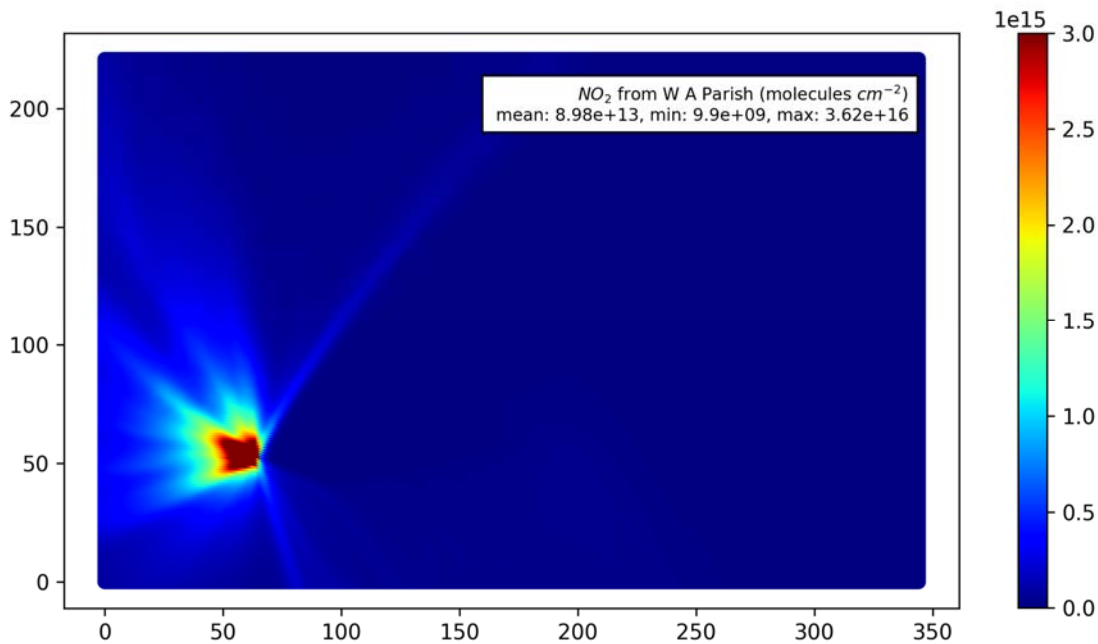


Figure 22-023-6. CAMx simulated source apportioned NO_2 columns from W A Parish power plant from between 8am and 5pm on GCAS flight days. Redder colors indicate higher NO_2 columns contributed by emissions from W A Parish in CAMx simulation while bluer colors indicate lower NO_2 columns. The x and y axes correspond to grid cells in the CAMx domain. Mean, minimum and maximum values are indicated in the top right.

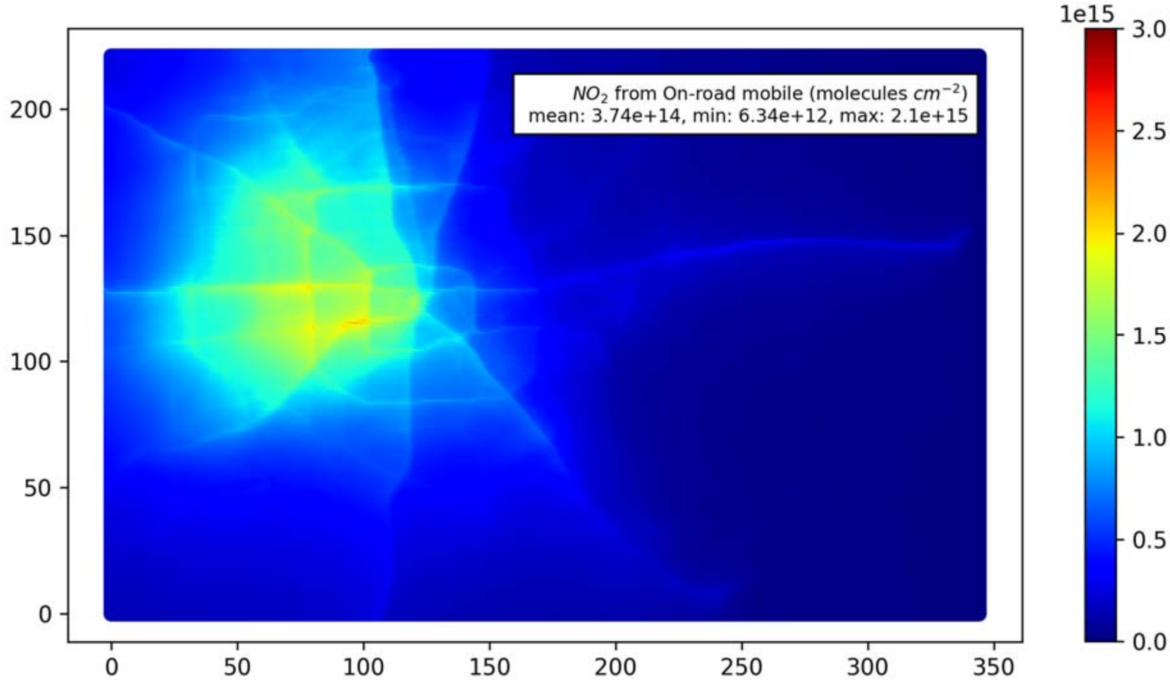


Figure 22-023-7. CAMx simulated source apportioned NO_2 columns from on-road vehicle emissions from between 8am and 5pm on GCAS flight days. Redder colors indicate higher NO_2 columns contributed by emissions from on-road vehicles in CAMx simulation while bluer colors indicate lower NO_2 columns. The x and y axes correspond to grid cells in the CAMx domain. Mean, minimum and maximum values are indicated in the top right.

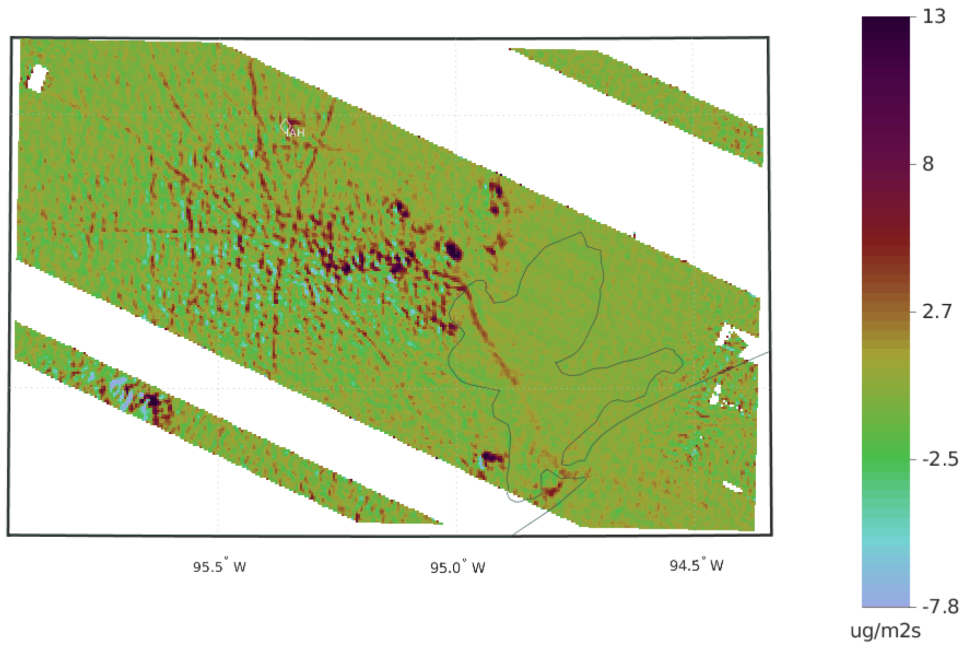


Figure 22-023-8. Flux divergence field using GCAS retrievals with CAMx Air Mass Factors. Point sources can be clearly seen, as well as the emissions from ship traffic through the bay and the signature from highways.

Data Collected: None.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments: Project approvals occurred later than anticipated. Development of the WRF-CAMx simulation was delayed by approximately 8-weeks. Model simulation output was delivered to the full team at the end of 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: Task 1 – The model output will continue to go through a QA/QC check and a comparison of the model output with the ground monitors will be completed.

Task 2 – Initial analysis completed. We will continue QA/QC and update analysis using the latest CAMx simulation in June.

Task 3 – Completed

Task 4 – NO_X emissions estimates from the point sources and using the flux divergence method will go through additional comparison with the CAMx simulation. This task should be complete in June 2023.

Task 5 – Intercomparison between the aircraft (GCAS), satellite (TROPOMI), and model (WRF-CAMx) will continue. This will constitute the majority of the work during June 2023.

Task 6 – This was initiated in May 2023

Detailed Analysis of the Progress of the Task Order to Date: Progressing as planned.

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 May 2023)

Budget Category	FY22 Budget	FY23 Budget	Total Budget	Remaining Balance
Personnel/Salary	$44,702.77	$51,800.00	$96,502.77	$16,931.97
Fringe Benefits	$13,812.96	$16,265.00	$30,077.96	$5,875.56
Supplies	$12,013.99	$1,755.00	$13,768.99	$11,683.59
Total Direct Costs	$70,529.72	$69,820.00	$140,349.72	$34,491.12
Authorized Indirect Costs *(10% of Salaries and Wages)*	$4,470.28	$5,180.00	$9,650.28	$1,693.20
Total Costs	**$75,000.00**	**$75,000.00**	**$150,000.00**	**$36,184.32**

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 May 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 May 2023)

Budget Category	FY22 Budget	FY23 Budget	Total Budget	Remaining Balance
Personnel/Salary	$38,000.00	$38,000.00	$76,000.00	$16,998.47
Fringe Benefits	$11,438.00	$11,932.00	$23,370.00	$5,632.78
Supplies	$3,012.00	$2,518.00	$5,530.00	$5,046.37
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	$31,427.62
Authorized Indirect Costs *(10% of Salaries and Wages)*	$3,800.00	$3,800.00	$7,600.00	$1,699.82
Total Costs	**$58,125.00**	**$58,125.00**	**$116,250.00**	**$33,127.44**

RESEARCH PROJECTS

All research projects have Subaward Agreements fully executed. Table 4 shows the FY 22-23 Research Project budgets and expenditures actually incurred on the UT account as of May 31, 2023. The FY 22-23 budget allocates $1,222,500.00 for research projects.

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

Project Number	Institution	Amount Awarded	Cumulative Expenditures	Remaining Balance
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	$97,063.90	$64,324.10
22-006	Aerodyne Research, Inc. (ARI)	$51,255.00	$17,001.97	$34,253.03
22-006	Baylor University	$57,225.00	$1,868.76	$55,356.24
22-008	University of Houston	$175,621.00	$26,827.73	$148,793.27
22-008	St. Edward's University	$6,103.00	$0.00	$6,103.00
22-010	Aerodyne Research, Inc.	$228,418.00	$32,393.56	$196,024.44
22-019	University of Houston	$131,366.00	$36,603.23	$94,762.77
22-020	Texas A&M University	$160,182.00	$44,283.93	$115,898.07
22-023	The George Washington University	$103,425.00	$25,239.09	$78,185.91
22-023	Ramboll	$144,721.60	$90,605.27	$54,116.33
FY 23 Total Contractual Funding Awarded		$1,219,704.60		
FY 23 Contractual Funds Expended (Init. Projects)			$371,887.44	
FY 23 Contractual Funds Remaining to be Spent				$239,362.56
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			**$371,887.44**	
Total Contractual Funds Remaining to be Spent				**$850,612.56**

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, August Kaiser
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