Air Quality Data Collection Support for TRACER-AQ in Houston

Final Report

Grant Number: 582-18-81339
Proposal for Grant Activities No. 582-21-22179-015
Tracking No. 2021-07 & 2021-24

Prepared for the Texas Commission on Environmental Quality (TCEQ)

Principal Investigators

James Flynn, University of Houston

Yuxuan Wang, University of Houston

Rebecca Sheesley, Baylor University

Sascha Usenko, Baylor University

Paul Walter, St. Edward's University

Mark Estes, St. Edward's University

November 30, 2022

Table of Contents

Executive Summary

The Department of Energy (DOE)'s Tracking Aerosol-Cloud Interaction Experiment (TRACER) project deployed the ARM Mobile Facility #1 to Houston in 2021 and conducted detailed meteorological and aerosol measurements for a year to examine the relationship of anthropogenic and natural aerosols and convection with an emphasis on thunderstorms and deep convection. To leverage the assets deployed in Houston for the DOE TRACER campaign, NASA's Tropospheric Composition program funded the TRACER-Air Quality (TRACER-AQ) campaign in September 2021 and made observations include: 1) ozone (O_3) profiles from the Goddard and Langley mobile ozone lidars, 2) columnar values of Nitrogen Dioxide (NO_2), O_3, and Formaldehyde (HCHO) from the ground-based Pandora spectrometers, and 3) aircraft observations by the Johnson Gulfstream-V research aircraft that carried a suite of instrumentation including the GEOCAPE Airborne Simulator (GCAS) for observations of O_3 precursors (NO_2 and HCHO columns) and the High Spectral Resolution Lidar-2 (HSRL-2) for O_3 and aerosols profiles. Other NASA programs also sent additional instrumentation into the field, including CIMEL Sun Photometers from the AERONET program and a micropulse lidar from the MPLnet program.

This TCEQ project, referred to as TRACER-AQ1, further leverages the DOE TRACER and NASA TRACER-AQ measurements by adding support for suites of in-situ atmospheric composition and meteorological measurements from ground-sites, mobile laboratories, boat platforms, and ozonesondes in summer, 2021. Three main universities, University of Houston (UH), Baylor University (BU), and St. Edward's University (SEU), were supported to conduct this research. Key sampling platforms included the UH Mobile Air Quality Laboratory #1 (MAQL1), the Baylor Mobile Air Quality Laboratory #2 (MAQL2), the UH pontoon boat in Galveston Bay, two commercial boats (a shrimp boat and the M/V Red Eagle) in the east side of the Galveston Bay and the Gulf of Mexico, respectively, and ozonesondes. This project also provided logistical support for the deployment of assets from NASA, University of Oklahoma (OU), and Virginia Tech.

This highly successful program, performed during COVID, included numerous significant findings. The overwater measurements have drawn particular attention with observations of high levels of O_3 in Galveston Bay and the Gulf of Mexico with the pontoon and automated sampling systems. A total of 56 ozonesondes were launched, and an additional 20 were supported by AQRP and 20 more by NASA. This project marked the first time that both MAQL1 and MAQL2 were deployed in tandem. Additional VOC measurement capabilities enhanced the measurement capacity of both labs. Together the labs found high levels of nighttime isoprene emissions near the ship channel and captured a high ethene event on September 27, 2021. MAQL1 was also able to document the evolution of Houston's urban plume as it developed and migrated across the area as well as identifying SO_2 emissions from the Parrish power plant. Drone based measurement capabilities were also established under this project and will be expanded upon in future work.

1. Introduction

The Department of Energy (DOE)'s Tracking Aerosol-Cloud Interaction Experiment (TRACER) project deployed the ARM Mobile Facility #1 to Houston in 2021 and conducted detailed meteorological and aerosol measurements for a year to examine the relationship of anthropogenic and natural aerosols and convection with an emphasis on thunderstorms and deep convection. The long-term goals of the DOE TRACER study include improving weather forecasts and the ability to better identify potential severe weather and flooding events in areas of high aerosol loadings such as Houston. The study was originally planned to be carried out from April 1, 2021 to March 31, 2022, with an intensive observation period (IOP) of June 1–September 30, 2021. COVID delays resulted in the shift of the project to a start date of October 1, 2021 and an IOP of June 1–September 31, 2022. These shifts in campaign dates did cause some projects that were originally scheduled to overlap with TRACER to be conducted with limited or partial overlap, including a project from the National Aeronautics and Space Administration (NASA).

To leverage the assets deployed in Houston for the DOE TRACER campaign, NASA's Tropospheric Composition program funded the TRACER-Air Quality (TRACER-AQ) campaign in September 2021 and made observations include: 1) ozone (O_3) profiles from the Goddard tropospheric Ozone (TropOz) and the Langley mobile ozone lidar (LMOL) systems, 2) columnar values of Nitrogen Dioxide (NO_2), O_3, and Formaldehyde (HCHO) from the ground-based Pandora spectrometers, and 3) aircraft observations by the Johnson G-V research aircraft that carried a suite of instrumentation including the GEOCAPE Airborne Simulator (GCAS) for observations of O_3 precursors (NO_2 and HCHO columns) and the High Spectral Resolution Lidar-2 (HSRL-2) for O_3 and aerosols profiles. Other NASA programs also sent additional instrumentation into the field, including CIMEL Sun Photometers from the AERONET program and a micropulse lidar from the MPLnet program. Many of these instruments have been left in the field in Houston in the care of the University of Houston (UH) for long-term measurements as we approach the launch of the Tropospheric Emissions: Monitoring Pollution (TEMPO) satellite. In fact, the TRACER-AQ project was partially developed to serve as "practice" for the upcoming campaigns in New York in 2023 which will be the first major campaigns to be used for calibration and validation of TEMPO after it launches.

This TCEQ project, referred to as TRACER-AQ1, further leverages the DOE TRACER and NASA TRACER-AQ measurements by adding support for suites of in-situ atmospheric composition and meteorological measurements from ground-sites, mobile laboratories, boat platforms, and ozonesondes in summer, 2021. Three main universities, University of Houston, Baylor University (BU), and St. Edward's University (SEU), were supported to conduct this research. Key sampling platforms include the UH Mobile Air Quality Laboratory #1 (MAQL1), the Baylor Mobile Air Quality Laboratory #2 (MAQL2), the UH pontoon boat in Galveston Bay, two commercial boats (the shrimp boat and the Red Eagle) in the east side of the Galveston Bay and the Gulf of Mexico, respectively, and ozonesondes. This project also provided logistical support for the deployment of assets from NASA, University of Oklahoma (OU), and Virginia Tech. The original TCEQ TRACER-AQ1 program included support for the NOAA TOPAZ scanning ozone lidar. However, COVID related travel issues prevented their participation in the field campaign. In response the project was amended to change the NOAA lidar support task to become development of a Rapid Science Synthesis report and extended the use of remaining funds to support preparations and limited operations for the 2022 TRACER-AQ2 campaign that was scheduled to run concurrently with the rescheduled TRACER IOP in 2022.

Despite the lack of official overlap with the DOE TRACER campaign, there were still several areas where overlap with NASA TRACER-AQ and this TCEQ TRACER-AQ1 project occurred. The main DOE site at the La Porte Municipal Airport began setup in August 2021with many instruments coming online for QA/QC checks in late August and early September. Although not publicly available, some data may be available from the individual instrument mentors upon request and with certain caveats. In addition, the TRACER forecast team took advantage of the opportunity to practice interpreting available data and generating both weather and air quality forecasts during September 2021. This month-long practice session provided our TRACER-AQ1 project with valuable daily planning information. The TRACER forecast team gained valuable insight into the various data products available in the Houston area. This also helped foster the development of a relationship with the Houston National Weather Service (NWS) office and a better understanding of the unique challenges that Houston's subtropical coastal environment presents.

2. Project Design and deployment

The TCEQ supported this TRACER-AQ1 measurement project with intensive operation periods beginning in late August and ran through the end of September 2021, overlapping with NASA's September 2021 deployment. The project design was done with specific attention to leverage as many measurements as possible and provide enhanced spatial coverage for air quality measurements. More than 10 research groups were involved with the TRACER-AQ1 IOP measurements in 2021, five from universities and six from NASA.

The TRACER-AQ1 project provided logistical support for the deployment of assets from NASA, OU, and Virginia Tech. The NASA Goddard TropOz ozone lidar was deployed at the TCEQ La Porte Airport site (C243). The Goddard lidar had very specific 3-phase power requirements that could not be met at most sites. However, the DOE facility at the La Porte Airport was able to provide the proper connections. Collocating the TropOz lidar in La Porte also placed the lidar near the enhanced meteorological measurements for TRACER as well as the coast of Galveston Bay, where unique complex mesoscale circulation patterns occur (Banta). It was hoped that the collocation of these measurements near the Galveston Bay would help further the understanding of the vertical structure related to these land-water interfaces.

The NASA Langley LMOL ozone lidar was deployed at the UH Launch Trailer (C1611) site on the UH main campus where power could be provided by the balloon launch trailer. This is collocated with the continuous measurements from the TCEQ supported HNET program (PGA # 582-21-21684-014), which provides surface measurements of O_3, nitric oxide (NO), nitrogen oxides (NO_X), NO_Y, carbon monoxide (CO), and meteorological variables, as well as the UH Pandora spectrometer. The third ozone lidar from NOAA would have been operated at the TCEQ Aldine site (C8), historically a design value site, had they been able to deploy.

The NASA Pandora deployments then were designed to complement the lidar sites. With the UH owned Pandoras at the UH Launch Trailer (C1611) site and at the TCEQ Liberty Sam Houston site (C1626), NASA and Virginia Tech supplemented the Houston area with 6 additional Pandora systems. Two were located on the UH trailer at the La Porte site in different scanning profiles, one atop the UH Moody Tower (C695), two at the Aldine (C8) site atop the UH/Baylor $(BC)^2$ (PGA # 582-21-22317-016) trailer, and an additional one on the UH Pontoon Boat. Upon the completion of the NASA TRACER-AQ campaign, the Virginia Tech and NASA Pandoras were removed, with the exception of two NASA systems in La Porte and Aldine bringing the number of long-term Pandoras in Houston to four. UH continues to operate and maintain all four Pandoras in Houston.

NASA AERONET and MPLnet leadership contacted UH and worked together to deploy additional Cimel Sun Photometers and an MPLnet micropulse lidar. Since the Liberty Sam Houston (C1626) site is becoming very well equipped to measure in situ aerosol properties through several programs (TCEQ HNET, TCEQ $(BC)^2$, and the National Science Foundation (NSF) funded Atmospheric

Science and Chemistry mEasurement NeTwork; ASCENT), the addition of vertical profiling remote sensing capabilities by the micro-pulse lidar was a natural fit. Because of the complimentary nature of the Cimel photometer and micropulse lidar, it was natural to include a Cimel at this location as well. UH had originally planned on installing one of UH-owned Cimel photometer at Liberty. However, AERONET offered an updated version that would pair well with the micropulse lidar for this site. The UH Cimel system was then relocated to the Aldine site to provide additional spatial coverage and compliment the $(BC)^2$ measurements there. Other sites which received temporary Cimel systems included the UH Smith Point (C1606) site, UH Coastal Center site, and UH Sugar Land site. These systems continued operation from summer 2021 through the end of the DOE TRACER campaign in 2022, except for the MPL at the Liberty Sam Houston (C1626) site, which is planned to stay for the foreseeable future, providing yet more complimentary measurements for the various TCEQ and NSF projects that operate there.

TRACER-AQ1 incorporated operations of several mobile/portable laboratories, i.e., the OU CLAMPS boundary layer profiling trailer, the UH MAQL1, and the Baylor MAQL2 during the IOP. The OU CLMAPS trailer and MAQL2 were operated in stationary phase, whereas MAQL1 was operated in both a mobile and stationary mode. The OU CLAMPS trailer was deployed to the Aldine site for boundary layer profiling with the intention of collocating with the NOAA TOPAZ system and to gain valuable experience with what to expect when deploying there for the TRACER intensive campaign in 2022. Although MAQL2 is capable of operating in a fully mobile fashion, it was decided to deploy it to the San Jacinto Battleground Historic Site located within the Houston Ship Channel area to better characterize volatile organic compounds (VOC) and ozone and ozone precursors in the VOC-intensive industrial region. Previous experience with the Battleground site during 2013 DISCOVER-AQ campaign was quite positive and they were once again receptive to hosting researchers and was chosen as the site to deploy MAQL2.

The UH MAQL1, which measures a suite of VOCs, trace gases, and meteorological variables, alternated between stationary, mainly at the La Porte site, and mobile measurements which were made across the Houston-Galveston-Brazoria (HGB) region. Rather than parking at the warehouse where it is stored on UH campus, MAQL1 was operated out of the La Porte Airport site. This allowed MAQL1 to supplement the measurements at the TCEQ and DOE sites at the airport. It also provided an important compliment to MAQL2 as many of the measurements in the two platforms overlap and emissions from the area between the La Porte and Battleground sites are of key interest to TCEQ. From La Porte, MAQL1 conducted 19 days of mobile measurements out of the 32-day deployment. The mobile measurements were prioritized on days when TRACER-AQ NASA aircraft was flying and days forecasted for interesting air quality. These driving days were focused on a variety of NASA and TCEQ objectives and included exploring spatial and temporal gradients of air pollutant concentrations, point source emissions, urban scale plume evolution, neighborhood scale sampling, and gradients at land-water interfaces. It should be noted that the support for MAQL1 during TRACER-AQ was largely supported through NASA funding rather than this project.

To further support the land-water gradient questions during TRACER-AQ, the three boats initially supported under the GO3 project (AQRP 20-004) were supplemented for continued operation. This includes two commercial boats operating on the east side of Galveston Bay out of Smith Point, TX (Larry Willis, commercial shrimper) and the offshore waters in the Gulf of Mexico adjacent to Galveston Island (Ryan Marine Services, the Red Eagle). A third boat, the UH owned and operated pontoon boat was operated for special studies in Galveston Bay out of Kemah, TX. Prior measurements in Galveston Bay were largely performed by larger NOAA research vessels and were constrained to the dredged ship channel due to their draft. The measurements in GO3 and TRACER-AQ1 represented the first time a concerted effort would be put forth to measure O_3, O_3 precursors, and boundary layer heights over a large portion of the Galveston Bay and off the coast of Galveston Island in the areas where ships anchor while waiting to enter Galveston Bay or to transfer petroleum products between larger and smaller ships.

While all of the measurements discussed so far are surface based in situ or remote sensing, additional vertical information was desired. This took shape as the acquisition of a small Uncrewed Aerial System (sUAS) (a.k.a. drone) and ozonesondes. Due to concerns over Chinese technology, the TCEQ and UH legal representatives determined that a TAA compliant platform should be used. UH purchased an Aurelia X6 Pro six-rotor system and replaced the Taiwanese flight control “brain” with a module produced in the United States. Measurements on the sUAS included meteorology and ozone, utilizing an ozonesonde system identical to those flown on free release balloons. Over 90 free release ozonesondes were launched during this campaign and were used primarily to provide in situ validations of ground and airborne ozone lidar measurements. The coordinated launch of these sondes, oftentimes within minutes of the NASA G-V overflights of a site, was an enormous task and required the support of 12 supported and volunteer students, staff, and often PIs themselves. Sondes were launched both from land (at the UH Launch Trailer (C1611) site, La Porte Airport (C243) site, and downwind of Houston) and over water from the UH pontoon boat in Galveston Bay and on select days from the Red Eagle commercial boat in the Gulf of Mexico.

It should be noted that although largely outside the scope of this project, Paul Walter volunteered to be the primary point of contact between all of the TRACER and TRACER-AQ sonde teams and the Federal Aviation Administration (FAA) and for coordinated use of the available sonde frequencies. This was key to the success of TRACER-AQ and future projects as it preserved the long relationship this collaboration has with the FAA in Houston and elsewhere in Texas and it ensured that on the busiest days for sonde launches, as many as 10 in one day, all the team members knew what frequencies were to be used for every launch. This was critical as there were often three or four balloons in the air transmitting at any given time and overlapping frequencies would have caused lost data for everyone on that frequency. Once the balloons are launched it cannot be changed remotely.

The operational range and flight profile of the NASA G-V, operating from Ellington Field, was also a consideration when laying out the sampling site locations and timing of the mobile measurements and sonde launches. Under ideal conditions the aircraft could complete three 3-hour raster mapping patterns per day. Figure 1 below shows the location of the various assets underneath the flight patterns. Because the GCAS instrument relies on reflected sunlight, their take-off and landing times were defined by the solar geometry and changes somewhat over the course of the project as the days grew shorter. Their flight pattern was generally laid out to accommodate the ground sites as well as take into consideration the prevailing winds which would transport ozone and ozone precursors to receptor sites in the metro area.

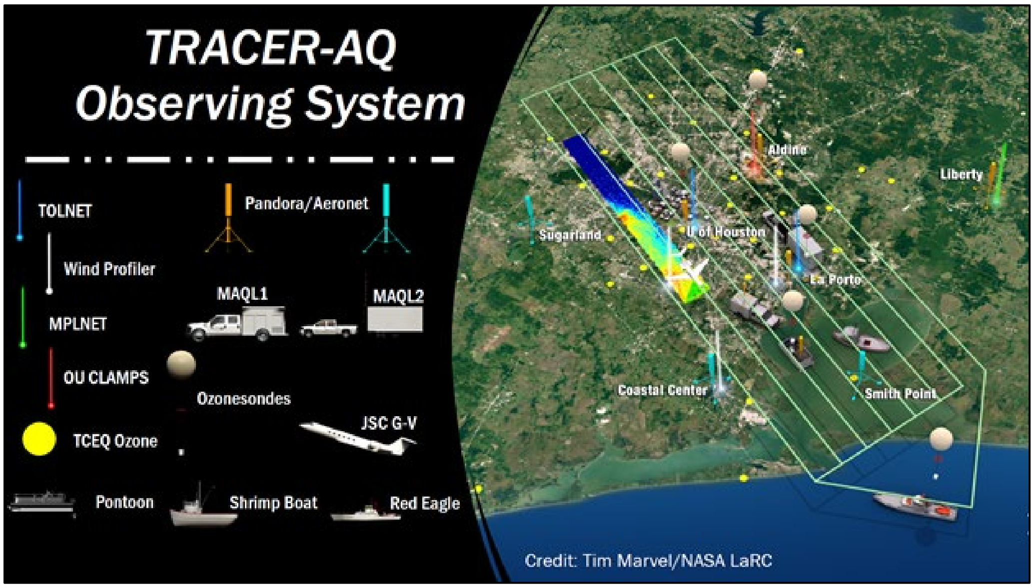
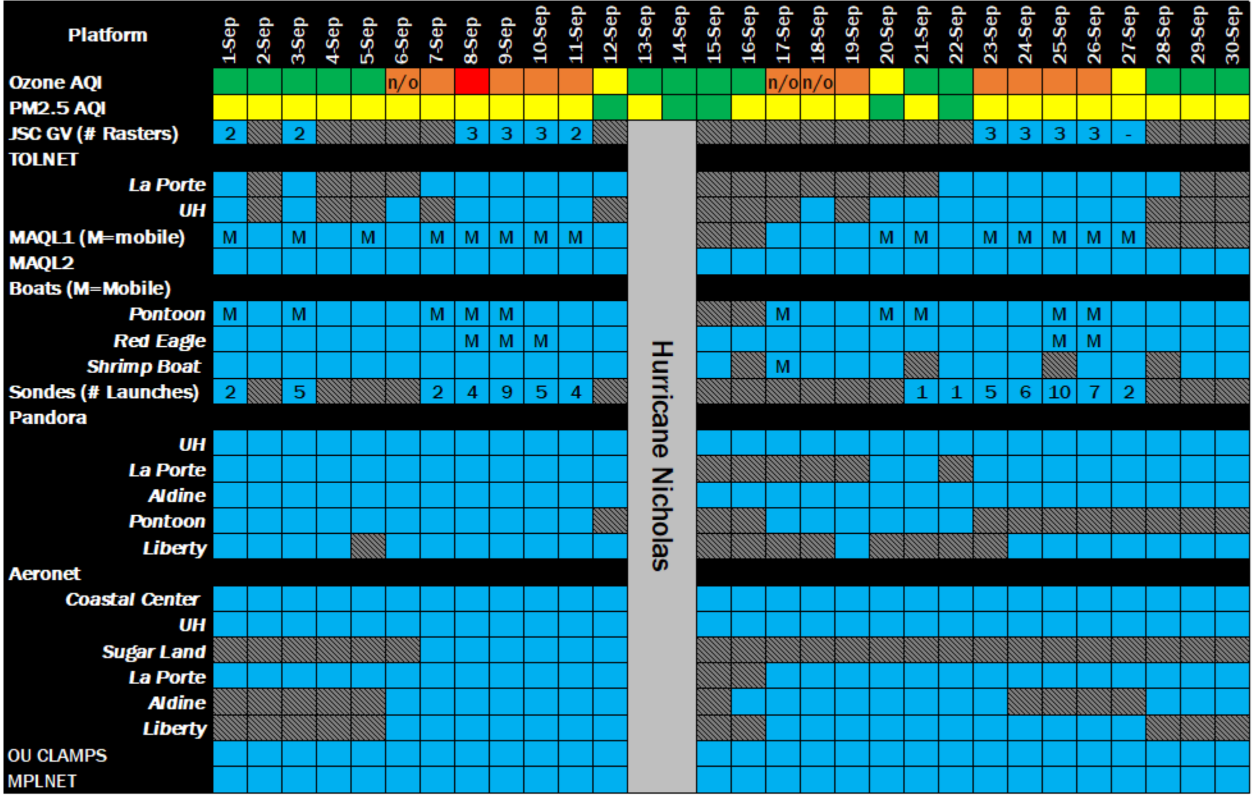


Figure 1: Location of the various assets underneath the NASA G-V flight patterns during TRACER-AQ.

A summary of measurements made during the September 2021 TRACER-AQ IOP is shown below (courtesy of Laura Judd and John Sullivan, NASA).

Table 1: Summary of observations during the September 2021 TRACER-AQ intensive period.



Platform	1-Sep	2-Sep	3-Sep	4-Sep	5-Sep	6-Sep	7-Sep	8-Sep	9-Sep	10-Sep	11-Sep	12-Sep	13-Sep	14-Sep	15-Sep	16-Sep	17-Sep	18-Sep	19-Sep	20-Sep	21-Sep	22-Sep	23-Sep	24-Sep	25-Sep	26-Sep	27-Sep	28-Sep	29-Sep	30-Sep
Ozone AQI	🟩	🟩	🟩	🟩	🟩	n/o	🟧	🟥	🟧	🟧	🟧	🟨	🟩	🟩	🟩	🟩	n/o	n/o	🟧	🟨	🟩	🟩	🟧	🟧	🟧	🟧	🟨	🟩	🟩	🟩
PM2.5 AQI	🟨	🟨	🟨	🟨	🟨	🟨	🟨	🟨	🟨	🟨	🟨	🟩	🟨	🟩	🟩	🟨	🟨	🟨	🟨	🟩	🟨	🟩	🟨	🟨	🟨	🟨	🟨	🟨	🟨	🟨
JSC GV (# Rasters)	2	▨	2	▨	▨	▨	▨	3	3	3	2	▨	Hurricane Nicholas		▨	▨	▨	▨	▨	▨	▨	▨	3	3	3	3	-	▨	▨	▨
TOLNET																														
La Porte	🟦	▨	🟦	▨	▨	▨	🟦	🟦	🟦	🟦	🟦	🟦			▨	▨	▨	▨	▨	▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦	▨	▨
UH	🟦	▨	🟦	▨	▨	🟦	▨	🟦	🟦	🟦	🟦	▨			▨	▨	▨	🟦	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	▨	▨	▨
MAQL1 (M=mobile)	M	🟦	M	🟦	M	🟦	M	M	M	M	M	🟦			▨	▨	🟦	🟦	🟦	M	M	🟦	M	M	M	M	M	▨	▨	▨
MAQL2	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Boats (M=Mobile)																														
Pontoon	M	🟦	M	🟦	🟦	🟦	M	M	M	🟦	🟦	🟦			▨	▨	M	🟦	🟦	M	M	🟦	🟦	🟦	M	M	🟦	🟦	🟦	🟦
Red Eagle	🟦	🟦	🟦	🟦	🟦	🟦	🟦	M	M	M	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	M	M	🟦	🟦	🟦	🟦
Shrimp Boat	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	▨	M	🟦	🟦	🟦	▨	🟦	🟦	🟦	▨	🟦	🟦	▨	🟦	🟦
Sondes (# Launches)	2	▨	5	▨	▨	▨	2	4	9	5	4	▨			▨	▨	▨	▨	▨	▨	1	1	5	6	10	7	2	▨	▨	▨
Pandora																														
UH	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
La Porte	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			▨	▨	▨	▨	▨	🟦	🟦	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Aldine	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Pontoon	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	▨			▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	▨	▨	▨	▨	▨	▨	▨	▨
Liberty	🟦	🟦	🟦	🟦	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦			▨	▨	▨	▨	🟦	▨	▨	▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Aeronet																														
Coastal Center	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
UH	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Sugar Land	▨	▨	▨	▨	▨	▨	🟦	🟦	🟦	🟦	🟦	🟦			▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨
La Porte	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
Aldine	▨	▨	▨	▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦			▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	▨	▨	▨	▨	🟦	🟦	🟦
Liberty	▨	▨	▨	▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦			▨	▨	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	▨	▨	▨
OU CLAMPS	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦
MPLNET	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦			🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦	🟦

3. Tasks

3.1. Ozonesonde Launches

A total of 72 ozonesonde launches supported by the TRACER-AQ1 measurement project were made. 56 ozonesonde launches were made in the Houston area between April 1, 2021 and October 31, 2021, and additional 16 during between May 1, 2022 and September 30, 2022, in coordination with the TCEQ Project Manager for:

1. Days that were forecast to meet certain air quality and/or meteorological conditions
2. To support the BC2 project during episodic smoke events
3. To support AQRP project 20-004 for measuring ozone offshore
4. To support TRACER-AQ aircraft missions
5. To support TRACER-AQ Lidar measurements; and/or
6. Other project goals as determined with the TCEQ Project Manager

3.1.1. Quality Control / Quality Assurance for Ozonesonde Launches

Ozone profiles for this project were measured using the electrochemical concentration cell (ECC) type ozonesonde instrument (Komhyr 1972; Komhyr 1986). All ozonesondes use 0.5% KI solution recommended by the Jülich Ozone Sonde Intercomparison Experiment (JOSIE), which found biases <5%, a precision of 3–5%, and an accuracy of 5–10% below 30 km (Smit et al. 2007; Thompson et al. 2019). The ozonesonde ECC cathode and anode solutions were prepared and provided by Brian Johnson (NOAA). Patrick Cullis (NOAA) maintains a website (https://www.patrickcullis.com/ozonesonde-instructions.html) that describes the ozonesonde conditioning and calibration procedures.

The campaign employed the InterMet iMet-4RSB radiosonde, which collects pressure, temperature, humidity, GPS location, and GPS-derived wind speed and direction. The radiosondes are connected to the ozonesondes and transmit data (~one data packet per second) that can be received by an antenna at the surface.

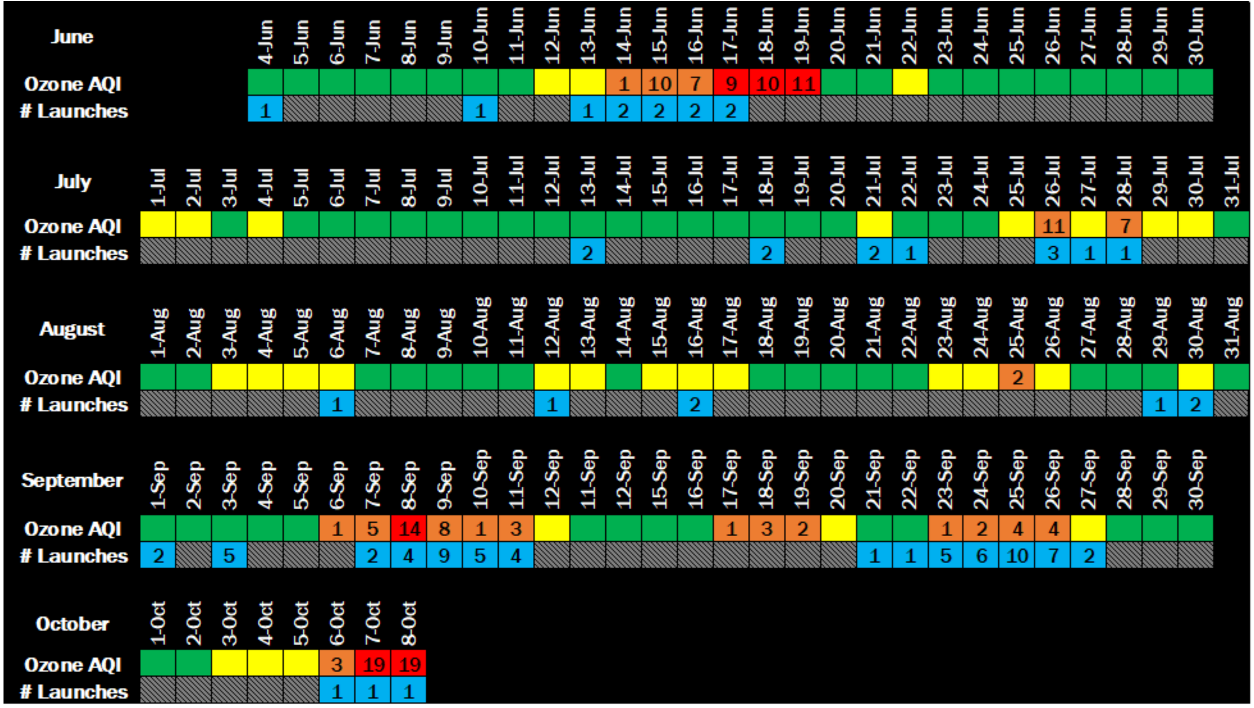
Our default balloon size is the 600-gram balloons that carry our payloads to 27–30 km before bursting. We used 350-gram balloons that carried our payloads to altitudes of 22–24 km before bursting in instances when a lower burst altitude had a more favorable expected landing site based on the balloon trajectory. On some occasions we used a type of 350-gram balloon that reached approximately 18 km prior to burst, which was again to accommodate a more favorable landing location.

Ozonesonde data is processed by Skysonde software. The data is then converted to the ICARTT format, which consists of a text file with a header followed by columns of data in comma separated values (csv) format, found on the NASA TRACER-AQ data archive (https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021?SONDE=1). In most cases, the data on the archive has been reprocessed to correct for a pressure offset of the radiosonde measurement (Stauffer et al., 2014).

3.1.2. Listing of all Ozonesonde Launches

In 2021, there were a total of 96 ozonesonde launches during TRACER-AQ, 63 of which occurred in the intensive period of September 2021. Table 2 summarizes all 2021 ozonesonde launches. Among all 96 launches in 2021, 56 ozonesondes were funded by TCEQ and 20 ozonesondes were provide by NASA, which are listed in Table 3 and Table 4, respectively. The remaining 20 ozonesondes were funded by the Texas AQRP 20-004 “Galveston Offshore Ozone Observations (GO3)” project. Information on those ozonesonde launches can be found in the final report for that project. This project also funded 16 ozonesondes launched in 2022, which are listed in Table 5.

Table 2: A summary of the 96 ozonesondes in 2021. The color code of the ozone air quality index (AQI) is shown for each day. For days where ozone concentrations exceeded the maximum daily 8-hour average (orange or red), the number of monitors in the Houston-Galveston-Brazoria (HGB) region in exceedance of the ozone standard (MDA8 [O3] > 70 ppbv) is shown.



June	4-Jun	5-Jun	6-Jun	7-Jun	8-Jun	9-Jun	10-Jun	11-Jun	12-Jun	13-Jun	14-Jun	15-Jun	16-Jun	17-Jun	18-Jun	19-Jun	20-Jun	21-Jun	22-Jun	23-Jun	24-Jun	25-Jun	26-Jun	27-Jun	28-Jun	29-Jun	30-Jun
Ozone AQI	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟨	🟨	🟧 1	🟧 10	🟧 7	🟥 9	🟥 10	🟥 11	🟩	🟩	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩
# Launches	1	▨	▨	▨	▨	▨	1	▨	▨	1	2	2	2	2	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨

July	1-Jul	2-Jul	3-Jul	4-Jul	5-Jul	6-Jul	7-Jul	8-Jul	9-Jul	10-Jul	11-Jul	12-Jul	13-Jul	14-Jul	15-Jul	16-Jul	17-Jul	18-Jul	19-Jul	20-Jul	21-Jul	22-Jul	23-Jul	24-Jul	25-Jul	26-Jul	27-Jul	28-Jul	29-Jul	30-Jul	31-Jul
Ozone AQI	🟨	🟨	🟩	🟨	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟨	🟩	🟩	🟩	🟨	🟧 11	🟨	🟧 7	🟨	🟨	🟩
# Launches	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	2	▨	▨	▨	▨	2	▨	▨	2	1	▨	▨	▨	3	1	1	▨	▨	▨

August	1-Aug	2-Aug	3-Aug	4-Aug	5-Aug	6-Aug	7-Aug	8-Aug	9-Aug	10-Aug	11-Aug	12-Aug	13-Aug	14-Aug	15-Aug	16-Aug	17-Aug	18-Aug	19-Aug	20-Aug	21-Aug	22-Aug	23-Aug	24-Aug	25-Aug	26-Aug	27-Aug	28-Aug	29-Aug	30-Aug	31-Aug
Ozone AQI	🟩	🟩	🟨	🟨	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟨	🟨	🟩	🟨	🟨	🟨	🟩	🟩	🟩	🟩	🟩	🟨	🟨	🟧 2	🟨	🟩	🟩	🟩	🟨	🟩
# Launches	▨	▨	▨	▨	▨	1	▨	▨	▨	▨	▨	1	▨	▨	▨	2	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	▨	1	2	▨

September	1-Sep	2-Sep	3-Sep	4-Sep	5-Sep	6-Sep	7-Sep	8-Sep	9-Sep	10-Sep	11-Sep	12-Sep	11-Sep	12-Sep	15-Sep	16-Sep	17-Sep	18-Sep	19-Sep	20-Sep	21-Sep	22-Sep	23-Sep	24-Sep	25-Sep	26-Sep	27-Sep	28-Sep	29-Sep	30-Sep
Ozone AQI	🟩	🟩	🟩	🟩	🟩	🟧 1	🟧 5	🟥 14	🟧 8	🟧 1	🟧 3	🟨	🟩	🟩	🟩	🟩	🟧 1	🟧 3	🟧 2	🟨	🟩	🟩	🟧 1	🟧 2	🟧 4	🟧 4	🟨	🟩	🟩	🟩
# Launches	2	▨	5	▨	▨	▨	2	4	9	5	4	▨	▨	▨	▨	▨	▨	▨	▨	▨	1	1	5	6	10	7	2	▨	▨	▨

October	1-Oct	2-Oct	3-Oct	4-Oct	5-Oct	6-Oct	7-Oct	8-Oct
Ozone AQI	🟩	🟩	🟨	🟨	🟨	🟧 3	🟥 19	🟥 19
# Launches	▨	▨	▨	▨	▨	1	1	1

Table 3: 56 TCEQ-funded ozonesonde launches made in 2021 during TRACER-AQ.

# of flights	Flight Number	Date	Time
1	RC624	6/4	afternoon
2	RC625	6/13	afternoon
3	RC626	6/14	morning
4	RC627	6/14	afternoon
5	RC628	6/15	morning
6	RC629	6/15	afternoon
7	RC630	6/16	morning
8	RC631	6/16	afternoon
9	RC632	6/17	morning
10	RC633	6/17	afternoon
11	RC634	7/26	afternoon
12	RC635	7/28	afternoon
13	RC636	8/6	afternoon
14	GB015	8/29	afternoon
15	LP002	8/30	afternoon
16	RC637	9/1	morning
17	LP009	9/10	morning
18	LP010	9/10	afternoon
19	GM005	9/10	noon
20	RC642	9/10	morning
21	RC643	9/10	afternoon
22	RC644	9/11	morning
23	LP011	9/11	noon
24	RC645	9/11	morning
25	LP012	9/11	noon
26	LP013	9/21	afternoon
27	LP014	9/22	afternoon
28	LP015	9/23	morning
29	LP016	9/23	noon
30	RC646	9/23	afternoon
31	LP017	9/23	afternoon
32	RC647	9/23	afternoon
33	LP018	9/24	morning
34	LP019	9/24	afternoon
35	GM006	9/24	afternoon
36	LP020	9/24	afternoon
37	LP021	9/25	raster 1
38	LP022	9/25	raster 2
39	LP023	9/25	raster 3
40	RC648	9/25	raster 1
41	RC649	9/25	raster 2
42	RC650	9/25	raster 3
43	GM007	9/25	raster 2
44	RC651	9/25	afternoon
45	GB023	9/24	raster 1
46	GB024	9/24	raster 3
47	LP024	9/26	dawn
48	LP025	9/26	afternoon
49	RC652	9/26	raster 2
50	RC653	9/26	raster 3
51	RC654	9/26	afternoon
52	RC655	9/27	dawn
53	RC656	9/27	morning
54	GB029	10/6	afternoon
55	GB030	10/7	afternoon
56	RC657	10/8	afternoon

Table 4: Additional 20 ozonesonde launches in 2021 during TRACER-AQ where the ozonesondes were provided by NASA.

# of flights	Flight Number	Date	Time
1	GB012	8/12	morning
2	LP001	8/30	morning
3	LP003	9/3	morning
4	GB017	9/3	morning
5	RC638	9/3	morning
6	LP004	9/3	afternoon

# of flights	Flight Number	Date	Time
7	RC639	9/3	afternoon
8	LP005	9/7	afternoon
9	GB018	9/7	afternoon
10	GM001	9/8	noon
11	GB019	9/8	noon
12	LP006	9/8	noon
13	GB020	9/8	afternoon
14	GM002	9/9	morning
15	LP007	9/9	noon
16	RC640	9/9	noon
17	GM003	9/9	noon
18	LP008	9/9	afternoon
19	RC641	9/9	afternoon
20	GM004	9/9	afternoon

Table 5: The first 16 ozonesondes funded by this project launched in 2022 during TRACER-AQ.

# of flights	Flight Number	Date	
1	GB031	5/26	Galveston Bay
2	GB032	6/2	Galveston Bay
3	RC658	6/24	UH
4	RC659	7/10	UH
5	RC660	7/10	UH
6	RC661	7/13	UH
7	ozonesonde for drone	7/20	UH
8	ozonesonde for drone	7/20	UH
9	GB033	7/25	Galveston Bay
10	GB034	7/27	Galveston Bay
11	RC662	7/28	UH
12	RC663	7/28	UH
13	GB035	7/30	Galveston Bay
14	ozonesonde for drone	8/3	UH
15	GB036	8/4	Galveston Bay
16	GB037	8/4	Galveston Bay

3.1.3. Problems Encountered and Corrective Actions for Ozonesonde Launches

There were two issues that were encountered with ozonesondes during the campaign. One issue was that at times the inlet straw that the ozonesonde pump draws air in through would occasionally become dislodged during the release of an ozonesonde. When this issue happened, it would occur when the ozonesonde shifted inside the styrofoam enclosure upon release when there was a jerk on the payload. It occurred more frequently during releases from Galveston Bay in the morning when the relative humidity was high and it was easier for the inlet straw to slip out. The fix was to add cardboard wedged between the styrofoam enclosure and the ozonesonde to prevent the ozonesonde from being able to shift during release, which addressed the problem and became part of our standard operating procedure when boxing up the ozonesondes before a release. The second issue that occurred occasionally was that some ozonesondes had a circuitry issue where the cell current measurement did not always work, or did not always work consistently, due to a manufacturer error. This was addressed by sending any ozonesondes exhibiting such issues in the lab during pre-flight preparations back to the manufacturer to be fixed or replaced.

Ozonesonde problems - although not explicitly a problem, the heavy focus of the ozonesondes on coordination with the NASA G-V meant that the sonde profiles were always in close spatial and temporal proximity to the HSRL2 measurements. This resulted in a robust data set to compare and support the measurements of the two groups, however the excellent agreement in the profiles likely means that it would have also been effective to do the coordinated launches in the beginning to gain the confidence in the comparability of the measurements or to spread them out throughout the campaign to ensure the representativeness of the sonde-lidar comparisons. Had either of these approaches been taken it would have been possible to launch the majority of the 90+ sondes either outside the aircraft area of operations, or between overpasses during flights. In the future, once the confidence of the sonde-lidar intercomparison is established it is recommended that the sondes be used to fill in the gaps left by the airborne measurements, such as early morning, late afternoon, overnight, outside the perimeter of the aircraft flight area, or between passes. It should also be noted that the aircraft measurements are not available at night, with low sun angles, or through clouds during partly cloudy days; these issues are not present in the ozonesondes.

3.1.4. Link for the Ozonesonde Data

The ozonesonde data for the 96 ozonesondes released in 2021 are located on the NASA TRACER-AQ data archive: https://www-air.larc.nasa.gov/cgi-bin/ArcView/traceraq.2021?SONDE=1.

3.2. TRACER-AQ Rapid Synthesis Report

The first phase of the Tracking Aerosol Convection Experiment – Air Quality (TRACER-AQ) study was carried out in the summer of 2021 in the Houston-Galveston-Brazoria (HGB) area. The purposes of the study included examining the chemical and meteorological factors affecting air quality in the HGB area and determining how well photochemical grid models and satellites are able to depict the observed air quality and its spatial and temporal variations. Converting the work of a field campaign into useful findings can be a long process, but regulatory agencies often must make decisions on more urgent timelines. Consequently, it is helpful for scientists involved in a field campaign to develop a Rapid Science Synthesis (RSS) document so that the preliminary findings of the scientific work can begin to benefit the regulatory process as soon as possible.

The RSS identified six air pollution episodes in HGB, from late July to early October 2021, which will provide a rich data set to study the causes of high air pollution in the HGB area. The RSS is intended to describe pertinent, preliminary observations collected during the TRACER-AQ study. At this point, only tentative findings can be described. Below is a listing of the most relevant of these tentative findings.

- High ozone concentrations have been observed at the surface over both Galveston Bay and the Gulf of Mexico. Previous modeling studies of the Houston area have suggested that high ozone could be present over the nearby bodies of water, but a lack of observational data prevented those simulations from being fully tested for accuracy. It remains to be seen if the models and observations match well, but the model can be adequately tested given the observations available.
- Sophisticated measurements of the meteorological factors affecting ozone formation, accumulation, and transport were made over land and water during the air pollution episodes, and these data should help researchers identify weather conditions most conducive to high ozone and determine which local and distant sources are responsible for the emissions driving high ozone and particulate matter.
- In the Gulf, relatively large ozone concentrations have been observed near the lightering and anchoring areas for ocean-going marine vessels. These new observations suggest a relationship between the emissions of these vessels and the high ozone concentrations.
- The MAQL1 and MAQL2 observed several unexpected VOC emission sources. MAQL1 observed an exceptionally high ethene emission event on September 27, which was corroborated by auto-GC data at two sites in Deer Park. MAQL2 observed very high isoprene concentrations that appear to originate from anthropogenic sources rather than biogenic sources. Further investigation of these data is warranted.

The findings in the RSS are preliminary, however, and may change as further analyses are carried out, data are quality checked, and intercomparisons among measurements are refined.

More complete analyses will be done in the follow-up TRACER-AQ1 Analysis project, but these RSS results can be used to focus attention on the lines of inquiry most likely to be fruitful. The RSS was submitted to the TCEQ on June 1, 2022. A link to the report and the Executive Summary can be found below:

http://hoth.geosc.uh.edu:5000/sharing/4jsvVD1Xm

3.3. VOC Measurements

3.3.1. Mobile Platforms - MAQL1 and MAQL2 Operations

An extensive suit of VOC measurements were made on two mobile labs, the UH MAQL1 and Baylor MAQL2, along with various trace gases and aerosol instrumentation as well as meteorological variables. MAQL1 was operated in both the stationary mode at the La Porte Airport site and mobile mode across the Houston-Galveston-Brazoria (HGB). MAQL1 conducted 19 days of mobile measurements out of the 32-day deployment region during TRACER-AQ1. The mobile measurements were prioritized on days when TRACER-AQ NASA aircraft was flying and days forecasted for interesting air quality. MAQL2 was deployed at the Battleground site in stationary mode. These deployment locations were determined in consultation with the TCEQ Project manager.

The UH MAQL1 is comprised of a 325-ft^3 fiberglass truck body in the bed of an UH-owned 2013 Chevrolet Silverado 3500HD Crew Cab pickup truck. The instrumentation installation was engineered to optimize the space and allow for performance of the full suite of measurements described below. Integrated in the shell are three air-conditioning systems (38,000 BTU cooling capacity), allowing for operation of instrumentation during warm weather. The truck and shell were wired to distribute power from a 50-A RV power outlet for stationary measurements; the power was supplied from a towed generator when in motion. Self-sampling of generator emissions were avoided through appropriate inlet design. The trace gas inlet box, aerosol inlet, and meteorological sensors (temperature, relative humidity, atmospheric pressure, and wind direction and speed) were mounted to the end of a 4-m articulating arm. When MAQL1 was in motion, the arm was lowered so that sampling was performed at a height of approximately 2 m. When stationary measurements were being made, the arm was raised such that measurements were made from approximately 6 m. Additionally, MAQL1 was equipped with wired and wireless network, dual 4G cellular internet connections, one hemispheric rooftop camera for cloud condition documentation, perimeter lighting for nighttime operations, and front and rear strobe lights for increased visibility.

MAQL1 was also adapted to house two remote sensing instruments from Dr. Elena Lind at Virginia Tech. Although her deployment and operating costs were supported by NASA, MAQL1 was modified slightly to accommodate her instrumentation. This included the addition of a platform on the roof to mount a Pandora Spectrometer sensor head as well as standoff brackets to allow the left rear access panel in the mobile lab's shell to be secured in a partially open position so that fiber optic and control cables could be securely routed into the shell. An additional remote sensing optic was clamped to the open door and its cables were routed into the shell as well. Rigid foamboard insulation, aluminum foil tape, and silicone caulk were then used to close off and seal the open gaps around the open door to prevent hot air and rain from entering the mobile lab.

MAQL2 is comprised of a BU-owned trailer and a BU-owned 2015 Ford F250 pickup truck to tow the equipment trailer. The trailer has a volume of ~22 m^3, which was sufficient for all of the equipment described subsequently, as well as area for team members to work when the trailer is not in motion. When operating in stationary mode at the Battle ground, MAQL2 was on utility power from a 50-A recreational vehicle (RV) power outlet. A telescoping tower was attached to the trailer to extend the sampling inlets well above the ground and trailer at ~ 10 m. The length of inlets from the trailer walls to the instruments were made as short as possible; these lengths of tubing were insulated to minimize wall loss and vaporization effects associated with temperature changes between outside and inside the trailer. MAQL2 was also equipped with wired and wireless network, dual 4G cellular internet connections. Additionally, the MAQL2 was equipped with the following: designated heated inlet for SRI-PTR/MS VOC measurements, designated stainless steel inlet with two size cutes for aerosol, designated trace gas inlet, walkable roof with safety railing and deployment of additional instrumentation, video monitor stations to display current measurements from multiple instruments, trailer air ride suspension system, storage space for calibration and maintenance tools, insulated walls and doors to stabilize temperature, stabilizing jacks, e-track for cylinder storage and rack space for calibration and guest instrumentation, full walkable ramp for instrument loading and unloading, two adjustable 4" Hilti (firestop sleeves) to serve as trailer sampling port, air compressor system, air-ride receiver hitch, AC and DC power, strobe lights and optional floodlights.

3.3.2. Instrumentation on mobile platforms

VOCs

Four VOC instruments were operated in MAQL1, which included the Peak Performer 1 Reducing Compound Photometer (PP1-RCP; Peak Laboratories, Edmond, OK) for isoprene measurement, a liquid-phase reaction and fluorescence light technique instrument from Aero-laser GmbH (Garmisch-Partenkirchen, Germany) for HCHO measurement, a Rapid Alkene Detector (RAD; Hills Scientific) that uses chemiluminescence for measuring highly reactive VOCs (HRVOC), and an AROMA VOC analyzer (AROMA; Entanglement Technologies, San Bruno, CA, USA) for select VOCs. The purchase of the AROMA VOC instrument was supported through this project via a cooperative agreement between Baylor PIs and Entanglement to work collaboratively on instrument development for select HR-VOCs and mobile applications. The RAD instrument detects several HRVOCs including ethene, propene, butadiene, and isoprene and measures the sum of these compounds as counts per second (cps). For reporting purposes, the RAD data is corrected with a propene response factor and presented as propene-equivalent cps. The AROMA was operated in rapid scan mode for bulk compound classes (e.g. aromatics, dienes, and chlorinated compound classes) during mobile measurements and the speciated mode for benzene, toluene, ethylbenzene, xylene, styrene, and isoprene, during stationary measurements. The deployment of multiple instruments in MAQL1 for various VOC measurements allowed improved spatial coverage of select VOCs in Houston during the TRACER-AQ field campaign.

VOCs on MAQL2 were measured using a Baylor-owned unit-mass resolution Proton Transfer Reaction Mass Spectrometer upgraded with a Selective Reagent Ionization (PTR-SRI-MS; Ionicon, Innsbruck Austria). The SRI upgrade was supported through this project. This upgrade allows for the use of O_2^+ and NO^+ as reagent ions (in addition to the current H_3O^+). This allowed for the routine measurement of the standard set of VOCs (measured using the traditional PTR-MS; H_3O^+), which include formaldehyde (*m/z 31*) (which requires an appropriate sample conditioner developed in previous work), acetonitrile (*m/z 42*), acetaldehyde (*m/z 45*), acetone (*m/z 59*), isoprene (*m/z 69*), methyl vinyl ketone plus methacrolein (*m/z 71*), benzene (*m/z 79*), toluene (*m/z 93*), styrene (*m/z 105*), C2-alkylbenzenes (*m/z 107*), C3-alkylbenzenes (*m/z 121*), C4-alkylbenzenes (*m/z 135*), and monoterpenes (*m/z 137*). With the addition of the SRI, HR-VOCS including propene, ethylene and 1,3- butadiene were also measured in this campaign.

Trace gases, aerosols, and meteorological parameters

Both the MAQL1 and MAQL2 had a suite of UH-owned instruments measuring trace gases including nitrogen oxide (NO), nitrogen oxides (NO_X)/nitrogen dioxide (NO_2), total reactive nitrogen (NO_Y), ozone (O_3), sulfur dioxide (SO_2), and carbon monoxide (CO). The NO and NOx/NO2 were measured using O_3 chemiluminescence and photolytic NO_2 converter, by a modified Air Quality Design instrument (Golden, Colorado) in MAQL1 and a Thermo Scientific 42C NO Analyzer and Thermo Scientific 42i NO_X analyzer in MAQL2. The NO_Y measurements were made using the Thermo Scientific (Waltham, MA) NOx Analyzer with heated molybdenum converter set at 315℃ in both mobile labs. Ozone in MAQL1 was measured with a Baylor-owned 2B Technologies (Boulder, CO) UV absorption O_3 analyzer, whereas that in MAQL2 used a UV absorption Thermo Scientific 49i Analyzer. Both SO_2 was measured with a pulsed fluorescence Thermo Scientific 43i TLE analyzer. A cavity enhanced absorption technique instrument from Los Gatos Research (San Jose, CA) was used for CO measurements in MAQL1 and an IR absorption Thermo Scientific 48C analyzer for CO in MAQL2. Both mobile labs used a Meteorologie Cosult GmbH filter radiometer to measure the NO_2 photolysis rate coefficient (jNO2). Meteorological parameters including wind direction, wind speed, relative humidity (RH), ambient pressure, ambient temperature, and GPS measurements were also made on both mobile platforms.

A Li-Cor (Lincoln, NE) LI7000 NDIR absorption instrument was used for CO_2 measurement in MAQL2. In the MAQL2, Baylor operated aerosol optical instrumentation including aerosol absorption a Tricolor Absorption Photometer (TAP 2901UV; Brechtel, Hayward, CA USA) and aerosol scattering using a TSI tricolor nephelometer 3563 (NEPH; TSI Incorporated, Shoreview, MN, USA). The aerosol optical measurements for TRACER-AQ duplicate measurements made for the TCEQ-sponsored BC2 network in Houston (sites in Galveston, Aldine, and Liberty).

3.3.3. Sorbent Tubes

VOC sample collection via sorbent tubes is a robust technique to capture and examine VOC atmospheric concentrations that has been employed for the last 15 years. Sorbent tubes are stainless steel tubes containing sorbents of varying affinities to retain a wide range of compounds (Figure 4). In this study, Material Emissions sorbent tubes from Markes International (Sacramento CA, USA) contained three different sorbents to capture $C_{4/5}$–C_{32} organic compounds. Ambient air was be drawn through a sorbent tube using a portable pump at a flow rate of 0.1 liters per minute for 10 minutes so as not to exceed the breakthrough volume (Figure 2). Afterwards, the tubes were transported back to the lab in coolers and placed in long-term storage at 5 °C for up to two weeks.

Sorbent tube samples were taken using the portable pump and tripod setup shown in Figure 2. This single-tube, portable setup was taken to multiple locations including the Battleground site, the La Porte and Aldine TCEQ sites on 9/11/21. A commercially available sampler, the Multi-Tube Sampler-32 (Markes International) was purchased and can sample up to 32 tubes without manual intervention between tubes (Figure 3).

An additional VOC sorbent tube-based sampler was constructed for use on the drone (Figure 4). The sampler enclosure has a small footprint to ensure feasibility with the drone size and is lightweight to increase future flight times by not weighing down the drone and putting strain on the batteries. Note, TRACER-AQ supported a significant fraction of the method development, and sampler purchasing and development as well as a pilot study of VOC measurements at the San Jacinto Battleground Historic Site. These samplers were finalized and used heavily during TRACER-AQ 2.

In the lab, VOCs captured on sorbent tubes were analyzed using a coupled Markes International thermal desorption unit with a Thermo gas chromatography-tandem mass spectrometry (TD-GC-MS/MS) system located in the Baylor University Mass Spectrometry Center (Figure 5). This system utilizes a two-stage desorption prior to chromatographic separation. Briefly, VOCs are extracted from tubes during the initial heating stage at 250°C and held for 8 minutes under a constant flow of He at 1 ml/min. VOC samples are then transferred along a 150°C flow path to a cold trap held at 20 °C where they are refocused before the GC. As the cold trap is heated, the desorbed sample is sent to the analytical column which is heated stepwise from 40°C to 255°C (total GC runtime: 36 min) prior to quantification using the MS/MS. This TD-GC-MS/MS system is capable of both targeted and non-targeted analysis through simultaneous collection of selective (Figure 6) and full scans. Selective ion scans allow for targeted analysis via calibration curve across a range of 10 ppb to 2 ppm and full ion scans allow for continued non-targeted analysis of previous samples.

Figure 2: Markes single pump system to sample sorbent tubes (September 2021) at the San Jacinto Battleground Historic Site

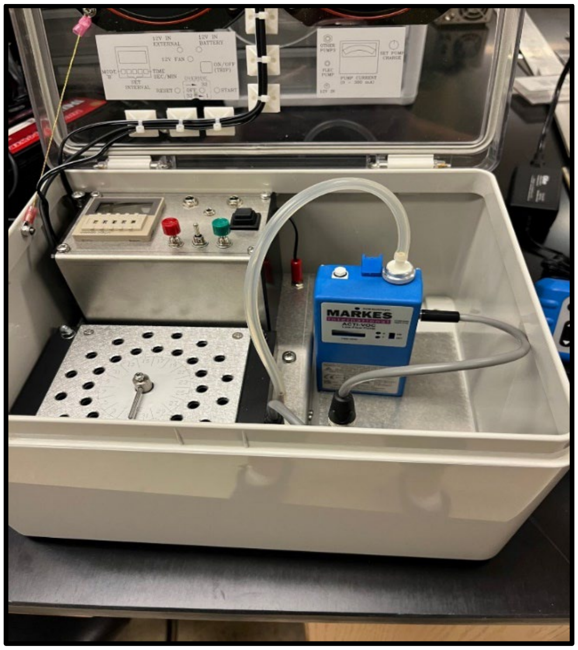


Figure 3: Multi-Tube Sampler (MTS-32: Markes International) capable of sampling up to 32 tubes.

Figure 4: VOC sampler (below drone) mid-flight with ozone monitor (above drone) near the San Jacinto Monument (2022).

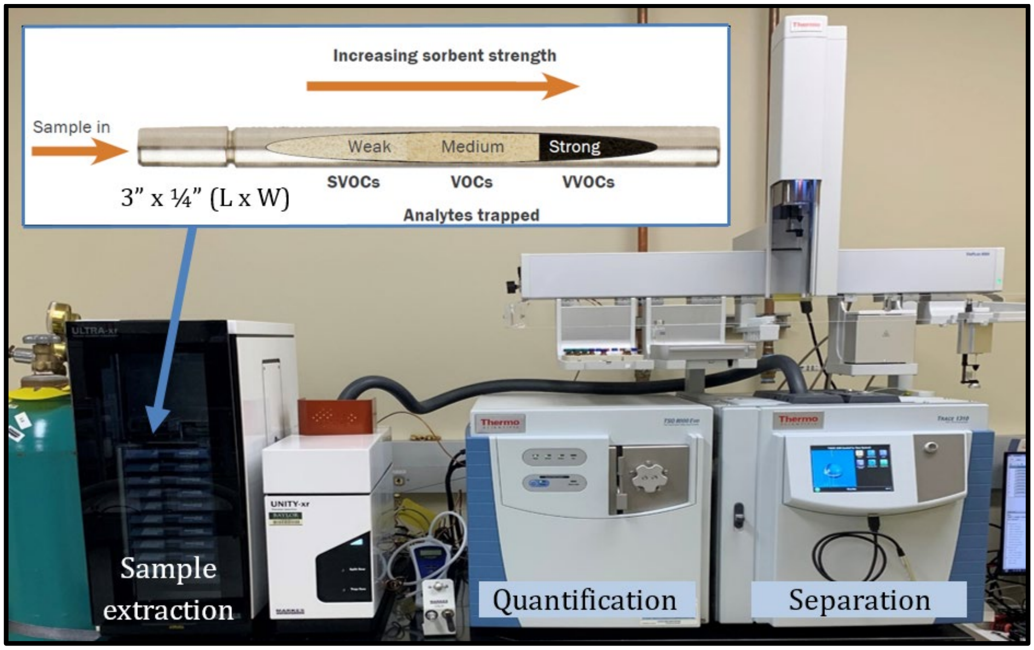


Figure 5: Triple-bed sorbent tube that captures volatile organic compounds (VOCs; C4/5–C32). MarkesTD-100xr system and Thermo Scientific TRACE 1310 GC coupled with Thermo Scientific TSQ8000 Evo Tandem MS/MS.

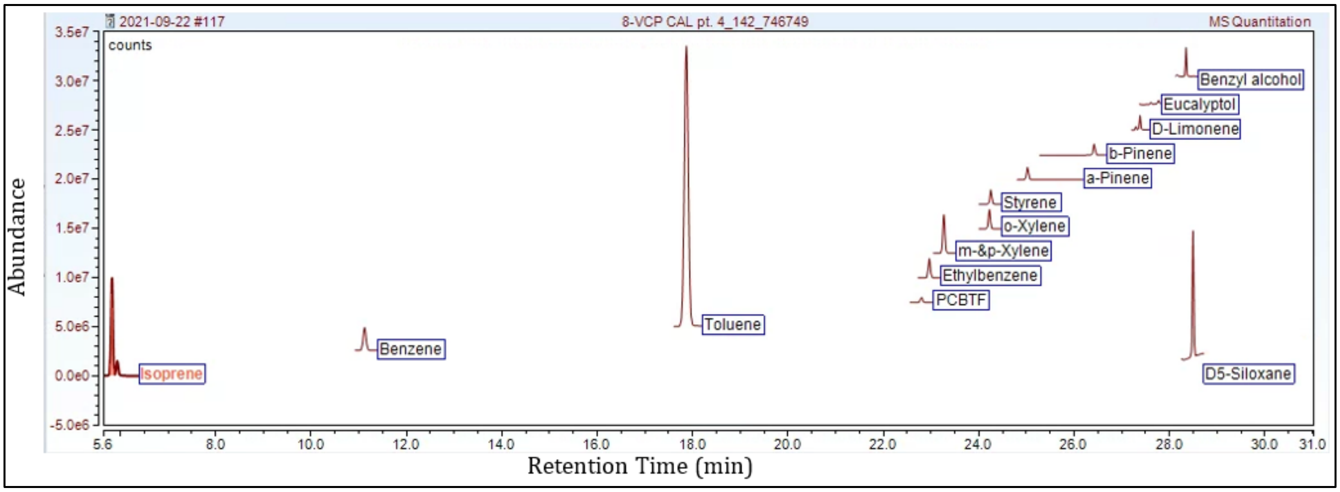


Figure 6: Chromatogram of analytical standards used to quantify target analytes in sorbent tube samples.

3.3.4. Quality Control / Quality Assurance for Measurements

The RAD instrument was calibrated using discrete cylinders of propene, ethene, isoprene, and 1,3-butadiene (Apel-Riemer Environmental Inc) before and after the sampling campaign to determine sensitivity factors for each gas. During the sampling period, the RAD instrument was calibrated with NIST traceable equipment and propene standard once ever few days to monitor instrument stability and changes in instrument sensitivity. The PP1 and AROMA were calibrated weekly with NIST traceable equipment and isoprene gas standard. All trace gas instruments were calibrated before, during, and after the sampling period. Multi-point calibrations were performed using NIST traceable equipment and gas standards.

For the PTRMS, a combination of single point and multipoint calibrations were used. Based on instrument stability at Battleground, multi-point calibrations were run every 2-4 days. Zero air was generated by passing laboratory air through a heated catalyst (alumina on palladium at 350 °C). The calibration gases included the following species: acetonitrile (m/z 42), acetaldehyde (m/z 45), acetone (m/z 59), dimethylsulfide (m/z 63), isoprene (m/z 69), methanol (m/z 33), methyl vinyl ketone (MVK) and methacrolein (m/z 71), methyl ethyl ketone (MEK) (m/z 73), hydroxyacetone (m/z 75), benzene (m/z 79), toluene (m/z 93), xylenes (m/z 107), C_3-benzenes (m/z 121), C_4-benzenes (m/z 135) and monoterpenes (m/z 137). The PTR-MS measurements reported in this study are obtained from the measured sensitivity using daily calibration of the individual masses against the known concentration of calibration mixture of VOCs. Calibrations and zeros were routinely analyzed for consistency and accuracy to ensure that the PTR-MS and calibration systems were operating properly. The raw signal from the PTR-MS is converted into a mixing ratio (ppbv) through a number of steps. First, the signal [Hz] for the VOC of interest, RH^+, is normalized to H_3O^+ (Mhz at m/z 21) to get a normalized signal [RH+ Hz/MHz m/z 21].

Second, the normalized background [RH^+ Hz/MHz m/z 21], which is the m/z signal (Hz) corresponding to the RH^+ measured during the periodic zeros (i.e., zero air), is subtracted from this normalized signal. Third, this background corrected normalized signal is divided by the sensitivity [RH^+ Hz/ (MHz m/z 21*ppbv of the calibration gas)] to result in a mixing ratio. The sensitivities are calculated from the periodic calibrations.

Field-based limits of detection (FLOD) were characterized as three standard deviations of the instrument background during SAFS. The instrument background was determined by grouping the signals from the zeros performed during the project and calculating the standard deviation from these data. The standard deviation was then converted into a mixing ratio by applying the methodology described above. FLOD for all the measured VOCs were calculated for each day during the campaign. The 5-minute average VOC concentrations below FLOD were not included in final calculations.

The trace gases instruments in MAQL1 (NO, NO_X, NO_Y, SO_2, and CO) and MAQL2 (NO, NO_X, NO_Y, SO_2, CO, and CO_2) were calibrated every other day. Multi-level calibration for NO_2 conversion efficiency and O3 for instrument were performed once every few days.

The uncertainty and limit of detection (LLOD) has been calculated for all VOC and trace gases for measurements made on MAQL1 and MAQL2 (Table 6 and Table 7). For MAQL1, the VOC and trace gas measurements were averaged to 300 s (i.e., 5 min) when the platform was in stationary mode and averaged to 10 s when the platform was mobile. The MAQL2 trace gas measurements were averaged to 300 s as the platform was stationary during full sampling period.

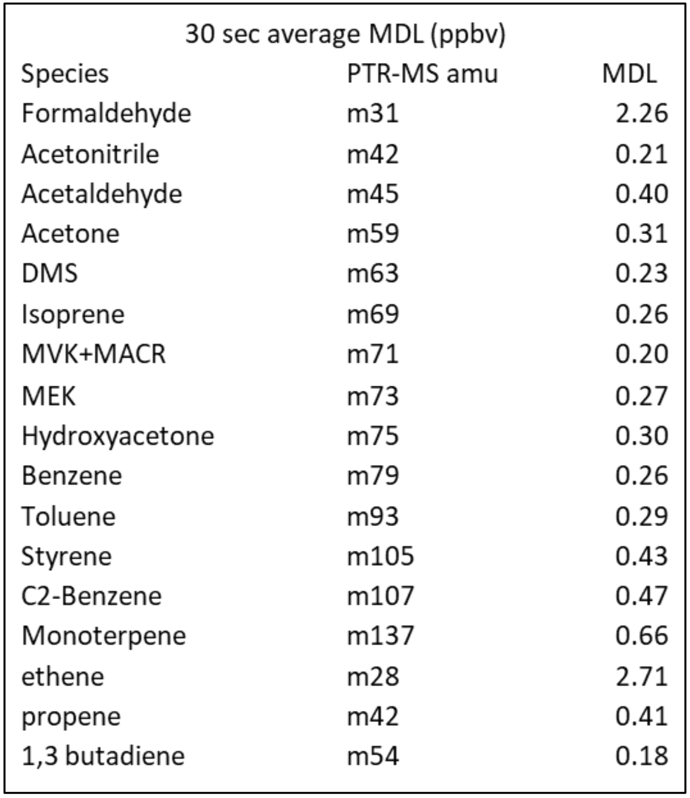
Table 6: Limit of Detection (LOD) for VOC measurements made in MAQL1.

VOC	Instrument	10s LOD (ppbv)	300s LOD (ppbv)	400 mL LOD (ppbv)
HCHO	AeroLaser	0.21	0.11	
Isoprene (PP1)	PP1-RCP	0.20*	-	
Propene Equiv.**	RAD	3.12	0.95	
Benzene	AROMA			0.0375
Toluene	AROMA			0.1875
Ethylbenzene	AROMA			0.375
Xylene	AROMA			0.375
Styrene	AROMA			1.875
Isoprene	AROMA			0.375

* For the isoprene measurements using the PP1 instrument, the sampling period is 50s followed by analysis period of 250s

** Rapid Alkene Detector measures sum response of several alkenes and isoprene. The propene correction is applied to RAD data as a default.

Table 7: Limit of Detection (LOD) for 30s averaged VOCs measurements using the Ionicon PTRMS instruments in the MAQL 2. Note that the 30s average MDL is higher than the 5 minute average MDL that would be used in future data analysis.



30 sec average MDL (ppbv)

Species	PTR-MS amu	MDL
Formaldehyde	m31	2.26
Acetonitrile	m42	0.21
Acetaldehyde	m45	0.40
Acetone	m59	0.31
DMS	m63	0.23
Isoprene	m69	0.26
MVK+MACR	m71	0.20
MEK	m73	0.27
Hydroxyacetone	m75	0.30
Benzene	m79	0.26
Toluene	m93	0.29
Styrene	m105	0.43
C2-Benzene	m107	0.47
Monoterpene	m137	0.66
ethene	m28	2.71
propene	m42	0.41
1,3 butadiene	m54	0.18

Table 8: Limit of Detection (LOD) and uncertainty for trace gas measurements made in MAQL1 and MAQL2, respectively.

		MAQL 1		MAQL 2	
Trace gas	**10s LOD (ppbv)**	**300s LOD (ppbv)**	**Uncertainty (%)**	**300s LOD (ppbv)**	**Uncertainty (%)**
NO	0.06	0.01	5.6	0.13	3.5
NO_2	0.07	0.02	7.3	0.38	7.3
NO_Y	0.43	0.21	5.8	0.66	6.3
O_3	4.73	3.04	4.4	1.06	2.0
SO_2	0.97	0.47	5.4	0.17	6.5
CO	0.51	0.27	3.2	16.4	4.2
CO_2	-	-	-	1.15 (ppmv)	5.2

VOC identification in sorbent tube samples was performed using TD-GC-MS/MS retention times (±0.05 min), their unique ions and ratios and comparison with the National Institute of Standards and Technology (NIST) database. Quantitation was performed using a 5-point external calibration curve containing analytical standards of target analytes. Liquid calibration solutions were spiked onto a set of tubes that did not undergo sampling using a calibration standard loading rig under N_2 gas flow at 50 mL/min for 5 minutes. Calibration solution spiking produced responses such as those observed in Figure 7 for α-Pinene and target analytes had an coefficient of determination (r^2) value of 0.97 or higher. Calibration curves were run before and after each sample batch and a continuing calibration verification standard was run throughout samples to ensure the linear relationship of analytes was upheld.

Table 9: Breakdown of target analyte identification and quantitation parameters and potential sources

Target Analyte	**Retention Time (min)**	**Ions (*m/z*)**	**Dynamic Linear Range (pg/uL)**	
			Lower limit	Upper limit
Benzene	11.13	52, 50, 77	11	1630
Toluene	17.81	91, 39, 65	11	1630
Ethylbenzene	22.94	91, 65, 39	11	1630
m-& *p*-Xylene	23.24	91, 65, 77	11	1630
o-Xylene	24.19	91, 65, 39	11	1630
Isoprene	5.85	67, 41, 65	10	1851
α-Pinene	25.00	77, 51, 91	11	1630
β-Pinene	26.40	77, 51, 91	11	1630
D-Limonene	27.37	67, 77, 91	11	1630
Eucalyptol	27.60	79, 39, 41	7	1001
Benzyl alcohol	28.34	77, 79, 107	11	1630
D5-Siloxane	28.49	250, 179, 267	7	1040
PCBTF	22.77	145, 130, 161	7	1469
Styrene	24.22	78, 77, 103	6	967

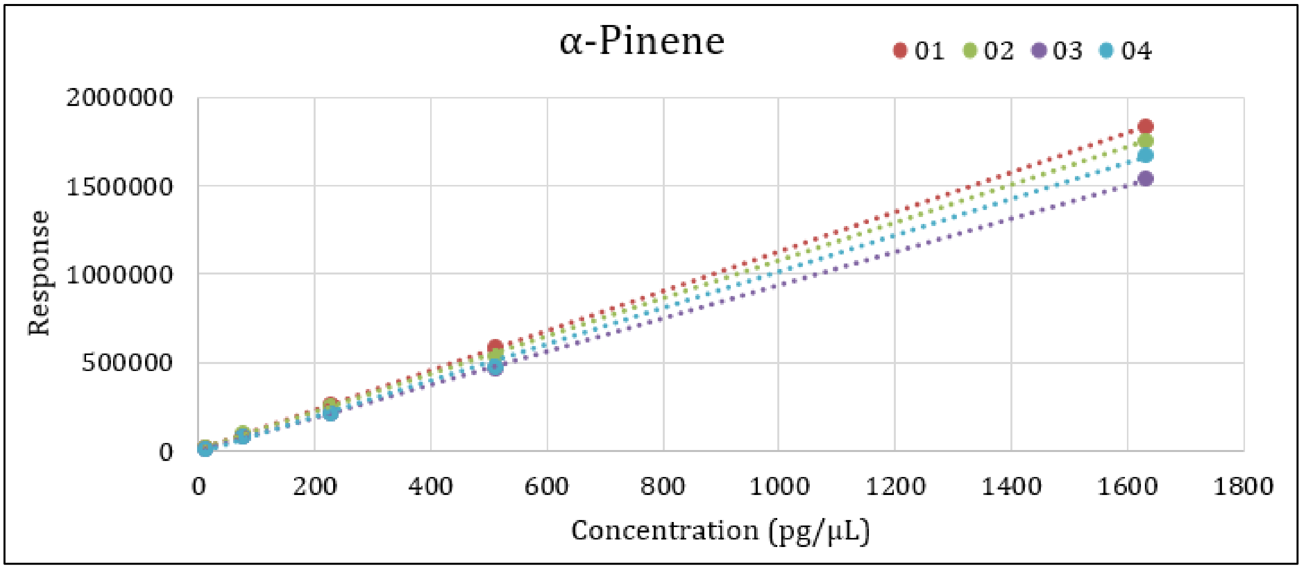


Figure 7: Responses from α-Pinene in 4 different spikes of VOC calibration curve after undergoing TD-GC-MS/MS analysis.

3.3.5. Results for Measurements

MAQL1

Deployment of MAQL1 was led by UH PI. There were several objectives for MAQL1's deployment including capturing urban plume photochemistry, industrial emissions, on-road emissions, land-bay breeze transitions, land-water gradients, storm outflows, intercomparing measurements made on MAQL2 and UH pontoon boat, and supporting TRACER-AQ NASA aircraft flights. MAQL1 made 32 total days of measurements (August 23 to September 12, September 9 to 27) where 19 had mobile measurements (August 23 to 26; September 1, 3, 5; September 7 to 11; September 20 to 21; and September 23 to 27). MAQL1 was stationed at the La Porte Airport site in the evenings to the early mornings and on non-mobile sampling days. Figure 8–Figure 11 shows an overview of the VOC and trace gas measurements of non-mobile MAQL1 at the La Porte Airport site. Diurnal profiles of hourly averaged isoprene, HCHO, NO, NO_2, NO_Y and O_3 are included in Figure 11.

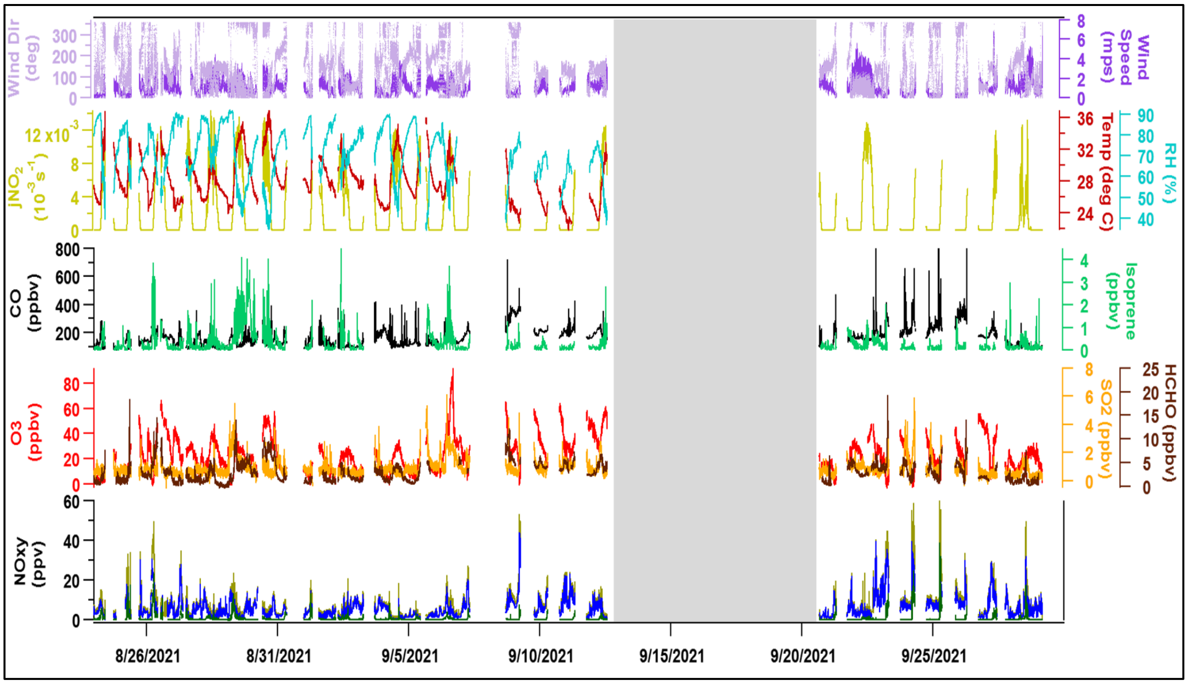


Figure 8: Time series of trace gases (NO, NO_2, NO_Y, O_3, SO_2 and CO), some VOCs (HCHO and isoprene), and meteorological (wind speed, wind direction, relative humidity, and ambient temperature) measurements made from the MAQL1 during stationary periods at La Porte Municipal Airport.

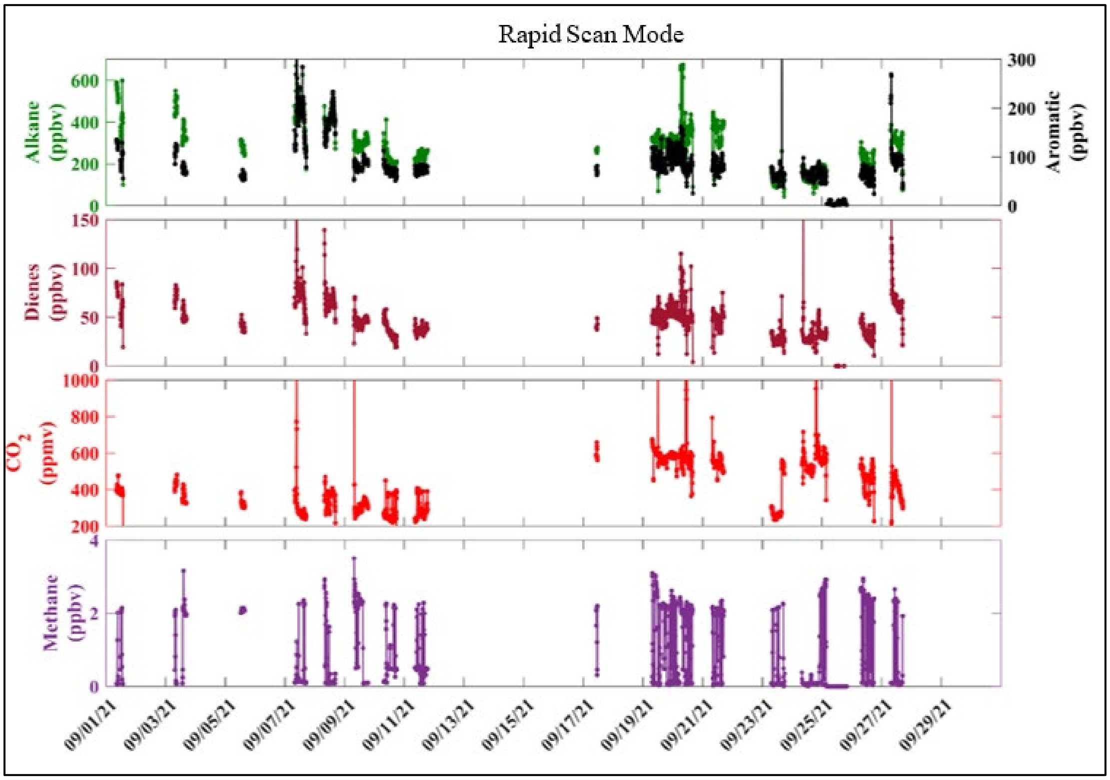


Figure 9: Time series of VOCs measurements made with the AROMA VOC instrument in rapid scan mode from the MAQL1.

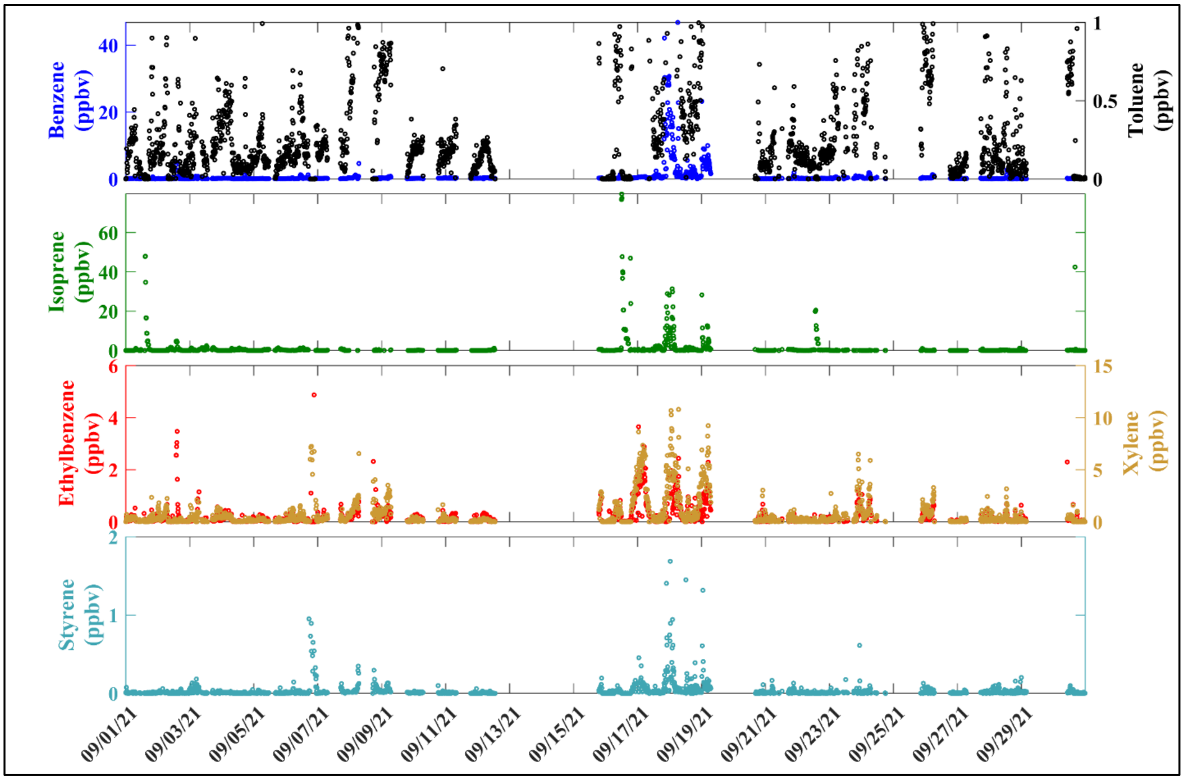


Figure 10*:* Time series of VOCs measurements made with the AROMA VOC instrument in speciated mode from the MAQL1.

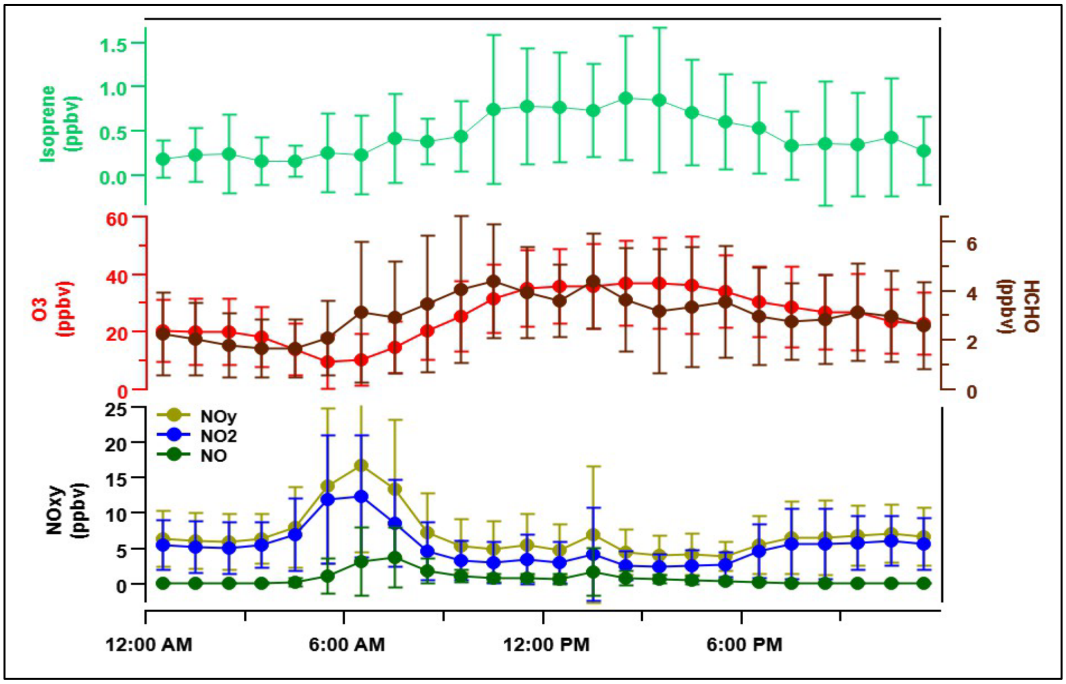


Figure 11: Diurnal profile of hourly averaged NO, NO_2, NO_Y, O_3, isoprene, and HCHO during stationary measurement at La Porte Municipal Airport from the MAQL1.

Figure 12 presents all mobile routes (in red) made during the campaign. The route for each MAQL1 mobile outing was preplanned to ensure that one or more objectives were met for the trip. During the campaign, MAQL1 was able to capture multi-day O_3 episodes while the platform was mobile and showed the progression of O_3 plume as the platform moved across Houston (Figure 13). Other MAQL1 mobile days highlighted emission impact from likely industrial and/or urban plumes (Figure 14 and Figure 15).

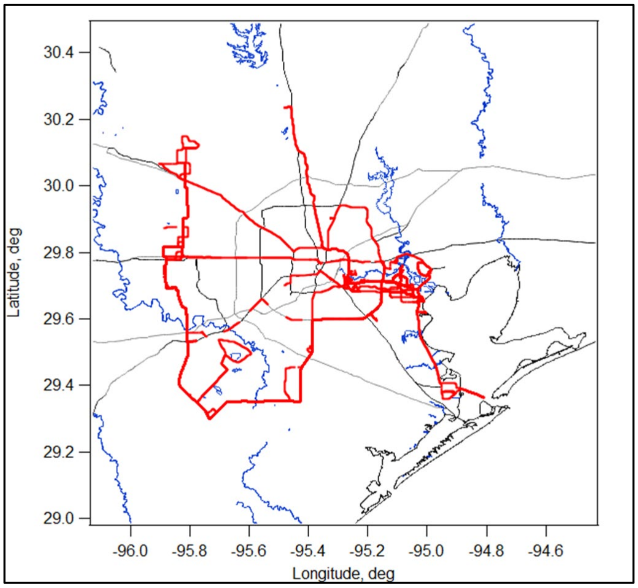


Figure 12: Spatial plot of all the mobile driving completed by MAQL1 during the full sampling period.

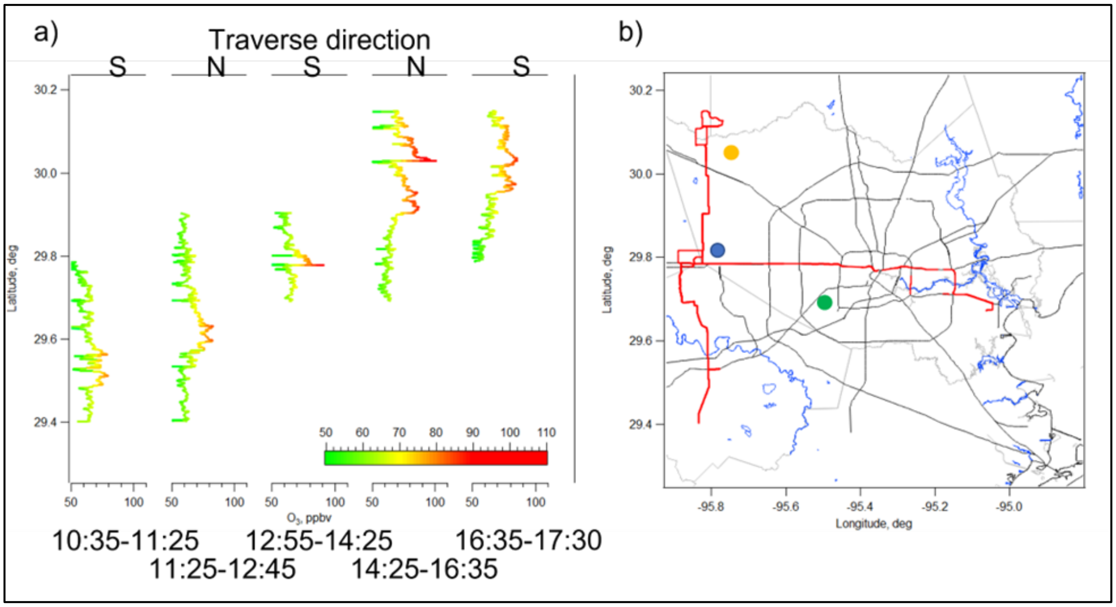


Figure 13: Measurements made Sept 1, 2021. a) the O3 concentrations during north and south traverses starting from 10:35 to 17:30 CST and b) spatial map of the mobile route on the day.

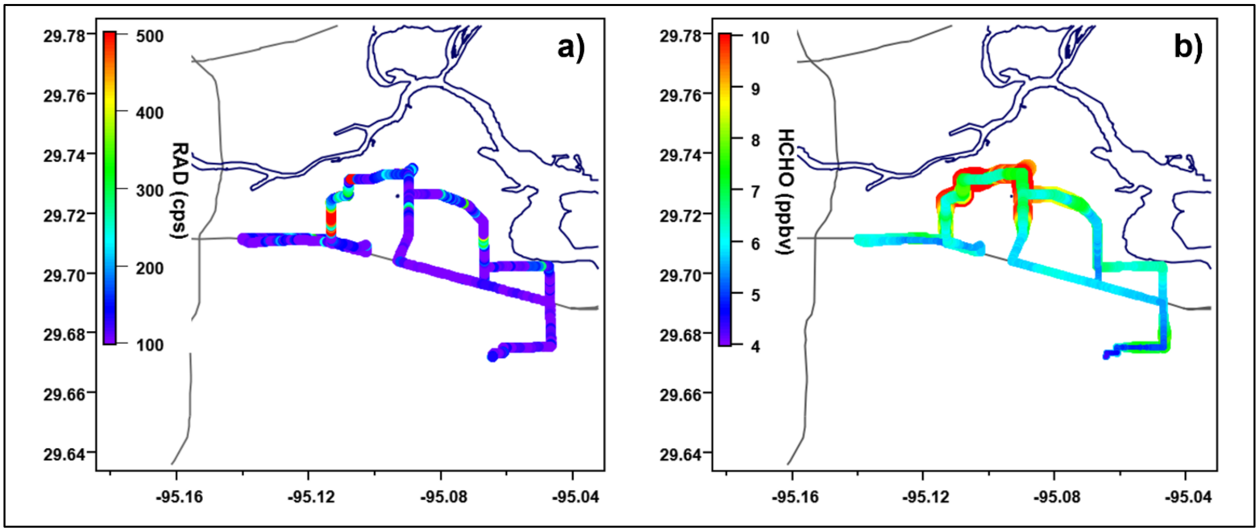


Figure 14: MAQL1 mobile sampling of industrial point sources near the Houston Ship Channel on Sept. 5 measuring a) bulk HR-VOCs as RAD (cps) and b) HCHO.

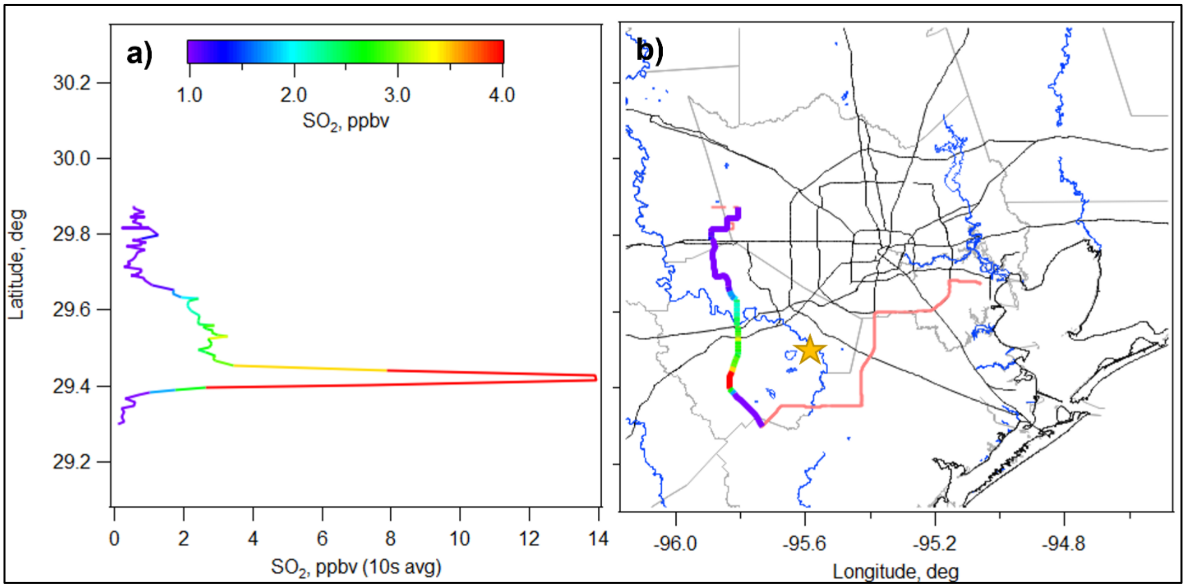


Figure 15: MAQL1 mobile a) sampling broad plume of SO_2 b) southwest of Houston and near a coal-fired power plant (gold star).

MAQL2

The deployment of the BU MAQL2 to the San Jacinto Battleground Historical Site for the month of September 2021 was led by Baylor PIs. The goal of this effort was to characterize the ship channel area, with specific emphasis on understanding local and industrial influences. The PTRMS with SRI was used during TRACER-AQ in September 2021 to measure the standard set of VOCs + ethylene, propene and 1,3 butadiene. These VOC measurements can be compared to VOCs measured using the AROMA (MAQL1) and the sorbent tubes. There were additional measurements of trace gases, aerosol absorption and scattering, and meteorological parameters. Specifically, the aerosol optical measurements were operated in the same manner as BC2 to enable identification of the influence of biomass burning during this intensive sampling period Figure 16–Figure *19* show the time series of all measurements made at the Battleground site in September 2021 during TRACER-AQ.

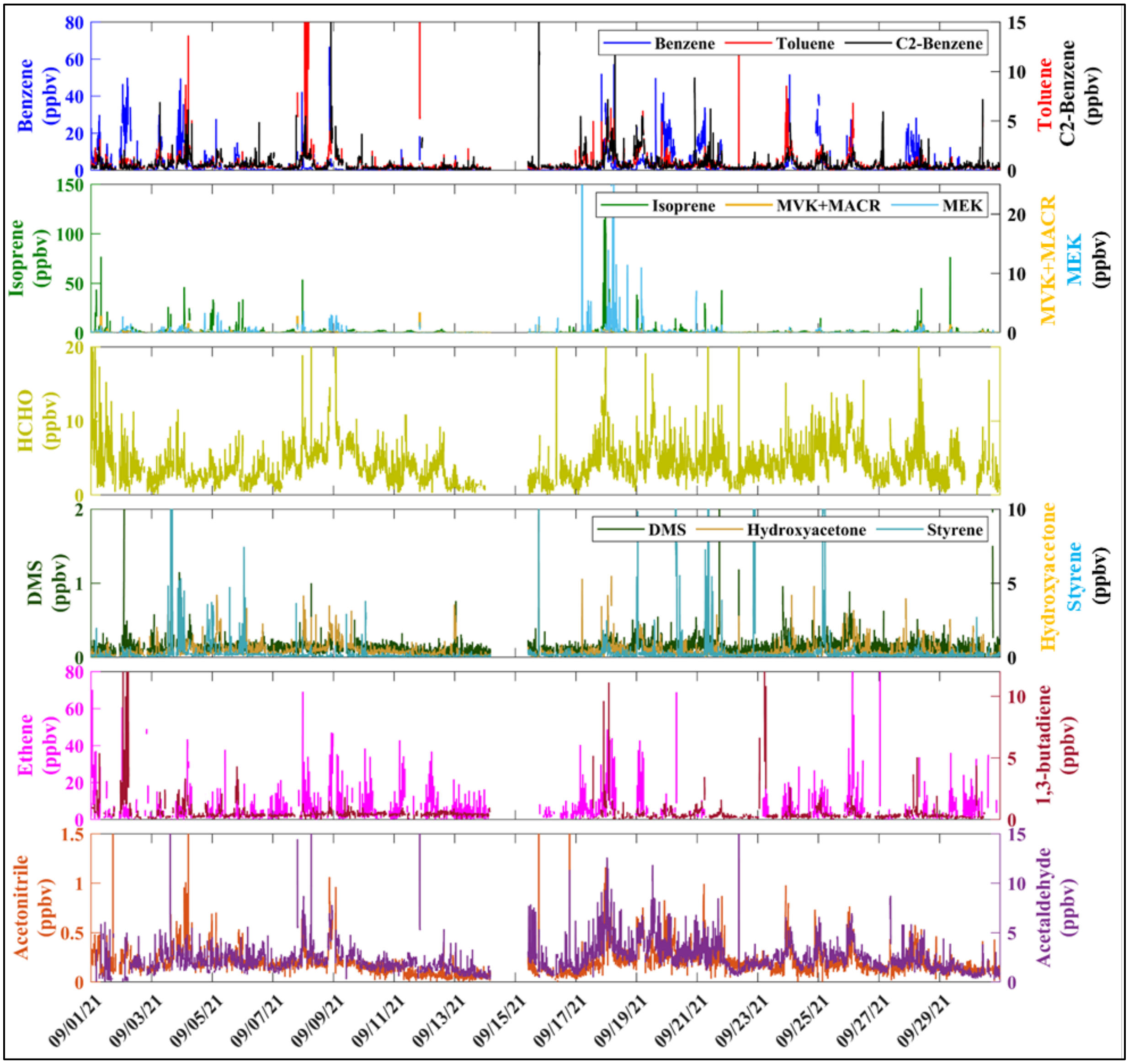


Figure 16: Time series of VOC measurements made from the MAQL2 at the San Jacinto Battleground Historic Site using the PTR-SRI-MS. The MAQL2 made a total of 30 days over the month of September 2021.

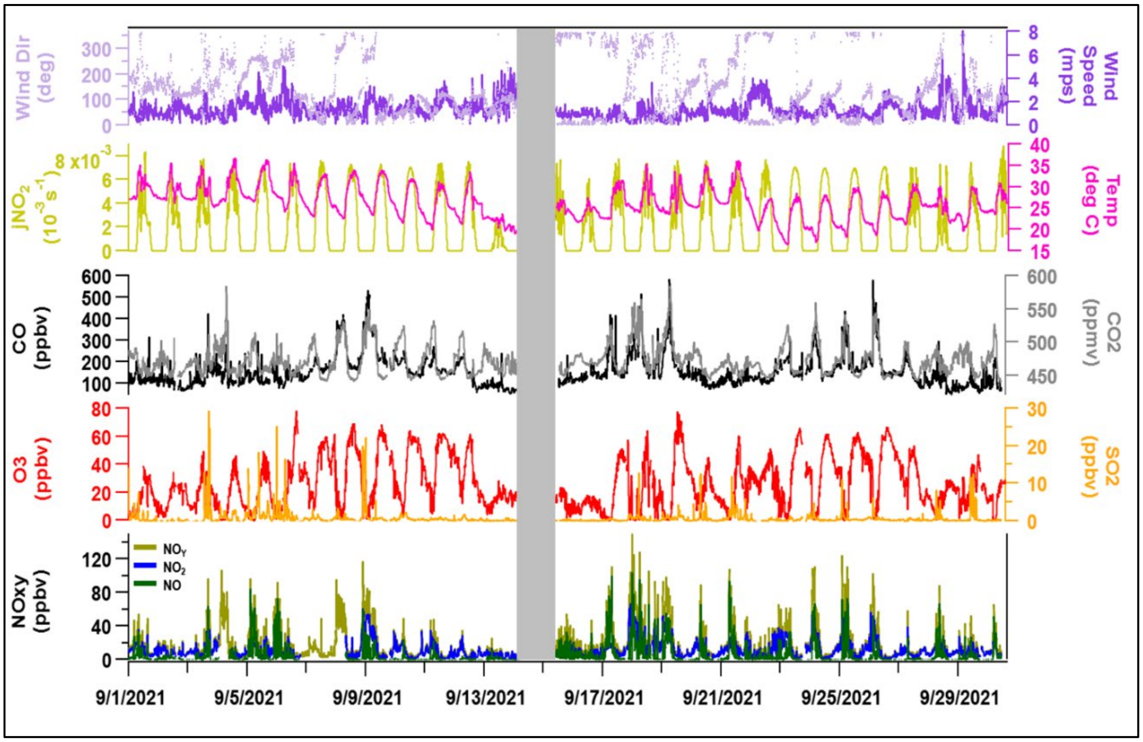


Figure 17: Time series of trace gases (NO, NO_2, NO_Y, O_3, SO_2, CO, and CO_2) and meteorological (wind speed, wind direction, and ambient temperature) measurements made from the MAQL2 at the San Jacinto Battleground Historic Site. The gray box was MAQL2 lost power during Hurricane Nicholas.

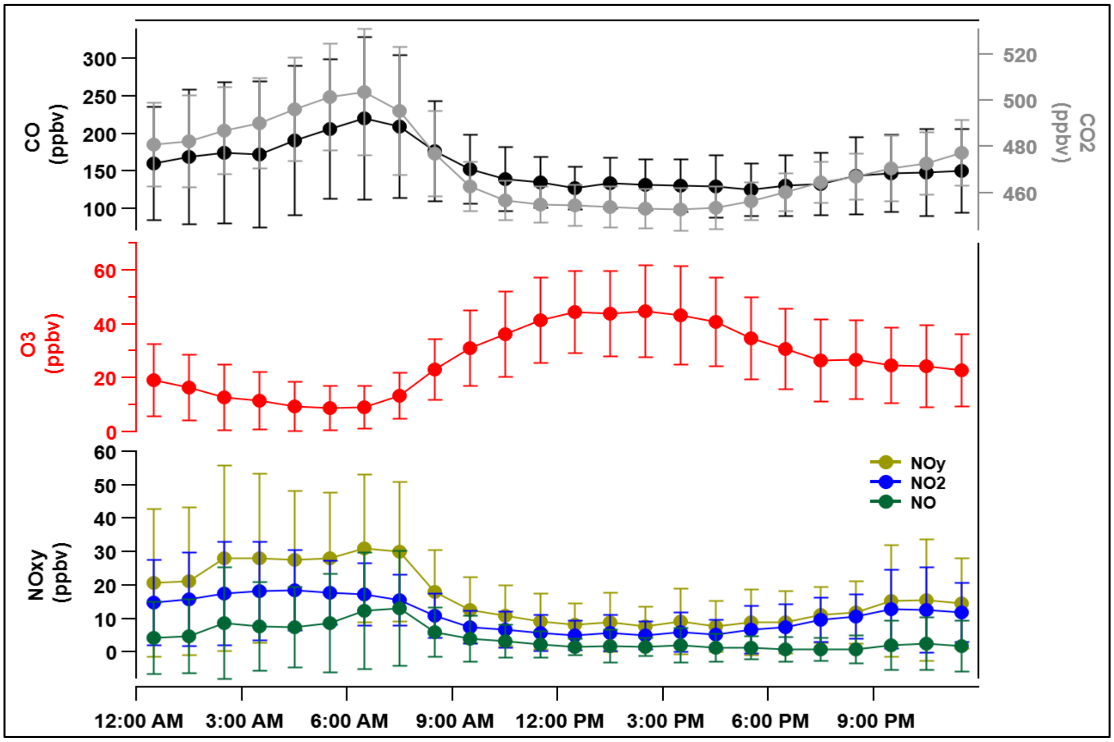


Figure 18: Diurnal profile of hourly averaged NO, NO_2, NO_Y, O_3, and CO measurements of instruments in MAQL2 at the San Jacinto Battleground Site.

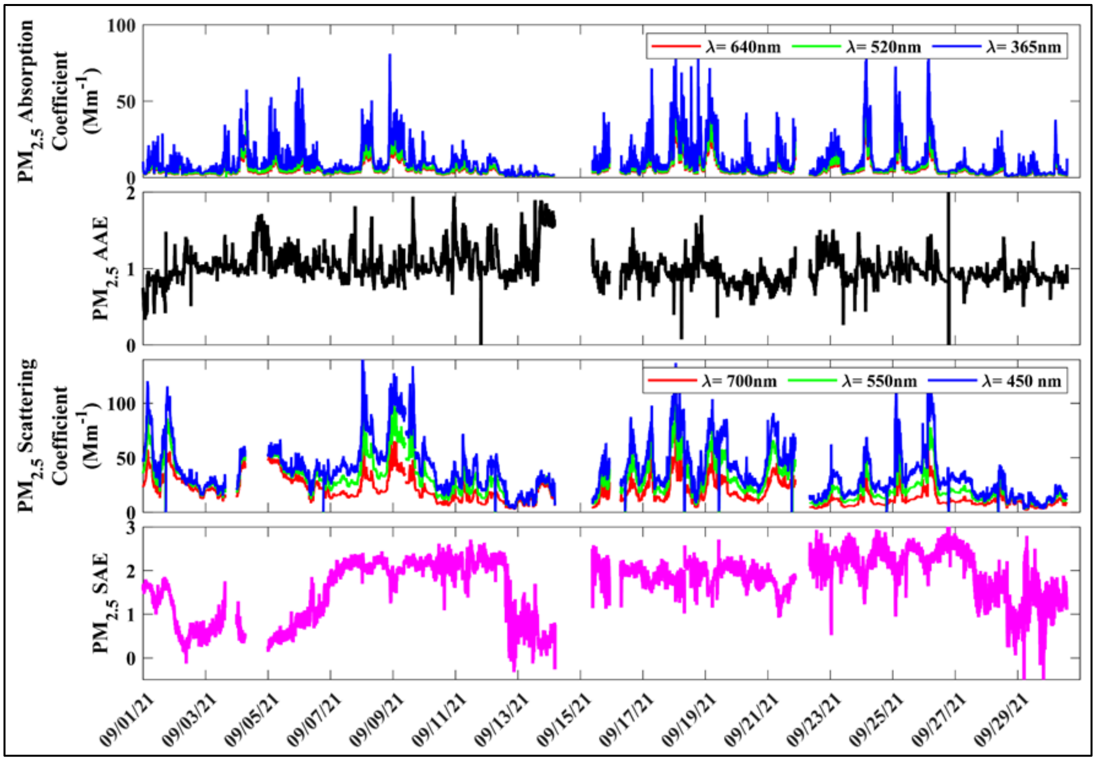


Figure 19: Time series of aerosol optical measurements made from the MAQL2 at the San Jacinto Battleground Historic Site. The MAQL2 made a total of 30 days over the month of September 2021. Aerosol absorption Ångstrom exponent (AAE) were calculated from the absorption coefficients, while the aerosol scattering Ångstrom exponent (SAE) were calculated from the scattering coefficients.

Sorbent tubes

Deployment of sorbent tubes during September 2021 and development of an offline analysis method were led by Baylor PIs. The objectives of sorbent tube deployments were to validate the sampling and analysis methods including sample collection, transport to BU, and quantification of ambient VOCs. Therefore, co-located samples were taken with the BU PTR-MS. An example of successful sorbent tube deployment and analysis is shown in Table 11 with observations from September 11th, 2021. Three tubes were sampled on the walkable roof of the MAQL2, and additional samples were taken at Brookglen Park and at the TCEQ Aldine site (CAMS 8). Winds were observed to be from the Northeast on 9/11. Most of the target analytes were identified in these samples and the sorbent tubes were able to speciate monoterpenes and C_8 isomers to support VOC measurements made in MAQL1 and MAQL2.

Table 10: Summary of preliminary VOC results taken using sorbent tubes on September 9th, 2021.

	Concentrations (ppbv)				
Target Analyte	10:13 - 10:23[a]	15:23 - 15:33[a]	15:31 - 15:41[a]	17:36 - 17:46[b]	19:18 - 19:28[c]
Isoprene	0.80	5.06	2.89	0.06	0.38
Benzene	0.14	0.89	1.23	0.87	1.31
Toluene	< DLR	1.89	2.17	< DLR	0.25
PCBTF	N.D.	< DLR	N.D.	N.D.	N.D.
Ethylbenzene	0.02	0.16	0.14	< DLR	0.10
m-& *p*-Xylene	< DLR	0.16	0.40	< DLR	0.04
o-Xylene	< DLR	0.14	0.12	< DLR	0.06
Styrene	< DLR	< DLR	< DLR	< DLR	< DLR
α- Pinene	0.04	0.22	0.16	0.04	0.09
β-Pinene	0.02	0.33	0.30	N.D.	0.05
D-Limonene	0.05	0.27	0.15	N.D.	N.D.
Eucalyptol	< DLR	0.01	0.01	N.D.	N.D.
Benzyl alcohol	< DLR	< DLR	0.03	< DLR	< DLR
D5-Siloxane	< DLR	0.13	0.66	< DLR	< DLR

[a] San Jacinto Battleground Historical site

[b] Brookglen Park

[c] Aldine TCEQ site

N.D. = non detect

DLR = dynamic linear range

3.3.6. Problems Encountered and Corrective Actions for Measurements

One of the main reasons for instrument downtown during the sampling project was due to Tropical Storm Nicholas. MAQL1 was brought back to campus and parked inside a warehouse-like facility on UH campus. MAQL2 was weather proofed and secured at the Battleground site. However, during this period there was a power outage from September 14 to 15. No major damages were incurred. Both MAQL1 and MAQL2 were quickly started back up and operating by September 16 and 17, respectively.

The problems encountered for sorbent tube operations pertained to the offline chemical analysis system and supply chain issues. When developing the offline analysis method, a benzene contamination in the TD-GC-MS/MS system was discovered and was concerning due to the compound being on the target analyte list. To resolve this issue, a service engineer from the thermal desorption company was called to BU and after two days of maintenance and flushing the system the cause of the carryover was determined to be the O-rings inside the desorption caps provided by the company. To stop the carryover contamination from recurring, the O-rings were swapped out with O-rings from another company and those from the thermal desorption company will no longer be used in the system.

The second issue slowed the progression of sampler development was global supply chain issues such as extended lead times and limited availabilities of specialty products. For example, the pumps and valves used in the VOC samplers were chosen because they are ruggedized, lightweight, and can operate at higher altitudes, but their lead time was 12 weeks. The items arrived in working condition and were successfully deployed. In the future these items should be ordered at least 4 months in advance of the intended sampling period to allow for preparation before sampling. In addition, the unavailability of lightweight materials to build the aerial sampler enclosure slowed its development. The sampler's external structure, internal wiring and accessibility were redesigned through a few rounds of development which resulted in a successful deployment in 2022

3.4. Offshore Air Quality Measurements

During the TRACER AQ campaign, the offshore vessel-based ozone, oxidant (O_3 and NO_2), and meteorological parameter monitoring from AQRP 20-004 was continued for September 2021. All instrument operation, maintenance, data collection, data validation, and safety processes from AQRP 20-004 were followed. All deployments were coordinated with the NASA TRACER-AQ science team and in consultation with the TCEQ.

Three active boats were outfitted with instrumentation to obtain the ozone, meteorological and boundary layer data. These boats, a 100' commercial ocean-going boat operated out of Galveston, TX that primarily services large marine vessel traffic offshore in the Gulf of Mexico (the Red Eagle boat), a commercial shrimper operated on the east side of Galveston Bay out of Smith Point, TX (the shrimp boat), and a UH-owned pontoon boat operated by the UH science team out of Kemah, TX were equipped to measure meteorological parameters and surface ozone. The pontoon boat and shrimp boat (July-August) were equipped with ceilometers to measure the boundary layer data. The pontoon boat also measured Ox (O_3 + NO_2) for six weeks and provided a platform to launch ozonesondes over Galveston Bay.

3.4.1. Platforms

Several different types of marine vessels and operators were considered for this project. The two chosen were based on their typical operating profiles and openness to working with the science team. In Galveston Bay, the commercial shrimper from Smith Point was chosen. As described to the science team, their operating pattern would follow the shrimp in the Bay as they slowly migrated through various portions of the eastern portion of the Bay, unlike oyster boats which visit fixed locations.

Figure 20 shows the shrimp boat with the mobile sampling package installed onto the roof of the pilothouse. A dedicated high output marine alternator and battery was installed for additional power to operate the science equipment while underway. State regulations dictate different seasons and legal catch amounts; however, except for bad weather, he was expected to be on the bay typically four days a week. Based on precampaign discussions, on a typical day he would leave the Smith Point area around dawn and return around 2:00 PM, depending on the season and catch. Mr. Willis based his boat at the basin in the RV park where the UH Smith Point monitoring site (C1606) is located, allowing for routine comparisons with the O3 monitor just 260 m east of the dock. The early season influence of fresh water in the Bay from local rains decreased the quality of catch this season and resulted in significantly lower number of outings and spatial coverage by the Shrimp Boat. COVID related issues also limited his ability to operate for a couple of weeks in August and September.

Figure 20: Shrimp boat operated in Galveston Bay by Larry Willis.

For the Gulf of Mexico, a charter boat, the M/V Red Eagle operated by Ryan Marine out of Galveston, TX (Figure 21), was selected as their operations would take them to the various anchoring and lightering areas off of Galveston Island frequently, sometimes multiple times per day. The Red Eagle is a 100’ long crew/utility vessel with two 40 kW 110/208V three-phase power generators. The typical operating profile for the Red Eagle was to depart the Galveston docks for the Galveston Anchorages and Lightering areas roughly every other day, depending on their clients’ needs. The Red Eagle also conducted some operations as far west as Matagorda Bay (one occasion) and north through the ship channel to the port of Houston. On occasion, the boat would go up to 50 miles offshore. These activities would occur at any time of day and in all weather conditions.

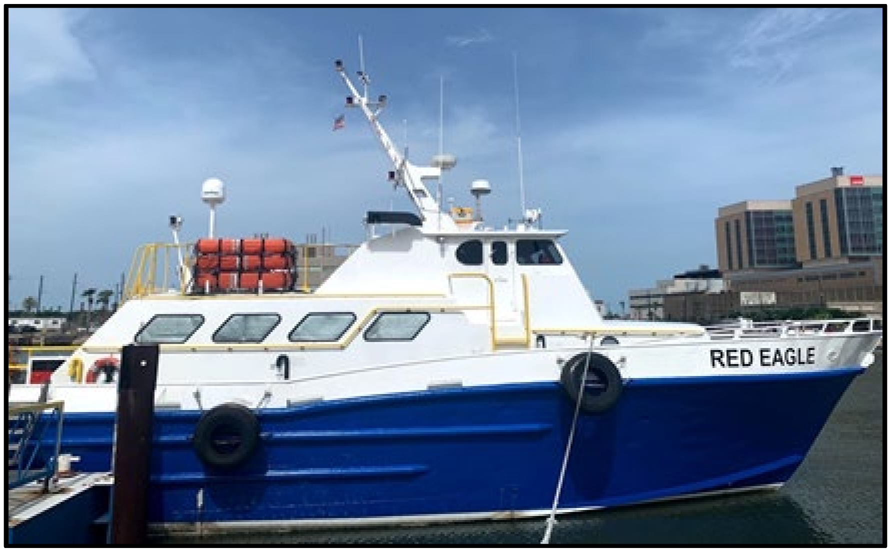


Figure 21: The M/V Red Eagle operated by Ryan Marine out of Galveston, TX in the Gulf of Mexico.

Additionally, the R/V Mishipeshu (Figure 22), a pontoon boat owned and operated by UH was deployed on selected days in July, August, September and October (outings listed in Table 1) in Galveston Bay. The pontoon boat was kept at the Portofino Harbour Marina in Kemah. This gated entry site allowed quick and easy access to the Bay for the pontoon and is adjacent to a fuel dock for refilling the boat and generator at the end of each day of operations on the water. By not having to trailer the boat from campus, launch, recover, and return the boat to campus each day of operation the crew was able to save 3-4 hours each day which were put towards sampling activities. Shore power (30A 120V) was also available at the marina, allowing the instrumentation on the boat to remain operational 24/7 and essentially providing a monitoring site in Kemah when not in use on the Bay. This also ensures that the instrumentation is warmed up prior to any activities on the Bay. The cost for the marina is approximately $300 plus miscellaneous fees and electrical usage.

Figure 22: The UH pontoon boat is owned by the University of Houston and operated in Galveston Bay.

Ozonesondes were launched from the Red Eagle and UH pontoon boat on select days of interest throughout the campaign period to determine the vertical distribution of O_3 and the marine boundary layer height. Together, the three boats characterized much of Galveston Bay and the offshore waters. This operational area and pattern provided a robust data set for analysis and evaluating model outputs.

3.4.2. Instrument Packages

All three active boats were outfitted with an automated instrument package (Figure 23). The automated instrument packages consist of a 2B Technology Model 205 dual-beam O_3 analyzer provided by St. Edward's University (Gary Morris, Co-PI), Global Positioning System (GPS), and a ruggedized industrial computer (PC). The PC was configured to boot and shut down with an external switch or with the application or loss of power which automatically started or stopped the instrumentation and data logging. A compact, all-in-one weather station was installed to measure temperature, relative humidity, pressure, and wind speed and direction. An internal digital compass was used with GPS data to correct winds for the motion of the boat. This equipment was installed into a light-colored (yellow) weatherproof enclosure to protect the instrumentation and reduce heat. Additional insulation and a radiant barrier further reduced solar heating. A thermoelectric heat exchanger attached to the enclosure further reduced heat and maintained a stable environment for the instrumentation. Desiccant bags were also used to help control internal relative humidity. This enclosure was secured to the boat exterior on top of the cabin. A Teflon sample line was run from the sample pump in the O_3 monitor to an elevated location on each boat for the sample inlet. A Teflon rain shroud prevented water from entering the 90 mm Teflon particle filter before being sampled. The relatively large area of the filter required less frequent access to the boat and equipment for filter changes.

Figure 23: Instrumented weatherproof enclosure installed on the two commercial boats showing the 2B Tech O_3 monitor (blue box, bottom left), dual-sim cellular router (small blue box above 2B), backup battery (black box, center), zeroing cartridge (orange and clear, left rear), rugged industrial computer (black box with fan on top, right), high efficiency 24VDC power supply (silver box, far right). The rear panel of the chassis provides space for the LabJack U3 data card (red, center rear), thermoelectric temperature controller (black with green screen, rear behind computer), and circuit breaker for the thermoelectric cooler system (black button on silver tab, right of temperature controller). Space for mounting the NO_2 photocells is reserved on top of the O_3 analyzer, near the cellular router and will be installed for future campaigns.

Data was logged internally and then transferred to servers at UH via integrated cellular modems when the boat was within the cellular coverage area. There was excellent cellular coverage over most of the areas where the boats operated in Galveston Bay, with the exception of spotty signal at Smith Point itself. Coverage in the Gulf was also present typically as far out as the main anchoring locations but not at the lightering area. The data, which included performance information such as instrument temperatures, pressures, and flows, was displayed on the same system used to visualize and edit data from the network of UH monitoring sites. The network connection also allowed investigators to log into the computers on the boat via LogMeIn to evaluate instrument performance and aid in troubleshooting.

Vaisala CL-51 ceilometers were installed on the UH pontoon boat and the Shrimp Boat. The ceilometers operated and collected data continuously, however the ceilometer on the UH pontoon boat suffered a failure on August 30th. Since the Shrimp Boat was not going out as frequently as hoped due to poor shrimping conditions, the team removed the ceilometer from the Shrimp Boat and installed it on the UH pontoon boat. The data, both mobile and stationary, is used to better understand O_3 processes in and around the Galveston and Trinity Bay area.

A NASA Pandora spectrometer was installed on the UH Pontoon boat on August 25, 2021 while the UH Pontoon boat was docked in the Portofino Marina. After the initial install the UH pontoon was deployed into Galveston Bay for testing. The Pandora instrument was able to successfully track the sun while mobile over Galveston Bay, with the best performance was achieved during smooth water conditions. The NASA Pandora continued observations until September 23, 2021. High heat and humidity in the Galveston Bay marine environment along with insufficient mitigation allowed condensation to form within the spectrometer and caused a short circuit.

The main shortcoming of the project was that the manufacturer failed to deliver working NO_2 photocells. Ultimately an alternate NO_2 photocell was installed during the downtime caused by Hurricane Nicholas and deployed on the UH pontoon boat system. The O_X measurement was captured from September 17 to October 25, 2021, the end of field measurements.

3.4.3. Quality Control / Quality Assurance for Offshore Air Quality Measurements

A valve was used to periodically route the sample through an ozone-destroying charcoal volume to assess the instrument baseline. Instruments were calibrated prior to and after deployment by comparison with O_3 standards directly traceable to the EPA Region 6 standard reference photometer for O_3. Data was also compared to other O_3 monitors when in proximity to TCEQ monitoring sites.

Comparisons of Measurements between the UH Pontoon Boat and TCEQ monitoring sites

Figure 24–Figure 25 show comparisons of ozone made by the UH pontoon boat stationary measurements and the nearest TCEQ monitor site, Seabrook (C45). Comparison between stationary ozone and mobile platforms generally shows good agreement.

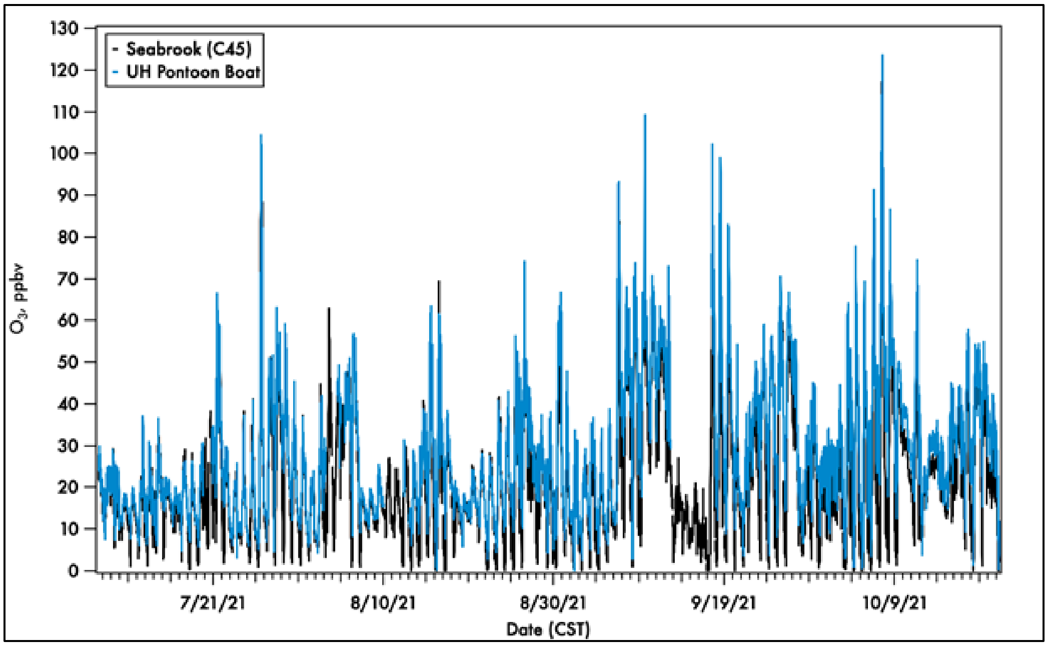


Figure 24: Time-series of 5-minute averaged ozone (O_3) concentration from the UH pontoon boat mobile monitor and the nearest TCEQ monitor, Seabrook (C45). Measurements are from July 7 to October 21, 2021.

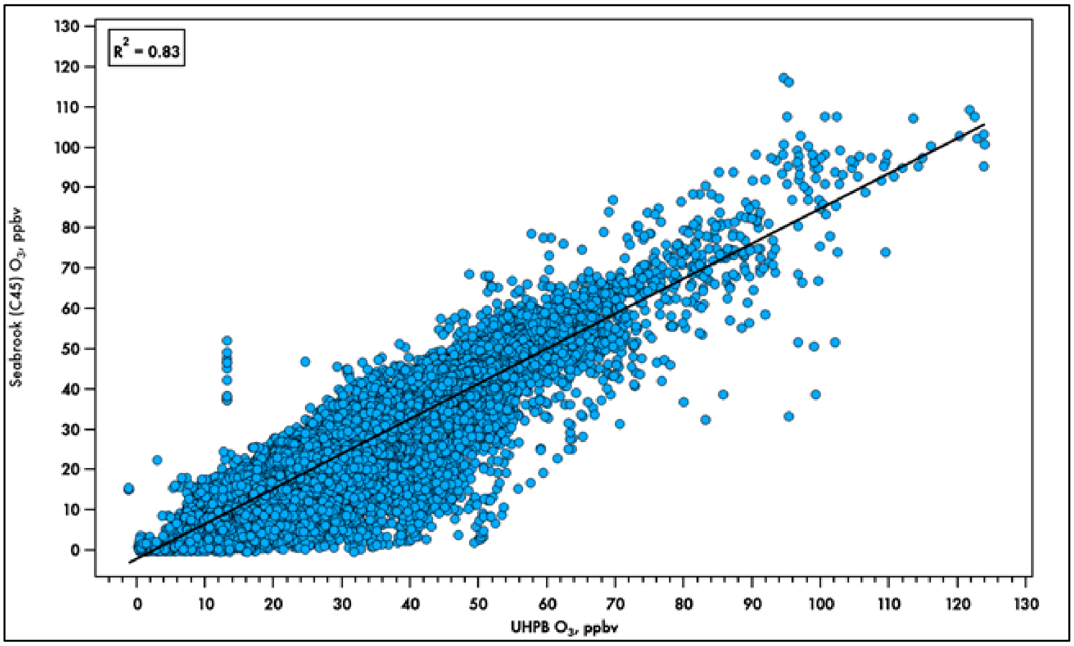


Figure 25: Scatter plot of 5-minute averaged ozone (O_3) concentration from the UH pontoon boat mobile monitor and the nearest TCEQ monitor, Seabrook (C45). Measurements are from July 7 to October 21, 2021.

Comparisons between the UH Pontoon boats calculated NO_2 with the stationary NO_2 monitors around Galveston Bay are shown in Figure 26–Figure 27, and appeared to be more variable. Generally, the closest TCEQ monitor to the UH pontoon boat was the Seabrook (C45) site, which also showed the closest agreement ($r^2 = 0.43$) to the UH pontoon boat. The Texas City site (C620) located near-shore on the SW side of the Bay showed some agreement with the UH Pontoon boat ($r^2 = 0.26$), but significantly less than the closer Seabrook site. The Smith Point (C1606) site located on the East side of Galveston Bay showed no agreement ($r^2 = 0.00$) with the UH pontoon boat. This comparison indicates the significant spatial variability of NO_2 across Galveston Bay.

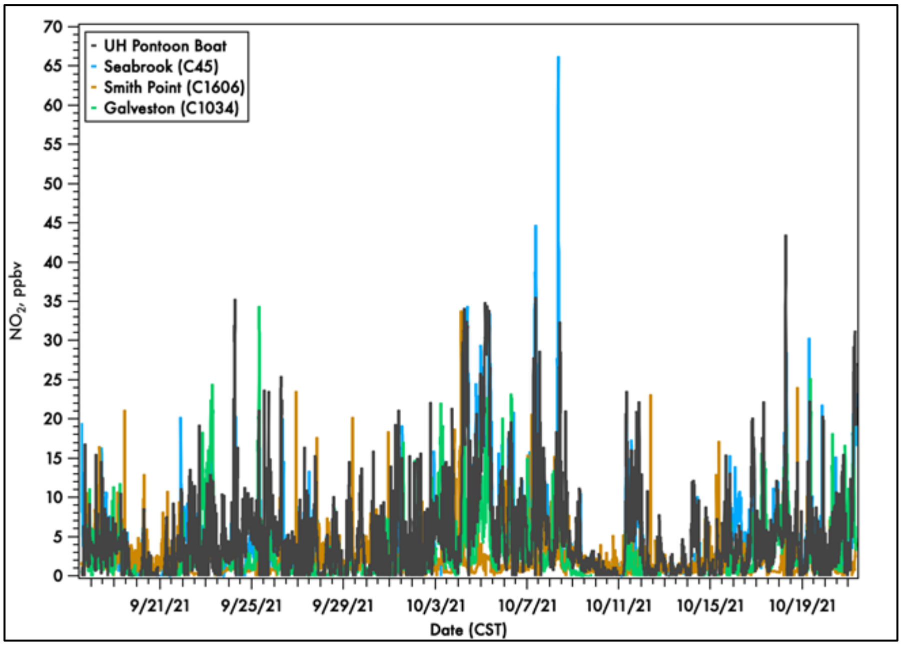


Figure 26: Time series of 5-minute averaged nitrogen dioxide (NO_2) concentration from the UH Pontoon boat mobile monitor and other stationary monitors around Galveston Bay.

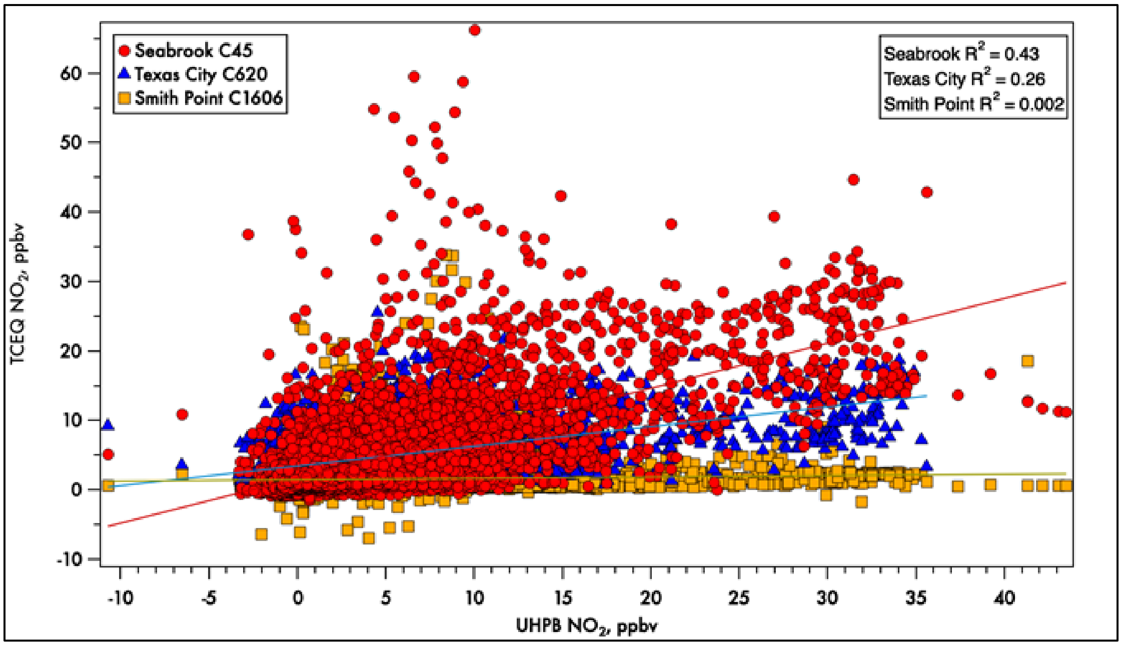


Figure 27: Scatter plot of 5-minute averaged nitrogen dioxide (NO_2) concentration from the UH Pontoon boat mobile monitor and other stationary monitors around Galveston Bay.

Comparisons of Measurements between the Red Eagle boat and TCEQ monitoring sites

The Red Eagle boat operating out of Galveston, TX, showed the weakest agreement between the nearest TCEQ monitor site, Galveston 99th St. (C1034), as seen in Figure 29. In this case, the variability between the two monitors is likely exacerbated due to the locations of the monitors. The Galveston 99th St. site is located on the Gulf side of Galveston Island and was not as likely to be impacted by titration due to local emissions. The Red Eagle, when at dock, was located on the Bay side of Galveston Island in a harbor that sees frequent ship traffic and was located adjacent to a moderately trafficked road (Harborside Dr.). Additionally, when maneuvering alongside the larger vessels that they service, the captain was not always able to position the Red Eagle in such a way as to avoid sampling the exhaust of the Red Eagle or other ships.

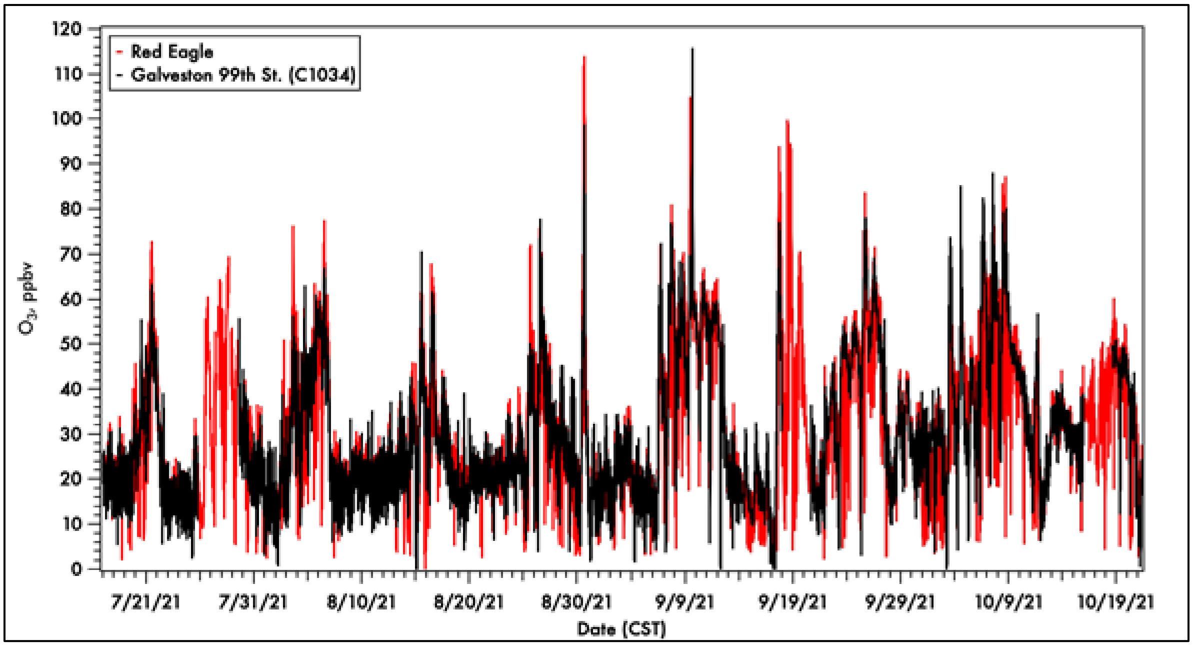


Figure 28: Time series of 5-minute averaged ozone concentration from the Red Eagle mobile monitor and the nearest TCEQ monitor, Galveston 99th St (C1034). Measurements are from July 17 to October 21, 2021.

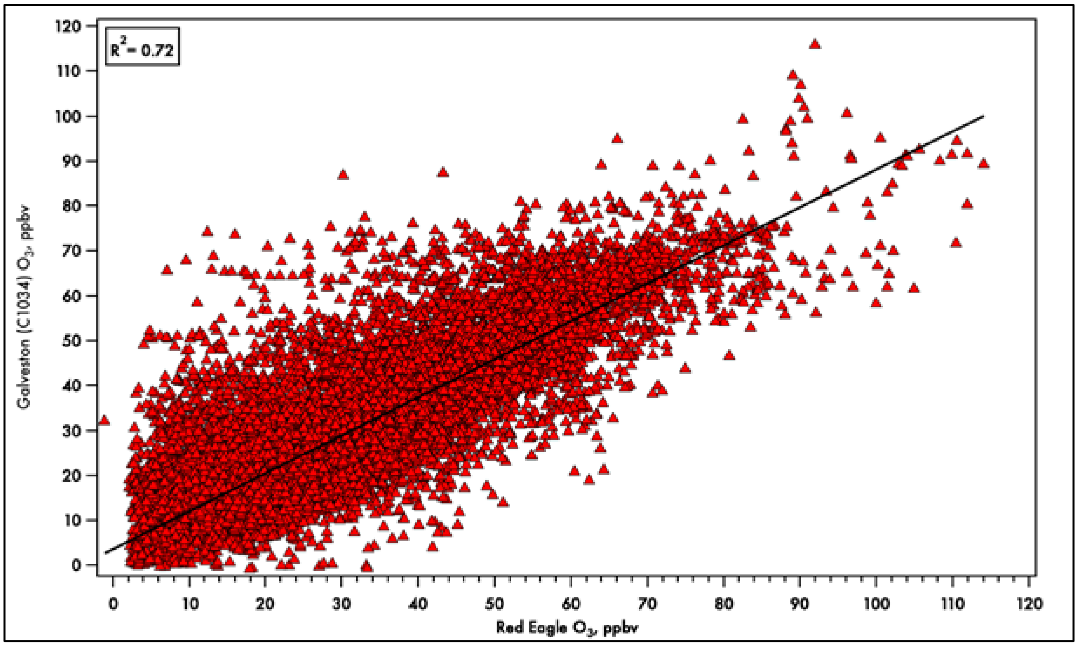


Figure 29: Scatter plot of 5-minute averaged ozone (O_3) concentration from the Red Eagle mobile monitor and the nearest TCEQ monitor, Galveston (C1034). Measurements are from July 7 to October 21, 2021.

Comparisons of Measurements between the Shrimp boat and TCEQ monitoring sites

The closest agreement between measuring sites was between the Smith Point monitor (C1606) and the Shrimp Boat mobile platform (Figure 31). These two locations were approximately 230 m apart when the shrimp boat was at dock. The shrimp boat also operated on a mobile basis the least frequently, due to a variety of reasons including poor shrimping due to the influence of fresh water from local rains and COVID-related recovery time. When the shrimp boat was operating, it also had the smallest spatial coverage of the three platforms, as seen in Figure 37. The strong correlation between these two measurements indicates that the C1606 monitor is representative of the O_3 conditions of the nearby Bay waters.

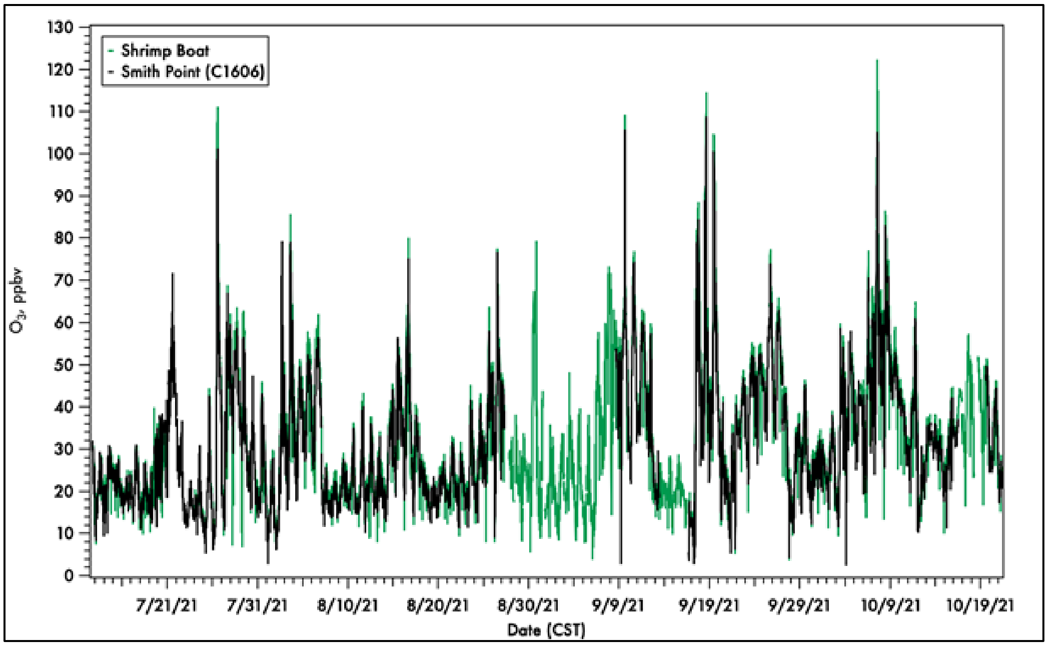


Figure 30: Time series of 5-minute averaged ozone concentration from the shrimp boat mobile monitor and the nearest TCEQ monitor, Smith Point (C1606). Measurements are from July 12 to October 24, 2021.

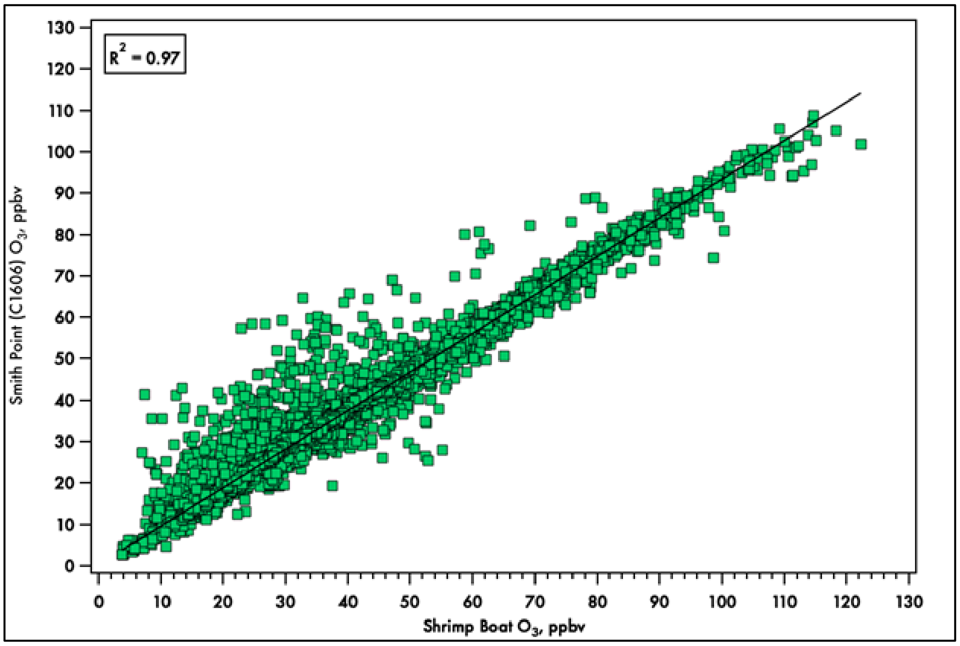


Figure 31: Scatter plot of 5-minute averaged ozone concentration from the shrimp boat mobile monitor and the nearest TCEQ monitor, Smith Point (C1606). Measurements are from July 12 to October 24, 2021.

3.4.4. Results for Offshore Air Quality Measurements

Trace Gas Measurements

An overview of all meteorological, O_3, and NO_2 collected by the three research vessels over the entire sample period are shown in Figure 32 to Figure 34. The time series, showed that periods of high ozone occurred over the water throughout the ozone season. The highest ozone periods over the water do generally coincide with a wind flow reversal shifting the winds from generally onshore (southerly flow) to generally offshore (northerly flow). This scenario would typically occur after the passing of a frontal boundary. The highest ozone of the sample period of 133 ppb was observed on October 7, 2021, approximately 4 days after the passing of a frontal boundary. This measurement was recorded by the UH pontoon boat during a mobile sampling period on Galveston Bay in the W/NW regions.

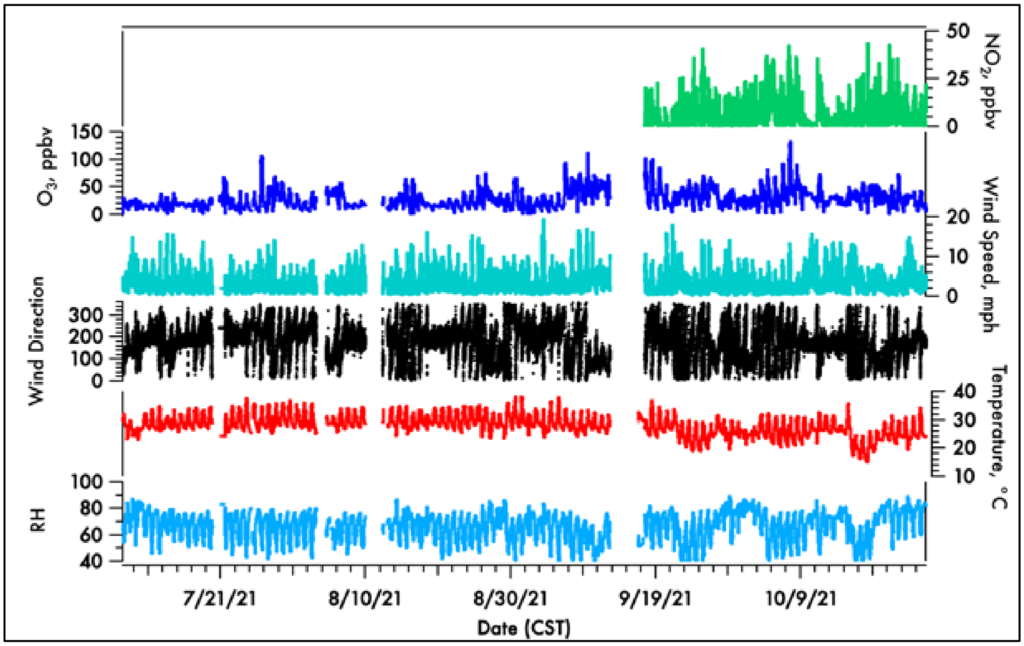


Figure 32: Ozone and Meteorological data collected on the UH pontoon boat operated by the University of Houston from July 13 to October 11, 2021.

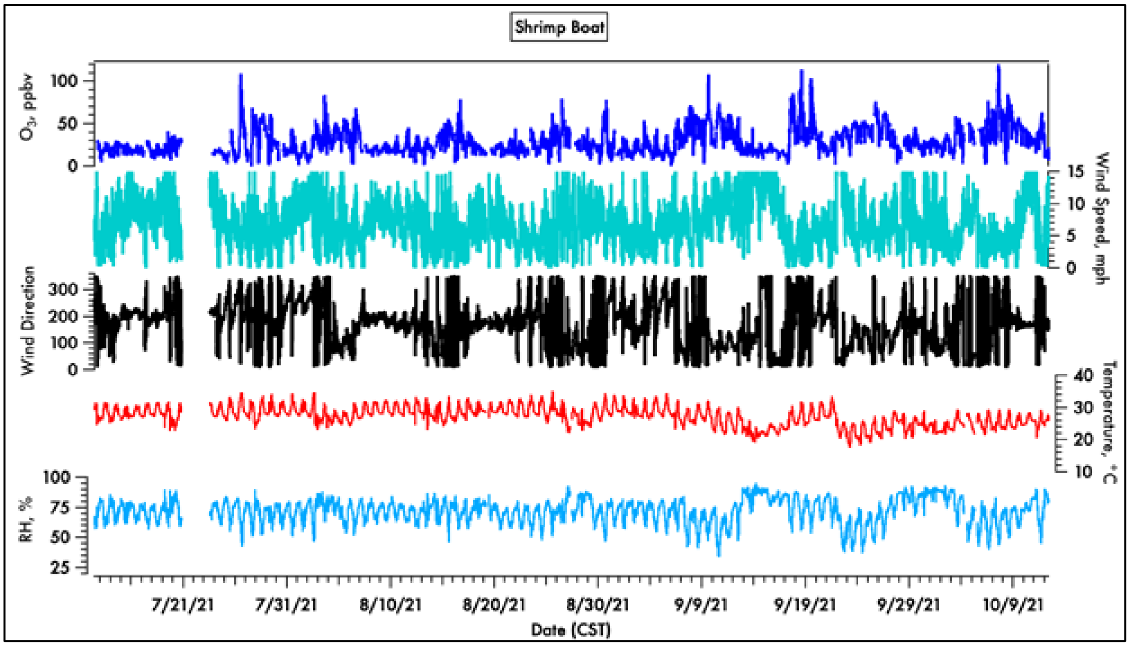


Figure 33: Ozone and Meteorological data collected on the Shrimp Boat operated by Larry Willis from July 12 to October 11, 2021.

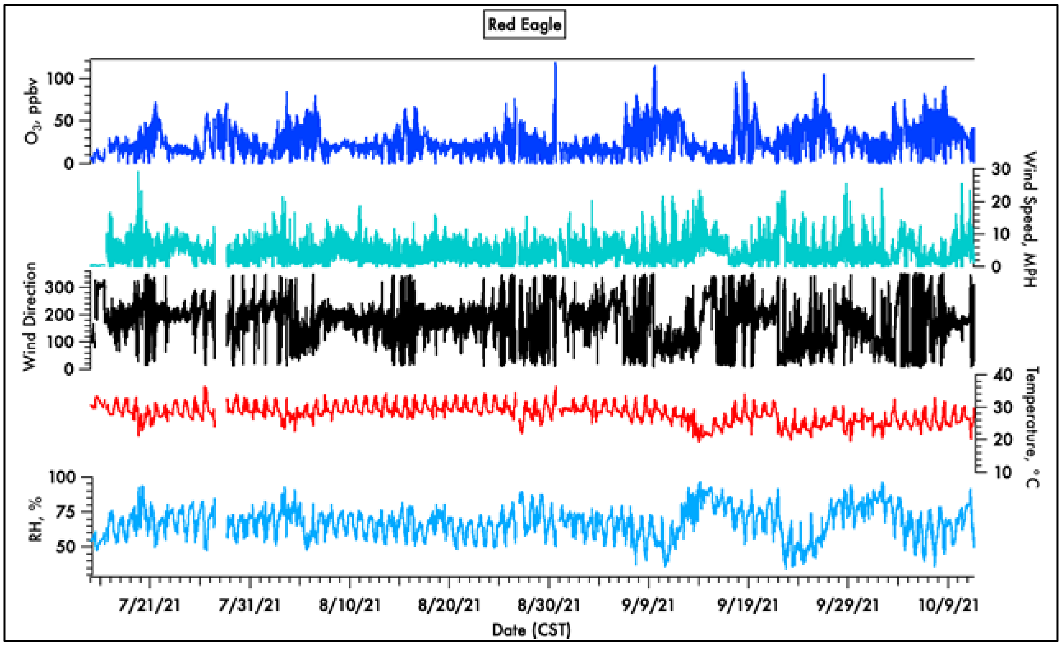


Figure 34: Ozone and Meteorological data collected on the Red Eagle operated by Ryan Marine from July 17 to October 11, 2021.

The spatial plots of O_3 and NO_2 (UH pontoon boat only) for the UH pontoon boat, Shrimp Boat, and the M/V Red Eagle are shown in Figure 35–Figure 38. The UH pontoon boat was docked in Kemah, TX, labeled in Figure 35, on the West side of Galveston Bay. The primary operating areas were on the west side of the Houston ship channel. The Shrimp Boat was docked at Smith Point when not being operated in Galveston Bay. The M/V Red Eagle, which primarily operated in the Gulf of Mexico, was docked on the bayside of Galveston Island when not being operated. The Red Eagle regularly serviced both anchorage locations, approximately 10 miles offshore, as well as the lightering area approximately 30 miles offshore. During the sample period, the Red Eagle also traversed the Houston ship channel to service clients near the port of Houston on two occasions.

The spatial plot of ozone collected during the sample period from the UH pontoon boat is shown in Figure 35. The spatial plot shows an overlapping picture of spatial and temporal ranges. However, some trends were apparent, specifically that high ozone was more frequently observed over Galveston Bay west of the ship channel and north of Kemah, TX, although sampling bias is likely influencing this observation. These areas are nearest to emissions sources and most likely subject to recirculation processes associated with the bay/sea breeze and potentially less affected by penetration of the Gulf breeze.

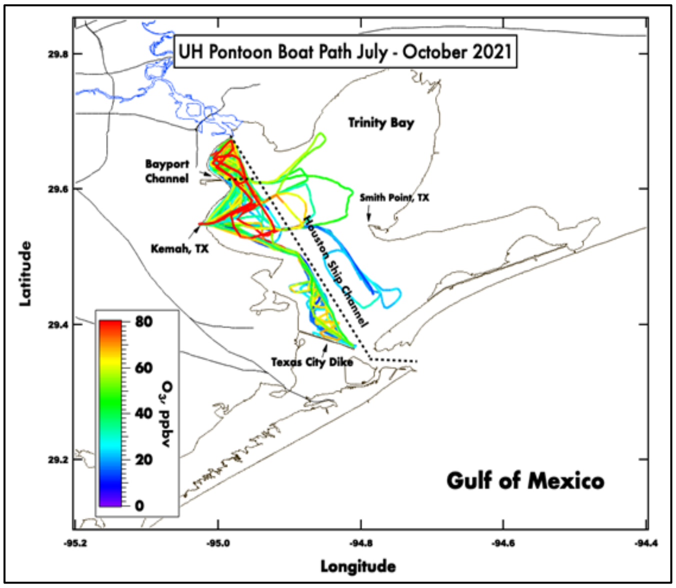


Figure 35: Spatial Map of ozone collected from July–October 2021 on the UH pontoon boat.

Regions of Galveston Bay near the Houston ship channel and nearest the urban and industrial emissions sources showed frequent spikes in NO_2, as shown in Figure 36. The sample period for NO_2 was considerably shorter (09/17/2021–10/24/2021) compared with the time period for the ozone data collection on the UH pontoon boat displayed in Figure 35.

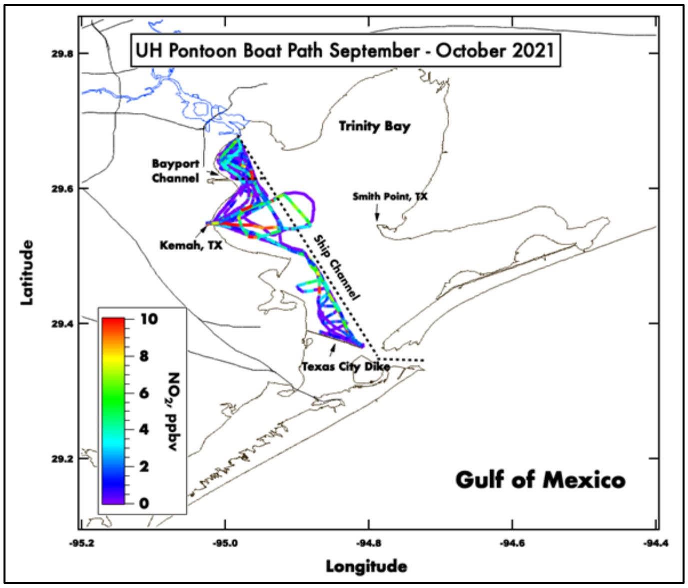


Figure 36: Spatial Map of NO_2 collected from September 17–October 11, 2021, on the UH pontoon boat.

The spatial overview for the shrimp boat, operated by Larry Willis out of Smith Point, is shown in Figure 37. The spatial plot shows less ozone variability in the coverage region, primarily around the Smith Point area on the East side of Galveston Bay. The shrimp boat operated less frequently than the Red Eagle or UH pontoon boat. Unfortunately, the shrimp boat did not operate out on the Bay during the majority of the high ozone episodes, staying at the dock at Smith Point.

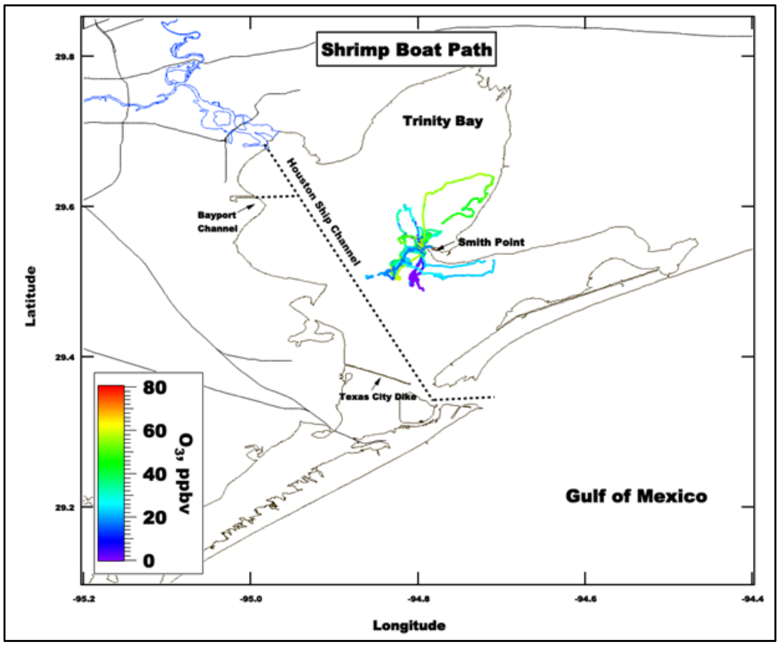


Figure 37: Spatial Map of ozone collected from July 12–October 11, 2021, on the Shrimp Boat operated by Larry Willis.

The M/V Red Eagle operated primarily in the offshore waters of the Gulf of Mexico, servicing large commercial vessels in the anchorage and lightering areas. The Red Eagle operated at any time of day or night and in most weather conditions. The wide spatial and temporal variability of ozone observed offshore, as seen in Figure 38, is an interesting feature. The highest ozone observed offshore was on September 9, 2021, with concentrations exceeding 110 ppbv. The high ozone observations typically occurred in the post-frontal environment with a flow reversal from onshore (southerly) to offshore (northerly).

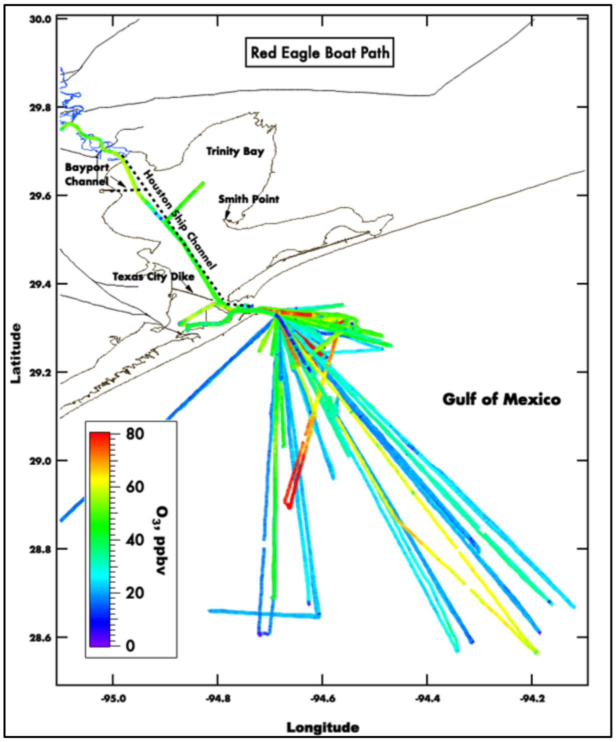


Figure 38: Spatial Map of ozone collected from July 17–October 11, 2021, on the Red Eagle operated by Ryan Marine.

Boundary Layer Measurements

For ozonesonde profiles, the boundary layer height is determined by examining gradients in relative humidity (RH), O_3, temperature, and potential temperature (θ) and is identified as the height at which most (if not all of) these variables show a sharp change in their vertical gradients. Typically, for an afternoon potential temperature profile, just above the surface $\partial\theta/\partial z < 0$, the air is unstable (due to surface heating). After the initial negative gradient near the surface, the potential temperature is approximately constant ($\partial\theta/\partial z = 0$) to the top of the boundary layer near 3.9 km AMSL on this day. A near-zero gradient in potential temperature is common. The atmosphere is generally stable above the boundary layer, as indicated by the positive potential temperature gradient ($\partial\theta/\partial z > 0$). The larger a positive potential temperature gradient is, the stronger the atmospheres stability at that altitude. The potential temperature will reach the same value that it is at the surface at the top of the PBL (Haman, Lefer, and Morris 2012). As with ceilometer data, when identifying the PBLH from ozonesonde profiles, in some cases, there are multiple possible layers present, and there is uncertainty based on which layer is chosen. An example is shown in Figure 39.

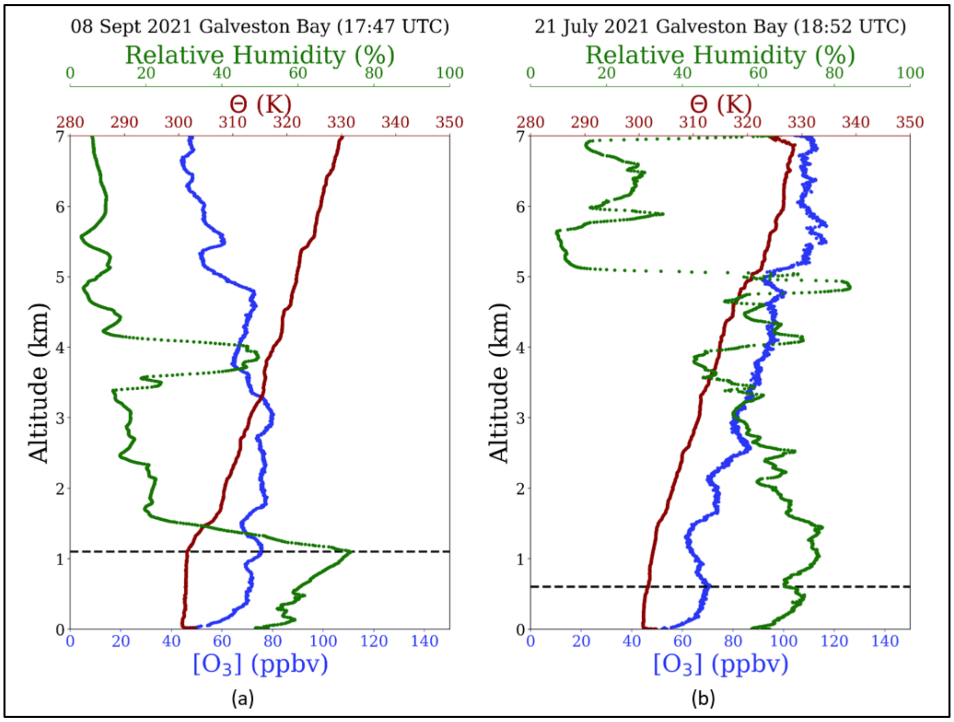


Figure 39: Vertical profiles of ozone (blue), relative humidity (green), and potential temperature (dark red) from two ozonesondes released from Galveston Bay. The top of the boundary layer is shown by the black dashed horizontal line at (a) 1.1 km and (b) 0.6 km. Profile (a) is an example of having somewhat higher confidence in the estimate of the top of the boundary layer than profile (b). In profile (b), other possible boundary layer estimates could be 0.95 km or 1.5 km. In profile (a) there is a clear transition in the potential temperature profile at 1.1 km and the relative humidity drops substantially just above the estimated boundary layer height of 1.1 km. In profile (b) the potential temperature does not have as pronounced a change at the estimated boundary layer height of 0.6 km and the relative humidity does not drop substantially until near an altitude of 5 km, both of which make the estimated boundary layer height in profile (b) a more difficult estimate.

For ozonesonde launches that occurred from the UH Pontoon Boat, a comparison of the boundary layer heights from the ozonesonde profiles versus the Vaisala CL-51 ceilometer first identified boundary layer height is shown in Figure 40. The trendline has a slope of 0.58 ± 0.12 and a y-intercept of 223 ± 129 with an r^2 value of 0.45.

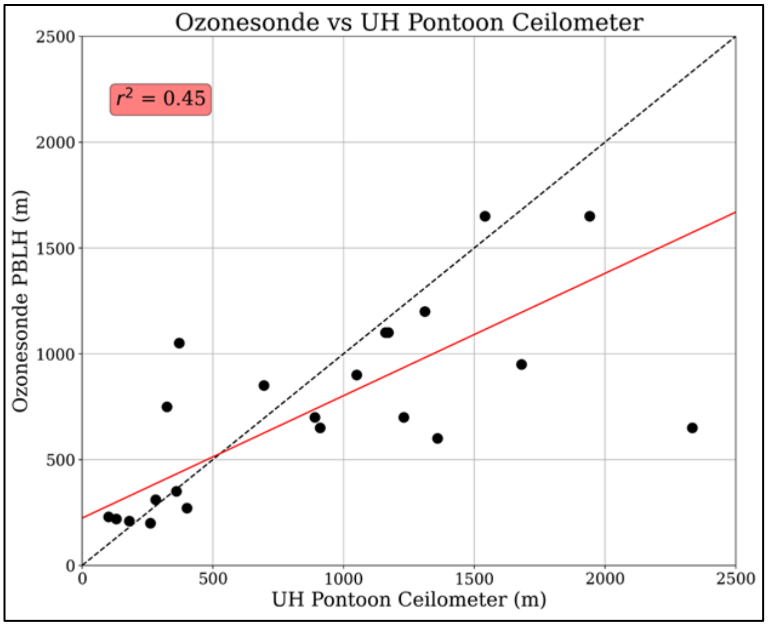


Figure 40: Comparison of boundary layer heights determined from profiles of collated ozonesonde launches versus the UH Pontoon boat Vaisala CL-51 ceilometer first identified boundary layer height. The red line shows a linear best fit with a slope of 0.58 ± .12 and a y-intercept of 223 ± 129. The dashed black line shows a 1-to-1 trendline.

In addition to the observations of the boundary layer height from the pontoon boat described above, measurements were also collected on the Shrimp Boat during the first stages of the campaign. As reported in the monthly reports, a short circuit damaged the ceilometer on the pontoon boat system. The system from the Shrimp Boat was removed and subsequently installed on the pontoon for the remainder of the campaign. This decision was largely based on the lack of movement in the Shrimp Boat. The CL-51 from the pontoon was returned to Vaisala for repair under warranty and was not returned before the conclusion of the campaign.

Data from the early portion of the project is shown below in Figure 40–Figure 43 as average diurnal profiles for the three layers identified by the instrument's software. Although the boats did operate out in the Bay to varying extents, the vast majority of the data was collected while in port. Therefore, these datasets are considered to be from either Smith Point (Shrimp Boat) on the east side of the Bay or Kemah (pontoon) on the western side. From Figure 41, we see significant differences in the two profiles, with the pontoon 200-400 m lower than the Shrimp Boat in the overnight hours but as much as 600-700 m higher than the Shrimp Boat in the afternoon. During the middle portion of the day, the two locations reported similar boundary layer heights. Aside from the clear differences in boundary layer height between the two sides of the Bay, each profile is interesting on its own. The profile from the Kemah location appears to be similar to other land-based boundary layer height measurements, with a minimum early in the morning and increasing throughout the day until shortly before sunset. On the other hand, the Smith Point profile shows a relatively stable boundary layer height near 1,000 m throughout the first half of the day and decreasing to around 500 m in the afternoon. The stability of the Smith Point profile in the first half of the day may be due to the relatively stable temperatures of the surrounding water. The decrease in boundary layer height in the afternoon period is interesting. An early hypothesis is that the effect seen here may be tied to the onset and retreat of a Gulf breeze moving in from the coast. However, at this time, a full analysis of this feature is beyond the scope of this project but may be included in future planned analyses. These features differ from those reported for Galveston at the C1034 site during DISCOVER-AQ in September 2013 (Figure 42), which found that the first layer was often around 200 m with a second layer near 700 m. Given the proximity of the Galveston measurements to the Gulf, the measurements here are likely more sensitive to the conditions over the Bay. In addition to the difference in year, season (September 2013 for Galveston and July-August 2021 for Smith Point and Kemah) may play a role in the observed differences. Both layers two (Figure 43) and three (Figure 44) for Kemah and Smith Point differ from layer 1 in that they are quite similar to each other despite being separated by over 20 km of water on opposite sides of the Bay. This seems to indicate that the lofted features may be regional in scale and less impacted by Bay or Gulf driven dynamics.

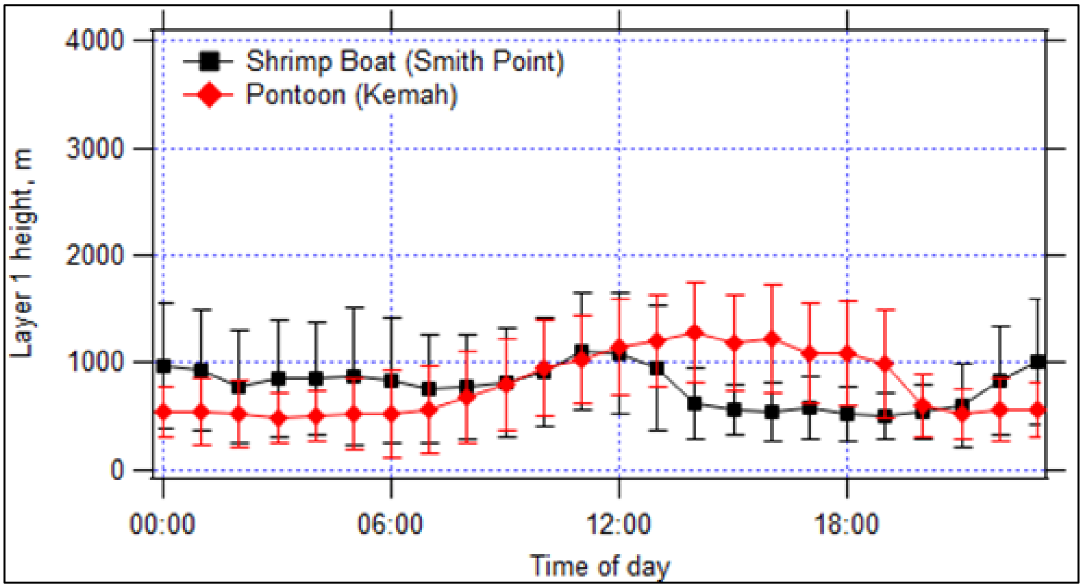


Figure 41: Diurnal profile (± one standard deviation) of the first identified layer height from the Shrimp Boat at Smith Point and the pontoon boat in Kemah. This layer is often considered the boundary layer height. Significant differences are seen between these two profiles, indicating variability in the boundary layer height over the Bay.

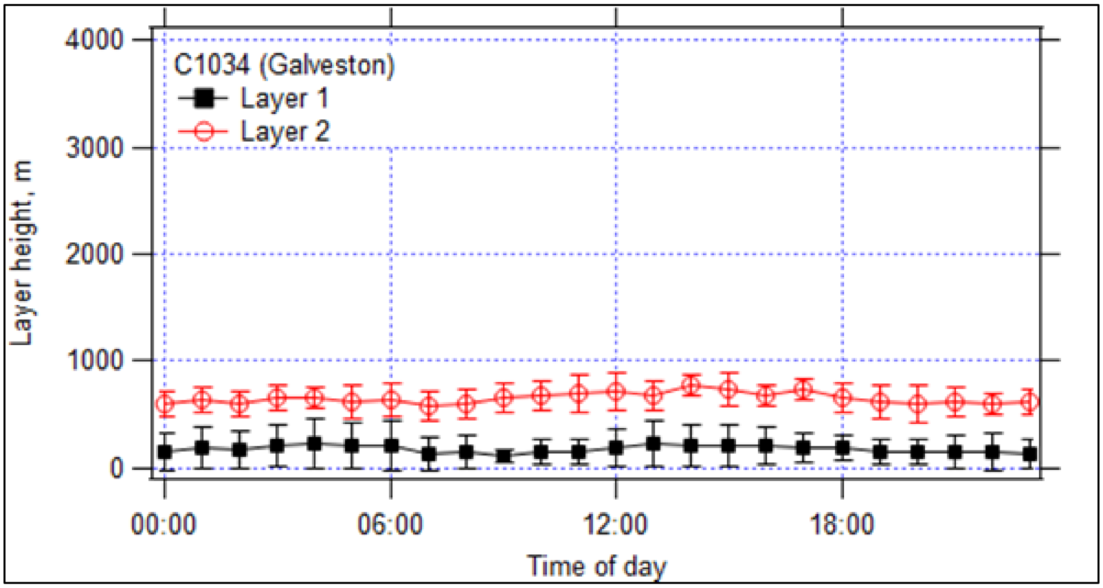


Figure 42: Diurnal profile of Layers 1 and 2 for Galveston (C1034) during DISCOVER-AQ in September 2013.

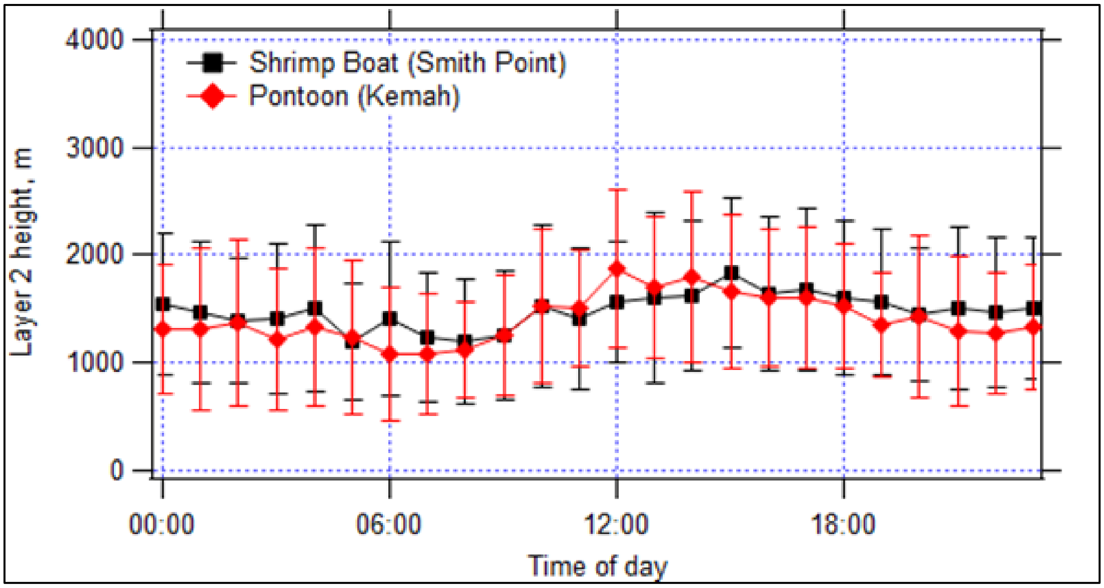


Figure 43: Diurnal profile (± one standard deviation) of the second identified layer height from the Shrimp Boat at Smith Point and the pontoon boat in Kemah. This elevated layer compares quite well between the two over the Bay.

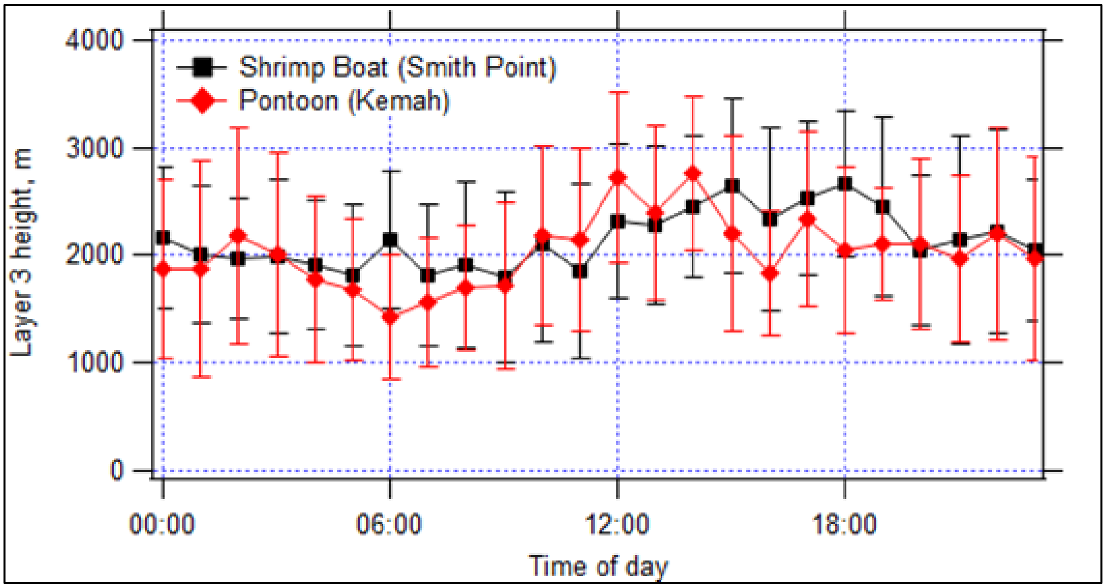


Figure 44: Diurnal profile (± one standard deviation) of the third identified layer height from the Shrimp Boat at Smith Point and the pontoon boat in Kemah. Like the second layer above, the third layer is consistent between the two platforms, indicating a uniform feature over the Bay.

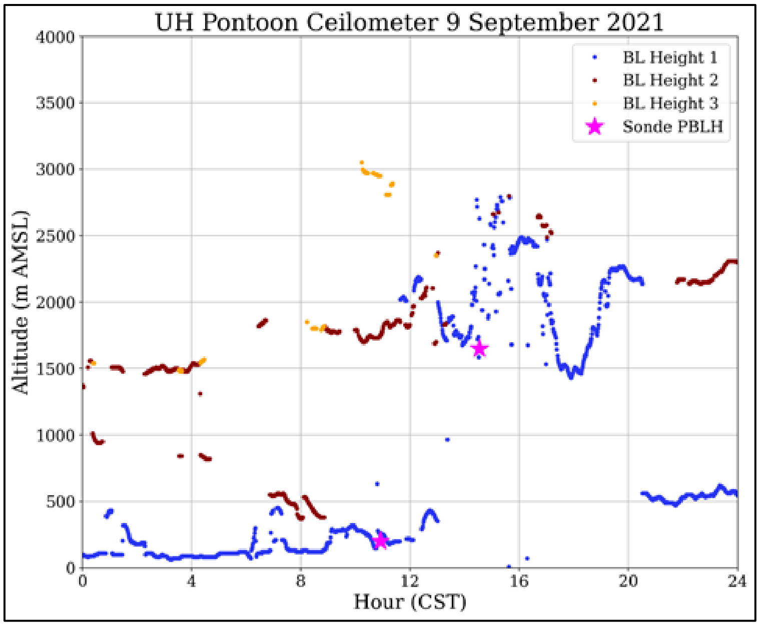


Figure 45: Ceilometer data from the pontoon boat on 9 September 2021.

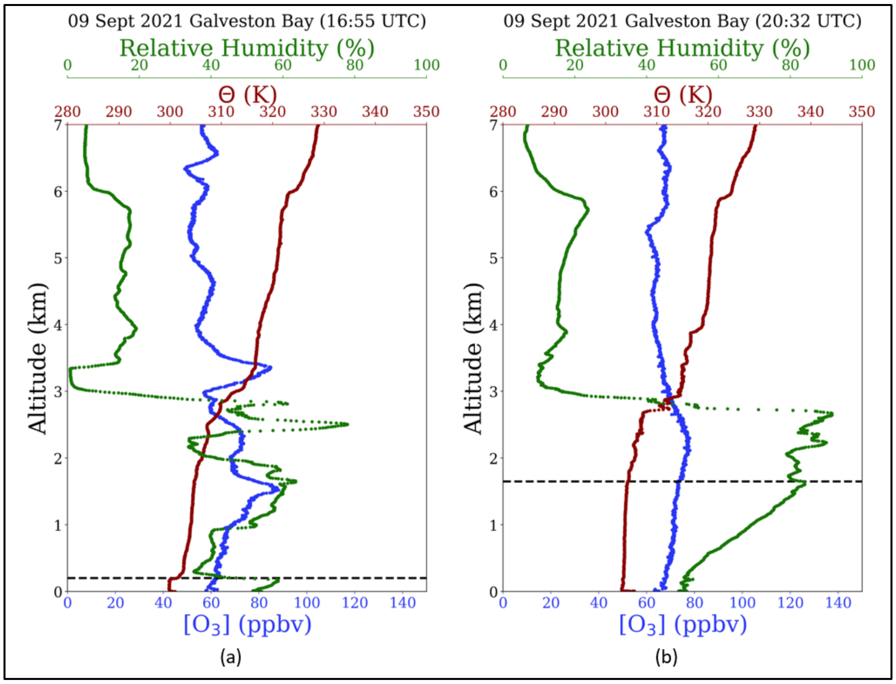


Figure 46: Vertical profiles of ozone (blue), relative humidity (green), and potential temperature (dark red) from two ozonesondes released on September 9, 2021 from Galveston Bay. The top of the marine layer is shown by the black dashed horizontal line at (a) 0.2 km and (b) perhaps near 1.65 km.

3.4.5. Problems Encountered and Corrective Actions for Offshore Air Quality Measurements

While this task ran relatively smoothly there were some occasional problems and things the team learned since this was a new method of sampling for the group. One of the first issues discovered was that the pontoon boat was very susceptible to a rough ride on choppy water because of the inherent design of this style boat. These boats tend to ride relatively flat, causing the bow to plow into waves when conditions were greater than the weather service's "slightly choppy" threshold. Plowing into the waves instead of riding over them also caused some damage to the mostly cosmetic sheet metal at the bow of the boat. During the campaign there was not much to be done about this so operations were restricted to calm days. Fortunately the boat was able to operate on most of the intensive days. To address this issue in preparation for the 2022 measurements, an additional 3/4 -length center pontoon was added in January 2022. This also incorporated an additional 35 gallon fuel tank which would allow for a full day of sampling rather than having to spend time coming in to refuel midday. The wave conditions also caused the spray guards, thin aluminum fins designed to deflect spray away from the occupants, began to break away from the pontoons. While this was not a safety issue it began to be fatiguing on the crew to get sprayed with water more frequently. To address this redesigned heavy duty fins were added during the offseason to prepare for the 2022 measurement season. Other improvements during the offseason to correct issues discovered in 2021 included reskinning and reinforcing the sheet metal at the bow and adding underskinning to the bottom of the deck between the pontoons. This last step aided in keeping water out of the pontoon with the fuel tank and reducing the slowing effect of waves hitting exposed crossmembers. In 2022, preseason testing demonstrated the performance gains from these corrective actions would result in the ability to successfully operate the boat on a greater number of days in 2022.

Another lesson learned was how quickly algae and barnacles began to grow on the pontoon tubes, and its effect on the boat's performance. Later in the season it became apparent that the growth was beginning to slow the pontoon's cruising speed by a few miles per hour. After the season was over the boat was thoroughly cleaned and a coating of anti-fouling paint was applied to slow the growth of algae and barnacles below the waterline. Plans were also made to have the boat hauled out periodically and pressure washed to remove any growth that was occurring.

The other platform related issue that arose was that the shrimp boat did not operate as frequently as expected. Other than one wire that had to be replaced in the instrument package's air conditioning system and the operator's occasional failure to plug the instrument power into the inverter after unplugging it from shore power, the main issue was the quality of shrimping conditions in the Bay. Early season rains caused an influx of freshwater into the Bay system, driving many of the shrimp from the Bay. The resulting poor shrimping conditions meant that outside of occasional scouting trips to check conditions, the boat remained mostly at the dock all season. Another issue that arose was that the operator contracted COVID during the summer. Since this was a single person operation they were unable to even attempt shrimping trips for several weeks. While this could not be addressed during the campaign, plans to correct this for 2022 measurements were developed. Given the impressive frequency of Red Eagle operations the team realized that partnering with industry serving operations would result in more consistent activities rather than single person operations which depend on fishing or shrimping conditions. Preparations for 2022 included reaching out to the Red Eagle operators and identifying the Victory, a boat that operates primarily in the industrialized portion of the Houston Ship Channel. The only operational issues on the Red Eagle was that the adhesive bases used to route and secure the instrument package power cable began to come loose in the summer heat. A quick trip down to replace and install additional bases were the extent of issues on that platform.

From an instrumentation standpoint, the ceilometer on the pontoon boat failed during the campaign and was sent back for repairs under warranty. Given the infrequent trips the shrimp boat was making, the decision was made to remove the ceilometer from the shrimp boat and install it on the pontoon instead. The other significant issue was that the manufacturer of the NO_2 photocells designed for the two commercial boat instrument packages had problems completing them in time for the ozone season. Issues with vendors and subsequent overheating issues during testing resulted in all three sampling platforms (Red Eagle, shrimp boat, pontoon) unable to sample NO_2 during the campaign. However, partway through the project when Hurricane Nicholas forced the team to bring the pontoon back to campus for safety, the team took the opportunity to install a second ozone instrument that had been modified with an older version of a photocell to measure Ox as initially planned. After the storm substantial debris was in Galveston Bay and many boat ramps were damaged, so the delay in being able to redeploy the boat was utilized to further test and verify the Ox measurements. The first day the boat was back in the water saw striking indications of NO_2 and plans are to integrate the older design of photocells into the commercial boat instrument packages for 2022.

3.5. Commercial Vessel to Ship Anchoring/Lightering Areas (Red Eagle Charters)

The chartered marine offshore crew vessel, the Red Eagle boat, used in AQRP 20-004 made 5 trips into the Gulf of Mexico to the ship anchoring and lightering areas outside the Houston Ship Channel opening in September 2021 during the TRACER-AQ campaign. The air quality and meteorological parameters used in AQRP 20-004 were measured during the entire trip. These trips were coordinated with the NASA aircraft and in consultation with the TCEQ Project Manager.

3.5.1. Quality Control / Quality Assurance for Commercial Vessel to Ship Anchoring/Lightering Areas Measurements

The instrument package installed on the Red Eagle boat, which collected observations in the ship anchoring/Lightering areas underwent a bench calibration before (07/02/2021) and after (11/4/2021) deployment with a 0.05% change in slope for the 2b Tech O_3 instrument (Table 11). Comparison of the Red Eagle data to the air quality monitoring site located in Galveston, TX (C1034) was also analyzed for the entire field campaign with suitable results (Figure 47). One note on that comparison is that the local air quality monitor (C1034) appears to have a sine function appearance to the observations possibly caused by a faulty Cell A/B issue in the instrument. This fault likely skewed the direct comparison to the negative.

Table 11: Calibration results for the 2b Tech O_3 instrument that was deployed on the commercial vessel Red Eagle.

Date	Slope	Offset	r^2
07/02/2021	0.987	-0.32	0.99
11/04/2021	0.987	-0.28	0.99

In addition to the calibrations, daily remote checks were also performed. Parameters such as instrument/case temperatures and humidity, flow rates and set points were monitored to assure instruments were in an optimal and stable environment for collecting measurements.

3.5.2. Results for Commercial Vessel to Ship Anchoring/Lightering Areas Measurements

The HGB region was in a post-frontal environment in an ozone episode from September 6–11, 2021 with light offshore winds and a reinforcing front on September 9, 2021. Air quality models forecast elevated O_3 concentrations offshore warranting the chartering of the Red Eagle for offshore ozonesonde launches on September 8, 9, and 10, 2021. Another post-frontal high O_3 episode occurred from September 23–26, 2021. Chartered science missions were executed on September 24th and 25th, 2021. Figure 48–Figure 57 show the surface weather station analysis data and surface O_3 concentrations during each of the chartered science mission trips into the Gulf of Mexico.

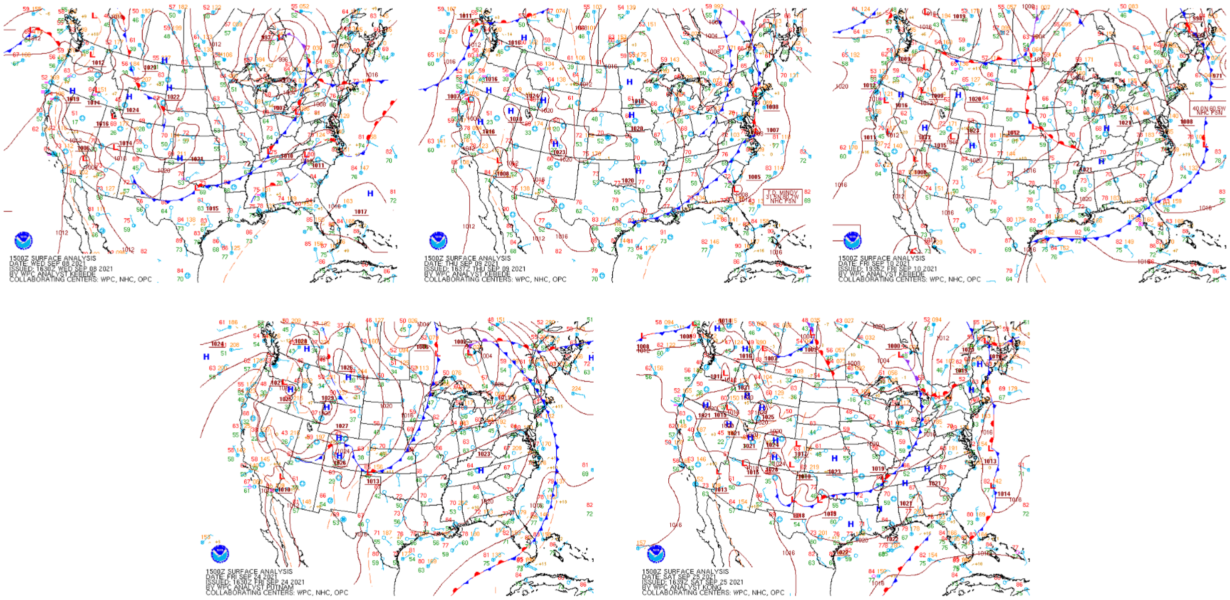


Figure 47: Surface weather station analysis for commercial vessel charter days.

September 8, 2021

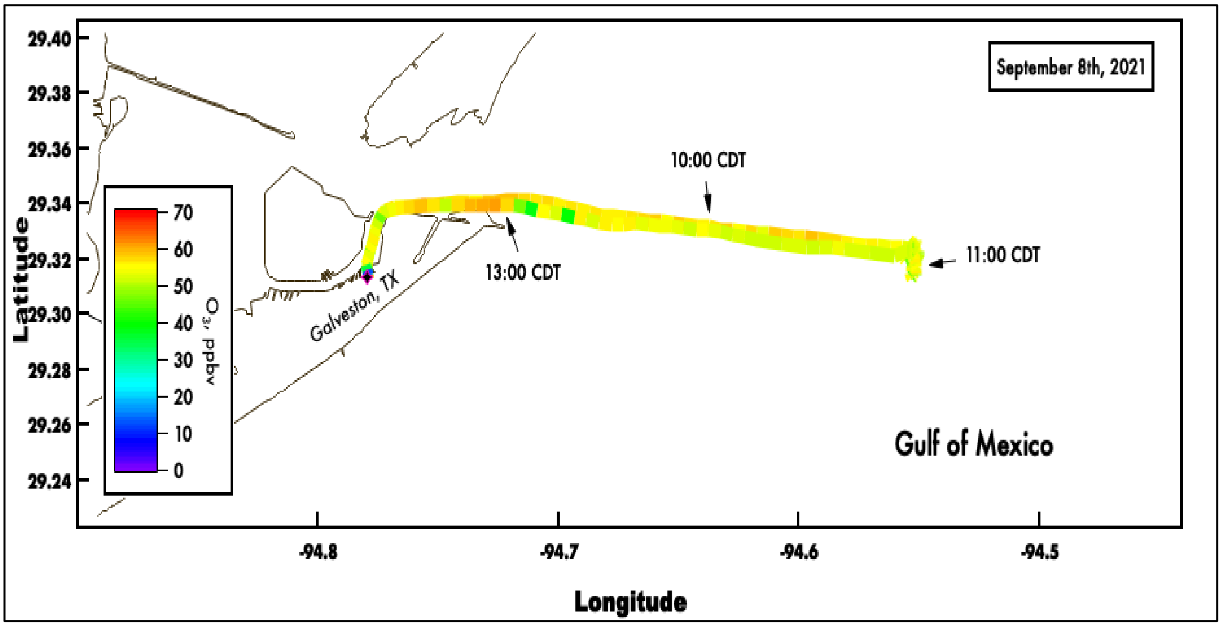


Figure 48: Surface ozone data from a chartered science mission on September 8, 2021.

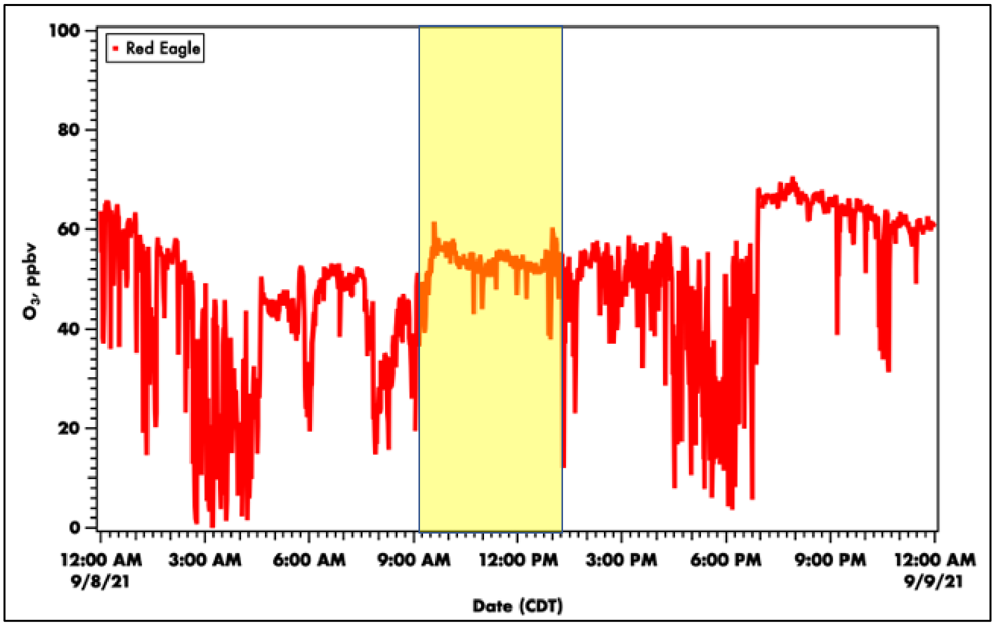


Figure 49: Surface ozone data from a chartered science mission on September 8th, 2021. The mobile portion of the data is highlighted in yellow.

September 9, 2021

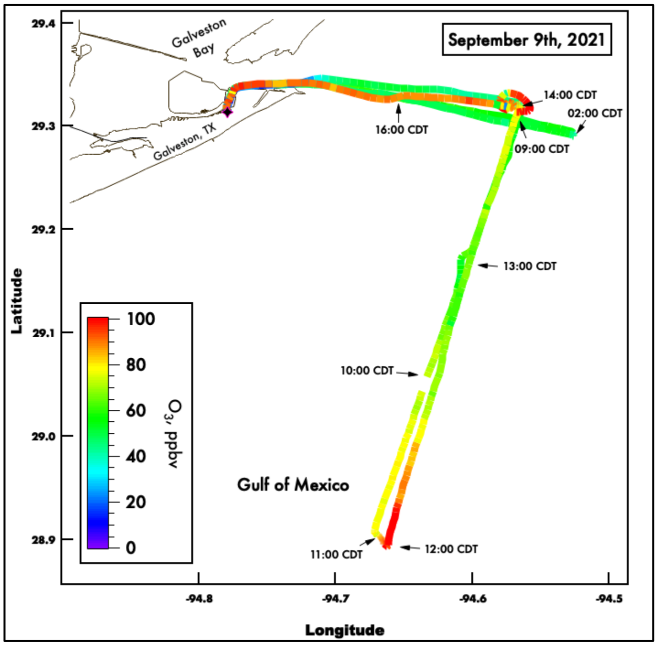


Figure 50: Surface ozone data from a chartered science mission on September 9, 2021. Note, the scale was increased from 0–70ppbv to 0–100ppbv to show the spatial gradient of ozone more clearly due to the higher O_3 observed.

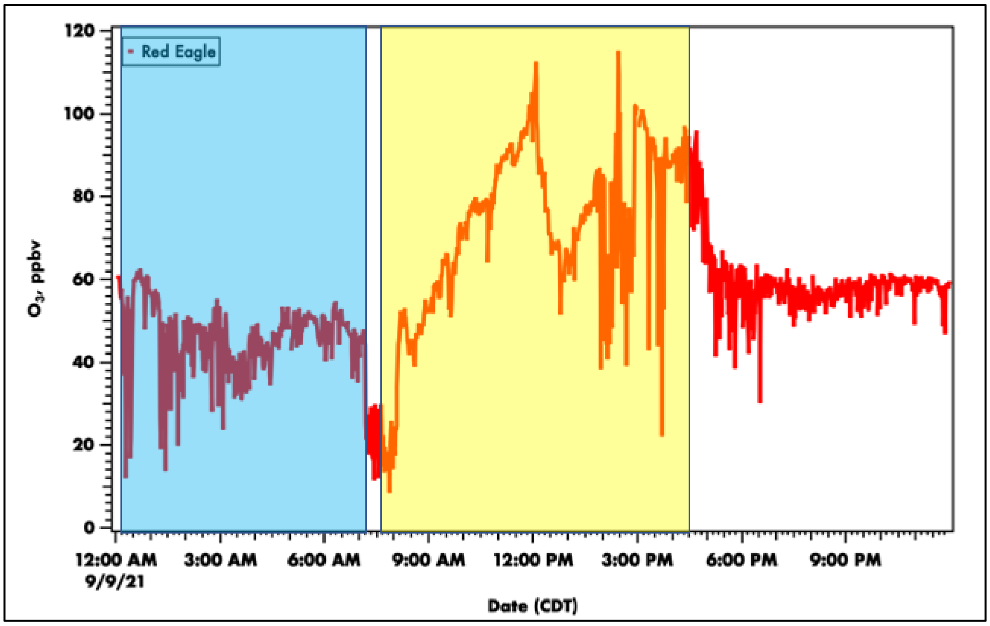


Figure 51: Surface ozone data from a chartered science mission on September 9th, 2021. The mobile portion of the science mission data is highlighted in yellow. A separate mobile period from regular operations of the commercial vessel is highlighted in blue.

September 10, 2021

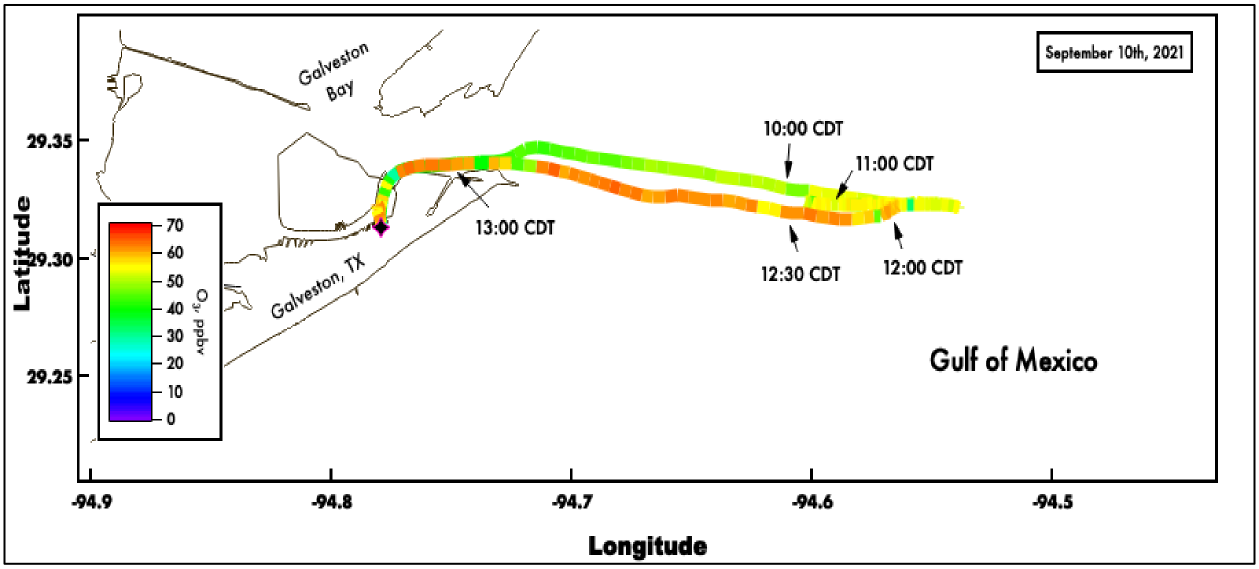


Figure 52: Surface ozone data from a chartered science mission on September 10th, 2021.

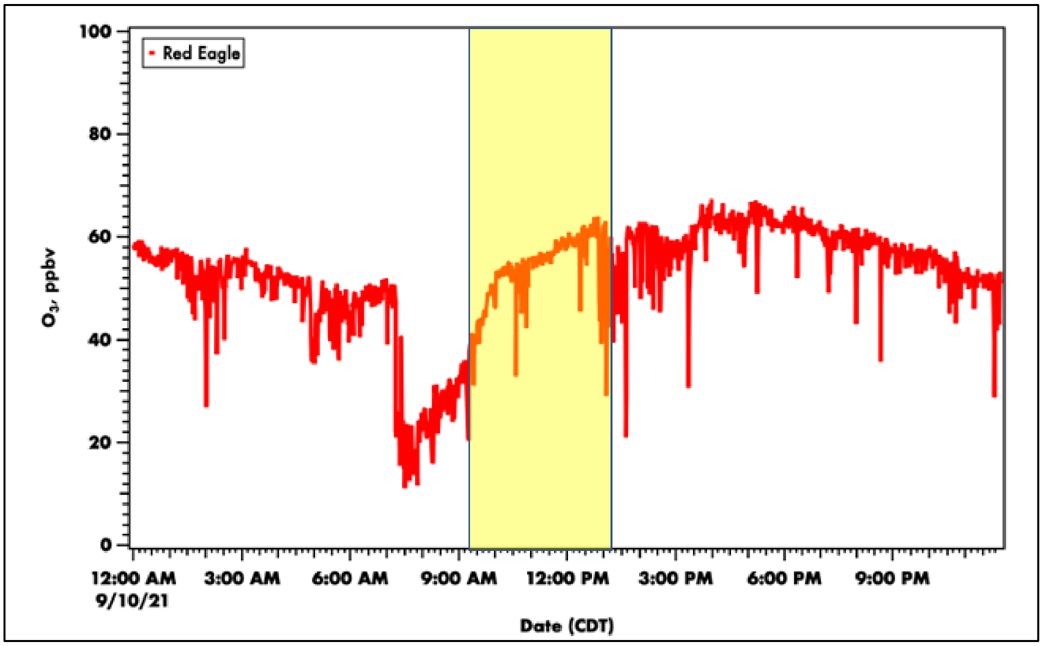


Figure 53: Surface ozone data from a chartered science mission on September 10th, 2021. The mobile portion of the data is highlighted in yellow.

September 24, 2021

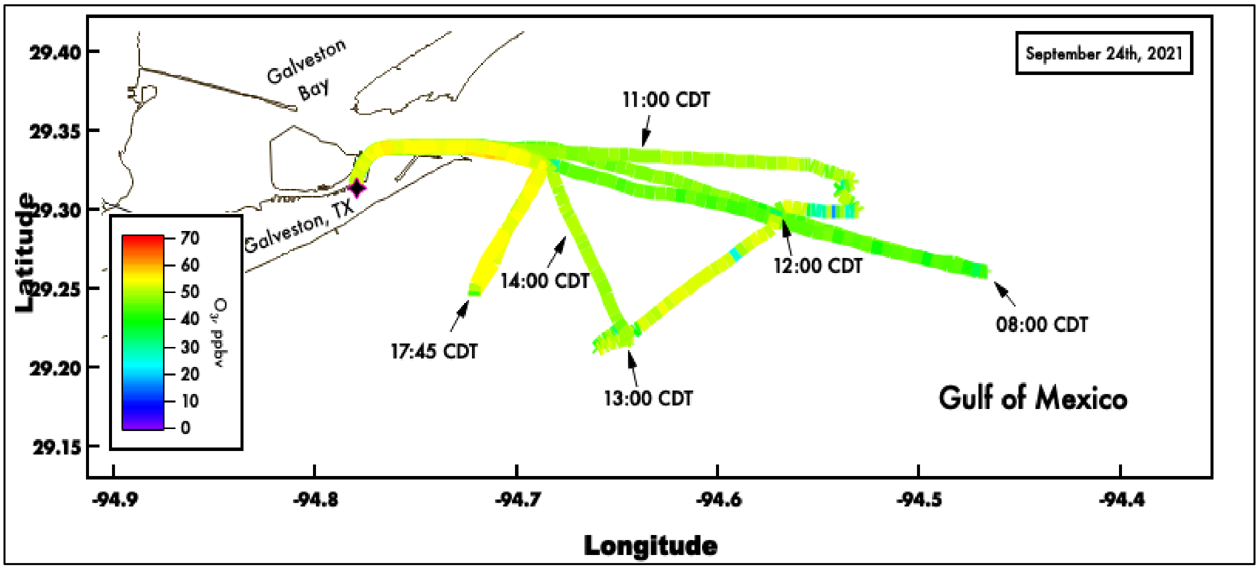


Figure 54: Surface ozone data from a chartered science mission on September 24th, 2021.

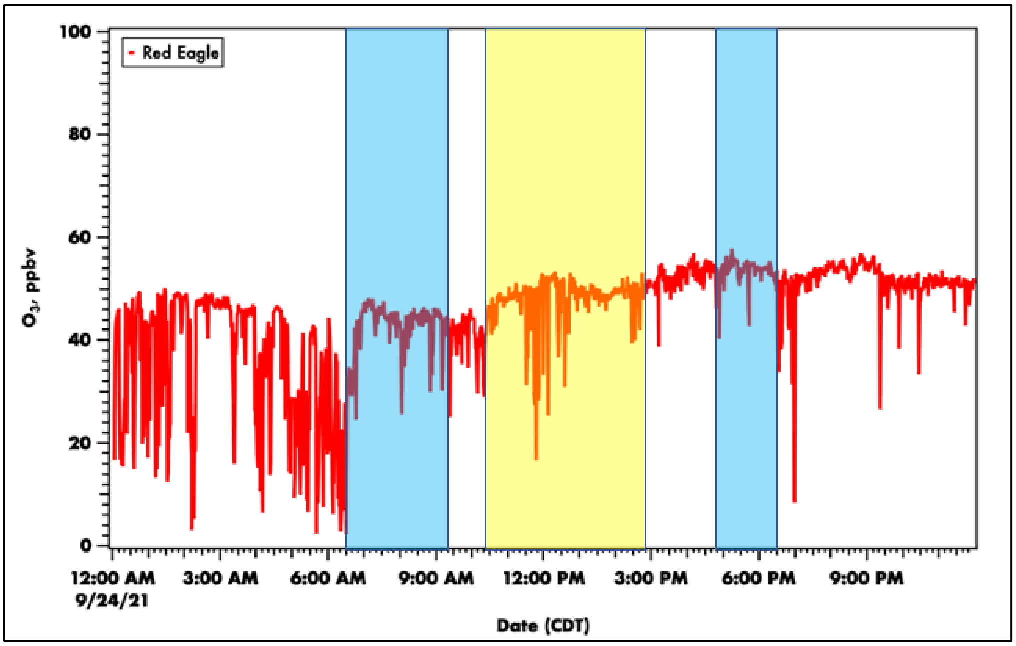


Figure 55: Surface ozone data from a chartered science mission on September 24, 2021. The mobile portion of the science mission data is highlighted in yellow. Separate mobile periods from regular operations of the commercial vessel are highlighted in blue.

September 25, 2021

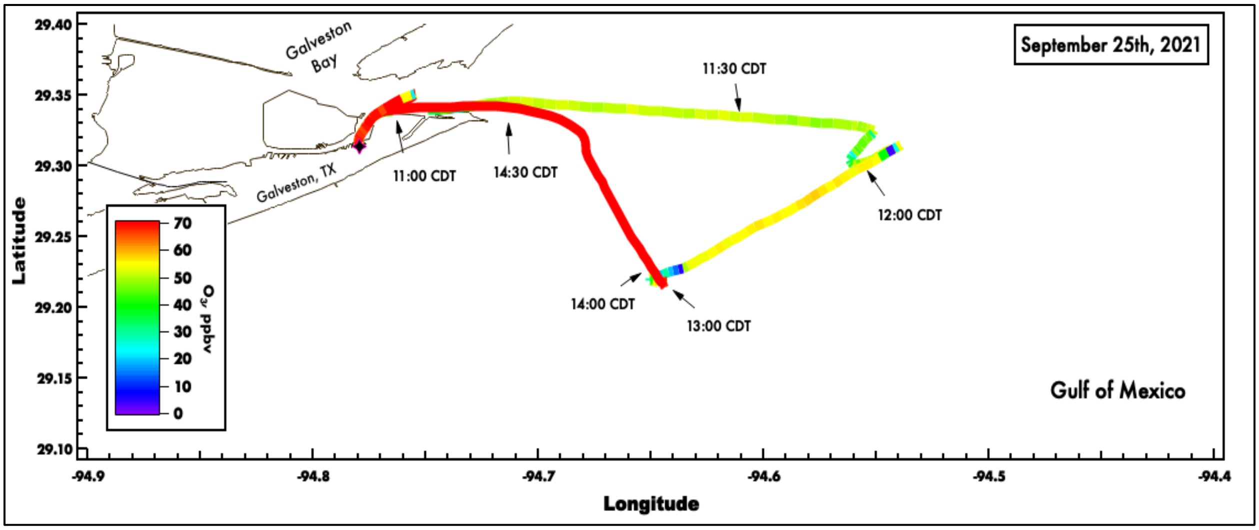


Figure 56: Surface ozone data from a chartered science mission on September 25th, 2021.

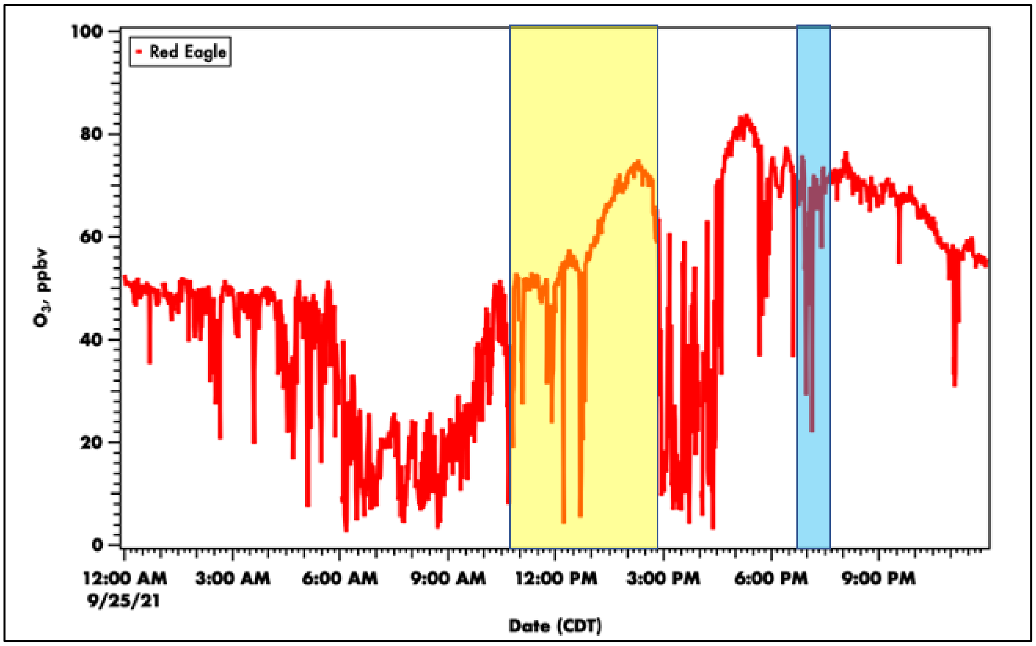


Figure 57: Surface ozone data from a chartered science mission on September 25, 2021. The mobile portion of the science mission data is highlighted in yellow. A separate mobile period from regular operations of the commercial vessel is highlighted in blue.

3.6. TRACER Monitoring Site Logistics

Under Task 8 of this project several sites were established, upgraded, or otherwise made available to support the Air Quality Data Collection Support for TRACER-AQ in Houston project. This section summarizes the sites that were available for this project.

3.6.1. Mobile Air Quality Lab 1

The UH MAQL1 was adapted to house two remote sensing instruments from Dr. Elena Lind at Virginia Tech. Although her deployment and operating costs were supported by NASA, the MAQL1 was modified slightly to accommodate her instrumentation. This included the addition of a platform on the roof to mount a Pandora Spectrometer sensor head as well as standoff brackets to allow the left rear access panel in the mobile lab's shell to be secured in a partially open position so that fiber optic and control cables could be securely routed into the shell. An additional remote sensing optic was clamped to the open door and its cables were routed into the shell as well. Rigid foam board insulation, aluminum foil tape, and silicone caulk were then used to close off and seal the open gaps around the open door to prevent hot air and rain from entering the mobile lab.

3.6.2. Portofino Harbour Marina

For AQRP 20-004 and this project the UH pontoon boat which measured O_3, Ox (O_3+NO_2), mixing layer height, and meteorological parameters in Galveston Bay was kept at the

Portofino Harbour Marina in Kemah. This gated entry site allows quick and easy access to the Bay for the pontoon and is adjacent to a fuel dock for refilling the boat and generator at the end of each day of operations on the water. By not having to trailer the boat from campus, launch, recover, and return the boat to campus each day of operation the crew was able to save 3-4 hours each day which was put towards sampling activities. Shore power (30A 120V) was also available at the marina, allowing the instrumentation on the boat to remain operational 24/7 and essentially providing a monitoring site in Kemah when not in use on the Bay. This also ensures that the instrumentation was warmed up prior to any activities on the Bay.

3.6.3. Aldine (C8)

The TCEQ's Houston Aldine site was expanded to include a second fenced site on the north side of the primary space. In 2020 under the TCEQ funded BC2 project UH established a new 200A 120/240V electrical service built to TCEQ specifications and with two 50A 120/240V RV connections. A trailer for the UH/Baylor BC2 project was parked inside the vacant northern space. For the 2021 TRACER-AQ campaign the trailer was relocated within the site to allow for a boundary layer profiling trailer from OU and an ozone lidar trailer from NOAA to deploy at the site. Power connections on the UH service was upgraded to include a 100A 120/240V pin-and-sleeve connector. The TCEQ power service was also upgraded to increase the available power from the previous 70A 120/240V maximum to better utilize the full 200A 120/240V service that was being provided by the utility company, an increase of 130A of usable power. At the same time that the upgraded meter and electrical panel were installed, an additional 50A 120/240V RV outlet was installed on the TCEQ service. All of the electrical upgrade costs were paid by UH through this grant. An all-weather access driveway was also installed in coordination with the Aldine School District's maintenance department to allow access to the gate at the northwest corner of the enclosure. This gate had been largely inaccessible due to the often-wet conditions that would result in damage and ruts in the adjacent school's grass were it to be used and would be required for the NOAA trailer to access the site. This new access drive was subsidized by the district and UH was asked to cover only less than 1/3 of the total cost. This expense was also paid by this project and should eliminate the need for significant remediation costs at this site upon completion of this project. In future years this access will be used by the OU profiling trailer as well as the UH and Baylor mobile labs (e.g. TRACER-MAP in 2022).

3.6.4. La Porte Airport (C243)

The TCEQ's La Porte Airport site was used in NASA's 2013 DISCOVER-AQ project to host a trailer from the EPA as well as the NOAA ozone lidar truck. Many of those improvements remain however the second 200A 120/240V electrical service that had been installed was no longer in service. Under this project UH reestablished service to this meter, inspected the system, and replaced breaker as needed due to age and weathering. In preparation for the joint TCEQ/DOE operation of the radar wind profiler, a small lab trailer was parked inside the TCEQ fence to house rain droplet measurement equipment to support the adaptive profiling measurement abilities to better characterize convective events when the traditional horizontal wind measurements were not possible due to precipitation. This also provided an opportunity for two NASA Pandora Spectrometers similar to the one at the UH Launch Trailer (C1611) site to be installed to further support the TRACER-AQ sampling project as well as the NASA Goddard ozone lidar and TCEQ/NASA ozonesonde launches at the adjacent DOE measurement site which is also collocated at the La Porte Airport. The reestablishment of power to the second meter at this site also provides a measurement location for the UH and Baylor mobile labs. The restoration of power and subsequent utilities were paid for under this project.

3.6.5. San Jacinto Battleground State Historic Site

Another measurement location in the Houston Ship Channel region was the San Jacinto Battleground State Historic Site in the caretaker section in the maintenance area. This area has roughly seven locations for the park hosts to keep their RVs and travel trailers while helping to maintain the park. These spots are rarely full and access to the sites was readily granted by the park's director. Upon initial set-up of the Baylor MAQL2, it was determined that the 50A 120/240V connections at the two most desirable pads had been degraded due to age and weather and would trip prematurely. These breakers were replaced and have not tripped since. This site will provide measurement space for both the Baylor and UH mobile labs this year and in the future (e.g. TRACER-MAP and TRACER-AQ2 in 2022).

3.6.6. UH Launch Trailer (C1611)

The UH Launch Trailer (C1611) site was operated under the HNET program, sponsored by the TCEQ. In addition to measuring trace gas and meteorological data this site has been instrumented with a Pandora Spectrometer for trace gas column measurements, similar to those collected by the TROPOMI satellite and upcoming TEMPO satellite. This location also serves as the radiosonde and ozonesonde launch site for UH campus and often acts as a hub for distributing supplies to other launch locations around the Houston area due to its ease of access. During this project NASA Langley reserved four parking spaces in the adjacent parking lot for their Langley Mobile Ozone Lidar (LMOL) trailer and were plugged into the Launch Trailer for power using a 50A 120/240V RV connection that was previously installed.

3.6.7. UH Moody Tower (C695)

The North Moody Tower rooftop at the UH main campus served as the elevated measurement site (70 m) as a compliment to the ground-based UH Launch Trailer (C1611) site under the HNET program. This site was the first of the UH measurement sites and has since hosted numerous of measurement campaigns. During this campaign, the site hosted a researcher from Virginia Tech who has deployed a Pandora Spectrometer which was operating a different profiling mode than the Pandora at the Launch Trailer.

3.6.8. UH ERP

Adjacent to the UH campus is the UH Technology Bridge, formerly known as the Energy Research Park (ERP). This site is still frequently referred to as the ERP since the change in names was relatively recent and is familiar to many of the field teams. This site provided shelter for many of the UH mobile labs, trailers, pontoon boat, and radar wind profiler when not in use or in the event severe weather such as a hurricane are expected to impact the area. The space was also used to prepare many of the assets since it has two 50A 120/240V RV outlets and six additional 20A 120V dedicated circuits in addition to outdoor space that was used for parking mobile labs and trailers for testing and operational measurements.

3.6.9. UH Coastal Center

The UH Coastal Center (UHCC) is an auxiliary research campus in La Marque, TX that is primarily used for atmospheric, biological, and geotechnical research. The research team maintains a 40’ converted shipping container for laboratory space. The interior of the lab is a finished research space with insulated and painted walls, floors, ample lighting, roughly 27 dedicated interior and outdoor 20A 120V electrical circuits, three 50A 120/240V RV outlets, gigabit internet service, and a 5-ton air conditioner. Power upgrades to supply a full 200A 120/240V service to the container were completed by UH after the trailer was installed to replace the previous lab which was damaged during Hurricane Harvey. For this project, UH’s new radar wind profiler was deployed to the site utilizing one of the 50A RV connections. During TRACER IOP the UHCC site hosted a boundary layer profiling trailer from NOAA’s National Severe Storm Laboratory, the NSF funded uTRACER project, and the DOE funded TRACER-UAS drone sampling program.

3.6.10. UH Sugar Land

In 2015, after several years of operating the UH Sugar Land HNET site out of a trailer in a remote parking lot at the UH Sugar Land campus the equipment was relocated to a rooftop mechanical room and a 10-meter sampling mast was installed on Brazos Hall. The 50A 120/240V RV connection which previously powered the sampling trailer was left in place and is still powered for use by UH and Baylor mobile labs. This site was also selected by the UT soil moisture team as a measurement location for the TCEQ until the DOE’s ancillary site in Guy, TX was completed for the TRACER campaign. The UH team worked with the management and administration at UH Sugar Land to renew and amend the MOU which would allow UT access to the site. This amendment also allowed NASA to install one of their Aeronet instruments on the roof of Brazos Hall for the duration of the TRACER campaign.

3.6.11. UH Liberty Sam Houston (C1626)

In late 2020 UH began the process of moving the UH West Liberty (C699) measurement site to a new location due to the nearby construction of State Highway 99, Houston's "Grand Parkway" and the subsequent sale of the property. The new site was established near the town of Liberty on an unused piece of land owned by the Texas State Library and Archives Commission adjacent to the Sam Houston Regional Library and Research Center. This site has a new 20' converted shipping container for laboratory space and serves as a measurement site for both the HNET and BC2 measurement programs. Due to the collection of equipment here a NASA Pandora Spectrometer and Aeronet instrument were installed, alongside a new micropulse aerosol lidar system from NASA Goddard during this project. In addition to the in situ and remote sensing equipment, the lab has two 50A 120/240V RV connections available and space within the site for at least two additional sampling trailers. The 10-year site agreement also has provisions to expand the 50' x 50' space to 100' x 100' without requiring additional permissions.

3.6.12. UH WG Jones Forest (C695)

The UH WG Jones Forest (C695) measurement site is operated under the HNET program funded by the TCEQ. In addition to the gas and meteorological measurements in 2015 Texas A&M and Rice colleagues helped to fund power upgrades to the site, including the installation of three 50A 120/240V RV connections for mobile lab usage. This site is available for, and has been used in the past by the UH and Baylor mobile labs as well as those from collaborating groups.

3.6.13. Galveston 99th Street (C1034)

Similar to the TCEQ La Porte Airport site, 50A 120/240V power connections for research labs were installed at the TCEQ Galveston 99th Street site in 2013 for the DISCOVER-AQ campaign. This power was checked and usage resumed in 2020 by the UH/Baylor team for the TCEQ funded BC2 program by parking the BC2 trailer outside the TCEQ fence yet within distance for easy connection to power. The siting of the trailer was performed in close coordination with the Monitoring Operations team to avoid any issues regarding distance to samplers. The second power connection here also serves as a point of connection for the UH and Baylor mobile labs during this project.

3.6.14. UH Smith Point (C1606)

The HNET site operated by UH at the Spoonbill RV Park at Smith Point measures trace gases to supplement the TCEQ's near-by meteorological station. This site was also selected to host one of the NASA Aeronet instruments for the TRACER campaign. The shrimp boat which carried one of the small, automated measurement packages under this and the AQRP 20-004 projects routinely docked at the dock roughly 100 m west of the sampling trailer, allowing for frequent QA/QC comparisons between the two systems.

3.6.15. sUAS sites

In compliance with the UH policies regarding usage of small unmanned aerial systems (sUAS, aka "drones") the project team set forth several locations for which UH was approved to operate. The listing of these sites is below in Table 12. Depending on the conditions and type of operations a typical deployment to one of these sites included the sUAS and supporting communication, batteries, chargers, communication equipment, payload sensors, folding table, pop-up canopy with anchors, fold-up chairs, rugged laptop, sUAS power tether, and generator (as needed).

All flights were conducted in accordance with FAR 107 and TX Code 423 and was not operate at night. Initial test flights occured at the UH ERP remote parking lots and at the UH Coastal Center. Operational flight location and dates were determined by science objectives, payload availability, personnel availability, and weather conditions.

Table 12: Drone approved operating sites

Site Name	Address	Lat, Lon	Dates	Notes
UH Campus	4800 Calhoun Rd	29.723889°, -95.339214°	July 6, 2021– October 31, 2021	Flights from vicinity of Building 486 to profile up to Moody Tower laboratory height to study observed gradients with height
UH ERP	5000 Gulf Freeway	29.716344°, -95.329903°	July 6, 2021– October 31, 2021	Test flights in open parking lots
UH Sugar Land	14000 University Blvd Sugar Land, TX 77479	29.573415°, -95.652463°	July 6, 2021– October 31, 2021	Flights in field behind UH-SL to study the Parrish Power plant plume
UH Coastal Center	5721 Highway 2004 La Marque, TX 77568	29.388237°, -95.042336°	July 6, 2021– October 31, 2021	Test flights and sampling
UH Smith Point	450 Old Dutchman Rd Anahuac, TX 77514	29.546110°, -94.780333°	July 6, 2021– October 31, 2021	Public land/water and/or coordination with Spoonbill RV Park where we already conduct research and maintain good relations with the owners
San Jacinto Battleground Park	3523 Independence Pkwy La Porte, TX 77571	29.742516°, -95.072979°	July 6, 2021 – October 31, 2021	Have met with director and he has offered to issue park permits as well as to block off parking lots for our use to prevent operating over non-participants
Texas City Dike	Dike Rd Texas City, TX 77590	29.364534°, -94.810641°	July 6, 2021– October 31, 2021	Over public waters to study the water-land gradients in coordination with the UH Mobile Lab and UH Pontoon boat measurements in Galveston Bay
TCEQ Aldine Site			July 6, 2021– October 31, 2021	TCEQ/UH measurement site to support NOAA vertical ozone lidar
Galveston Island beaches (outside exclusion zone)	14901 FM3005 Galveston, TX 77554 San Louis Pass beach	29.191744°, -94.954531° 29.085304°, -95.113483°	July 6, 2021– October 31, 2021	Sample vertical structure of air coming into the TX coast to extend ground level measurements conducted at San Luis Pass in 2016

3.7. Remediation of Property Upon Decommissioning of Research Sites

Due to site preparations as part of Task 8: TRACER Monitoring Site Logistics, the site remediation tasks under Task 9 were quite minimal. Ultimately the only site remediation required was to fix ruts at the La Porte Airport. The NASA Goddard TROPOZ ozone lidar trailer, a converted 40' 18-wheeler trailer, was removed upon completion of the field campaign. Because of saturated ground the driver of the truck hired to return the trailer to Goddard got stuck in soft ground, requiring a heavy-duty wrecker to extract the truck and trailer from the grass/mud and onto the hard-packed road. This resulted in ruts which a local landscape company repaired. No other remediation was required for any of the TRACER monitoring sites.

3.8. Monitoring Air Quality by Use of Small Unmanned Aerial Vehicle (sUAS)

Task 10 of the TRACER-AQ support project was to purchase and operate a small unmanned aerial system (sUAS, aka "drone") measurement platform to support the TRACER-AQ research program, which was conducted in September 2021. During TRACER-AQ several flights were conducted to collect vertical profiles of O_3, temperature, relative humidity, and pressure at the UH campus.

Figure 58: Ozone and meteorological sensors mounted to upper platform alongside voltage regulators.

Figure 59: Drone in flight with sensors mounted to the lower platform.

3.8.1. Operation of the sUAS

The drone can operate in several modes. For the purposes of this project, flights were primarily focused on vertical profiles although horizontal flights will be explored in future work. All flights can be flown either manually or automatically if the flight profile is loaded into the integrated autopilot. The autopilot is capable of all flight operations, including automatic take-off and landing, as well as executing lost communication safety protocols. Since the relays that were added to the drone are controlled through the autopilot, they can also be controlled through the preprogrammed route allowing for samples to be taken consistently at the same location (i.e. water treatment tanks, within an industrial complex, within a forest for biogenic emissions, etc.) with a high degree of repeatability. This can also be applied to the vertical profile flights where samples could be taken at preset altitudes. While some flights were flown using preprogrammed plans, most flights to date were hand flown. There are several tools to assist the pilot, however. The loiter setting was used most often, allowing the drone to be flown to a specific location and altitude and hover with no additional inputs by the pilot. In this mode the drone remains stable and holds horizontal and vertical positions within less than half the diameter of the drone, even under changing wind conditions and turbulence. Another manual flight mode briefly explored was altitude hold where the drone was allowed to maintain a constant altitude but would then drift with the wind. This mode will be explored more in future work as a possible way to estimate wind speed and direction using the GPS motion of the drone, similar to how winds are measured from weather balloons, but may require a large open area to ensure an undisturbed wind field, as well as room for the drone to drift and collect a representative estimate of the winds. It should be noted that this is still an area of exploration and may not be feasible in practice.

3.8.2. Sensor Chassis Construction

TCEQ executed an amendment which allowed remaining TRACER-AQ support to extend into 2022 to cover sUAS-related preparations for TRACER-AQ2.

To make better use of the drone in 2022, a new sensor chassis for the drone's primary payload was required. The primary payload planned for the drone included ozone, temperature, pressure, and humidity sensors. However, the chassis also needed the flexibility to accommodate additional sensors as research needs evolve.

For 2022, the primary purpose of drone flights was to measure ozone in the range of 0 to 400 feet above ground level (AGL). However, it was also hoped to have SO_2 and NO_2 measurements from the drone after some further development. Therefore, it was important to construct a sensor chassis with space to accommodate instrumentation for all three of these measurements. If all three were to occur simultaneously, the chassis would need room for three sondes, a dryer, a blue light converter (BLC), two filters, and the associated tubing, electrical wiring, and switches.

All components needed to fit within the weight limit of 11lbs as well as the spatial restrictions of the drone. Figure 61 highlights the spaces above and below the drone in which the payload could sit. Also, the chassis had to work around the power tether module mounted semi-permanently to the bottom of the drone. Everything had to be clear of the LiDAR rangefinder also on the bottom of the drone, which is part of the drone's system to sense altitude. It is necessary for smooth and safe flying and for automated failsafe sequences that land the drone in the event of communication loss, low voltage, or other failures that can occur during flight.

Another important consideration for the chassis design was the ease of alteration. The chassis was required to be capable of supporting ozone, SO_2, and NO_2 sondes simultaneously, but that did not mean that it would always need to carry them all. If only ozone needed to be measured on a given flight, it would not make sense to carry the extra components as that would unnecessarily diminish flight time. Furthermore, the team wanted to have the option of mounting the payload on either the top or bottom of the drone. That way, adjustments could be made to carry additional instruments or change weight distribution for flight stability.

The area beneath the drone presented the tightest spatial restrictions. Therefore, the chassis was designed with the assumption that it would be mounted below-whatever fits there could easily fit on the top of the drone. With this in mind, components of ozone, SO_2, and the proposed NO_2 sondes were gathered and measured. These dimensions, along with measurements of the space beneath the drone, were used to create a 3-dimensional model (shown in Figure 60) using the TinkerCAD software from Autodesk. While 2-dimensional diagrams were also drawn, the 3-D model proved helpful during design and construction.

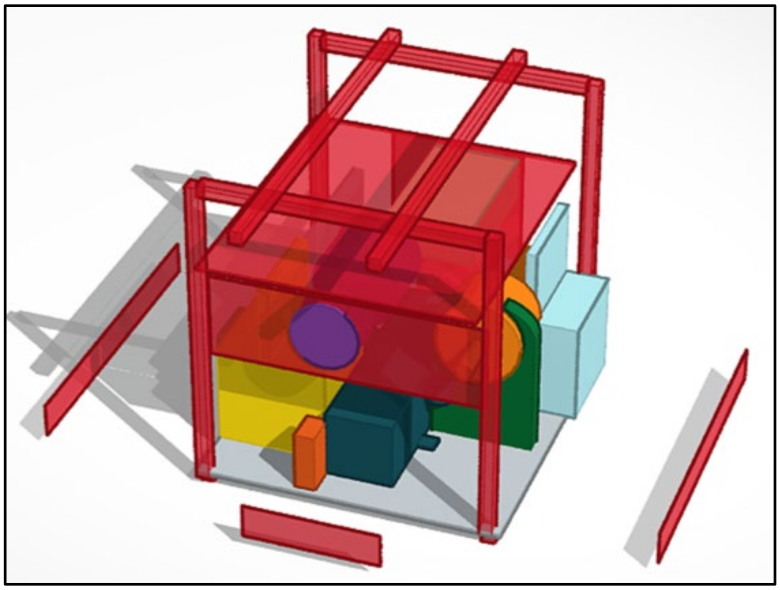


Figure 60: The 3-dimensional model of the payload created with TinkerCAD. The thin red rectangular shapes at the edges marked the boundary of the space available between the landing supports on the drone.

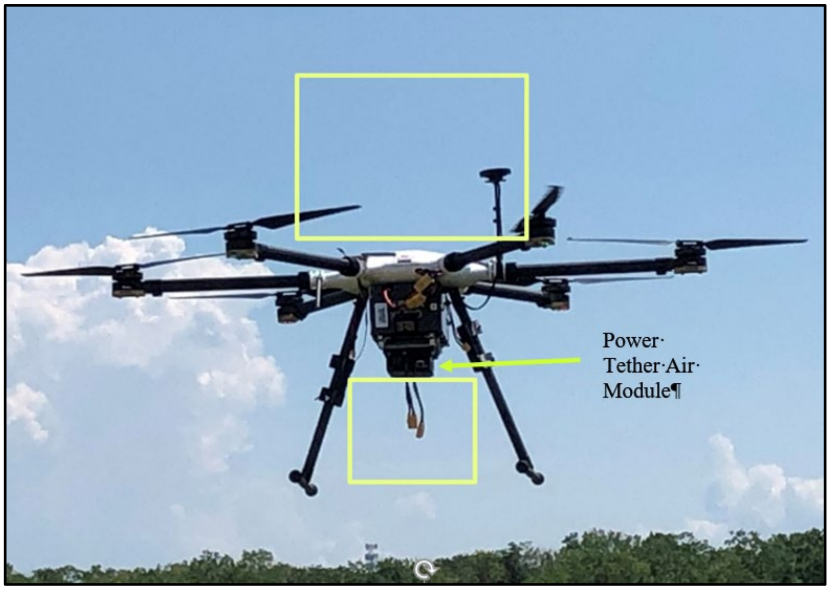


Figure 61: The highlighted rectangles indicate the spaces above and below the drone that payloads may be mounted. The power tether Air Module is mounted to the bottom of the drone’s battery compartment frame. The cables hanging below the power tether are for payload power connections.

The chassis was constructed primarily of aluminum to meet weight and durability requirements. The miniature T-slotted aluminum framing used was convenient and effective since it was used for other drone modifications and is light and easy to work with. Forming the floor, ceiling, and half-walls of the chassis, aluminum perforated sheets provided some structure without severely limiting airflow. The large perforations also allow 1/8” tubing, wires, cable ties, and screws to be passed through wherever necessary, providing excellent versatility. The drone pilot constructed the chassis in the University of Houston lab in the spring of 2022.

When completed, the chassis was weighed and tested with a full mockup of the anticipated payload to ensure it could hold all sensor components. The chassis alone (pictured in Figure 62) weighed approximately one pound, and Table 13 shows the payload weights when loaded with various sensors. Additionally, the chassis fits beneath the drone (see Figure 63) or above the drone (see Figure 64).

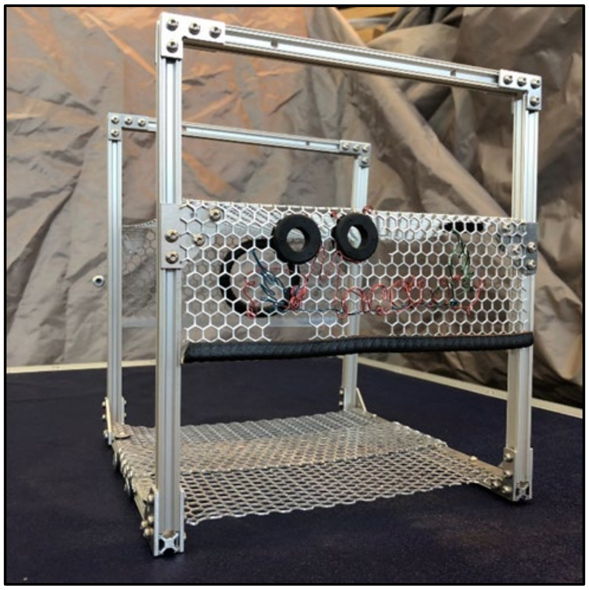


Figure 62: Drone sensor chassis constructed primarily of aluminum.

Table 13: Weights of the chassis and components for various sensor combinations

Sensors Onboard	Weight (lb)
None	1.0
Ozone	1.5
Ozone and SO_2	3.3
Ozone, SO_2, and NO_2	6.6

Figure 63: Chassis mounted to the bottom of the drone.

Figure 64: Chassis mounted to the top of the drone

3.8.3. Flight Preparation

A remote pilot in command must be present and possess a valid Remote Pilot Certificate from the Federal Aviation Administration (FAA) to fly a drone weighing over 0.55 lb for any purpose other than pure recreation. Therefore, to prepare for the 2022 TRACER-AQ2 project, the anticipated drone pilot studied for the FAA Part 107 Unmanned Aircraft General - Small (UAG) knowledge test throughout the winter and spring. The Remote Pilot Certificate was issued on May 10, 2022, after the pilot passed the proctored knowledge test at the Aviation Institute of Maintenance in Houston, TX.

In addition to federal regulations, University of Houston's drone policies also affect all drone operations conducted by research groups within the UH system. Thankfully, much of the work involved in complying with these policies was completed in 2021. For 2022 operations, the drone pilot needed only to submit the Remote Pilot Certificate to the University of Houston Police Department (UHPD) and take the Recreational UAS Safety Test (TRUST) from an FAA-certified test administrator. The TRUST certificate of completion was earned on June 9, 2022, from the Academy of Model Aeronautics. Additional requirements from UH included maintenance of a drone insurance policy with $1M liability coverage and notification to UHPD of intentions to fly at least one day before flights.

As an added layer of sensible preparation, a professional drone instructor was hired to ensure the new drone pilot would be comfortable flying the Aurelia X6 Pro. Although the principal goal of the training was to allow the primary pilot to gain hands-on experience flying, several other team members including the Principal Investigator also joined the class so that multiple people would have at least basic familiarity with the drone. The class was held for approximately five hours at the UH Technology Bridge in Houston on July 8, 2022.

3.8.4. Quality Control / Quality Assurance for Monitoring Air Quality by Use of sUAS

The primary quality control checks for the O3 measurements on the sUAS during 2021 measurements were performed as part of the ozonesonde preparation process which followed the procedures described in the QAPP for ozonesondes. Beyond this, the data were checked for reasonableness by making qualitative comparisons to nearby monitors, as is standard with ozonesonde operations.

3.8.5. Results for Monitoring Air Quality by Use of sUAS

Due to a variety of reasons such as weather, pilot availability, and staff prioritization (in coordination with the TCEQ program manager) measurements from the drone platform were unfortunately limited during the 2021 TRACER-AQ field campaign. On September 11, 2021 the drone was flown at the UH Launch Trailer (C1611) site in coordination with the NASA Langley Mobile O_3 Lidar (Figure 65 and Figure 66). Due to FAA altitude restrictions the flights were limited to 80 m (200 ft.) above ground. Figure 67 below shows the vertical profiles of O_3 between 10 and 80 m. During this flight, the drone climbed at to incremental heights and was allowed to loiter for several minutes before increasing height again. Descents were handled in a similar fashion. Due to the battery endurance, the drone was landed between vertical profiles to exchange the batteries for freshly charges ones. Later profiles climbed and descended in larger increments to speed up the profile and reduce the impact of temporal changes. In the first profile the positive gradient in the O_3 signal indicates that the lowest 80 m is not well mixed and titration from surface NO_X emissions may be reducing O_3 at the surface. Subsequent profiles show two things, that the

O_3 levels increased as the day progressed and that the 10-80 m height above ground became well mixed.

Figure 65: Drone in flight at the UH Launch Trailer (C1611) hovering near the inlet height for comparison of ozone measurement.

Figure 66: Drone in flight over the UH Launch Trailer (C1611).

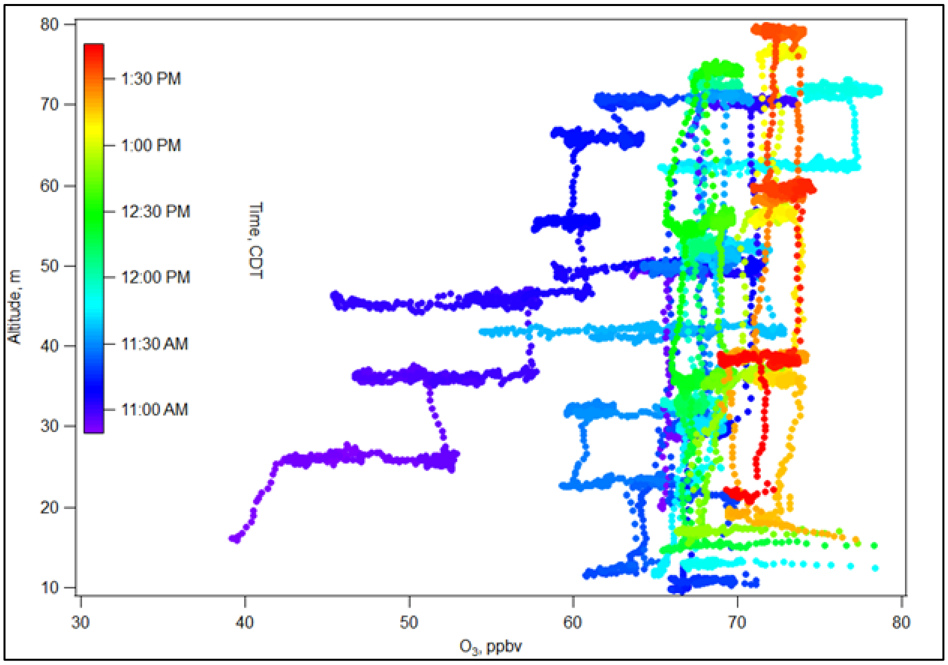


Figure 67: Vertical profiles of O_3 measured by the sUAS at the UH Launch Trailer (C1611) site On September 11, 2021, showing an increase in O_3 with altitude in the earliest profile, with higher O_3 and a well-mixed profile as the day progressed.

Table 14 and Table 15 show the results of the comparison of the drone measurements to those from Moody Tower (70 m) and Launch Trailer (6 m). The measurements compare quite well, particularly when the uncertainty in the O_3 sonde of ±5-20% (Sterling, et al., 2018) are considered. Additionally, the Moody Tower measurements are collected roughly 1 km south of the flight location. Future work will incorporate more comparisons of the drone data with both O_3 sondes, which were launched from the same location, and O_3 lidar results, which begin at a few hundred meters. This type of measurement profile should allow for the drone data to be incorporated into the O_3 lidar data and extend the profile to the surface.

Table 14: Comparison of drone measurements to O_3 data from the nearby Moody Tower at a height of 70 m above ground.

Time	Drone Alt (m)	Drone O_3 (ppbv)	Moody Tower O_3 (ppbv)
11:15	70	63.4	60.5
11:52	72	76.9	72.7
12:30	75	68.7	71.1
13:00	77	72.7	61.9
13:31	79	72.4	60.0

Table 15: Comparison of drone measurements to O_3 data from the UH Launch Trailer (C1611) with a measurement height of 6 m above ground.

Time	Drone Alt (m)	Drone O3 (ppbv)	Launch Trailer O3 (ppbv)
10:50	16	39.2	47.2
11:20	11	67.9	60.1
11:50	13	68.1	66.9
12:20	17	67.4	73.7
13:20	19	70.5	61.8

3.8.6. Problems Encountered and Corrective Actions for Monitoring Air Quality by Use of (sUAS)

The primary issue encountered during the 2021 measurement program was the availability of personnel while suitable weather conditions were present. Due to the complex nature of the various tasks under this PGA, the decision was made in coordination with the TCEQ program manager to prioritize sending staff on the Red Eagle during the charter tasks. Because of the duration of the charter trips only certain staff and students were available and ultimately meant that the drone crew was sent on the charters rather than to fly the drone on high ozone days. Additionally, the pilot was a student worker who underestimated the workload from his classes as well as commitments to his family's business. As a result, the drone was not able to be flown on non-charter days. To correct this for 2022, a new pilot was hired full time and tasked with attaining her Part 107 license from the FAA, learning to fly the sUAS first with a toy-grade quadcopter, and then with a professional coach when transitioning to the actual sUAS platform, as well as designing and building the sensor chassis, as described above. These steps, as well as hiring additional support staff for the 2022 measurement season under TRACER-AQ2, helped ensure that adequate personnel would be available for the TRACER-AQ2 project.

4. Conclusions

This project was without a doubt the most complex project this group of researchers has coordinated. Through the massive efforts of everyone on the team from the TCEQ project managers, PIs, staff, postdocs, and students from UH, Baylor, and St. Edward's this project was a huge success. Not only were there the TCEQ supported tasks described above assets from NASA and the Department of Energy also played a massive role in the TRACER-AQ study. NASA initiated the TRACER-AQ project by funding the deployment of the GCAS and HSRL2 instruments aboard the Johnson Space Center's Gulfstream-V aircraft to provide satellite-like observations of NO_2, HCHO, O_3, and aerosols. NASA further supported these measurements by deploying two ground based O_3 lidar systems from the Goddard and Langley research centers as well as five Pandora spectrometers and four Cimel sun photometers from the AERONET system. It should be noted that due to the impending launch of the TEMPO satellite NASA has opted to leave two of the Pandoras and two Cimels with UH for long term operation in Houston, bringing the total number to four of each. Through the Goddard O_3 lidar group NASA supported an additional 20 ozonesondes and provided personnel to aid with launches at the DOE's La Porte site. DOE support not only included providing the site access and 3-phase power for the Goddard lidar system, the TRACER science team also provided operational support by organizing daily weather and air quality forecast calls. Though unfunded, these calls helped the TRACER-AQ teams determine the optimal plans for the coming days and helped the forecast team gain an understanding of the needs and questions that the field teams would bring during the main intensive operation period in 2022. It is also worth noting that other than the aircraft operations themselves, the TCEQ and UH played a role in every other aspect of the project whether directly through site access or funding or through the continued support of the UH, Baylor, and St. Edward's teams.

Though the 2021 calendar year proved to be a very busy year for this research group it was one that ultimately saw the capabilities of this collaboration grow significantly. The year began with the conversion of the Baylor MAQL2 from a portable measurement system into a truly mobile air quality lab with the addition of an air-ride suspension and other provisions for over the road measurements and a 10 meter tower which can quickly loft the sampling inlet above the trailer when stationary. This was first deployed for a 7-week AQRP measurement project in Corpus Christi and San Antonio and then again a short few months later in Houston at the Battleground site for this project. The MAQL2 was previously deployed as a portable laboratory fpr the AQRP San Antonio Field Study in 2019, the AQRP and TCEQ $(BC)^2$ measurements in El Paso (2019) and Houston (2020). This project also marked the first time both the UH MAQL1 and Baylor MAQL2 were deployed simultaneously and demonstrated the utility of being able to selectivly Another unique capability developed in 2021 were the AQRP supported overwater measurements on the UH pontoon and small sampling cases whose operations were continued under this program and provided platforms for instrumentation as well as for launching ozonesondes in Galveston Bay and the Gulf of Mexico. Drone measurements were also introduced under this project where a six-rotor sampling platform was outfitted with a radiosonde and ozonesonde to collect vertical profiles of ozone and meteorology.

Beyond the overall complexity of this project, all of the 2021 projects and the preparation they required took place under varying levels of COVID restrictions and risks. Fortunately all preparations and field measurements were able to be conducted with minimal disruption.

A total of 72 onzonesondes were launched through support by the TRACER-AQ measurement project, 56 in 2021 and additional 16 during 2022. Many of these were launched in coordination with overflights of the NASA G-V aircraft to validate the vertical profile measurements from the downward looking HSRL2 O_3 lidar. As a result they were preferentially launched midday on days with moderate to high ozone. Multiple launch locations around the area, including the pontoon boat in Galveston Bay and the Red Eagle in the Gulf of Mexico, resulted in as many as 7-10 launches on the most active days. These profiles helped to identify layers of elevated O_3 above the boundary layer, within the marine boundary layer offshore, and validate the boundary layer heights over water. Lidar measurements of O_3 are fairly robust, therefore future campaigns may choose to prioritize spatial and temporal coverage of the area rather than focusing on supporting the lidar measurements. For instance, rather than timing many of the launches to occur under the aircraft track when it is overhead, the launches could instead be used to characterize the vertical structure of O_3 outside the flight track area or before and after the flight takes off and lands.

Task 4, the Rapid Science Synthesis report, was introduced through an amendment in response to the NOAA TOPAZ lidar not being able to deploy as originally planned due to the Houston area's COVID situation and health concerns of certain required team members. As a result, a report was developed to consolidate the preliminary key findings. Among these were that for the first time extensive observations exist for Galveston Bay and the coastal Gulf of Mexico that can be used to test models and provide empirical boundary conditions. These measurements also highlighted the complex interaction of meteorology, emissions, and photochemistry and the need for additional measurements with more complete sampling systems. High O_3 levels were found in the Gulf of Mexico using small, automated sampling systems installed on commercial support boats. On land, the two mobile labs captured a particularly interesting ethene event on September 27, 2021 where measurements reached approximately 13 ppmv at La Porte and were well correlated with high HCHO. Future analyses will seek to identify the source of the event.

The two mobile labs, MAQL1 and MAQL2, were deployed to supplement the exiting monitoring network during TRACER-AQ. The MAQL1 was based at the TCEQ site at the La Porte airport and conducted mobile sampling drives on 19 of 32 days. These drives, primarily funded by NASA, had objectives which included supporting the spatial measurements of the G-V aircraft, examining point, mobile, and area source emissions, urban plume emissions, and storm outflow boundary impacts on pollutant distribution. The MAQL2 focused on VOC measurements and was operated in a stationary mode at the Battleground Park caretaker's area at the southwest corner of the park behind the headquarters. Key findings here were early signs of the high ethene event, high levels of nighttime isoprene emissions verified with four different instruments and techniques, and the identification of potential influence of biomass burning events. Under this task Baylor also acquired new VOC capabilities such as a switchable reagent ion source to allow the PTR-MS to measure a broader suite of compounds including HRVOCs, an Aroma-VPC instrument (deployed in MAQL1), and the further development of using resin tubes to collect VOCs for offline laboratory analysis.

The overwater measurements were highly successful, collecting a robust set of data, and demonstrating that small sampling systems can be reliably deployed on commercial boats. Furthermore, traditional instrumentation can be deployed on a dedicated research boat and operated safely in Galveston Bay to collect O_3, Ox, boundary layer height, meteorological data, and serve as a platform for launching radiosondes and ozonesondes. Through careful calibration of the Ox and O_3 instruments, an estimate of NO_2 was possible, revealing that in addition to discrete plumes from passing boats and ships, broad areas of NO_2 were occasionally present over the Bay. Changes in the partitioning of O_3 and NO_2 resulted in apparent gradients in O_3 that were not as pronounced when examining Ox and would have otherwise been misrepresented. This further underscores the importance of understanding O_3 and NO_2, particularly in and around urban areas where titration can play a significant role. Charters of the Red Eagle in the Gulf allowed for targeted sampling as well as the opportunity to loiter and launch ozonesondes in the Gulf, an area the pontoon cannot reach safely.

Measured boundary layer heights over the Bay differed from the model and between the two measurement locations on the east and west sides of the Bay. While the second and third measured layers agreed quite well, the lowest layer did not and interestingly portrayed nearly opposite diurnal profiles. On the western side, the pontoon boat measured from a marina in Kemah presented a more traditional diurnal profile of boundary layer height, lowest overnight and in the early morning with a peak in mid-late afternoon before decreasing again with the loss of solar heating. In contrast, the Smith Point site on the east side showed a consistent and higher boundary layer between midnight and noon, with a significant decrease in the afternoon. The current hypothesis is that this could be related to the onset of the Gulf breeze. However more study is needed before any definitive conclusions can be drawn.

Data from this project collected by the Red Eagle, Shrimp Boat, and the UH pontoon boat over the Gulf of Mexico and Galveston Bay could inform future modeling studies by providing measurements to compare model boundary conditions. It could also be used to determine the proper parameters to use in CAMx in order for the model results to better represent the observations. Additionally, to better represent coastal ozone and meteorology in the WRF-GC model, two major improvements could be implemented for the current model settings. One is to adopt fine resolution (e.g. 1–4 km) emissions with detailed emission patterns for major roads and the Shipping Channel for Houston-Galveston region, replacing the current 10 km-resolution emissions in the model. The second is to test the best practice for model physics schemes, particularly PBL schemes, that may work best over land vs. water. Additional sensitivity tests employing results from this and the prior halogen study results may allow for additional improvements in the modeling of O_3 over water on the Texas coast.

With the successful deployment of the instrument packages, continued measurements over the Gulf of Mexico and Galveston Bay with these systems would be useful to follow up on the trends and spatial patterns observed in O_3, Ox, and boundary layer heights. These measurements could be incorporated into intensive campaigns or as part of routine measurements, such as with the HNET program of monitoring sites.

While the pontoon remains a solid and reliable platform for conducting atmospheric research, it's design inherently limits it to good conditions in Galveston Bay and the Houston Ship Channel. To expand on the success of the pontoon, UH is purchasing and outfitting a larger, faster, and more rugged research boat that will be capable of carrying more research instrumentation and will be capable of conducting operations in the Gulf of Mexico, as much as 50 miles offshore. This new capability, either on it's own or in addition to the other commercial and pontoon boats, can carry instrumentation to measure O_3, NO, NO_X, NO_Y, CO, SO_2, VOC, aerosol, meteorological and boundary layer instrumentation in addition to the ability of launching radio- and ozonesondes. These measurements will help further our understanding of the causes of high O_3 over water and characterize the precursor and secondary products to aid in identifying sources influencing these high O_3 conditions.

The MAQL2 had a successful measurement season at Battleground with a full package of trace gas, met, VOC and two size fractions of aerosol optical properties. The location offered an opportunity to better understand and characterize the difference in emission sources between the industrial Ship Channel area and the rest of metro Houston. Unique trends in the VOC and trace gas (i.e. potential local sources) will be investigated in the data analysis project. With larger trans-boundary events, the aerosol optical instrument suite at Battleground allowed for identification of potential influence of transported emissions (e.g. dust and biomass burning) to the Ship Channel area. The deployment of the MAQL2 to Battleground while MAQL1 was mobile was a new strategy, both containing a similar set of measurements, was a new strategy with potential to be employed in future air quality campaigns in Texas.

Tasks 7 and 8 dealt with the preparation and remediation of research sites. Power was installed at the TCEQ Aldine site to accommodate the research trailers that were slated to operate there, as was an all-weather road to access the site from the west side. Additional accommodations were made in MAQL1 to accept exterior mounted remote sensing instrumentation. These upgrades were left in place at the conclusion of the project and will be available for future use. The only remediation task was to have a landscape company repair ruts left at the DOE's site at the La Porte airport. These ruts were caused when the truck which came to retrieve the Goddard O_3 lidar, housed in an 18-wheeler trailer, got stuck in soft ground and had to be towed out.

While there were disappointments in the number of flights that were conducted during TRACER-AQ, the basic platform and measurement system demonstrated that it is possible to collect quality O_3 measurements from the sUAS purchased for this project. Additionally, the cost to procure and operate the system, which can collect samples in the first three layers of most photochemical grid models such as CAMx, CMAQ, and WRF-GC, is much less than the costs of constructing antenna style towers to sample from, and with the enhanced benefit that it can be flown when and where the science objectives dictate. Going forward, the addition of other sensors such as NO_2 and SO_2, both of which are or have been developed at UH, will further enhance the utility of these measurements, particularly when studying early morning gradients in O_3 and determining the role of NO_2 to better understand the partitioning of Ox with respect to vertical structure and mixing of the residual layer into the boundary layer.

5. References

Banta, R. M., Senff, C. J., Nielsen-Gammon, J., Darby, L. S., Ryerson, T. B., Alvarez, R. J., Sandberg, S. P., Williams, E. J., & Trainer, M. (2005). A Bad Air Day in Houston, *Bulletin of the American Meteorological Society*, 86(5), 657-670. Retrieved Nov 30, 2022, from https://journals.ametsoc.org/view/journals/bams/86/5/bams-86-5-657.xml

DOE, 2020. Tracking Aerosol Convection Interactions Experiment (TRACER), DOE ARM, https://www.arm.gov/research/campaigns/amf2021tracer, September 2020.

Haman, C. L., Lefer, B., & Morris, G. A. (2012). Seasonal Variability in the Diurnal Evolution of the Boundary Layer in a Near-Coastal Urban Environment, *Journal of Atmospheric and Oceanic Technology*, *29*(5), 697-710. Retrieved Nov 29, 2022, from https://journals.ametsoc.org/view/journals/atot/29/5/jtech-d-11-00114_1.xml

Komhyr, Walter D. 1972. "Electrochemical Concentration Cell for Gas Analysis." Google Patents.

Komhyr, W D. 1986. "Operations Handbook-Ozone Measurements to 40-Km Altitude with Model 4A Electrochemical Concentration Cell (ECC) Ozonesondes (Used with 1680-MHz Radiosondes)." National Oceanic and Atmospheric Administration, Silver Spring, MD (USA ….

National Aeronautics and Space Administration (NASA), 2020. Tracking Aerosol Convection Interactions Experiments-Air Quality (TRACER-AQ), NASA TolNET, https://www-air.larc.nasa.gov/missions/tracer-aq/index.html, September 2020.

Smit, Herman G J, Wolfgang Straeter, Bryan J Johnson, Samuel J Oltmans, Jonathan Davies, David W Tarasick, Bruno Hoegger, Rene Stubi, Francis J Schmidlin, and T Northam. 2007. "Assessment of the Performance of ECC-ozonesondes under Quasi-flight Conditions in the Environmental Simulation Chamber: Insights from the Juelich Ozone Sonde Intercomparison Experiment (JOSIE)." *Journal of Geophysical Research: Atmospheres* 112 (D19).

Stauffer, R M, G A Morris, Anne Mee Thompson, E Joseph, G J R Coetzee, and N R Nalli. 2014. "Propagation of Radiosonde Pressure Sensor Errors to Ozonesonde Measurements."

Thompson, Anne M, Herman G J Smit, Jacquelyn C Witte, Ryan M Stauffer, Bryan J Johnson, Gary Morris, Peter von der Gathen, Roeland Van Malderen, Jonathan Davies, and Ankie Piters. 2019. "Ozonesonde Quality Assurance: The JOSIE–SHADOZ (2017) Experience." *Bulletin of the American Meteorological Society* 100 (1): 155–71.