Air Quality Data Collection for TRACER-AQ-2 Field Campaign in Houston

FINAL REPORT

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List of Abbreviations and Acronyms

Abbreviation	Definition								
AAE	Absorption Ångström Exponent								
ADS-B	Automatic Dependent Surveillance-Broadcast								
AGL	Above Ground Level								
AQI	Air Quality Index								
BC2	Black and Brown Carbon								
BTEX	Benzene, toluene, ethylbenzene and xylene								
amu	atomic mass unit								
BTU	British Thermal Unit								
BU	Baylor University								
CAMS	Continuous Ambient Monitoring Station								
CAMx	Comprehensive Air Quality Model with Extensions								
CDT	Central Daylight Time								
CO	Carbon Monoxide								
COA	Certificate of Waiver or Authorization								
CO_2	Carbon Dioxide								
COVID	Coronavirus Disease 2019								
CSV	Comma Separated Values								
CU	Colorado University								
DOE	Department of Energy								
DOAS	Differential Optical Absorption pectrometer								
ECC	Electrochemical Concentration Cell								
EN-SCI	Environmental Science- Ozonesonde manufacturer								
FAA	Federal Aviation Administration								
FEL	An ANSI standard 1000 watt quartz halogen lamp; lamp-type								
	designation (not an acronym)								
ft	Feet								
GCO	Ground Control Operator								
GPS	Global Positioning System								
НСНО	Formaldehyde								
HGB	Houston-Galveston-Brazoria								
HNET	Houston Network of Environmental Towers								
HRVOC	Highly Reactive VOC								
HSC	Houston Ship Channel								
ICARTT	International Consortium for Atmospheric Research on Transport and								
	Transformation								
IOP	Intensive Observation Period								
IR	Infrared radiation								
jNO ₂	NO ₂ photolysis rate coefficient								
JOSIE	Jülich Ozone Sonde Intercomparison Experiment								
km	Kilometer								
LAANC	Low Altitude Authorization and Notification Capability								
LED	Light-Emitting Diode								
LiDAR	Light Detection And Ranging								

LOD	Limit of Detection
m	Meter
m ³	Cubic meter
MAQL1	Mobile Air Quality Lab 1
MAQL2	Mobile Air Quality Lab 2
MAQL3	Mobile Air Quality Lab 3
MAX-DOAS	Multi-Axis Differential Optical Absorption Spectrometer
MeFTIR	Mobile extractive Fourier Transformed Infrared Spectrometer
MeDOAS	Mobile extractive White cell DOAS
MEK	Methyl ethyl ketone
MDA8	Maximum Daily 8-hour Average
MDL	Method Detection Limit
ML	Mixing layer
mph	Mile Per Hour
MS	Mass Spectrometry
m/s	Meter per second
MVK+MACR	Methyl vinyl ketone + methacrolein
m/z	Mass-to-change-ratio
NAAOS	National Ambient Air Quality Standard
NaN	Not a Number
NASA	National Aeronautics and Space Administration
NDIR	Non-Dispersive Infra-Red
NIST	National Institute of Standards and Technology
nm	Nanometer
NO	Nitrogen Oxide
NOAA	National Oceanic & Atmospheric Administration
NO ₂	Nitrogen Dioxide
NOx	Nitrogen Oxides
NOy	Total Reactive Nitrogen
N ₂	Nitrogen
OŪ	Oklahoma University
Ox	Ozone + Nitrogen Dioxide
O ₃	Ozone
PCBTF	Parachlorobenzotrifluride
PGA	Proposal for Grant Activities
PGN	Pandonia Global Network
PM _{2.5}	Particle matter that are 2.5 microns or less in diameter
POPS	Printable Optical article Spectrometer
ppbv	Parts per billion by volume
ppm	Parts per million
PP1-RCP	Peak Performer 1 Reducing Compound Photometer
PTR-MS	Proton Transfer Reaction – Mass Spectrometry
PTR-SRI-MS	Proton Transfer Reaction Mass Spectrometer upgraded with a Selective
	Reagent Ionization
QA/QC	Quality Assurance / Quality Control
RAD	Rapid Alkene Detector

RH	Relative Humidity
RPIC	Remote Pilot In Command
RSS	Rapid Synthesis Report
RV	Recreational Vehicle
r^2	Coefficient of determination
SARP	Student Airborne Research Program - NASA
SEU	St. Edward's University
SkyDOAS	Differential Optical Absorption Spectroscopy
SOF	Solar Occultation Flux
sUAS	small Uncrewed Aerial System
SO_2	Sulfur Dioxide
SO _X	Sulfur Oxide
TAP	Tricolor Absorption Photometer
TAQ1/T-AQ1	TRACER-AQ1 (see below)
TAQ2/T-AQ2	TRACER-AQ2 (see below)
TCEQ	Texas Commission on Environmental Quality
TD-GC-MS/MS	Thermo Scientific Gas Chromatography-tandem mass spectrometry
TEMPO	Tropospheric Emissions: Monitoring Pollution
TRACER	Tracking Aerosol-Cloud Interaction Experiment
TRACER-AQ	Tropospheric Composition program funded the TRACER-Air Quality
TRACER-AQ1	Air Quality Data Collection Support for TRACER-AQ in Houston study
	funded by TCEQ
TRACER-AQ2	Air Quality Data Collection for TRACER-AQ-2 Field Campaign in
	Houston study funded by TCEQ
TRACER-MAP	Mapping Aerosol Across Houston
TX	Texas
μg/m3	Microgram per cubic meter
UH	University of Houston
UPS	Uninterruptible Power Supply
USB	Universal Serial Bus
UTC	Coordinated Universal Time
UV	Ultra Violet
VCP	Volatile Chemical Products
VOC	Volatile organic compounds
VT	Virginia Tech
WRF-GC	Weather Research and Forecasting Model coupled with GEOS-Chem
	chemistry

Executive Summary

The TRACER-AQ 2 study in Houston was designed as a follow-up study to the 2021 TCEQ and NASA funded TRACER-AQ study. The TRACER-AQ 2 study's intensive operation period (August-September 2022) overlapped with the Department of Energy's TRACER intensive operation period (June-September 2022) in order to leverage the additional meteorological land aerosol observations by DOE and the other participating federal and academic partners. This report focuses on the data collection, QA/QC, and data summaries for the TRACER-AQ 2 campaign. A TCEQ funded follow-on study in which this data will be more deeply analyzed is underway with all of the field participants as well as including a modeling component.

The University of Houston, Baylor University, St. Edward's University, Virginia Tech, and FluxSense deployed a wide variety of instrumentation in Houston including three mobile laboratories, an instrumented pontoon boat, two automatic sampling packages on commercial boats, a drone, and 65 ozonesonde launches. The Mobile Air Quality Lab 1 (MAQL1) was based at the TCEQ site at the La Porte airport with sampling objectives including locating and following the Houston urban plume, point source sampling from industrial and power plants, and complimentary sampling with the pontoon boat to characterize ozone and precursor gradients over land and water. The Mobile Air Quality Lab 2 was located at the San Jacinto Battleground State Historic Site in September as it was in 2021. This location is essentially surrounded by petrochemical facilities and refineries and had the most sensitive speciated VOC instrumentation deployed during this project. The third mobile laboratory was operated by FluxSense which focused on industrial emission sources using remote sensing instrumentation to quantify estimated mass fluxes and emission rates of key VOC species. Through TCEQ and other funding sources FluxSense has participated in numerous campaigns in the Houston area since the mid 2000's, providing a rich data set to evaluate spatial and temporal changes in emissions.

The pontoon boat was kept in a slip near Kemah, TX where Clear Lake connects to Galveston Bay and was equipped with in situ O₃, NO/NO₂, CO, and met measurements as well as serving as a platform to launch ozonesondes. It also carried remote sensing instrumentation for boundary layer height measurements and a Pandora spectrometer (on loan from NASA) for formaldehyde and NO₂ column measurements. The pontoon operated throughout the summer of 2022, primarily on days when high ozone or a land-bay breeze circulation was forecast. The two automated instrument packages were installed on commercial boats, one operated primarily in the industrial portion of the Houston Ship Channel and the other operated in the coastal Gulf of Mexico. These instruments allowed measurements of O₃, NO₂, meteorology, and boundary layer height (Gulf boat only) while the boats conducted their normal commercial operations. As a result, the spatial and weather conditions which were explored are more variable than the targeted measurements of the pontoon. An instrumented drone flew many mornings with an ozonesonde to probe gradients in O₃, occasionally reaching the residual layer above the nocturnal boundary layer. Sixty-five ozonesonde launches from varying locations on land and over the water were conducted in coordination with 64 additional ozonesonde launches from La Porte supported by the DOE TRACER study. Together these sondes and drone flights allow for the characterization of early morning mixing of the surface and residual layers as well as evaluating potential mixing between the boundary layer and free troposphere.

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 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. To leverage the assets deployed in Houston for the DOE TRACER campaign, National Aeronautics and Space Administration (NASA)'s Tropospheric Composition program funded the TRACER-Air Quality (TRACER-AQ) campaign in September 2021 and made various observations. 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.

To further leverages the DOE TRACER and NASA TRACER-AQ measurements, the TCEQ supported TRACER-AQ1 measurement project took place in summer 2021 and added suites of insitu atmospheric composition and meteorological measurements from ground-sites, mobile laboratories, boat platforms, and ozonesondes. This project, the TCEQ supported 2022 TRACER-AQ2 study, provided a follow up to the 2021 TRACER-AQ field study in the Houston area that was conducted in partnership with the DOE and NASA. The TRACER-AQ2 project conducted air quality measurements from stationary and mobile platforms from April through October 2022.

Project Design and Deployment

The TCEQ supported this TRACER-AQ2 measurement project beginning in April 2022; instruments were placed at stationary sites and on shipping vessels for "passive" measurements. Ozonesondes, balloons with ozone and meteorological instruments were launched from land and ships to evaluate the vertical profile of ozone, temperature, pressure, moisture, and wind speed/direction. During the TRACER-AQ2 intensive monitoring period of August and September 2022, more active measurement were conducted from mobile labs and shipping vessels.

The TRACER-AQ2 project provided support for the deployment of assets from Virginia Tech (VT). A multi-axis differential optical absorption spectrometer (MAX-DOAS) system comprised of light collecting optics and individual spectrometers were deployed on the mobile air quality laboratory #1 (MAQL1) to collect hyperspectral UV-Visible scattered solar radiation. The DOAS remote sensing technique was used to derive formaldehyde (HCHO) and NO₂ tropospheric gas columns during August and September 2022.

TRACER-AQ2 incorporated operations of several mobile/portable laboratories, i.e., the UH MAQL1 (mobile air quality laboratory #1), the Baylor MAQL2 (mobile air quality laboratory #2), and the FluxSense mobile laboratory during the IOP. The MAQL1 housed a suite of trace gas, VOC, aerosol optical, and meteorological measurements and made mobile measurements across the Houston-Galveston-Brazoria (HGB) region during most days. It was stationed overnight at the La Porte Airport (29.672141, -95.064676) from August 1, 2022 to September 20, 2022. The MAQL2 was stationed at the San Jacinto Battleground State Historic Site (29.752248, -95.091320) located along the Houston Ship Channel from September 3 to September 30, 2022. The MAQL2 platform also housed instruments to measure trace gases, VOCs, aerosol optical properties, and meteorological parameters. The FluxSense van employed an advanced mobile air pollution measurement lab equipped with four optical instruments for gas monitoring: SOF (Solar Occultation Flux), SkyDOAS (Differential Optical Absorption Spectroscopy), MeFTIR (Mobile extractive Fourier Transformed Infrared spectrometer) and MeDOAS (Mobile extractive White cell DOAS). A wind lidar was also positioned nearby the measurement location so that the winds, when coupled with the remote sensing measurements, can calculate a mass flux of selected VOCs, including alkanes, alkenes, and trace gases. The ground level measurements were also capable of VOC measurements and in some cases can continue to operate well even with overcast conditions that disrupt the solar/remote sensing methods.

To further support the land-water gradient questions during TRACER-AQ2, the overwater measurements were operated between April and October 2022 on three different platforms, the UH Pontoon Boat, the *Red Eagle*, and the *Victory*. The UH Pontoon Boat included an instrument package of O₃, NO, NO₂, NOx, CO, jNO₂, Ceilometer, Pandora, meteorological parameters and ozonesondes. The UH Pontoon Boat traversed the Houston ship channel north of Galveston Bay to the federally restricted waters at the San Jacinto Monument with VOC resin tubes taken on selected days. The latter two marine commercial service vessels were operated by Ryan Marine

Services and equipped to autonomously monitor ozone (O_3) , oxidants $(O_3 + NO_2)$, and meteorological parameters from April through October 2022. The *Victory* was sampling primarily in the industrial portion of the Houston Ship Channel (HSC) and the *Red Eagle* was primarily operated offshore in the coastal waters of the Gulf of Mexico. The *Red Eagle* also had a ceilometer to measure boundary layer heights over the water. There were 386 unique trips between the three boat platforms in 2022.

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. Measurements aboard the sUAS included ozone and meteorological measurements at the Battleground, UH Coastal Center, and the UH campus sites. Resin tube sampling of VOCs were also included for select days at the Battleground site. A total of 65 TCEQ TRACER-AQ2 free release ozonesondes were launched during this campaign and were used primarily to provide in situ validations of ground and airborne ozone lidar measurements. Sondes were launched both from land and over water. A separate DOE TRACER-Sonde project included 64 ozonesondes (32 days, twice-daily morning releases at ~6:00 and 10:00 LT) from La Porte.

Figure 1 shows an overview of the data collected during the TAQ2 campaign as well as the ozone air quality index (AQI). Days that had a Continuous Ambient Monitoring Station (CAMS) exceed the National Ambient Air Quality Standard (NAAQS) of Maximum Daily 8-hour Average (MDA8) ozone concentration of 70 ppbv are shown along with the number of monitors in the Houston-Galveston-Brazoria region that exceeded the standard.

May	1-May	2-May	3-May	4-May	5-May	6-May	7-May	8-May	9-May	10-May	11-May	12-May	13-May	14-May	15-May	16-May	17-May	18-May	19-May	20-May	21-May	22-May	23-May	24-May	25-May	26-May	27-May	28-May	29-May	30-May	31-May
High Monitor						91					71	83				72	73								89	77		78			
# Exceedances						2					1	3				2	1								3	8		1			
TCEQ Sondes	_					-																			-	1					
UH Pontoon																															
June	1-Jun	2-Jun	3-Jun	4-Jun	5-Jun	6-Jun	1-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	
High Monitor				77												79				97	73		73			78	71				
# Exceedances				3												4				18	1		1			6	1				
TCEQ Sondes		1																						1							
UH Pontoon																															
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																															
TCEQ Sondes										2			1												1		1	2		1	
DOE Sondes					2	2						2	2	2		2											2		2	2	
UH Pontoon																															
UH Drone																															
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
High Monitor										73	73																				
# Exceedances										1	1																				
TCEQ Sondes				2							2					2										3					1
DOE Sondes				2	2	2	2	2	2	3										2	2	2					2	2			
UH Pontoon				voc							voc					voc									voc						
UH Drone																															
September	Sep)-Sep	-Sep	-Sep	-Sep	H-Sep	i-Sep	o-Sep	-Sep	3-Sep)-Sep	0-Sep	-Sep	2-Sep	3-Sep	t-Sep	5-Sep	5-Sep	7-Sep	3-Sep	9-Sep	0-Sep									
	1-	2-	ċ	4	ù	ė	7.	Ġ	ъ	10	11	12	13	14	15	16	17	18	19	20	21	2	23	2	29	26	27	28	29	3(
High Monitor													89	11	75					84	92	76	81	78	71	74					
# Exceedances								-	-	-	-		8	4	3					4	14	3	8	2	1	1					
ICEQ Sondes		4				1		2	2	3	5	4	2	1	1				-	1	4	4	3			3			2	2	
DOE Sondes						2			2	2	2	2	2						2	2	2								2	2	
UH Pontoon	_								VOC								-				VOC	VOC	VOC		-	<u> </u>	-				
Chartered Red Eagle																	-				VOC	VOC	VOC		-						
UH Drone	_					-				VOC			voc	voc	VOC												-				
MAQL2@Battleground																															
October	1-Oct	2-Oct	3-Oct	4-Oct	5-Oct	6-Oct	7-Oct	8-Oct	9-Oct	10-0ct	11-0ct	12-0ct	13-0ct	14-0ct	15-0ct	16-0ct	17-0ct	18-0ct	19-0ct	20-0ct	21-0ct	22-0ct	23-0ct	24-0ct	25-0ct	26-0ct	27-0ct	28-0ct	29-0ct	30-0ct	31-0ct
High Monitor	72				72	73	88	87	78					80	72																
# Exceedances	1				2	3	5	11	2					3	1																
TCEQ Sondes						1																									
UH Pontoon																															
UH Drone																															

Figure 1: Operations during the TRACER-AQ 2 campaign.

Tasks

3.1 Task 3 - Ozonesonde Launches

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.

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.

3.1.2 Results for Measurements

There were 65 TCEQ TAQ2 ozonesondes with a breakdown of those from Galveston Bay (25), Gulf of Mexico (10), Southwest of Houston (10), University of Houston (14), La Porte (1), Beach City (1), Galveston (1), and those used by the UH sUAS (3). A separate DOE TRACER-Sonde project included 64 ozonesondes (32 days, twice-daily morning releases at ~6:00 and 10:00 LT) from La Porte. The number of ozonesondes released each day are shown in **Figure 1**. Of the 126 free-release balloon ozonesondes, 47 occurred in the early morning (profiles of residual layer ozone), 47 occurred in the late morning (profiles of the developing boundary layer), 30 during the afternoon (profiles near peak afternoon ozone), and two in the early evening near sunset (profiles of the collapse of the boundary layer). There were 23 ozonesondes released in September from La Porte while the MAQL2 was stationed at the nearby Battleground site.

A few cases of days with ozonesonde launches include:

• August 26, 2022: The UH Pontoon Boat measured ozone concentrations in Trinity Bay as high as 90 ppbv, which it also had the day before. We released 3 ozonesondes on August 26, two from the UH Pontoon Boat in Trinity Bay (Figure 2, bottom left and bottom middle panels) and one from Beach City (Figure 2, bottom right panel). The ozonesonde profile from 11:35 am CDT (16:35 UTC) shows elevated ozone of 85 ppbv in the boundary layer in the late morning. The last ozonesonde showed that while ozone was 55 ppbv at the surface in Beach City at the time of release (2:38 pm CDT) there was an enhancement just above the boundary layer that reached 85 ppbv. It also shows that the ozone levels in Trinity Bay had decreased by the time the sonde from Beach City landed approximately two hours after being released.



Figure 2: Boat and ozonesonde measurements from August 26, 2022. In the top left panel, the orange shows the path and altitude of each balloon during the ascent and the magenta shows the descent.

• September 21, 2022: Six ozonesondes were released on September 21, 2022 (**Figure 3**), a day in which 14 monitors exceeded the ozone standard and the highest monitor had a MDA8 ozone concentration of 92 ppbv. The last profile observed 110 ppbv of ozone in the boundary layer southwest of Houston.



Figure 3: Boat and ozonesonde measurements from September 21, 2022.

• Evening Ozonesondes (Collapse of the Boundary Layer): An ozonesonde was released at sunset on September 11 from the La Porte airport and on October 6 from near the C84 Manvel Croix monitoring station. **Figure 4** shows the initial 7 km of the ozonesonde profiles. The goal of releasing an ozonesonde near sunset is to observe a snapshot of the collapse of the boundary layer in the evening. In the right panel of **Figure 4**, the top of the boundary layer is shown by the thick dashed line near 2.3 km. The thin dashed line near 450 meters shows the top of a (potential surface) layer.



Figure 4: Ozonesonde profiles on two days where they were released just after sunset to observe the collapse of the boundary layer.

3.2 Task 4 - Guest Researchers Located at Monitoring Sites

During TRACER-AQ-2 there was one guest researcher involved in this project, Dr. Elena Lind from Virginia Tech. Dr. Lind deployed two Pandora spectrometer systems on the MAQL1. This work built on the NASA supported deployment on MAQL1 by Dr. Lind in 2021 for the initial TRACER-AQ project and prior work this group performed during the 2018 Kilauea eruption. In 2021 a single system installed using a fixed mount pointing vertical (zenith) on a plate attached to structure on the roof of MAQL1. In 2022, Dr. Lind was supported through this project for a more robust measurement system which again utilized the same mounting system as in 2021 however for this project two separate Pandoras were deployed on robotic trackers. These trackers were used to point the spectrometer collection optics at multiple directions and elevations. One system was oriented such that it pointed to the rear of the mobile lab and scanned vertically at three angles to collect measurements nominally along the path of the mobile lab (along roadways) while the second system was oriented such that it scanned perpendicular to the first and would collect data over areas adjacent to the road. This work is quite novel in several aspects. The installation of a remote sensing instrument such as the Pandora on a fully instrumented research laboratory has only been accomplished on land by this group. The use of two systems to scan in different directions simultaneously while driving has never been attempted prior to this project.

While this deployment was successful, there were some unexpected challenges. First, the data file sizes were too large for routine transfer across the cellular internet connection and had to be periodically transferred via USB hard drive and uploaded to Virginia Tech offsite. To prevent

damage to the fiber optic cables, the Pandora systems are designed to reset the tracker motors if the current torque is too large. In a normal installation, this may indicate a cable being caught on an obstruction and prevents the tracker from damaging or breaking fibers. On the MAQL1 the wind loads from driving on interstates created enough of a strain on the trackers that the current limits were reached and the systems reset. This has also been seen in other areas such as mountain installations where winds can get strong. Fortunately, the systems can be reset remotely, and this issue was discovered fairly early. The mitigation for this was to limit the MAQL1 speed to \sim 50 mph during the daytime when the Pandoras were operating. No speed restrictions were required at night with the trackers in the parked position.

3.2.1 Quality Control / Quality Assurance

Two Pandora instruments deployed during TRACER-AQ 2 were calibrated at the Virginia Tech Laboratory using the standard to Pandonia Global Network (PGN) calibration procedures and equipment. 1000W Hydrogen Tangsten Lamp (FEL) was used to characterize detector signal linearity, pixel response non-uniformity, filter transmissions and radiometric temperature sensitivity. Six atomic emission light sources were used to determine instrument transfer function and pixel-to-wavelengths mapping of the spectrometers. Spectrometer stray light was characterized using Princeton Instruments 750 mm monochromator and multi-wavelengths LEDs. In addition, field calibration of the zenith sky measurements were conducted to evaluate changes in wavelengths relative to the lab measurements. Dark current was characterized at different temperatures and integration times. For this study quality assurance and control follows the PGN established procedures and flags (combined effect of wavelengths shift, temperature, and optical depth DOAS fitting residuals) for the tropospheric columns retrieved from the sky scan measurements (https://www.pandonia-global-network.org/wpcontent/uploads/2021/09/BlickSoftwareSuite Manual v1-8-4.pdf). Uncertainties for NO₂ and HCHO differential slant columns are less than 5 and 15 % of the measurements (based on 10 sec integration time) and for columns (up to 3-4 km) are 15% and 30% respectively.

3.2.2 Results for Measurements

Conducting measurements along a roadway and perpendicular to it can help characterize pollution spatial heterogeneity due to the remote sensing "air sampling volume". Figure 5 shows tropospheric direction derived from the simultaneous Pandora measurements along and across of MAQL1 direction (August 23 to September 30, 2023). Considering the different sources and chemistry of NO₂ and HCHO in the atmosphere, their distribution and temporal changes are different during the campaign.

Clear differences in NO₂ tropospheric columns were observed depending on the direction while driving on busy roads and through locations with local sources (**Figure 5** lower left panel). Practically no spatial difference was observed in NO₂ at the more remote locations (e.g. 10 September 2023)

Surprisingly, no significant difference in HCHO columns were observed along the road compared to the perpendicular to the road remote sensing measurements. Suggesting that vehicular emissions of HCHO are relatively small compared to photochemically produced HCHO.



Figure 5: Left panel: NO_2 tropospheric columns derived from Pandora solar radiance measurements on top of MAQL1 pointing along the mobile lab path (looking backwards) and perpendicular to the path (looking to the left relative to the mobile lab direction); Right panel: HCHO tropospheric columns derived from Pandora solar radiance measurements pointing along the mobile lab path (looking backwards) and perpendicular to the path (looking to the left relative to the mobile left relative to the mobile lab direction); Right panel: HCHO tropospheric columns derived from Pandora solar radiance measurements pointing along the mobile lab path (looking backwards) and perpendicular to the path (looking to the left relative to the mobile lab direction)

3.3 Task 5 - Mobile Lab Measurements

3.3.1 Mobile Platforms - MAQL1 and MAQL2 Operations

An extensive suit of trace gas, VOC, aerosol optical, and meteorological measurements were made on two mobile labs, the UH MAQL1 and Baylor MAQL2. MAQL1 was operated in both the stationary mode at the La Porte Airport site and mobile mode across the Houston-Galveston-Brazoria (HGB) (**Figure 6**a). MAQL2 was deployed at the Battleground site in stationary mode (**Figure 6**b). These deployment locations were determined in consultation with the TCEQ Project manager.



Figure 6: Spatial plot and location of the mobile laboratories: a) MAQL1's routes and b) MAQL2's stationary site at the Battleground site during TRACER-AQ2.

The UH MAQL1 is comprised of a 325-ft³ 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

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.

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 $\sim 22 \text{ m}^3$, 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 Battleground, 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

3.3.2.1 Real-time VOC measurements

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 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.

3.3.2.2 Sorbent Tubes

VOC sample collection via sorbent tubes is a robust technique to capture and quantify VOC atmospheric concentrations using sorbents of varying affinities to retain a wide range of volatile compounds (**Figure 10**(a)). In this study, Material Emissions sorbent tubes from Markes International contained three sorbents to capture $C_{4/5}$ – C_{32} organic compounds. Ambient air was drawn through a sorbent tube using a portable pump at a flow rate of 0.1 liters per minute for up to 10 minutes (1 L total sample volume) not to exceed the breakthrough volume. After field sampling, the tubes were transported back to the lab in coolers and placed in long-term storage at 5 °C for up to two weeks before chemical analysis.

Ambient VOC sampling was completed using a combination of commercially available and custom-built sorbent tube samplers by BU. The commercially available sampler (i.e., Multi-Tube Sampler-32 from Markes International, **Figure 7**) was suitable for ground-based sampling without manual intervention between samples. This system was employed to conduct overnight sampling on top of the MAQL2 at Battleground. However, the large footprint and power requirements precluded its use during mobile, marine, and aerial sampling. Thus, lightweight, small-footprint samplers were constructed, such as the drone sampler that was constructed using the same lightweight material as the UH trace gas sampler and could interface with the internal drone communication system for the pilot to sample up to four tubes per flight (**Figure 8**). Additional sample collection was completed using the portable BU-built samplers and tripod setup shown in **Figure 9**.

In the lab, VOCs captured on sorbent tubes were analyzed using a coupled Markes International thermal desorption unit with a Thermo Scientific gas chromatography-tandem mass spectrometry (TD-GC-MS/MS) system located in the Baylor University Mass Spectrometry Center (**Figure 10**). 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 helium at 1 ml/min. VOC samples are then transferred along a 150°C flow path to a cold trap held at 20 °C and are refocused before GC injection. As the cold trap is heated, the

desorbed sample is sent to the analytical column that is heated stepwise from 40°C to 255°C before 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 11**) 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 7: MTS-32 setup to sample overnight on 9/22/22



Figure 8: VOC sampler (below drone) mid-flight with ozone monitor (above drone) at the San Jacinto Monument



Figure 9: Custom-built sorbent tube sampler atop the MAQL2 at Battleground location



Figure 10: Triple-bed sorbent tube for VOC sampling $(C_{4/5}-C_{32})$ *(a). MarkesTD-100xr system and Thermo Scientific TRACE 1310 GC coupled with Thermo Scientific TSQ8000 Evo Tandem MS/MS.*



Figure 11: Chromatogram of analytical standards used to quantify target analytes in sorbent tube samples

3.3.2.3 Trace gases 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 (NO₂), total reactive nitrogen (NO_Y), ozone (O₃), sulfur dioxide (SO₂), and carbon monoxide (CO). The NO and NO_X/NO₂ were measured using O₃ chemiluminescence and photolytic NO₂ converter, by a modified Air Quality Design instrument (Golden, Colorado) in MAQL2 and a Thermo Scientific 42C NO Analyzer and Thermo Scientific 42i NO_X analyzer in MAQL1. The NO_Y measurements were made using the Thermo Scientific (Waltham, MA) NOx Analyzer with heated molybdenum converter set at 315 °C in both mobile labs. Both mobile labs measured O₃ with an UV absorption Thermo Scientific 49i Analyzers. Both SO₂ 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 MAQL2 and an IR absorption Thermo Scientific 48C analyzer for CO in MAQL1. Both mobile labs used a Meteorologie Cosult GmbH filter radiometer to measure the NO₂ 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 CO₂ measurement in MAQL2.

3.3.2.4 Aerosol measurements

Both MAQL1 and MAQL2 housed aerosol optical measurements including absorption and scattering made using a tricolor absorption photometer (TAP 2901UV; Brechtel, Hayward, CA USA) and TSI tricolor nephelometer 3563 (NEPH; TSI Incorporated, Shoreview, MN, USA).

3.3.3 Quality Control / Quality Assurance for Mobile Lab Measurements

3.3.3.1 Real-time trace gas measurements

The method detection limit (MDL) values are shown below for the PTRMS in MAQL2 (**Table 1**). The reported PTR-MS amu values are the values at which each compound is identified by the PTR-MS. Uncertainties for each compound were calculated using the calibration settings most utilized. Concentrations below the MDL have been removed.

Campaign	Average 5-min	MDL and	Uncertainty
Species	PTR-MS amu	MDL	Uncertainty (%)
Acetonitrile	m42	0.18	11.47
Acetaldehyde	m45	0.42	9.91
Acetone	m59	0.55	10.26
DMS	m63	0.18	9.86
Isoprene	m69	0.18	10.02
MVK+MACR	m71	0.35	9.73
MEK	m73	0.53	10.37
Benzene	m79	0.17	10.48
Toluene	m93	0.25	9.94
Styrene	m105	0.35	12.14
Xylene	m107	0.33	10.49
C3-Benzene	m121	0.22	16.09
C4-Benzene	m135	0.29	16.90
Monoterpenes	m137	0.19	11.73
Formaldehyde	m31	2.08	47.24

Table 1: Method Detection Limits for each compound measured by the PTR-MS.

The RAD instrument was calibrated using discrete cylinders of propene, ethene, isoprene, and 1,3butadiene (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. The trace gases instruments in MAQL1 (NO, NO_X, NO_Y, SO₂, and CO) and MAQL2 (NO, NO_X, NO_Y, SO₂, CO, and CO₂) were calibrated once every few days. Multi-level calibration for NO₂ conversion efficiency and O₃ for instrument were performed once every week. The uncertainty and limit of detection (LOD) has been calculated for trace gases made on MAQL1 and MAQL2 (**Table 2**). For MAQL1, the 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 stationary during full sampling period.

Table 2:	Limit of Detect	tion (LOD) and	d uncertainty j	or trace	gas	measurements	made ir	ı MAQL1	and
MAQL2,	respectively.								

		MAQL 1		MAQL 2			
Trace gas	10s LOD (ppbv)	300s LOD (ppbv)	Uncertainty (%)	300s LOD (ppbv)	Uncertainty (%)		
NO	0.34	0.15	3.8	0.08	7.0		
NO ₂	0.96	0.30	4.8	0.13	9.1		
NO _Y	0.40	0.14	2.9	0.10	3.3		
O ₃	0.75	0.37	2.3	0.26	2.4		
SO_2	0.58	0.10	3.2	0.11	3.4		
СО	50.8	5.28	3.1	0.21	2.9		

3.3.3.2 Sorbent tubes

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 N₂ gas flow at 50 mL/min for 5 minutes. Calibration curves were run before and after each sample batch, and a coefficient of determination (r²) value of 0.97 or higher for each analyte's response was required before samples were run. A continuing calibration verification standard was run throughout samples to ensure the analytes' linear relationship was upheld.

The target analyte list of the sorbent tube samples includes VOCs from different emission sources, including transportation, biogenic, cleaning and personal care products, and industrial applications (Table 3). Historically, anthropogenic VOC emissions in urban inventories have predominately originated from automotive sources, including compounds such as benzene, toluene, ethylbenzene, and xylene (McDonald et al., 2018). However, recent studies have observed the emergence of nonvehicular sources as major contributors to urban VOC emission inventories (McDonald et al., 2018; Gkatzelis et al., 2021). These emission sources, known as volatile chemical products (VCPs), include cleaning and personal care products, pesticides, printing inks and adhesives, paints, and coatings (McDonald et al., 2018). Several modeling studies have observed enhanced ozone and secondary organic aerosol production in population-dense cities due to increasing contributions from VCP emissions (Khare and Gentner, 2018; Dunkera et al., 2019; Coggona et al., 2021; Pennington et al., 2021; Oin et al., 2021; Seltzer et al., 2021a; Seltzer et al., 2021b). In the context of Houston, the city is uniquely situated at the apex of increasing consumer product usage as the population grows, and it contains a booming petrochemical manufacturing industry, which may lead to changes in primary emissions and subsequent atmospheric processing within the region in the coming years. VCP emissions encompass many reactive species, and to focus monitoring efforts tracer compounds have been identified in previous studies (Gkatzelis et al., 2021; Stockwell et al., 2021), and were included in the target analyte list as follows: monoterpenes (*i.e.*, α -pinene, β -pinene, and limonene) for fragrances, octamethylcyclotetrasiloxane (D4 siloxane) for adhesives, decamethylcyclopentasiloxane (D5 siloxane) for personal care products, para-chlorobenzotrifluride (PCBTF) and Texanol for solvent- and water-based coatings, respectively.

Target Analyte	Retention Time (min)	Ions (m/z)	Dynamic Linear Range Lower limit (pg/uL)	Dynamic Linear Range Upper limit (pg/uL)	Potential Sources
Benzene	9.45	52, 50, 77	13	100	Transportation emissions
Toluene	13.18	91, 39, 65	13	100	Transportation emissions
Ethylbenzene	15.95	91, 65, 39	13	100	Transportation emissions
m-& p-Xylene	16.16	91, 65, 77	13	100	Transportation emissions
o-Xylene	16.85	91, 65, 39	13	100	Transportation emissions
Isoprene*	5.07	67, 41, 65	14	9	Biogenic emissions
α-Pinene*	17.46	77, 51, 91	13	8	Biogenic emissions
β-Pinene*	18.64	77, 51, 91	13	8	Biogenic emissions
Limonene*	19.48	67, 77, 91	13	8	Cleaning & personal care products
D4 Siloxane	18.06	249, 73, 205	20	12	Cleaning & personal care products
Benzyl alcohol	20.39	77, 79, 107	13	8	Cleaning & personal care products
D5-Siloxane	20.5	250, 179, 267	20	13	Cleaning & personal care products
Texanol	23.45	56, 71, 41	20	13	Cleaning & personal care products
PCBTF	15.79	145, 130, 161	11	7	Industrial emission
Styrene	16.91	78, 77, 103	19	12	Industrial emission

 Table 3: Breakdown of target analyte identification, quantitation parameters, and potential sources

*Analytes are also known to be used in manufacturing processes

3.3.4 Results for Measurements

3.3.4.1 Real time measurements of VOCs

Summary: Among the mobile measurement days, Alkanes had the highest average concentration of 103.5 ppb on September 2, Aromatics had the highest average concentration of 105.6 ppb on September 20, Dienes had the highest average concentration of 13.02 ppb on September 23, and Methane had the highest average concentration of 4.5 ppm on September 2. The Aroma instrument had some measurement issues during mobile measurement where it could not measure VOC concentrations for a notable period. For instance, Dienes was measured either for a negligible amount of time or in negative values for ten days out of 20 mobile days.

During TRACER-AQ1, isoprene proved to be a compound of interest at the San Jacinto Battleground (Battleground) site. The concentrations of isoprene previously exceeded concentrations of 50 ppbv at night, and those exceedances were also seen during TRACER-AQ2

(Figure 12). Concentrations of isoprene typically range below 5 ppbv from natural sources such as vegetation, these vegetative emission trends can be seen in Figure 13. Future investigations into isoprene and likely emission sources in the Battleground area will be conducted.

The acetaldehyde and acetonitrile in **Figure 14** can be used to identify biomass burning in certain scenarios. Aromatics in **Figure 15–Figure 16** often peak in the nighttime and indicate additional anthropogenic activities. The MEK is often different than the MVK and methacrolein, indicating different sources (**Figure 17**). **Figure 18** includes xylenes and toluene, which also often peak overnight and indicate other anthropogenic activities including industry and combustion.



Figure 12: Isoprene concentrations for the month of September 2022 at Battleground.



Figure 13: A closer look at isoprene trends for the month of September 2022 at Battleground.



Figure 14: Acetaldehyde and acetonitrile concentrations for the month of September 2022 at Battleground.



Figure 15: Benzene concentrations for the month of September 2022 at Battleground.





Figure 16: C4-Benzene and C3-Benzene concentrations for the month of September at Battleground.

Figure 17: Methyl ethyl ketone (MEK) and methyl vinyl ketone + methacrolein (MVK+MACR) concentrations for the month of September 2022 at Battleground.



Figure 18: Xylene, styrene, and toluene concentrations for the month of September 2022 at Battleground.

Select VOC classes (Alkanes, Aromatic, and Dienes) and Methane were measured in MAQL1 using an AROMA during September 2022, which included 20 days of mobile measurements. **Figure 19** shows the daytime average concentration of VOCs during the mobile period. **Figure 20** through **Figure 23** show the spatial variation of VOC concentrations in and around the Houston metropolitan region, Texas, on September 22, 2022. A large range in concentration is evident for the VOC classes during this drive; the areas with peak methane concentration did not always match the trends seen for other VOC classes on this day.

Alkanes (ppb)		Aromatic (ppb)			Dienes (ppb)			Methane (ppm)				
1-Sep	100.2	- 100	1-Sep	35.4	100	1-Sep	6.72	13	1-Sep	4.17		
2-Sep	103.5		2-Sep	74.17	- 100	2-Sep	3.21	12	2-Sep	4.5		4.4
6-Sep	89.77	- 90	6-Sep	29.62	00	6-Sep		12	6-Sep	4.23		
8-Sep	62.67		8-Sep	20.29	90	8-Sep		- 11	8-Sep	3.75		4.2
9-Sep	70.25	- 80	9-Sep	29.84	80	9-Sep	6.45		9-Sep	3.74		
10-Sep			10-Sep		00	10-Sep		- 10	10-Sep	3.7		4
11-Sep	55.57	- 70	11-Sep	15.05	- 70	11-Sep			11-Sep	3.85		
رم ^{12-Sep}	49.81		12-Sep	21.65	10	12-Sep		- 9	12-Sep	3.62		3.8
🚡 13-Sep	59.31	- 60	13-Sep	23.38	- 60	13-Sep	4.55		13-Sep	3.47		į
р 14-Sep	40.7		14-Sep	18.02	00	14-Sep	3.17	- 8	14-Sep	3.62		3.6
ig 15-Sep	72.2	- 50	15-Sep	26.9	- 50	15-Sep	3.97		15-Sep	3.93		900
Sep 20-Sep	56.25		20-Sep	105.6		20-Sep	5.54	- 7	20-Sep	4.22		3.4 0
21-Sep	64.7	- 40	21-Sep	26.66	- 40	21-Sep	10.98		21-Sep	3.18		
22-Sep	54.38		22-Sep	16.33		22-Sep	11.44	- 6	22-Sep	3.24	1.	3.2
23-Sep	57.48	- 30	23-Sep	16.96	- 30	23-Sep	13.02		23-Sep	3.37		0.2
24-Sep	65.78		24-Sep	17.7		24-Sep		- 5	24-Sep	3.79		3
26-Sep	49.72	- 20	26-Sep	17.85	- 20	26-Sep			26-Sep	2.63		3
27-Sep	13.28		27-Sep	8.15		27-Sep		- 4	27-Sep	2.69		
28-Sep	7.64	- 10	28-Sep	7.7	- 10	28-Sep			28-Sep	3.04		2.8
29-Sep	13.79	NaN	29-Sep	7.55	NaN	29-Sep		NaN	29-Sep	3.03		

Figure 19: Average concentration of VOCs (Alkanes, Aromatic, Dienes, and Methane) during the driving period of MAQL2 mobile measurement in September 2022. The NaN values are associated with either the VOC concentration data collected for a negligible time (< 1 hour) or a negative value.



Figure 20: Spatial variability of Alkanes during the mobile measurement on 09/22/2022 in Houston.


Figure 21: Spatial variability of Aromatic during the mobile measurement on 09/22/2022 in Houston.



Figure 22: Spatial variability of Dienes during the mobile measurement on 09/22/2022 in Houston.



Figure 23: Spatial variability of Methane during the mobile measurement on 09/22/2022 in Houston.

Tricolor absorption photometers (TAP) and Nephelometer were used to measure the aerosol optical properties of particulate matter ($PM_{2.5}$ in the MAQL2 and PM_5 in the MAQL1); only the MAQL2 had a nephelometer. The MAQL2 was stationed at San Jacinto Battleground from September 3 to September 30, and MAQL1 was mobile in and around Houston metropolitan region during September. The TAP to measure absorption coefficients of PM_5 in MAQL1 was installed on September 7.



Figure 24: Number of days the aerosol optical properties of PM measured in MAQL1 (mobile) and MAQL2 (stationary) during September 2022.

3.3.4.2 Aerosol Optical Measurements

Summary: Smoke influence was identified by MAQL 1 and 2 on September 29 for ~5 hours 45 minutes (00:30 to 06:15). During this time, all three TAPs in both MAQL 1 and 2 experienced smoke influence

MAQL 2 was stationed at San Jacinto Battleground for 28 days, from September 3 to September 30, to measure the aerosol optical properties of PM_{2.5} (**Figure 24**).

TAP and Nephelometer measured the absorption and scattering coefficient of $PM_{2.5}$ for 28 days. A time series plot of the 5-minute average aerosol optical data of $PM_{2.5}$ is shown in **Figure 25**. The data gaps in the time series plot are associated with either a TAP filter change or a power outage. Possible biomass-burning events were identified from September 27 at ~17:00 to September 28 at ~02:00 and September 28 at ~22:00 to September 29 at ~16:00 at San Jacinto Battleground. The average AAE for the given period, shown with the faint orange shaded strip in the figure, has risen above the AAE threshold. The AAE average plus one standard deviation of September data determines the AAE threshold.



Figure 25: Time series plot of 5-minute average aerosol optical data of $PM_{2.5}$ measured by TAP and Nephelometer and calculated angstrom exponents at San Jacinto Battleground during the TRACER- AQ2 campaign, September 2022. The time is in CST. The AAE average plus one standard deviation of September data is used as the AAE threshold to identify possible biomass-burning events.

In **Figure 26** we plotted the biomass burning period with the data from the BC² network (Black and Brown Carbon network; Baylor and UH network funded by TCEQ). This highlights that the event seen at La Porte and Battleground is also seen at Aldine, Liberty and Galveston; this indicates a broad impact across the Houston-Galveston metropolitan area.



Figure 26: Time series plot of the 5-minute average calculated AAE at (top) San Jacinto Battleground (MAQL2) and La Porte (MAQL1) and (bottom) BC^2 sites (Aldine, Galveston and Liberty) during a potential biomass burning event in September 2022. The time is in CST. The AAE average plus one standard deviation of September data is used as the AAE threshold to identify possible biomass-burning events.

MAQL1 was mobile to measure the spatial variability of the absorption coefficient in and around the Houston metropolitan region for 14 days during September 2022.

TAP was used to measure the absorption coefficient of PM₅ for 23 days, in which 14 days were mobile measurements, as shown in **Figure 24**. A time series plot of the 5-minute average aerosol optical data of PM₅ is shown in **Figure 27**. MAQL1 was stationed at La Porte Municipal Airport, TX, during a possible biomass-burning event.

The data gaps in the time series plot (**Figure 27**) are associated with either a TAP filter change or a power outage. Possible biomass-burning events were identified from September 27 at \sim 21:10 to September 28 at \sim 03:10 and September 29 at \sim 00:15 to September 29 at \sim 06:15 at La Porte. The average AAE for the given period, shown with the faint orange shaded strip in **Figure 27**, has risen above the AAE threshold. The AAE average plus one standard deviation of September data determines the AAE threshold. Mobile measurement times were shown by a gray patch in **Figure 27**.



Figure 27: Time series plot of the 5-minute average absorption coefficient of PM_5 measured by TAP in MAQL1 and calculated AAE during the TRACER- AQ2 campaign, September 2022. The time is in CST. The AAE average plus one standard deviation of September data is used as the AAE threshold to identify possible biomass-burning events. MAQL1 was stationed at La Porte Municipal Airport during a possible biomass-burning event.

Figure 28 through **Figure 31** show the spatial variation of the absorption coefficient and calculated AAE in and around the Houston metropolitan region, TX, on 09/22/2022.



Figure 28: Spatial variability of the absorption coefficient of PM_5 at 640 nm (Red) during the mobile measurement on 09/22/2022 in Houston.



Figure 29: Spatial variability of the absorption coefficient of PM_5 at 520 nm (Green) during the mobile measurement on 09/22/2022 in Houston.



Figure 30: Spatial variability of the absorption coefficient of PM_5 at 365 nm (Blue) during the mobile measurement on 09/22/2022 in Houston.



Figure 31: Spatial variability of the calculated AAE of PM₅ during the mobile measurement on 09/22/2022 in Houston.

Future works:

- Analysis of the identified smoke influence periods of the TRACER-AQ2 campaign and compare those with those identified in the BC2 campaign.
- Compare VOC data measured by Aroma to VOC data measured by other VOC instruments and trace gas data.
- Statistical analysis of aerosol optics data and VOC data.

3.3.4.3 Trace Gas Measurements

The MAQL1 made mobile measurements during most days and was stationed overnight at the La Porte Airport (29.672141, -95.064676) from August 1, 2022 to September 20, 2022. Figure 32 highlights spatial plots of select trace gases and VOCs measured in the MAQL1 during the sampling period. High alkene signals, using the propene equivalent from the RAD instrument, were regularly seen in La Porte, near the Houston Ship Channel. The MAQL1 identified strong O₃ plumes to the west (max: 123 ppbv) and south of Houston (max: 141 ppbv) (Figure 32 and Figure 33), including along the coast near San Luis Pass. Maximum O₃ concentration (10s average) was 106 ppbv. There were also multiple intercepts of the Parrish Power Plant plume as indicated by SO₂ plumes measured on the September 12, 2022 measurement (Figure 34). Maximum SO₂ concentration (10s average) was 42 and 40 ppbv measured near the Houston Ship Channel and Parish Power Plant, respectively.



Figure 32: Spatial plots of O₃, SO₂, Propene Equivalent, and HCHO of MAQL1 mobile measurements during the TRACER-AQ2 sampling period.



Figure 33: Spatial plots of O_3 on select passes during the mobile measurements of TRACER-AQ2 by MAQL1



Figure 34: East and west transects of SO₂ measurements (10s averages) made in MAQL1 southwest of Houston urban center, downwind of the WA Parish Power Plant on Sept. 12, 2022.

The MAQL2 was located near the San Jacinto Monument in the Houston Ship Channel area from September 3 to 30. From 19–25 September, O₃ concentrations increased each day, rising from 20–30 ppb up to nearly 100 ppb (**Figure 35**). The highest MDA8 (68 ppbv) and peak O₃ concentration 94 ppbv (5-min average) for MAQL2 during this period were measured on 25 September (**Figure 35**).

Wind direction data during this period shows a diurnal cycle of veering winds from 20 September to 23 September, during which wind direction shifts gradually in a clockwise manner during the day. The pattern is interrupted on 24 September, when the winds are southeasterly much of the day. Note that NO_{XY} concentrations are lower on this day, and that the nighttime ozone is not titrated to near zero during this period. The veering pattern resumes on 25 September, when the highest ozone concentration is reached.



Figure 35: Time series of trace gases (NO, NO₂, NO₃, O₃, SO₂ and CO) and meteorological (wind speed, wind direction, relative humidity, and ambient temperature) measurements made from the MAQL2 at the Battleground Site.

3.3.4.4 VOCs from Sorbent Tubes

Sample collection, Sampling Platforms, and Detection Frequency

Sorbent tubes were deployed and successfully measured VOCs during T-AQ2 across four sampling platforms (**Table 4**). VOC samplers were developed and outfitted for use on two marine, one terrestrial, and one aerial platform. One hundred and twenty-five total samples were taken across the four platforms as follows: during eight pontoon (n=58) and three Red Eagle

(n=12) outings, a colocation with the MAQL2 at Battleground (n=39), and on four flight days on the drone (n=16). Of the 125 total samples, 58 samples were associated with a sampling intensive which spanned across three platforms and occurred from 9/21 to 9/23. This intensive sampling was designed to explore the spatial gradients of ozone precursor species across the marine environment and included 10 min samples collected hourly coordinated across the MAQL2, pontoon, and Red Eagle platforms. At Battleground, this intensive sampling was expanded to assess temporal profiles and subsequent night vs day chemistry.

Date	Platform	Number of Samples			
8/4/2022	Pontoon	11			
8/16/2022	Pontoon	7			
8/25/2022	Pontoon	11			
9/9/2022	Pontoon	5			
9/11/2022	Pontoon	11			
9/21/2022	Pontoon	5			
9/22/2022	Pontoon	5			
9/23/2022	Pontoon	3			
9/21/2022	Red Eagle	4			
9/22/2022	Red Eagle	4			
9/23/2022	Red Eagle	4			
9/21/2022	MAQL2	5			
9/22/2022	MAQL2	11			
9/23/2022	MAQL2	11			
9/24/2022	MAQL2	6			
9/30/2022	MAQL2	6			
9/10/2022	Drone	3			
9/13/2022	Drone	5			
9/14/2022	Drone	4			
9/15/2022	Drone	4			
	Total	125			

Table 4: T-*AQ2* sorbent tube sampling dates, platforms used, and number of samples from the specific day.

VOCs were detected in samples on all platforms, and the detection frequency of each analyte is shown in **Figure 36**. The Battleground site had the highest detection frequency of analytes and is situated in the terrestrial/marine interface along the Houston Ship Channel. Comparatively, the detection frequency of anthropogenic species (*e.g.*, BTEX) decreased in the marine environment (**Figure 37**), and this trend was mirrored by traditionally biogenic species (*e.g.*, isoprene and monoterpenes, **Figure 38**) as well. This variability may reflect differences in proximity to sources (*e.g.*, industrial manufacturing, on-road traffic, shipping traffic, *etc.*), time of day, and meteorological conditions. It is important to note that the Red Eagle sampling occurred primarily

near the coast and outside shipping lanes, hence these samples may not reflect the VOC concentrations associated with this activity.



Figure 36: Detection frequency of target analytes using sorbent tubes across all sampling platforms during *TAQ2*.



Figure 37: Detection frequency of benzene, toluene, ethylbenzene, and xylenes (*BTEX*) using sorbent tubes across all platforms during *T*-AQ2.



Figure 38: Detection frequency of traditionally biogenic VOCs (isoprene, a-pinene, b-pinene, and limonene) using sorbent tubes across all platforms during T-AQ2.

Total VOC concentrations

Total VOC concentrations of pontoon, Red Eagle, and drone samples are shown in (Figure 39– Figure 42). Pontoon observations from August and September show changes in total VOC concentrations across sampling days as well as rapid changes in samples across a single deployment (Figure 39 and Figure 40). For example, on the 9/23 pontoon deployment, the total VOC concentration decreased by an order of magnitude over the course of two hours (*i.e.*, the 12 pm and 2 pm samples) (Figure 41). In addition, the VOC composition changed as well, as the 12 pm sample contained 75% contribution from benzene and toluene, as compared to the 2 pm sample that was dominated (i.e., 64%) by the industrial species D5 siloxane and Texanol. Similarly, changes in VOC contribution and concentrations were also captured in Red Eagle measurements along the Gulf Coast. Based on wind direction in the region, primary emissions may originate from the industrial area and undergo transport out over Galveston Bay, or they may be transported inland from origins in the marine environment. To explore the influences on this dynamic mixing of primary emissions and downwind interactions, we can match up with trace gas, meteorological, and ship tracking datasets. Finally, total VOC observations on the drone (**Figure 42**) highlighted composition changes on the sub-hour timescale throughout flight days, which may provide insight into the vertical distribution of VOCs in the first few 100 m. Using this distribution, the extent to which the gradient impacts ozone chemistry can be explored.



Figure 39: Operational days for sorbent tubes on the UH pontoon vessel 8/4 (a), 8/16 (b), and 8/25 (c).



Figure 40: Operational days for sorbent tubes on the UH pontoon vessel 9/21 to 9/23 (a). The inlay contains chemical composition data for the outing on 9/23. Samples were taken at the front of the vessel, which was upwind from the ship exhaust. Contributions < 5% are not labeled.



Figure 41: Operational days for sorbent tubes on the Red Eagle vessel during T-AQ2 (a). The inlay contains chemical composition data for the outing on 9/23. Samples were taken at the front of the vessel, which was upwind from the ship exhaust.



Figure 42: Operational days for sorbent tubes on the UH drone during T-AQ2 (a). The inlay contains chemical composition data for the morning flights on 9/15 (b and c). Samples were taken on the descent of the drone.

Day vs Night concentrations

During the sorbent tube sampling intensive from 9/21 to 9/24, sorbent tubes experiments conducted at Battleground were successfully able to quantify changes in VOC concentrations across specific daytime (12:00 to 5:00 pm) and nighttime (12:00 to 6:00 am) periods (**Figure 43**). Battleground VOC data showed large differences between day and night in the magnitude and contribution of key VOCs. Daytime samples were strongly dominated by isoprene, in addition to a wide range of other VOCs contributing to the composition (**Figure 44**). Following a reduction in biogenic production of isoprene at night, the contribution from those other species increased in the nighttime samples (**Figure 45**). In combination with the increased magnitude of nighttime samples, the shift in composition highlights several species that may be playing key roles in nighttime chemistry within the nocturnal boundary layer.



Figure 43: Operational days for sorbent tubes at Battleground during T-AQ2. Day and night samples were taken during this period and are shaded accordingly.



Figure 44: Chemical composition of daytime samples on 9/21/22. Contributions < 5% are not labeled.



Figure 45: Chemical composition of nighttime samples on 9/22/22. Contributions < 5% are not labeled.

Key findings and next steps

- On a broad spatial scale, Battleground total VOC observations were higher than the marine platforms. Proximity to source, meteorological conditions and time of day may impact VOC concentrations.
 - With this new insight into VOC spatial variability, how does that help improve our understanding on major source regions or improve modeling efforts?
 - How does this variability impact ozone formation chemistry in the region?
- VOC concentrations over Galveston Bay vary by orders of magnitude over relatively short time periods (e.g., hours). The bay also experiences influence from both primary emission and transport from known sources regions such as the ship channel to the north and the Gulf to the south.
 - What is the major source of VOC variability across the three surface-level platforms? Wind direction, distance, time of day, trace gases?
 - How does this data help improve our understanding of critical ozone chemistry associated with the terrestrial/marine interface?
- VOC measurements captured on the Red Eagle along the Gulf Coast provided an additional spatial component to land and bay profiles.
 - To what extent do anchoring areas in the Gulf impact ozone production in the marine environment?

- Based on preliminary data, as changes in shipping traffic and port delays occur, what is the impact on VOCs emissions and consequent ozone production chemistry within the Houston-Galveston area?
- VOC measurements captured on the drone highlighted vertical concentration and composition differences.
 - Based on the limited number of vertical VOC datasets, how does this dataset combine with ozone datasets to provide insight into chemistry occurring in the first 100 m of the atmosphere and help improve modeling efforts?
- Day and night VOC profiles, collected via sorbent tubes, were able to successfully capture identify nighttime activities, which showed elevated total VOC as compared to daytime.
 - Are these night vs day differences drive by changes in activity or changes in atmospheric chemistry?
 - How does this temporal variability impact ozone chemistry, particularly during the enhanced ozone days from 9/21 9/24?
- Speciated VOC data from sorbent tubes was able to highlight key biogenic species apinene and b-pinene.
 - How can speciated a- and b-pinene help improve modeling efforts of VOCs and ozone chemistry from anthropogenic BVOC emission profiles in heavily industrialized areas?

3.4 Task 6 - Galveston Bay Offshore Air Quality Measurements

3.4.1 The UH Pontoon Boat and Instrumentation On-Board

The UH Pontoon boat is a 24' aluminum pontoon boat owned and operated by the University of Houston within Galveston/Trinity Bay and the Houston shipping channel. The vessel was powered by a 125 hp two-stroke engine. The boat was upgraded with an aluminum under skin and a third polyurethane pontoon with included 35 gallon auxiliary fuel tank. The UH Pontoon boat was capable of carrying 75 gallons of fuel and could make a maximum of 15 knots fully loaded. This fuel capacity allowed the UH science team to operate mobile for up to 8 hours covering as much as 75 miles in a day. The UH Pontoon boat included an expanded suite of instrumentation for the TAQ2 field campaign compared to the previous year's TAQ1 campaign. Instruments included a 2b Technology O₃ analyzer, a Thermo 42iQ NOx analyzer, a Thermo 48iQ CO analyzer, a $_{\rm JNO2}$ radiometer, a Vaisala CL-51 ceilometer, and an Airmar 220wx all-in-one meteorological station with GPS. Additionally, the UH Pontoon boat hosted a NASA Pandora instrument with dedicated sun-tracking camera from August–October 2022. Details of the instrument deployment dates and total missions/hours logged during the 2022 deployment are shown in **Table 5**.

Platform	Date Deployed	Date Completed	Mobile Hours	Missions	O 3	NO, NO2, NOX	Met. Station	Mixing Layers	jno2
UH Pontoon Boat	20 April 2022	17 October 2022	220	42	X	X	X	X	Х

 Table 5: Attributes of the UH Pontoon sampling package during TRACER-AQ2

Instrumentation was securely mounted into shipping cases with shock absorbing racks. In addition to the instruments a PC and monitor were used to monitor and record incoming data. An Uninterruptible Power Supply (UPS) battery backup was installed in the cases to allow smooth power switches from shore to the on-board generator power. While not operating over Galveston Bay the UH Pontoon boat was docked in the Seabrook Marina off the channel between Clear Lake and the western entrance to Galveston Bay (**Figure 46**). This setup allowed for continuous measurements on the UH Pontoon boat platform both at dock and mobile.



Figure 46: (*Left*) UH Pontoon boat docked at the Seabrook Marina. (*Right*) Instrument case used on the UH Pontoon boat while open in the lab.

3.4.2 Quality Control / Quality Assurance for UH Pontoon Data

The UH Pontoon boat was lab calibrated before and after deployment. Additionally, the lab calibration system and calibration gases were brought to the boat in the field on a quarterly basis for a calibration of all trace gases to ensure accurate data was collected. The UH Pontoon boat was also visited weekly for a site visit, which included a change of the Teflon inlet filter and weekly calibration of the CO and NO gases using an on-board calibration system. Daily remote checks on instrument health were also performed remotely to assure internal temperatures, pressures, and flow rates were within a normal operating range.

Upon completion of the data collection a comparison of observed data at the UH Pontoon while docked, was compared with the closest TCEQ monitoring site, Seabrook C45, approximately 3.3 km to the NE. Results from the comparison are shown in **Figure 47** and **Figure 48**.



Figure 47: UH Pontoon boat 5-minute averaged ozone values while docked plotted against the nearest TCEQ ozone monitor, Seabrook C45, from April – October 2022.



Figure 48: UH Pontoon boat 5-minute averaged NO₂ values while docked plotted against the nearest TCEQ monitor, Seabrook C45, from April –October 2022.

The results from the comparison of the UH Pontoon Boat and the nearby Seabrook C45 monitor showed a good overall comparison with respect to O_3 and NO_2 values. There is some high bias observed in both the O_3 and NO_2 values at the UH Pontoon Boat site, which may be a result of site locations relative to local emissions and/or differences in instrument calibrations.

3.4.3 Results for Measurements

The UH Pontoon boat was deployed on 18 April 2022 and began continuously collecting data on 20 April 2022. During the operational period the UH Pontoon boat deployed 42 separate days recording 220 mobile hours over Galveston Bay (**Figure 49**).



Figure 49: Operational days for the UH Pontoon boat during TAQ2 from April –October 2022. The highest regional AQI and number of MDA8 ozone exceedances is listed and color coordinated.

Continuous meteorological (atmospheric pressure, wind speed, wind direction, air temperature and relative humidity), trace gas (NO, NO₂, CO and O₃) and jNO₂ data was collected on board the UH Pontoon boat throughout the April–October 2022 period except for a 6-day period from 14–20 July 2022 (**Figure 50 & Figure 51**). The data outage during this period was due to mechanical failure of the UH Pontoon boat's stator which caused it to be inoperable and ultimately needed to be removed from the Marina to be repaired at a local mechanic shop.



Figure 50: Time-series of meteorological measurements (atmospheric pressure, wind speed, wind direction, air temperature and relative humidity) collected by the UH Pontoon Boat from April – October 2022.



Figure 51: Time-series of trace gas measurements (NO, NO₂, CO and O₃) and JNO₂ collected by the UH Pontoon Boat from April–October 2022.

The spatial extent of the UH Pontoon boat operations was throughout Galveston and Trinity Bays and north into the Houston Ship channel to the federally restricted marker near the San Jacinto Monument. Plots of the areas covered by the UH Pontoon boat with associated ozone concentrations and Mixing Layer (ML) heights are shown in **Figure 52** & **Figure 53**, respectively. Some areas of Galveston and Trinity Bays are too shallow or impeded by oil and gas infrastructure to navigate safely, primarily in the NE and SE areas, and were avoided during operational periods.



Figure 52: Spatial plot of all areas covered by the UH Pontoon boat with associated ozone values from *April –October 2022.*



Figure 53: Spatial plot of all areas covered by the UH Pontoon boat with associated PBL heights determined by the internal algorithm used by the Vaisala CL-51 from April–October 2022.

3.5 Task 7 - Commercial Vessel Offshore Air Quality Measurements

3.5.1 Commercial Vessels and Instrumentation

Commercial vessels (**Figure 54** and **Figure 55**) were chosen to host the instrument platforms due to reliable operations and ability to operate without dependence on individual schedules. A company, Ryan Marine, out of Galveston, Texas was willing to collaborate and provide a constant source of power to operate the instrument packages continuously during all operations of the vessels, both docked and mobile.



Figure 54: Picture of the RMS Victory which hosted a portable instrumentation case from April–October 2022.

The RMS Victory is a 27m long service utility and supply vessel with two 30kw diesel generators capable of making a maximum speed of 11 knots fully loaded. The RMS Victory stayed within Galveston Bay shipping channels typically servicing ports from the Bayport channel to the turning basing near the 610-loop highway. The operating time was most often during the business hours of the servicing ports but could occur 24-hours a day and during most weather conditions. The instrument package for the RMS Victory included meteorological data (RH, pressure, temperature, wind speed/direction and GPS location) from an Airmar 220wx all-in-one weather station, O₃ from a 2B tech instrument and attached photocell to measure Ox.



Figure 55: Pictured is the Red Eagle, which operated offshore in the Gulf of Mexico. This vessel hosted a portable instrumentation case and ceilometer from April –October 2022.

The Red Eagle is a 37m long crew/utility vessel with two 40 kW 110/208V three-phase power generators capable of making a maximum speed of 19 knots fully loaded. The typical operating profile for the Red Eagle was to depart the Galveston docks to service larger vessels in the Galveston Anchorages and Lightering areas, depending on their customer's needs. The Red Eagle

on occasion conducted operations as far west as Matagorda Bay and north into Galveston Bay and through the ship channel to the port of Houston. The Red Eagle would go up to 50 miles offshore, if needed, and these activities would occur 24-hours a day and in all weather conditions. The instrument package for the Red Eagle included meteorological data (RH, pressure, temperature, wind speed/direction and GPS location) from an Airmar 220wx all-in-one weather station, O₃ from a 2B tech instrument and attached photocell to measure Ox. Additionally, a Vaisala CL-51 ceilometer was mounted to the deck and data collected was logged through the PC in the instrument case.

3.5.2 Quality Control / Quality Assurance for Commercial Vessels

The commercial vessel instrument packages were lab calibrated before and after deployment. Additionally, a monthly site check was performed at each vessel which included: checking instrument case was firmly secured, checking for water ingress, confirming orientation of meteorological station, replacing internal desiccant pack, changing inlet particulate filter and checking with crew on board the vessel. Furthermore, a daily check was performed remotely where the instrument and case health check were examined, which included checking internal temperatures, pressures and flows. The measured data was then compared against nearby TCEQ continuous air monitoring stations for verification of reasonable results as shown in **Figure 56**–**Figure 59**.



Figure 56: The Red Eagle boat 5-minute averaged ozone values while docked plotted against the nearest *TCEQ* ozone monitor, Galveston C1034, from April–October 2022.

The comparison between ozone values at the Red Eagle and Galveston C1034 monitors overall shows good agreement. Periods of high ozone were occasionally observed at one monitor but not the other, which is attributable to the different locations (10.25km apart) the sites are located at, with the C1034 monitor only 850m from the shore and the Red Eagle docked near the urban center in a busy pier.



Figure 57: The Red Eagle boat 5-minute averaged, calculated NO2 values while docked plotted against the nearest TCEQ NO₂ monitor, Galveston C1034, from April–October 2022.

The comparison in NO_2 values between the Red Eagle and C1034 does show a relationship, with a high bias observed at the Red Eagle site. This difference is not unsurprising when considering the nature and location of the two sites. The Red Eagle, which is located near the urban center, shipping channel and in a well-used pier would tend to be exposed to more local emissions relative to a site (C1034) located within 900m of the shore of the Gulf of Mexico.



Figure 58: The RMS Victory boat 5-minute averaged ozone values while docked plotted against the nearest TCEQ ozone monitor, Lynchburg Ferry C1015, from Apri –October 2022.

Comparison of ozone values between the RMS Victory and the Lynchburg Ferry (C1015) site showed a good consensus, with a wide spread about the linear fit. The location of these sites along the main Houston Ship Channel would likely promote large differences between sites, even in close proximity, through the formation and titration of ozone due to local emissions.



Figure 59: The RMS Victory boat 5-minute averaged ozone values while docked plotted against the nearest TCEQ ozone monitor, Lynchburg Ferry C1015, from April–October 2022.

Comparing the NO₂ values at the RMS Victory and Lynchburg Ferry (C1015) site shows extremely high values impacting the RMS Victory that are not observed at the Lynchburg Ferry site (**Figure 59**). These observations are likely due to the dock the RMS Victory site is located at being downwind from large tanker vessel docks and an aggregate sorting yard working with dredging material from the Houston Shipping Channels. Periods in direct exhaust flow of heavy machinery and large ships due to this location were not uncommon.

3.5.3 Results for Measurements

The Red Eagle and RMS Victory boats both had successful campaigns logging more than 1,000 hours and 300 unique science missions between the platforms (**Table 6**). Both platforms were deployed in April and removed in October of 2022 (**Figure 60**). Once deployed, the systems collected data continuously both stationary and mobile.

The only sustained outage in the data was from 26 May–14 June, 2022 at the Red Eagle platform. This outage was due to a failure of the battery backup power supply which was not allowing the data acquisition PC to boot up. Ultimately, this issue was resolved by removing the battery backup system, which was also deemed unnecessary to the setup due to the constant power received at the site.

Platform	Date Deployed	Date Completed	Mobile Hours	Missions	O ₃	Ox	NO ₂ (Calc.)	Met. Station	Mixing Lavers
Red Eagle	21 April 2022	26 October 2022	842	175	Х	Х	X	Х	X
RMS Victory	27 April 2022	26 October 2022	292	169	Х	Х	Х	Х	

 Table 6: Attributes of the commercial vessel sampling packages during TAQ2



Figure 60: Operational days for the commercial vessels during TAQ2 from April – October 2022. The highest regional AQI and number of MDA8 ozone exceedances is listed and color coordinated. The five chartered science missions on board the Red Eagle in September are marked with an asterisk.

The Red Eagle platform logged a total of 842 hours of mobile operations across 175 unique missions, going as far as 187 km (about 116.2 mi) from port and 97 km (about 60.27 mi) offshore (**Figure 61**). A range of ozone conditions were observed during the operational period, including multiple high ozone episodes with < 70 ppbv ozone observed both at the dock and while over water (**Figure 62**).



Figure 61: Spatial plot of all area covered by the Red Eagle vessel with associated ozone values from *April* –October 2022.



Figure 62: Overall trace gas dataset with O_3 , $O_3 (O_3 + NO_2)$ and calculated NO_2 for the Red Eagle platform.

The RMS Victory platform logged a total of 292 hours of mobile operations across 169 unique missions. This platform generally did not go further south than the Bayport Channel Terminal on the Northwest side of Galveston Bay. Although did log one trip to Galveston, Texas for Coast Guard certifications and inspections (**Figure 63**). Additionally, missions on this platform tended to have a shorter duration compared with the Red Eagle. The docking location for the RMS Victory is in a region with numerous and complicated local emissions, and periods of greater than 100 ppbv NO₂ (calculated) were observed regularly. Additionally, multiple air quality episodes with periods of ozone exceeding 70 ppbv were observed at the dock and while mobile, including periods of high ozone that the Red Eagle and UH Pontoon boat did not observe (**Figure 64**).



Figure 63: Spatial plot of all areas covered by the vessel RMS Victory with associated ozone values from April –October 2022.



Figure 64: Overall trace gas dataset with O_3 , O_X ($O_3 + NO_2$) and calculated NO_2 for the RMS Victory platform.
3.5.4 Red Eagle Chartered Science Missions

In addition to the routine operations performed by the Red Eagle vessel during the TAQ-2 field campaign, five days were selected to charter the Red Eagle for targeted science routes during air quality events that took place in September of 2022 (Figure 65–Figure 69). The on-board instrumentation was operating during these missions with multiple ozonesonde launches accompanying the surface measurements at designated locations along the selected routes.



Figure 65: Spatial tracks from 11 September 2022 during a chartered science mission on-board the Red Eagle platform (Left) observed Ozone values (Right) observed NO2 values.



Figure 66: Spatial tracks from 12 September 2022 during a chartered science mission on-board the Red Eagle platform (Left) observed Ozone values (Right) observed NO₂ values.



Figure 67: Spatial tracks from 21 September 2022 during a chartered science mission on-board the Red Eagle platform (Left) observed Ozone values (Right) observed NO₂ values.



Figure 68: Spatial tracks from 22 September 2022 during a chartered science mission on-board the Red Eagle platform (Left) observed Ozone values (Right) observed NO₂ values.



Figure 69: Spatial tracks from 23 September 2022 during a chartered science mission on-board the Red Eagle platform (Left) observed Ozone values (Right) observed NO₂ values.

3.6 Task 8 - Remediation of Property Upon Decommissioning of Research Sites

Under this PGA (#582-22-32022-021) to support measurements for the TRACER-AQ2 measurement project in Houston, Task 8 provided for the remediation of property upon decommissioning of the research sites. Largely because of the successes in the 2021 measurement campaign supported by TCEQ (PGA # 582-21-22179-015) and NASA and the DOE supported TRACER-MAP campaign which immediately preceded this project, modifications to field sites were not needed during this campaign.

The few modifications which took place were completed under the TRACER-MAP project and were primarily replacing electrical breakers at sites for the mobile air quality labs (MAQL1 and MAQL2) including Battleground, Jones Forest, and La Porte. At Aldine, the 50A RV circuit on the TCEQ panel was unable to hold the load for the Baylor MAQL2. Rather than potentially disrupt service to the TCEQ monitoring site an adapter and temporary subpanel were installed on the UH electrical service there, taking advantage of the 100A pin and sleeve connector installed the previous year for the NOAA TOPAZ (Tunable Optical Profiler for Aerosol and oZone) ozone lidar system. This allowed the (BC)², boundary layer profiling trailer from the University of Oklahoma, and MAQL2 to operate on the UH service at the TCEQ La Porte site which have the same 100A connection to provide power for one or more mobile labs as the availability of mobile labs in Texas grows, expanding the abilities for collaboration to address air quality issues in the future.

3.7 Task 9 - Monitoring Air Quality by Use of Small Unmanned Aerial Vehicle (sUAS)

3.7.1 Quality Control / Quality Assurance for sUAS Flights

The principal goal of the sUAS operations during the Air Quality Data Collection for TRACER-AQ-2 Field Campaign in Houston (TRACER-AQ-2) was to measure vertical profiles of ozone (O₃), temperature, pressure, and humidity with the possibility of expanding to other measurements. These measurements included sulfur dioxide (SO₂), nitrogen dioxide (NO₂), and volatile organic compounds (VOCs). Another aim was to prove the utility of using sUAS for air quality measurements, as the platform offers several advantages over balloons or towers.

The small unmanned aerial system (sUAS) used for TRACER-AQ-2 measurements included an Aurelia X6 Pro hexacopter, and associated ground station components. The equipment was purchased in 2021 by the University of Houston (UH) under the TCEQ funded Air Quality Data Collection Support for TRACER-AQ in Houston (TRACER-AQ) grant (PGA# 582-21-22179-015) as a platform for air quality measurements. The sUAS, aka "drone", was purchased along with five sets of 21,000 mAh 22.2 VDC batteries and an Elistair SAFE-T power tether station. The hexacopter drone is capable of up to 55 minutes of flight in ideal conditions without a payload on a set of two batteries. However, using the power tether, it can maintain flight for hours without the need to land.

The primary payload for the Aurelia X6 Pro consisted of an aluminum sensor chassis (described thoroughly in TRACER-AQ Deliverable 10.2), two step-down DC-DC converters, a grounding busbar, and a relay board with six relays that can be controlled from the ground via the sUAS transmitter. The sensor chassis and these components are pictured attached to a perforated aluminum platform in **Figure 70**. The platform was designed to mount to the top of the drone, as shown in **Figure 71**. An EN-SCI ozonesonde is connected to an extended inlet tube was mounted to the chassis. The ozonesonde connected to an iMet-1 RSB Research Radiosonde which could transmit the ozone data as well as the temperature, pressure, and humidity measurements from the radiosonde's probe. These components made up the standard payload with enough space to incorporate SO₂ and NO₂ sensors. The payload was mounted to the top of the sUAS as in **Figure 72**, though it could also be bottom-mounted.

On four of the sUAS flights, a VOC instrument from Baylor University was integrated into the power relay system onboard the sUAS and carried along with the standard ozonesonde and iMet payload. The VOC payload, shown in **Figure 73**, could carry up to four sample tubes independently controlled in-flight using the sUAS transmitter.

Preparations and testing for the sUAS began in 2021 to ensure both the X6 Pro and the research team were prepared for the 2022 TRACER-AQ-2 program. As part of those preparations (detailed in the 2021 TRACER-AQ Deliverables 10.1 and 10.2) arrangements were made with University of Houston in 2021 to ensure compliance with policy and establish procedure for all sUAS flights.

According to the agreement with University of Houston, the sUAS could be flown in the predetermined locations specified in **Table 7**. Due to Federal Aviation Administration (FAA) regulations, the remote pilot could fly the sUAS to altitudes of only 121 m (400 ft) (AGL). However, at some locations, altitude is restricted further to only 60 m (200 ft), depending on the airspace regulations. **Table 7** indicates what altitudes were permissible at each location.

The flight crew for sUAS operations typically consisted of two people, the Remote Pilot In Command (RPIC) and a Ground Control Operator (GCO) to help ensure safety, efficiency, and data quality. Direct line-of-sight visual observation of the sUAS is required by FAA regulations, and both crewmembers participated in visual monitoring of the airspace, sUAS, and ground below the flight area to be sure the sUAS was functioning as expected and the area was free of hazards. To aid in situational awareness, the crewmembers also used the FlightAware app and adsbexchange.com to view local air traffic.

In addition to acting as a visual observer, the RPIC possessed the FAA Remote Pilot Certificate and acted as the sUAS pilot. The RPIC was accountable for all sUAS activities and used B4UFly and Aloft (recently updated to Air Control) apps to check the airspace and weather conditions and request Low Altitude Authorization and Notification Capability (LAANC) authorizations before flights. LAANC authorizations are provided by an automated system developed in collaboration with the FAA. LAANC approval is not required in uncontrolled airspace but can provide instant authorization up to a predetermined altitude in controlled airspace. For example, flights can be automatically approved through the LAANC system for up to 60 m (200 ft) at the UH Main Campus.

During flight days, the Ground Control Operator focused on setting up and monitoring the ground control computer, a heat-tolerant, waterproof Panasonic Toughbook. The computer ran opensource Ardupilot Mission Planner software used to monitor the sUAS status, plan automated missions, and modify flight parameters (e.g., speed, failsafe limits, battery capacity). The computer also ran Skysonde, which allowed the iMet radiosonde to transmit data from the payload in real-time. The GCO monitored the data and informed the RPIC of any irregularities. If there were any problems with the data transmission, the RPIC could land the sUAS immediately to address the issues. When the power tether was in use, the GCO also watched the T-monitor app on a cellular device. The app displays data from the power tether, such as power output, cable speed, and alerts that help ensure the safe operation of the tether.

In addition to aiding with sUAS setup, battery changes, and battery charging, recordkeeping was another key responsibility of the GCO. Maintaining a detailed log of events was critical to successful long-term operations. The notes on environmental conditions supplemented the data collected by the payload, and the log of precise launch and landing times allowed flight hours to be tracked, which helped the RPIC monitor long-term battery health and maintain the flight logs that are submitted to Aurelia. The Aurelia log tracked total flight hours on the drone and could also be used to demonstrate patterns in performance issues. Maintenance performed on the sUAS was also recorded. Careful recordkeeping helped to keep the system in peak operating condition, ensuring the safety and success of data collection.

The use of ozonesondes to collect data on the sUAS was motivated by the low weight (~240 grams) and relatively low cost of the instruments. Furthermore, the team had extensive experience using them on weather balloons. Ozonesondes have been used for decades to make tropospheric and stratospheric ozone measurements as balloon payloads, however they are not typically used for extended periods for near-surface data collection. To demonstrate that the sUAS ozonesonde data were in reasonable agreement with other nearby measurements, several sUAS flights were conducted at UH Main Campus at the launch trailer which measures ozone at an altitude of 6 m above ground level and provides a good comparison for low-altitude drone measurements. Moody Tower is roughly 1 km south of the flight location and measures ozone at an altitude of 70 m. **Figure 74** shows ozonesondes measurements made during flights that took place at the launch trailer. The measurements compare well, particularly when considering the \pm 5-20% ozonesonde uncertainty (Sterling et al., 2018).

Python script was used to process the data from the ozonesondes and radiosonde. The script first eliminated extreme values that resulted from missing data points and sensor errors. GPS altitudes, latitudes, and longitudes that were outside of a reasonable range for the location were also flagged as erroneous data. Then, as plots were generated, the altitude above ground level was calculated by finding the lowest GPS altitude measured by the iMet radiosonde not flagged as missing data and used the minimum as the ground level.



Figure 70: Aluminum sensor chassis and electrical system components attached to a platform that can be mounted to the top of the drone.



Figure 71: The Aurelia X6 Pro with the sensor chassis, electrical system components, and the upper platform mounted to the top of the drone.



Figure 72: The standard payload, including an ozonesonde (in the center of the chassis) and an iMet-1 RSB radiosonde (white box on top of the chassis), mounted to the top of the sUAS and connected to the sUAS power and relay input systems. The arms and compass of the sUAS are folded down.



Figure 73: The Aurelia X6 Pro flying at San Jacinto Battleground Park. The primary payload is mounted on top and the VOC payload is mounted on the bottom.

Site Name	Address	Lat, Long	Max Altitude (m)	
UH Campus	4800 Calhoun Rd Houston, TX 77204	29.723889°, -95.339214°	60	
UH ERP	5000 Gulf Freeway, Houston, TX 77204	29.716344°, -95.329903°	60	
UH Sugar Land	14000 University Blvd Sugar Land, TX 77479	29.573415°, -95.652463°	60	
UH Coastal Center	5721 Highway 2004 La Marque, TX 77568	29.388237°, -95.042336°	121	
UH Liberty	404 FM 1011 Liberty, TX 77575	30.0966°, -94.7634°	121	
UH Smith Point	450 Old Dutchman Rd Anahuac, TX 77514	29.546110°, -94.780333°	60	
San Jacinto Battleground Park	3523 Independence Pkwy La Porte, TX 77571	29.742516°, -95.072979°	121	
Texas City Dike	Dike Rd Texas City, TX 77590	29.364534°, -94.810641°	60	
TCEQ Aldine Site	4510 1/2 Aldine Mail Rd Houston, TX 77039	29.900917°, -95.326175°	121	
Galveston Island beaches (outside exclusion zone)	14901 FM3005 Galveston, TX 77554 San Louis Pass beach	29.191744°, -94.954531° 29.085304°, -95.113483°	60	

 Table 7: Locations and altitudes that the sUAS was permitted to fly in 2022.



Figure 74: Ozonesonde mixing ratios compared to data from Moody Tower (70 m) and Launch Trailer (6 m). Sonde values compared to Moody Tower are shown as circles colored by altitude of the sonde when the measurement was made. Sonde values compared to the launch trailer are shown as squares colored by altitude of the sonde.

3.7.2 Results for Measurements

Twenty-five flight days occurred during the TRACER-AQ-2 August-October 2022 intensive operating period where reliable ozone, temperature, humidity, and pressure data were collected. **Table 8** shows the date and location of each flight, as well as what was measured using the sUAS each day. On September 10, the VOC instrument from Baylor University was flown with the standard ozonesonde and iMet payload. On September 20, an SO₂ sonde was added to the standard payload and flown at Battleground Park. The sonde was calibrated in the lab prior to the flight, and the flight was a successful test of operations. However, further data analysis and refinement of the procedure and instrument was necessary. The SO₂ sonde was only flown once, and an NO₂ sonde was not attempted because it was determined that the amount of development necessary for them would distract from the primary goals of collecting the ozone and meteorological data to characterize ozone formation and observe the mixing of air layers. Further work on the new sondes is planned and SO₂ sonde measurements will be carried out onboard the sUAS in 2023.

The timing of flights was determined by the conditions and objectives of each day, which also affected whether the sUAS was powered by batteries or the power tether. Many flight days were dedicated to observing a vertical ozone gradient (see example in **Figure 75**). Therefore, these flights took place in the early morning as the gradient typically dissipates as the sun rises and the air becomes well mixed. These flights were powered by batteries so that the maximum altitude

was not restricted by the 80 m length of the power tether. For other flights aiming to observe ozone formation later in the day, the power tether was a more practical choice. Since the air was typically already well mixed between 0 and 121 m, it was better to avoid the interruptions of battery changes at the cost of some height. Once connected to the power tether, the sUAS could fly an automated mission to make continuous vertical profiles without the need for frequent landings (see **Figure 76** for a flight example). While the sUAS was landed periodically for inspection, an upper limit of flight duration for the sUAS on the power tether was not discovered during this campaign. The ozonesonde was the limiting factor rather than the sUAS or power station, as the solutions inside the sonde evaporate and become too concentrated after approximately 6 hours of use.

Flights that measured the vertical gradient, such as in **Figure 75**, provided important data for understanding ozone surface titration and deposition and photochemical production. **Table 9** below shows the ozone values for the first two ascent profiles of the August 26 flight shown in **Figure 75**. On descents when a gradient was present, ozone values were generally higher than on the way up because the sUAS was passing through a column of its own disturbed air due to rotor wash (see Figure 4 in McKinney et al., 2019 for diagrams depicting the effects of rotor wash). The air sampled on the way down was pulled from a higher altitude relative to the sUAS compared to what was sampled while the sUAS was moving upward. Therefore, only ascent measurements are reported in the tables below.

Note that the altitude values reported are from the radiosonde GPS system, which has inherent uncertainty of up to several meters. During flights, altitude above ground level was monitored by the sUAS's own LiDAR rangefinder and internal GPS system, which more accurately determines the vertical distance above ground level to ensure that the sUAS stayed within the permitted boundaries for each site. However, those altitudes were recorded on a separate system from the science data and were therefore not used in the analysis.

The August 26 flight measured a difference of up to 15 ppb between 10 m AGL and the maximum altitude. That range varied from day to day. The gradient was often much shallower, such as in **Figure 77** and **Table 10**, and was absent on some days. Other days, however, showed a much larger gradient. The highest difference in ozone mixing ratios was measured on October 7. This flight is shown in **Figure 78** and **Table 11**.

For each flight, the iMet radiosonde collected temperature, humidity, and pressure data to complement the ozone data. An example from the October 7 flight is shown in **Figure 79**, where the gradient was present in more than just the ozone mixing ratios. Very similar patterns were observed in the relative humidity and temperature. The pressure was also recorded, though it showed a typical linear decrease from approximately 1020 mbar at the surface to 1006 mbar at 120 m, consistent with other flights throughout the campaign.

Flights at San Jacinto Battleground Park yielded patterns in ozone that were distinct from other locations. Rather than smooth increases and decreases in ozone, values were highly variable (see **Figure 80**). This was particularly true on days with Easterly winds coming across the Houston

Ship Channel. Localized titration of O_3 may be the cause of these variations. Adding NO_2 measurements to the payload may shed more light on these kinds of features in the future. Sulfur dioxide is another likely source of variance since it interferes with the ozone measurement in the cells of the ozonesondes. Battleground Park flights were typically carried out in the late morning to evening hours, and VOCs were also sampled on four of those days. The flight team also took advantage of the presence of the Mobile Air Quality Lab 2 (MAQL2) at the park and frequently compared ozone values. When conditions were relatively stable, values at low altitudes were typically within a few ppb of MAQL2.

During the final two weeks of September, sUAS operations overlapped with Colorado University (CU) Boulder and their fixed-wing sUAS, Raven. On September 29 and 30, the Aurelia hovered at heights of 50 m and 30 m towards the end of Raven's 1.5-hour flights in the hopes that data could be compared between the sUASs while they were sampling at similar altitudes within the same field (approximately 200–600 meters away). Comparisons of this data will be made at a later date after the Raven data is available.

Additionally, the UH sUAS flew in close proximity to Oklahoma University's sUAS Coptersonde on September 21. The Coptersonde was flown to an altitude of 609 m (2000 ft), then back down at speeds greater than the Aurelia, but the possibility of data comparison and future collaborations have been discussed.

The sUAS proved a valuable measurement platform for air quality and meteorology studies. Altitudes of up to 121 m could be easily reached, allowing the project team to collect data at heights typically only reachable using a tower or a weather balloon. Tower systems can cost hundreds of thousands of dollars and can only measure from one location. The sUAS, on the other hand, could be deployed at whichever site was most conducive to research efforts on that day, and the entire system was a fraction of the cost of a tower (approximately \$30,000 at the time of purchase in 2021). Weather balloons have similar mobility but cannot be controlled after launch and do not provide continuous measurements in the 0–121 m range as the sUAS can. Balloons usually rise at 5–6 m/s through this range, providing less than 30 s of data. Furthermore, most components of a weather balloon flight are one-time use, even if the payload is recovered after landing; a typical ozonesonde launch costs around \$1000. With the sUAS, there is no need to use resources such as helium, balloons, and parachutes. The radiosonde can be powered with the sUAS and used indefinitely, and the ozonesonde solutions can be refilled so that they can be reused many times over. The longest running sonde on the sUAS was used on eighteen flight days throughout August, September, and October.

The sUAS provided an opportunity to move through up to three photochemical model layers used to analyze TRACER-AQ observations. Models such as CAMx and WRF-GC utilize many vertical layers in additional to horizontal grid cells. The lowest layers of the CAMx model have tops at 34, 86, and 173 m, while WRF-GC has layers with tops at 31, 108, and 212 m. Most atmospheric measurements are made near the surface in the first layer, but the sUAS maximum height of 121

m allowed for repeated data collection in the second and third layers for both models at multiple locations.

During the TRACER-AQ-2 measurement intensive, certain conditions often coincided with strong ozone gradients. At the UH Coastal Center, the presence of early morning fog was an indicator that there would be a notable gradient. **Figure 81** and **Figure 82** show two examples of when this combination occurred. Gradients were also likely when the wind was carrying emissions from nearby traffic since vehicle emissions contain plenty of NO, which reacts with ozone near the surface to form NO₂. In the presence of sunlight, that NO₂ is later converted back to ozone, which along with vertical mixing and the development of a convective boundary layer explains much of the decrease in ozone gradient and a general increase in ozone as each day progresses.

Date	Location	Temperature, Humidity, Pressure	Ozone	VOCs	SO ₂
7/26	UH ERP	Х	Х		
8/15	UH Campus	Х	Х		
8/16	UH Campus	Х	Х		
8/23	UH Coastal Center	Х	Х		
8/26	UH Coastal Center	Х	Х		
8/31	UH Coastal Center	Х	Х		
9/1	UH Coastal Center	Х	Х		
9/2	UH Campus	Х	Х		
9/6	UH Campus	Х	Х		
9/8	UH Campus & UH Coastal Center	Х	Х		
9/9	San Jacinto Battleground Park	Х	Х		
9/10	San Jacinto Battleground Park	Х	Х	Х	
9/11	UH Coastal Center	Х	Х		
9/13	San Jacinto Battleground Park	Х	Х	Х	
9/14	San Jacinto Battleground Park	Х	Х	Х	
9/15	San Jacinto Battleground Park	Х	Х	Х	
9/20	San Jacinto Battleground Park	Х	Х		Х
9/21	UH Coastal Center	Х	Х		
9/23	San Jacinto Battleground Park	Х	Х		
9/26	UH Coastal Center	Х	Х		
9/27	UH Coastal Center	Х	Х		
9/28	UH Coastal Center	Х	Х		
9/29	UH Coastal Center	Х	Х		
9/30	UH Coastal Center	Х	Х		
10/7	UH Coastal Center	Х	Х		

Table 8: Date, location, and measurements made during each flight day of the 2022 campaign.



Figure 75: Graph showing the first three profiles of data collection on August 26 at the UH Coastal Center. These profiles provide an example of the strong vertical ozone gradient often present in the early mornings. Official sunrise occurred at 11:55 UTC.

Table 9: Ozone values for the first three profiles of the August 26, 2022 flight at UH Coastal Center where a strong vertical gradient was observed.

Time (UTC)	Altitude (m)	Ozone (ppb)	Time (UTC)	Altitude (m)	Ozone (ppb)
12:25	10	7.4	12:37	105	24.7
12:30	60	20.7	12:46	10	6.9
12:32	111	23.5	12:49	60	21.5
12:35	10	8.5	12:51	90	24.9
12:36	60	17.4	12:55	105	27.1



Figure 76: A time series showing ozone concentrations by color measured while the sUAS was connected to the power tether. For this flight, the sUAS stayed in the air for 2 hr 18 min.



Figure 77: *Graph of ozone mixing ratio data collected on September 28 at the UH Coastal Center. On this day there was a very shallow gradient with a range of only a few ppb. Sunrise occurred at 12:13 UTC.*

Table 10: Ozone values for the first four profiles of the September 28, 2022 flight at UH Coastal Center where a very weak vertical gradient was observed.

Time (UTC)	Altitude (m)	Ozone (ppb)	Time (UTC)	Altitude (m)	Ozone (ppb)
13:03	10	27.2	13:36	12	29.5
13:07	60	29.5	13:40	60	31.8
13:12	113	30.4	13:45	120	32.9
13:21	10	29.4	13:55	15	31.5
13:25	60	29.6	13:58	60	31.7
13:28	106	30.5	14:01	99	31.4



Figure 78: Graph showing the strong vertical ozone gradient often present in the early mornings. The gradient is reduced as the day progresses and the air becomes well mixed. The flights between 12:50 UTC and 15:15 UTC were powered by batteries to achieve altitudes up to 121 m. Later flights were restricted to 73 m due to the constraint of the 80 m power tether.

Table 11: Ozone values for the first four profiles of the October 7, 2022 flight at UH Coastal Center where a strong vertical gradient was observed.

Time (UTC)	Altitude (m)	Ozone (ppb)	Time (UTC)	Altitude (m)	Ozone (ppb)
12:55	10	9.8	13:54	14	14.7
12:57	60	24.8	13:58	60	23.2
13:00	120	54.8	14:03	120	57.6
13:16	14	8.6	14:12	12	27.2
13:24	60	20.9	14:28	60	32.5
13:28	120	56.6	14:33	120	42.1



Figure 79: Relative humidity (left) and temperature (right) data from the October 7 flight. These data were collected at the same time as the ozone data displayed in *Figure 78*. Trends in humidity and temperature are very similar to those seen in the ozone mixing ratio.



Figure 80: Ozone mixing ratios measured on September 14 at Battleground Park. Values were highly variable, most likely due to emissions coming across the Houston Ship Channel.



Figure 81: The sUAS flying at UH Coastal Center on August 26, 2022 at 07:30 CDT (12:30 UTC) with a surface fog layer (left). The ozone data from the same flight showing an ozone gradient of up to 20 ppb (right).



Figure 82: The sUAS flying at UH Coastal Center on October 7, 2022 at 08:12 CDT (13:12 UTC) with a surface fog layer (left). The ozone data from the same flight showing an ozone gradient of up to 50 ppb (right).

3.8 Task 10 - TRACER-AQ-2 Rapid Synthesis Report

The TRACER-AQ 2022 study observed air quality and meteorological parameters in the Houston-Galveston region during the summer of 2022. Over 70 ozone exceedances occurred at HGB area monitoring stations during this period. Here is a preliminary summary of notable findings.

- The mobile MAQL1 platform has regularly observed high alkene signals at Miller Cutoff and Independence Parkway in La Porte, and Bayway Drive between Baytown Ave and Bayvilla Drive in Baytown. Given that very high propene concentrations have also been observed at the HRM7 site throughout 2021 and 2022, there appear to be some large sources of propene and/or other alkenes in the eastern Ship Channel and Baytown areas. Since alkenes are HRVOCs, their presence in high concentrations indicates that rapid ozone formation remains a strong possibility in the HGB area.
- FluxSense measured recorded ethene and propene fluxes that were higher than the modeling emissions inventories (EI) used by the TCEQ. While the EI ethene fluxes were within the confidence intervals of the measurements, the EI propene fluxes were outside the confidence intervals at the low end, suggesting that actual propene fluxes are higher than those being modeled. This observation appears to be consistent with the MAQL1 and HRM7 observations.
- FluxSense measured large excursions in alkane fluxes that appear to be consistent with an emission event on September 26.

- The MAQL2 platform, which spent most of the field campaign on site at Battleground, observed SO₂ spikes on numerous occasions, usually accompanied by elevated NOx concentrations.
- Ozonesonde measurements during 2022 confirm the frequent presence of a temperature inversion at about 3 km altitude over the HGB area during much of the summer. The depth of the mixed layer under this inversion varies depending upon the synoptic scale factors, sometimes dropping as low as 1.5 km when strong subsidence is present. The mixed layer over the Gulf is consistently lower than over the land or over Galveston Bay.
- Ozone and NO_X measurements by boats over Galveston Bay and the Gulf of Mexico have detected elevated ozone concentrations present over the bodies of water. Of particular interest is the high ozone observed in the Gulf near the areas where large vessels congregate offshore. There is some evidence that these high ozone concentrations can move ashore, generally affecting monitoring sites near the coast.
- Drone flights can effectively quantify ozone variations within the lowest ~150 m of the atmosphere. Some days have especially strong ozone gradients within these lowest layers.

The findings in the RSS are preliminary, however, and may change as further analyses are carried out, data are quality checked, and intercomparison among measurements are refined. More complete analyses will be done in the follow-up TRACER-AQ2 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, 2023. A link to the report can be found below:

https://hoth.geosc.uh.edu:5001/sharing/RU5259oTW

3.9 Task 11 - FluxSense Mobile Laboratory Monitoring

FluxSense (Inc. and AB) and in cooperation with Chalmers University, has conducted emission measurement campaigns for VOCs, HRVOCs, SO_X, NO_x, in Houston since 2006 (Johansson et al. 2014, Mellqvist et al. 2010, Rivera et al. 2010) and formaldehyde since 2009. During TRACER-AQ2, an advanced mobile air pollution measurement lab equipped with four optical instruments for gas monitoring: SOF (Solar Occultation Flux), SkyDOAS (Differential Optical Absorption Spectroscopy), MeFTIR (Mobile extractive Fourier Transformed Infrared spectrometer) and MeDOAS (Mobile extractive White cell DOAS) was employed. Measurements were conducted from 2–28 September 2022. A total of 20 measurement days were logged out of 26 days where personnel and instrumentation were in place. Extractive measurements within the HSC area including Channelview, Mont Belvieu and Bayport are shown in Figure 83 for alkanes and toluene. Full details on the background, measurement conditions, instrumentation, quality assurance and control, as well as measurement results can be found in the measurement report previously submitted to TCEO. link to the report can be found А at https://hoth.geosc.uh.edu:5001/sharing/7kzBN762v



Figure 83: Extractive measurements made by MeFTIR and MeDOAS showing alkane and toluenece concentrations (enhancement above background in $\mu g/m^3$). Apparent heights of the curves in the overlay are 1 m/µg m⁻³ for alkanes and 6 m / µg m⁻³ for toluene. Max alkane height is clipped to 1000 m (1000 µg m⁻³)

Conclusions

This project was one of 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, St. Edward's, Virginia Tech, and FluxSense this project was a huge success.

The sUAS is a versatile and economical mobile platform for atmospheric measurements. It collected over 44 hours of in-flight data across 25 flight days during the 2022 TRACER-AQ-2 campaign. Measurements included ozone, temperature, humidity, pressure, VOCs, and SO₂, and the sUAS can carry additional sensors for future work. It was instrumental in observing the early morning ozone gradient and the changes in ozone, temperature, humidity, and pressure as the air became well mixed. Future work could delve more deeply into these ozone gradients and may include some evening or night flying when the gradients reappear. Currently, experiments to test stability of the sUAS with an inlet that extends farther up from the top of the vehicle are planned in an effort to sample air less affected by rotor wash.

The UH sUAS was restricted by regulation to a maximum height of 121 m, but it is physically capable of altitudes well beyond that. The OU and CU Boulder sUAS teams were both authorized for up to 609 m, and with a Certificate of Waiver or Authorization (COA), the UH sUAS may be able to achieve the same. Due to the wait time involved in receiving a COA, it was not possible for 2022 operations. However, a COA can be requested from the FAA several months in advance of future operations to expand the capabilities of this platform.

Another improvement to operations that would be especially helpful if a COA is obtained is an Automatic Dependent Surveillance-Broadcast (ADS-B) receiver. The ADS-B is a device that broadcasts an aircraft's identification number, location, speed, and altitude to other aircraft and ground control stations. The Aurelia X6 Pro is equipped with such a device, as are other sUAS that fall into the same regulatory category. Presently, the UH sUAS team can use apps and websites like FlightAware and adsbexchange.com to see some air traffic, but as these rely on data submitted by people with their ADS-B receivers, not all aircraft show up on these tools. With a simple Raspberry Pi system, the team could set up an ADS-B receiver and enhance situational awareness and safety during UH operations in high traffic areas or at higher altitudes.

The versatility and maneuverability of unmanned aerial vehicles offer significant advantages over other platforms, and further payload improvements will enhance the value of the sUAS as an atmospheric measurement platform. Development of the NO₂ and further refinement of the SO₂ sondes will allow for a greater understanding of the ozone data and its relationship to local conditions. These would be especially useful at locations like Battleground Park, where local emissions dramatically affect measurements. If O_3 , NO₂, and SO₂ were to be measured simultaneously it can be more easily determined when variations in ozone concentrations are caused by NO_x titration or SO₂ interference versus other possible influences. Measuring these

compounds and other pollutants such as VOCs alongside ozone would provide a much more complete picture of what is happening in the atmosphere.

The mobile lab measurements programs were also a strong success, demonstrating the utility of using them both as a portable lab such as the Baylor MAQL2, which was able to set up quickly at Battleground after having been moved around Houston several times in the months prior during the TRACER-MAP study, and in the mobile mode as was the primary focus of the UH MAQL1 which was able to conduct emissions surveys as well as urban plume evolution studies. Going forward, a third mobile laboratory will be added to the resources available to this research group. This new, larger mobile lab (MAQL3) can carry the same instrumentation as the other two while still providing ample room for guest researchers and new collaborators. The first deployment of this new mobile lab took place in June 2023 to the NASA SARP program where much was learned both scientifically as well as how to utilize the truck. Lessons learned from this deployment will be applied to the upcoming 2023 mobile measurement campaign for TCEQ. Although this new mobile lab marks a significant increase in group capabilities, the existing mobile laboratories will continue to be available for use. Future work could include adding MAQL1 or MAQL2 to more routine operations such as the HNET program where a mobile lab could be stationed at an RV park or other similar venue to fill potential gaps in the current monitoring network yet still be available for special studies such as during high ozone episodes or unusual pollution or weather events. The use of a mobile lab such as this could be complimentary to the existing TCEQ mobile labs which are more focused on emissions and events rather than photochemistry.

The boat based measurements yet again proved themselves to be valuable by providing an economical and viable method of collecting a unique set of data over the water. The two commercial boat sampling systems conducted 344 separate trips along the Houston Ship Channel and into the Gulf of Mexico. In addition to transitioning these observations into a more "operational" program by incorporating them into the HNET program, the program could have the suite of measurements expanded to include aerosols. The 2023 mobile and offshore research program will incorporate a Printable Optical article Spectrometer (POPS) on MAQL3 and the new UH research boat. The results from these small, lightweight, and power efficient sensors could be packaged along with other appropriate aerosol samplers to complement the existing $O_3/Ox/meteorology$ sampling systems. These could add valuable information about overwater conditions in times of international transport such as smoke from biomass burning and Saharan dust.

The UH pontoon boat performed well for two consecutive years and will continue to be a valuable asset to the research group. Similar to the new mobile lab, a larger research boat has been purchased and will be deployed for the first time during the 2023 mobile and offshore research project sponsored by the TCEQ. This larger boat will carry a much more complete payload for studies of primary and secondary pollutants in and around the Texas Gulf Coast. Of particular interest, this will provide a much more economical way of reaching source regions like the

lightering and anchoring areas along the coast. Although the Red Eagle was available for charter, budget limitations prevented the boat from being chartered for extended periods or as frequently as may have been desired. The reduced operating cost, increased payload, and higher availability of the new boat will provide many opportunities to study the offshore emissions that reach the Texas Gulf Coast. In particular, establishing baseline conditions which can be compared to future scenarios are key to determining what impacts may occur from the proposed offshore terminals for petroleum products and container platforms that are being proposed in Texas' waters. Additional state and federal activities in the Gulf such as offshore wind, carbon capture and sequestration, and critical minerals mining activities will all increase vessel traffic as well as the emissions that accompany the increase in traffic. The coming years are likely the best opportunity to characterize the baseline conditions prior to these activities ramping up.

An additional offshore study which could be conducted would be to partner with Ramboll to evaluate the mobile emissions estimates which are generated using vessel specifications coupled with Automated Information Systems. The pontoon demonstrated that through careful positioning it is possible to sample emissions from individual ships within Galveston Bay. The new more fully equipped research boat can be operated in a way to sample specific ships and the measurement data compared to the emissions estimates as a way to validate and improve the emission inventory.

Finally, the payload and performance of the new research boat makes it a more useful platform to conduct sampling missions within the Houston Ship Channel itself. Prior communications with local law enforcement indicated that they would be willing to coordinate and collaborate with the research teams to provide access to the Houston Ship Channel for environmental monitoring purposes.

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