

Quality Assurance Project Plan

Project Title: “Quantifying the Emissions and Spatial/Temporal Distributions of Consumer Volatile Chemical Products (VCPs) in the Greater Houston Area”

Project Leader: Yue Zhang (Texas A&M University, TAMU)

Unfunded Collaborator: Qi Ying (TAMU)

RFA Name & Number: AQRP 22-23 Proposal Call

Grant Number: AQRP 22-020

Texas A&M University (TAMU)

2022.09

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the Quantifying the Emissions and Spatial/Temporal Distributions of Consumer Volatile Chemical Products (VCPs) in the Greater Houston Area project. The Principal Investigator for the project is Yue Zhang (and Co-PI is Qi Ying).

Electronic Approvals:

This QAPP was approved electronically on 09/02/2022 by Elena McDonald-Buller, The University of Texas at Austin.

Elena McDonald-Buller

Project Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 09/02/2022 by Vincent Torres, The University of Texas at Austin.

Vincent Torres

Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 09/13/2022 by Bipin Sharma, Texas Commission on Environmental Quality.

Bipin Sharma

Project Liaison, Texas Commission on Environmental Quality

QAPP REQUIREMENTS FOR THIS PROJECT

1. PROJECT DESCRIPTION AND OBJECTIVES

1.1. Problem Definition/Background

Air pollution is the fifth largest cause of death in the world.¹ Volatile organic compounds (VOCs) can also undergo chemical reactions with atmospheric oxidants to form major atmospheric pollutants, such as photochemical ozone (O₃) and particulate matter (PM).^{2, 3} Traditionally, a significant portion of the VOCs from the urban environment comes from traffic and tailpipe emissions, power plants, and residential combustion.⁴ During the past few decades, as VOC emission reduction strategies have been successfully implemented, traffic related VOC emissions have decreased rapidly, leading to an increase of the relative contribution of other types of VOCs.⁵ With this changing emission profile of carbonaceous compounds in urban areas, volatile chemical products (VCPs) have become one of the most significant sources of anthropogenic VOCs.^{4, 6, 7}

As the fourth largest city in the US, with more than 7 million people in the surrounding areas, Houston has no reported ambient measurements of the VCP to our knowledge, highlighting the urgent need to measure VCP emissions and update the VCP emission inventory in the Greater Houston Area validated by ambient measurements with detailed spatial and temporal resolution. The recent VCPy emission inventory also shows higher than expected VCP emissions in the Greater Houston Area,⁴ further demonstrating the need to use real-world measurements to constrain the uncertainties in model parameterization. An improved understanding of VCPs in the Houston area may also improve predictions of O₃ concentration in the Greater Houston Area, bridging the gap between modeled and measured O₃ concentration.

1.2. Project/Task Description

Based on the research gap listed above, our primary hypothesis is that the VCPs in the Greater Houston Area account for a significant portion of the total VOC emission and have important implications on the regional ozone concentrations that were previously not captured by the emission inventory and models. To address this hypothesis, our primary goal is to use existing field measurement data to provide temporal, spatial, and seasonal information of the VCPs in the Greater Houston Area and use a high spatial resolution regional chemical transport model with a detailed photochemical mechanism to further improve the VCP emission inventory and understand the impacts of VCP on air quality, including ozone.

To address our overarching study hypothesis above, we have 3 specific project objectives (tasks):

Objective (Task) 1: conduct field measurements of a broad range of VOCs, including oxygenated VOCs and monoterpenes, in the Greater Houston area using the Vocus Chemical Ionization Time-of-Flight Mass Spectrometer (Vocus CI-MS) on a mobile platform. In October-November, the PI will use the TRAM van to circle around Houston for 10-15 days to capture VCP emission patterns. In January-February 2023, the PI's team will again sample VCP emission patterns using the mobile platform in the winter.

Objective (Task) 2: characterize seasonal difference of VCP concentrations in Houston. To understand the seasonal differences of VCP emissions, we will analyze the VCP emission data collected from the Texas A&M Measurement van that cover both VCP emission profiles of the

Houston Area at different seasons. The data collected from these two time periods will be analyzed to compare the VCP composition, concentration, and spatial distributions to understand the differences of VCPs in the ambient environment between seasons in a metapolitical areas.

Objective (Task) 3: improve understandings of how VCP affect air quality in the Houston, including MDA8 O₃. In this study, emissions of major primary VOCs from different sources, including the oVOCs and explicit monoterpenes, will be tracked using different model species. By this approach, the contributions of VCPs to the ambient VOC concentrations can be directly determined.

2. ORGANIZATION AND RESPONSIBILITIES

2.1 Project Personnel

This research project involves researchers from the Texas A&M University (TAMU). TAMU is the lead institution on this project. The Lead PI for this project is Dr. Yue Zhang from TAMU, with Dr. Qi Ying as the unfunded collaborator from TAMU. Dr. Zhang will serve as the primary decision makers for this project, but will do so in close consultation with our unfunded collaborator Dr. Qi Ying (TAMU). The Lead PI and unfunded collaborator are responsible for implementation of this project.

Dr. Zhang will ensure the implementation of all specified QA/QC procedures with the assistance of Dr. Ying. They will oversee the performance of all laboratory and field analyses in accordance with standard methods and standard operating procedures (SOPs), the regular calibration of all laboratory instruments and equipment, and the documentation and reporting of all laboratory and field activities. He will ensure complete documentation of all SOPs and ensure all SOPs are available along with results in resulting publications. Dr. Zhang will also oversee the completion and implementation of the HR-ToF-CIMS, SP-HR-ToF-AMS and OFR QA/QC protocols in all objectives, including calibrations and data analysis.

2.2 Schedule

This project brings together two teams from the field of experimentalist/measurement (Zhang) with atmospheric chemistry modeling (Ying) to jointly understand an increasingly important group of species, VCP, their emission inventory, and their atmospheric implications. Monthly meetings will be held to discuss progress/plans for ongoing and future work related to our project objectives and milestones, as outlined in our proposed timeline for meeting these objectives shown in Table 1. Full-day virtual meetings will be held once every 3 months to discuss results and outline potential publications. We expect to deliver (1) spatial and temporal distributions of VCPs in the Houston area; (2) characterize seasonal difference of VCP concentrations in Houston; (3) impacts of VCP on local air quality such as ozone; and (4) 2-3 publications related to the project objectives described above.

Table 1. Timetable and Milestones of Proposed Work

Tasks	Year 1											
	Sept	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug
Task 1: Mobile Lab Field Deployment												
Deployment Preparation												
Urban VCP Measurement												
Laboratory Calibration and Quantification												
Data Analysis												
Task 2: VCP Season Difference												
Measurement Analysis												
Inventory Improvement												
Task 3: The Impacts of VCP on Urban Air Quality												
Effects of VCP on Ozone												
Sensitivity Analysis												
Publications												

3. SCIENTIFIC APPROACH

3.1 Experimental Design

Specifically, Texas A&M University Rapid Measurements Van (TRAM van) will be deployed to measure the urban climate and atmospheric composition across the Greater Houston Area (GHA). The TRAM van includes a Vocus 2R Chemical Ionization Mass Spectrometer (Vocus 2R CI-MS) and Vocus Inlet for Aerosols (VIA). We will follow prior studies which has already demonstrated that Vocus 2R CI-MS and VIA are capable of providing a comprehensive chemical characterization of atmospheric VCPs.^{7, 8} In addition, other atmospheric relevant parameters, including the temperature, relative humidity, aerosol mass loading, and O₃, will also be recorded by the meteorological station and a Soot Particle Aerosol Mass Spectrometer (SP-AMS).

During TRACER campaign and this project, the TAMU mobile lab will drive from the upwind direction of Houston to the downwind direction for the whole 4 month-time of the summer. Typically, the mobile van will start sampling from the northwest part of Houston, driving across the downtown area, and then reach the southeast part of Houston by early afternoon, then returning to the northern part of Houston by early evening (blue line in Figure 2), based on the pre-defined TRACER deployment plan. In October-November, the PI will use the TRAM van to circle around Houston based on the blue- and green-shaded routes in Figure 2 for an additional 10-15 days to capture additional VCP emission patterns. In January-February 2023, the PI's team will again sample VCP emission patterns using the mobile platform.

3.2 Process Measurements and Target

Table 2 shows the process measurements and the specific targets for each sample we plan to achieve for this project.

Table 2. Geographic Location of Tasks & Measurements (Work) Targets

Objective (Task) #	Geographic Locations	Measurement Targets by Texas A&M Team
1 - Detection and Calibration of VCP Standards	College Station, TX (Texas A&M)	i.) Ammonium (NH ₄ ⁺), nitrosonium (NO ⁺) and hydronium (H ₃ O ⁺) reagent ions for detection and calibration of gas- and particle-phase VCP standards measured by the Texas A&M VIA-HR-ToF-CIMS ii.) Particle-phase measurements of low-volatility

		VCP standards by Texas A&M SP-HR-ToF-AMS
2 - Mobile Lab Deployment of Newly Developed HR-ToF-CIMS Methods w/ SP-HR- ToF-AMS	Houston, TX	i.) Sample at different locations of Houston using the Texas A&M VIA/HR-ToF-CIMS method on the Texas A&M mobile platform ii.) Collect GPS and weather data iii.) Collect real-time ambient aerosol sizing data using a nano-SMPS (TSI, Inc.) and SEMS (BMI, Inc.) iv.) Obtain 10-15 days of data for each deployment

3.3 General Approach and Test Conditions

The calibration and field measurement work will be performed based on previous studies that detect two hundred major VCP species.^{7, 8} The Vocus, VIA, and SP-AMS will be analyzed at the same time under ambient pressure and 10-30 °C ambient testing conditions.

4. SAMPLING PROCEDURES

4.1 Site-specific sampling procedures

During this project, the TAMU mobile lab will drive from the upwind direction of Houston to the downwind direction for the whole 4 month-time of the summer. Typically, the mobile van will start sampling from the northwest part of Houston, driving across the downtown area, and then reach the southeast part of Houston by early afternoon, then returning to the northern part of Houston by early evening (blue line in Figure 1), based on the pre-defined TRACER deployment plan. In October-November, the PI will use the TRAM van to circle around Houston based on the blue- and green-shaded routes in Figure 2 for an additional 10-15 days to capture additional VCP emission patterns. In January-February 2023, the PI's team will again sample VCP emission patterns using the mobile platform based on the blue and green-shaded routes in Figure 1 below.

4.2 Sample Instruments and Procedure

Vocus CIMS instruments: The Vocus CIMS ionizes the gaseous analyte via gas-phase ion-molecule reactions. In this study, we will use 5 ionization schemes as described in Table 1 where the VCP will react with the ions through the ion-molecule reactions. The Vocus uses a quadrupole RF field in the reactor to collimate ions onto the central axis and improve the detection limit, while maintaining similar collision conditions for conventional drift tubes in the meantime. The reagent-ion source consists of two conical surfaces between which a plasma is produced.

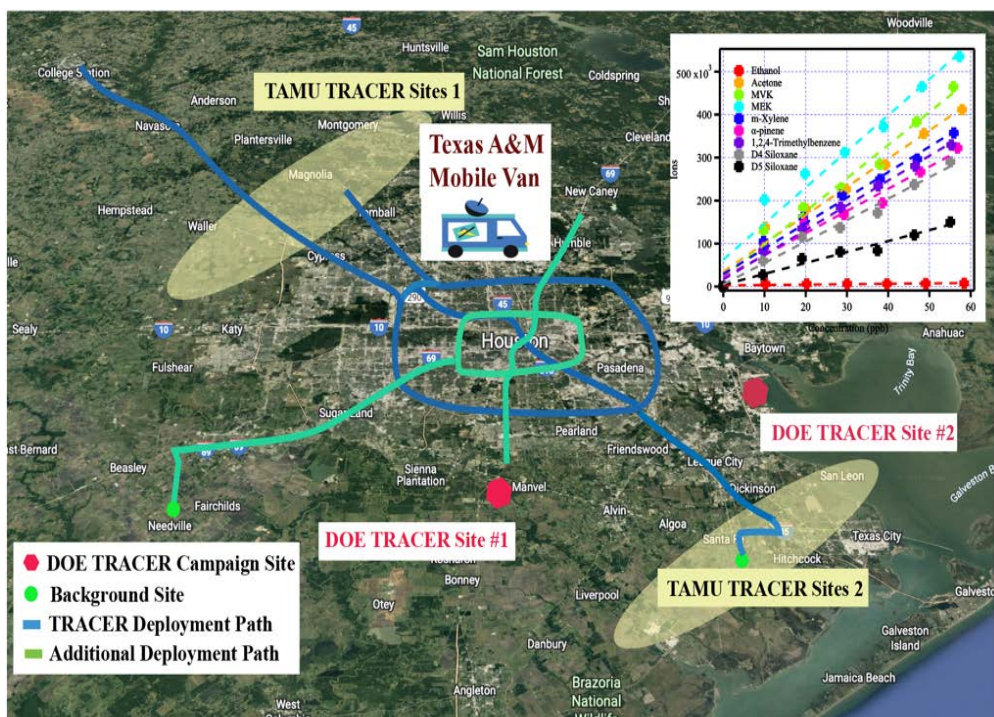


Figure 1. Field deployment map of the Texas A&M Mobile Van. The blue line represents the deployment route during the TRACER campaign. The green line represents the additional deployment path immediately after TRACER, to further capture VCP emissions. The green solid dots are background sites where there is limited VCP emission compared with urban areas. The van will sample at two background sites for each deployment. Inset is the preliminary calibration data of VCPs using Vocus 2R CI-MS.

The corresponding vapor will enter the focusing ion-molecule reactor (FIMR). The discharged current is regulated to be 1.5 – 2.0 mA. The sampling air will enter the FIMR with a pressure of 1 mbar, which is controlled by a valve between the reactor and a mechanical pump. The FIMR consists of a 10 cm glass tube and a homogeneous electric field will be generated. At the end of the FIMR, the adduct ions are sampled into a time-of-flight mass spectrometer for detection. The ions from FIMR first enter a big segmented quadrupole (BSQ) region to focus the ion beam, and then enter the primary beam (PB) region, and finally the ToF chamber. The BSQ acts as a high-pass band filter that ions smaller than specific mass-to-charge ratio (m/z) determined by the voltage setting will be detected at a much lower efficiency. Such setting could help prevent the degradation of the microchannel plate detector due to the very high reagent ion intensities.

For VIA-Vocus, a Vocus-Inlet-for-Aerosols will be added at the front of the Vocus-HR-ToF-CIMS. The VIA is an add-on for Vocus that could expand its capabilities to particle phase with ng/m^3 detection limits. An active charcoal denuder at the front of the VIA will remove the VOCs in the sampling air, and the VIA will be heated up to 230 °C to evaporate the particle phase species for Vocus detection. To reduce the potential aerosols accumulation in the VIA and maintain a good intensity in the meantime, a 3 liter per minute flow rate and a $10 \mu\text{g}/\text{m}^3$ aerosol loading could be adapted. Organic species with different volatility will be analyzed;

SP-HR-ToF-AMS: The AMS consists of three main sections, including the aerosol sampling chamber, particle sizing chamber, and particle composition detector chamber. In the aerosol

sampling chamber, the AMS has an aerodynamic lens coupled with the vacuum that will focus the aerosol into a narrow beam from the atmospheric air samples. The narrow beam is approximately 1 mm in diameter and particle transmission efficiency to the detector of nearly 100% for the particle size range of 70 to 500 nm. The focused beam exiting the sampling chamber is directed to the particle sizing chamber. The particle sizing chamber is maintained at approximately 10^5 torr by a 550 L/s turbo pump. The particles are directed in this chamber through a skimmer cone and the aerosol beam is modulated in this chamber by a rotating wheel chopper. The aerodynamic diameter is obtained from particle velocity, which is given by time-resolved detection of particles coupled with known flight distance. Particles with different sizes will travel at different speeds after the chopper and are focused into the detection chamber. The particle detection chamber is isolated from the sizing chamber by an aperture with 4 mm diameter. A molecular turbo pump is used to pump this chamber differentially at 250 L/s. A diaphragm pump operating at inlet pressure of 1.2 torr and 60 L/min is used to back the turbo pump of the particle detection chamber. The particles are directed to a resistively heated close end tube, where semivolatile/volatile constituents in the particle vaporize at 600 °C. The vaporized gasses are then ionized with an electron beam of 70 eV using the electron impact ionization method. After the ionization, the ion fragments will be analyzed using a quadrupole mass analyzer. The instrument is connected to the computer system for data acquisition which processes the data in real time.

The AMS data obtained from the experiment will be analyzed using the data analysis software IGOR. The file in .h5 format is imported into the software for the analysis. First the m/z calibration is done for the selected run followed by the baseline correction of the peak. This is followed by pre-processing the data. After pre-processing, peak shape corrections are done to get a gaussian fit. This process is unit mass resolution (UMR) analysis and prepares raw spectra for HR analysis. UMR processing is followed by high resolution (HR) fit. For HR fitting the peak shape is corrected again to get HR gaussian fit. This process is called HR fit preparation. After this, the HR fit for a selected run number is done by selecting the appropriate ions for each m/z value, generally up to m/z 200. This is followed by HR-MS calculation.

4.3 Sample Information

Table 3 below shows the sample collected from each instrument. We expect to collect 10-15 days of samples during each deployment.

Table 3: Examples of instruments, data, and inferences

Instrument	Parameter	Inferences and Caveats
SP-HR-ToF-AMS	peak area	VCP-derived Particle mass loading. The quantification of the VCP mass loading can be used to understand how much VCP can be oxidized in the atmosphere to form aerosols.
HR-ToF-Vocus CIMS Instruments	peak area	VCP concentration. The quantification of VCP can be used to calculate VCP emissions and chemical transformations in the atmosphere.

4.4 Sample Preservation

We use online analysis so there is no need for sample preservation.

4.5 Sample Numbering

We will number the sample based on date and time, with the collector's initials. For instance, for samples collected on Nov. 8, 2022 at 3 pm, will be named as: 20221108_1500_YZ.

4.6 Sample Packing and Shipping

We use online analysis so there is no sample packing and shipping.

5. MEASUREMENT PROCEDURES

HR-ToF-Vocus CIMS instruments: Vocus CIMS instruments will mainly sample either gas-phase or particle-phase VCP. For gas-phase VCP standards, they will be diluted with nitrogen gas to the desirable level and then injected into the Vocus using PTFE tubing. For particle-phase VCP, similar to the AMS measurements described above, a stainless-steel tubing or conductive tubing will be used to minimize particle losses. Flow rate can be monitored either by a flow meter or the inlet pressure of the Vocus CIMS instruments.

SP-HR-ToF-AMS: AMS will mainly sample particle-phase VCP-containing aerosols in real time. The aerosol samples will be directed to AMS using either stainless-steel tubing or conductive tubing to minimize particle loss. A flow meter will be used to measure the inline flow to AMS to ensure the flow rate is between 1-2 LPM to reduce particle loss in the tubing. All AMS measurements will be recorded in lab notebooks during each lab experiment with VCP standards and during field measurements.

6. QUALITY METRICS (QA/QC CHECKS)

6.1 QC Check for each method

SP-HR-ToF-AMS: The quality control of AMS data will include the following steps. Firstly, before the operation, calibration procedures will be performed. The detailed calibration methods are described in section B7. Briefly, IE calibration will be performed at an interval of two weeks. Flow rate calibration will be performed along with the IE calibration every two week. Particle time of calibration will be performed if the instrument is moved to a new measurement site, the chopper wheel is perturbed or if there is a shift in vaporizer. Secondly, during the operation, m/z calibration will be performed once daily before starting the analysis. Thirdly, after the experiments, the data will be imported into the PIKA Igor analysis software, where the flow rate and all voltages of the instrument during the operational period will be examined. We will identify any bad data points based on these benchmark values and remove them from the analysis software.

HR-ToF-Vocus CIMS Instruments: The quality control of Vocus CIMS data will include the following steps. Firstly, before the sampling, the calibration procedure as described in section B7 will be performed weekly under laboratory conditions. Secondly, prior to daily sampling, while the Vocus is sampling ambient air, the obtained mass spectrum should have specific ions as the highest. Under the PTR mode, the highest ions would be m/z 55 ($(\text{H}_2\text{O})_2\text{H}_3\text{O}^+$), m/z 59 ($\text{C}_3\text{H}_7\text{O}^+$),

m/z 37 ((H₂O)H₃O⁺), and m/z 73 ((H₂O)₃H₃O⁺). With NH₄⁺ mode, the highest ions would be m/z 76 ((C₃H₆O)NH₄⁺), m/z 36 ((H₂O)NH₄⁺), m/z 35 ((NH₃)NH₄⁺), and m/z 54 ((H₂O)₂NH₄⁺). Thirdly, after the experiments, the data analysis of Vocus will be performed using the Tofware package (version 3.2.3) running in the Igor Pro. The status of the instrument will be examined during the data processing, and any bad data points based on the benchmark values will be removed from the data set.

6.2 Additional QA Objectives

For this project, we will also perform the additional calibration to ensure the data pass the QA objectives. The calibration procedures are:

AMS: IE calibration. The atomizer is used to generate the aerosols of ammonium sulfate/nitrate which is followed by the diffusion dryer. The aerosols generated are made monodisperse by passing them through differential mobility analyzer (DMA). After this the fraction of aerosols is sampled by the AMS and condensation particle counter (CPC). The aerosols are analyzed at a minimum of five concentrations. The aerosol concentration is controlled by the dilution system installed before the AMS and the CPC. This method is used to calibrate the particle size dependent TOF measurement, so as to determine the particle collection or particle detection efficiency of the AMS. The IE calibration will be carried out every two weeks. The acquired data will be analyzed using IGOR software to generate calibration curves.

M/z calibration of the instrument will be carried out once daily before the start of the sample analysis. The m/z calibration is done automatically by the data acquisition software when sampling. Generally, the ion peaks by N₂, O₂ and W are used for the m/z calibration. The N₂ peak is the largest peak at m/z 28 followed by the O₂ peak at m/z 32. Opposed to the ambient ion peak of N₂ and O₂, W ion peak at m/z 184 is caused by the heating material in the instrument. It is included to ensure validity for higher m/z values. From the m/z calibration panel of the software we can also follow peak properties like peak shape, peak intensity and peak position.

Particle time of flight calibration of the instrument is done by using polystyrene latex spheres. This calibration is done only if the instrument is moved to a new measurement site (such as from laboratory to field campaign), if the chopper wheel is perturbed or there is a shift in position of the vaporizer. In the calibration procedure the PSL spheres of diameter generally in the range of 50 nm to 1000 nm are atomized and are passed through a diffusion dryer. The particles are monodispersed using DMA prior to AMS sampling and are sampled one diameter at a time. The instrument is run in the PTOF mode and the acquired data is analyzed using IGOR software.

Flow rate calibration can be performed at the same interval as for IE calibration. The sample flow rate is measured by the AMS instrument with a pressure meter situated near to the exit of the aerodynamic lens. The instrument translates the output voltage of this pressure meter linearly into the flow rate. The linear relationship between output voltage and flow rate is utilized to carry out the calibration. The flow is controlled by the needle valve by setting the valve. The flow measured using Gillibrator is noted down along with the corresponding voltage.

HR-ToF-Vocus CIMS instruemnts: The Vocus CIMS ionization efficiency calibration will be done weekly for lab experiments and per 3 hours during the field campaign with a calibration gas

cylinder including ethanol, acetonitrile, acetone, acrylonitrile, isoprene, methyl vinyl ketone, methyl ethyl ketone, benzene, m-xylene, α -pinene, 1,2,4-trimethylbenzene, octamethylcyclotetrasiloxane, decamethylcyclopentasiloxane, and β -caryophyllene. The calibration gases are around 1000 ppb in the cylinder and will be diluted into VOC-free air produced by a zero-air generator to around 10 ppb. The diluted calibrants will be measured by the Vocus CIMS, and the sensitivity factor for each compound will be derived with the unit cps (count per second)/ppb.

7. DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

7.1 Data Reporting Requirements

The combined data from the mobile van facility, the Vocus 2R CI-MS, VIA, and other mobile van measurements, including AMS, will provide crucial key information in understanding the spatial and temporal variabilities of the VCP and their oxidation products in the Greater Houston Area. We will average the species-specific data based on each day and each season for the final report. The raw data can also be requested from the PI.

7.2 Data Validation

AMS: Data will be analyzed and reviewed using IGOR. The description of IGOR data analysis is discussed before in the section B4. The software has two inbuilt checkpoints to identify any deviation within any of the runs during the experiment. First check happens while correcting the baseline of the peak in UMR data processing. The second check happens during the correction step which is done after pre-process in UMR. If the software gives a negative value during the correction step, then the corresponding run number for that point can be found and blacklisted from the data analysis. IGOR also helps to identify if background ions like N_2 and CO at m/z 28 and m/z 44 respectively are selected during the ion selection while carrying out the HR fit of the mass spectra. All these internal checks by the data analysis software helps to review, verify and validate the data obtained from the experiment. To further verify and validate the data collected from the AMS, the results will be cross compared with the data acquired using GC-MS, LC-MS, SMPS, and Vocus.

Vocus:

Data cleaning will be performed in order to remove all the potential contaminated field data. For instance, when the instrument status is fluctuating due to the mobile lab vibration, environment temperature change, etc.

Regarding the VCP standards, their Vocus CIMS ionization efficiency calibration factors (in cps/ppbv), and detection limits (in pptv) would be compared with previous literature. The field data will be quantified with the VCP standards calibration results obtained during the laboratory experiments. The HR-ToF-CIMS Vocus instruments will be calibrated every three hours during the field campaign. For the VCP compounds we do not have a standard, they could be quantified according to their chemical composition (i.e., their proton-transfer rate coefficient) and the ionization efficiency calibration results based on known compounds.

In addition, we will use the calibration procedures described above to provide acceptance criteria for data validation, as shown below in Table 4.

Table 4: Example data validation checks for instruments and sampling

Instruments	QC Check	Frequency	Data Summary	Data Validation Acceptance Criteria	Action if values are unacceptable
SP-HR-ToF-AMS	Mass calibration using aerosol standards such as ammonium sulfate particles	Before each session	plot linear regression	linear response, $r^2 > 0.95$	repeat calibration or perform maintenance
VOCUS CIMS Instruments	Mass to charge calibration and VCP mass calibration using VCP standards	Before each session	plot linear regression	linear response, $r^2 > 0.95$	repeat calibration or perform maintenance

As shown in Table 5 below, the parameters we expect to measure are shown, including units, expected range, accuracy, and precision. VCP measurements from lab- or field-based samples will be validated by comparison to authentic standards (when available). Since the purpose of this project is to develop new real-time HR-ToF-Vocus CIMS instruments for measuring both gas- and particle-phase VCP, we will compare these quantitative measurements with more established methods that have been used to measure VCP;. We will also quantify VCP from samples using authentic VCP and correct for losses using mass-labelled internal VCP standards.

Table 5: Examples of Measurement Quality Criteria

Parameter	Units	Expected Range ¹	Accuracy (%)	Precision (%)	Complete (%)
VCP Conc.	ppt	0.1-300	+/-100	+/-50	80
OA aerosol mass loadings	$\mu\text{g}/\text{m}^3$	1-100	+/-10	+/-10	90

7.3 Data Summary

Any collected data will be analyzed within the first six months of acquisition. For SP-HR-ToF-AMS and HR-ToF-Vocus CIMS instruments, the teams will use Aerodyne-developed data analysis software to analyze the raw mass spectrometry data, and then plot the analyzed results in Igor Pro software.

When presenting the data, a master table will all the VCPs and their daily concentrations as well as their seasonal concentrations will be reported. In addition, the standard error of these

concentrations will be reported as well.

7.4 Data Storage

Data acquired will be saved on the hard drive during the experiments and backed up to the MS cloud service as well as a redundant hard-drive by A&M teams every week by working with the IT offices of both universities. For AMS and Vocus, there are specific Aerodyne-developed Igor-based software to acquire the data collected through the instruments and it is rare to encounter collection errors. If there are collection errors, the teams from TAMU will repeat the experiments to generate the data again.

8. REPORTING

8.1 Deliverables

The deliverables of this project include: (1) provide the VCP concentrations from the Greater Houston areas during two field deployments; (2) provide seasonal differences of VCP concentrations in the Greater Houston Areas; (3) estimate the contribution of ozone from the VCP in the Greater Houston areas; (4) mentor 2 graduate students through this project and foster collaborations between Texas A&M, AQRP, UH, and UT Austin.

Monthly report and quarterly report will also be submitted to AQRP. The deliverables are listed below.

Abstract

At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities and will be written for a non-technical audience.

Due Date: Ten (10) business day after notice of intent to fund

Quarterly Reports

The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 3 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	August, September, October 2022	October 31, 2022
Quarterly Report #2	November, December 2022, January 2023	January 31, 2023
Quarterly Report #3	February, March, April 2023	April 30, 2023
Quarterly Report #4	May, June, July 2023	July 31, 2023

DUE TO PROJECT MANAGER

Monthly Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the [Monthly Technical Report](#) Template.

Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start - August 31, 2022	September 10, 2022
Technical Report #2	September 1 - 30, 2022	October 10, 2022
Technical Report #3	October 1 - 31, 2022	November 10, 2022
Technical Report #4	November 1 - 30, 2022	December 10, 2022
Technical Report #5	December 1 - 31, 2022	January 10, 2023
Technical Report #6	January 1 - 31, 2023	February 10, 2023
Technical Report #7	February 1 - 28, 2023	March 10, 2023
Technical Report #8	March 1 - 31, 2023	April 10, 2023
Technical Report #9	April 1 - 30, 2023	May 10, 2023
Technical Report #10	May 1 - 31, 2023	June 10, 2023
Technical Report #11	June 1 - 30, 2023	July 10, 2023
Technical Report #12	July 1 - 31, 2023	August 10, 2023

DUE TO PROJECT MANAGER

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQR Grant Manager (RoseAnna Goewey, r.goewey@ceer.utexas.edu) by each institution on the project using the [FSR Template](#).

Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start - August 31, 2022	September 15, 2022
FSR #2	September 1 - 30, 2022	October 15, 2022
FSR #3	October 1 - 31, 2022	November 15, 2022
FSR #4	November 1 - 30, 2022	December 15, 2022
FSR #5	December 1 - 31, 2022	January 15, 2023
FSR #6	January 1 - 31, 2023	February 15, 2023
FSR #7	February 1 - 28, 2023	March 15, 2023
FSR #8	March 1 - 31, 2023	April 15, 2023
FSR #9	April 1 - 30, 2023	May 15, 2023
FSR #10	May 1 - 31, 2023	June 15, 2023
FSR #11	June 1 - 30, 2023	July 15, 2023
FSR #12	July 1 - 31, 2023	August 15, 2023
FSR #13	August 1 - 31, 2023	September 15, 2023
FSR #14	Final FSR	October 15, 2023

DUE TO GRANT MANAGER

Draft Final Report

A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Due Date: August 1, 2023

Final Report

A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Due Date: August 31, 2023

Project Data

All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information.

AQRP Workshop

A representative from the project will present at the AQRP Workshop in the first half of August 2023. The selected date will be updated.

8.2 Final Products

We will provide monthly report and a final report for this project, as well as publish 1-3 peer-reviewed journal articles. Results of the audits of data quality will be included in the final report. In addition, we will also present the above work at least one national scientific conference.

9. REFERENCES

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