Abstract

Project 24-007
Texarkana Intensive Campaign

The Texarkana Texas (TX)-Arkansas (AR) metropolitan area has recently become an area of concern due to elevated fine Particulate Matter ($PM_{2.5}$) aerosol loadings. The area is forested and contains a few large paper mills which are one potential source of the PM. These paper mills are located in Texas, Arkansas, and Louisiana. There are other possible industrial sources of $PM_{2.5}$ and it is possible that the $PM_{2.5}$ is being advected into the area from sources well outside of the area. The upcoming changes to regulatorily acceptable $PM_{2.5}$ levels necessitate a better understanding of the cause of these enhanced $PM_{2.5}$ levels in the Texarkana area. A comprehensive study of the particle and gas phase chemical species associated with these $PM_{2.5}$ exceedance episodes will assist in interpreting the source of these air masses.

A three-week field deployment in Texarkana, TX during the February-March 2025 time period to examine the sources of high $PM_{2.5}$ loadings in the Texarkana area will be conducted. This study will obtain information regarding the chemical species present in these high loading events in both particle and gas phase. This information will better inform policymakers with respect to the health hazards associated with these higher aerosol loading events.

Objectives for this study include

1. Characterize selected $PM_{2.5}$ and Volatile Organic Compound (VOC) point sources in the Texarkana area.
2. Evaluate background $PM_{2.5}$ conditions in the vicinity, including upwind of the Texarkana TX-AR metropolitan area. Given the location of the metropolitan area this will likely involve measuring areas outside of the state of Texas but would not emphasize detailed emission factors for out-of-state sources.
3. Any highly local effects which might be present and impacting the measurement of $PM_{2.5}$ at the Texarkana New Boston Station (C1031) will be examined.

The University of Houston, Baylor University, and Aerodyne are nationally recognized for their experience in development and deployment of mobile air quality labs. These customizable, comprehensive, and dynamic platforms provide on-the-go monitoring and analysis of aerosol, VOCs, trace gas, boundary layer height and meteorological parameters. Texarkana's air quality is impacted by local sources, photochemical processing and transport from multiple regions. This complexity can be overcome with the deployment of mobile air quality laboratories which have several advantages in study areas such as Texarkana. These advantages include real-time monitoring, flexibility in sampling location and time, response to plumes or events (e.g., potential aerosol or precursor plumes), source characterization (e.g., upwind vs downwind), repeat measurements, and accessibility in complex environments.

Quality Assurance Project Plan

Project 24-007
Texarkana Intensive Campaign

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September 12, 2024
Version #2

The University of Houston has prepared this QAPP following Environmental Protection Agency (EPA) guidelines for a Quality Assurance (QA) Category III Project: Requirements for Measurement Projects. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan.

QAPP Requirements: Project Description and Objectives, Organization and Responsibilities, Scientific Approach, Sampling Procedures, Measurement Procedures, Quality Metrics, and Management, Reporting, References.

QA Requirements:	Technical Systems Audits - Not Required for the Project
	Audits of Data Quality – 10% Required
	Report of Findings from Audits of Data Quality– Required in Final Report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the Texarkana Intensive Campaign project. The Principal Investigator (PI) for the project is James Flynn and the Co-PIs are Sascha Usenko, Rebecca Sheesley, Edward Fortner, and Brian Lerner.

Electronic Approvals:

This QAPP was approved electronically on 2024-09-20 | 10:13:01 PDT
by Vincent M. Torres, The University of Texas at Austin.

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Project Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 2024-09-20 | 10:13:01 PDT
by Vincent M. Torres, The University of Texas at Austin.

DocuSigned by:
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Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 2024-09-20 | 13:57:04 CDT
By Chola Regmi, Texas Commission on Environmental Quality.

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E85D613535774AC...

TCEQ Liaison, Texas Commission on Environmental Quality

This QAPP was approved electronically on 2024-09-20 | 10:43:52 PDT
By James Flynn, Ramboll

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013AFCC6369247A...

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1. PROJECT DESCRIPTION AND OBJECTIVES

1.1. PROCESS AND/OR ENVIRONMENTAL SYSTEM TO BE EVALUATED

The Texarkana Texas (TX)–Arkansas (AR) metropolitan area has recently become an area of concern due to elevated fine Particulate Matter ($PM_{2.5}$) aerosol loadings. The area is forested and contains a few large paper mills which are one potential source of the PM. These paper mills are in Texas, Arkansas, and Louisiana. There are other possible industrial sources of $PM_{2.5}$ and it is possible that the $PM_{2.5}$ is being advected into the area from sources well outside of the area. The upcoming changes to regulatory acceptable $PM_{2.5}$ levels necessitate a better understanding of the cause of these enhanced $PM_{2.5}$ levels in the Texarkana area. A comprehensive study of the particle and gas phase chemical species associated with these $PM_{2.5}$ exceedance episodes will assist in interpreting the source of these air masses.

1.2. PURPOSE AND OBJECTIVES

The purpose of this project is to examine the sources of high $PM_{2.5}$ loadings in the Texarkana area to be conducted during a three-week field deployment in Texarkana TX during the February-March 2025 time period. This study will obtain information regarding the chemical species present in any high loading events, for both the particle and gas phase. This information will better inform policymakers about the potential sources and consequent health hazards associated with these higher aerosol loading events. Objectives for this study include:

1. Characterize select $PM_{2.5}$ and Volatile Organic Compound (VOC) point sources in the Texarkana area.
2. Evaluate background $PM_{2.5}$ conditions in the vicinity, including upwind of the Texarkana TX-AR metropolitan area. Given the location of the metropolitan area this will likely involve measuring areas outside of the state of Texas but would not emphasize detailed emission factors for out-of-state sources
3. Investigate any highly local effects which might be present and impacting the measurement of $PM_{2.5}$ at the Texarkana New Boston Station (C1031).

The University of Houston (UH), Baylor University (BU), and Aerodyne are nationally recognized for their experience in development and deployment of mobile air quality labs. These customizable, comprehensive, and dynamic platforms provide on-the-go monitoring and analysis of aerosol, VOCs, trace gas, boundary layer height and meteorological parameters. Texarkana's air quality is impacted by local sources, photochemical processing and transport from multiple regions. This complexity can be overcome with the deployment of mobile air quality laboratories which have several advantages in study areas such as Texarkana. These advantages include real-time monitoring, flexibility in sampling location and time, response to plumes or events (e.g., potential aerosol or precursor plumes), source characterization (e.g., upwind vs downwind), repeat measurements, and accessibility in complex environments.

2. ORGANIZATION AND RESPONSIBILITIES

2.1. KEY PERSONNEL

James Flynn, Principal Investigator (PI), Research Associate Professor, Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas, USA, jhflynn@Central.uh.edu.
Responsible for overall project management and reporting as well as providing oversight for instrument preparation and deployment. Will coordinate all team efforts as well as ensure the field measurements and truck are maintained and operated in a responsible manner.

Sascha Usenko, Co-PI, Associate Professor, Department of Environmental Science, Baylor University, Waco, Texas, USA, Sascha_Usenko@baylor.edu.
Responsible for leading the AMS deployment in MAQL3 and providing operational support to the science team and for providing quality assurance oversight on Baylor measurements collected during this project.

Rebecca Sheesley, Co-PI, Associate Professor, Department of Environmental Science, Baylor University, Waco, Texas, USA, Rebecca_Sheesley@baylor.edu.
Responsible for leading the aerosol optical measurement collection, analysis, and interpretation of the aerosol data and the apportionment of dust and biomass burning sources.

Edward Fortner, Co-PI, Principal Scientist, Center for Aerosol and Cloud Chemistry Aerodyne Research, Inc., Billerica, Massachusetts, USA
Responsible for leading the minAML deployment. Will assist in project planning and coordination of daily deployment plans.

Brian Lerner, Co-PI, Principal Scientist, Center for Aerosol and Cloud Chemistry Aerodyne Research, Inc., Billerica, Massachusetts, USA
Responsible for VOCUS operation and VOCUS data analysis and interpretation. Will assist in project planning and for providing quality assurance oversight on Aerodyne measurements collected during this project.

Sergio Alvarez, Quality Assurance, Researcher 4, Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas, USA, slalvare@central.uh.edu.
Responsible for providing quality assurance oversight on University of Houston measurements collected during this project. Will assist in project planning, operations, and reporting.

2.2. PROJECT SCHEDULE

The project timeline is given below. Note that this schedule does not include the items described in the Deliverables section below, as those Deliverables will be provided in addition to the performance of the tasks prescribed here.

Task description	Timeline
Develop Work Plan	August 9–23, 2024
Project preparations	Receipt of Notice to Commence through the beginning of field deployment
Field Deployment	Three consecutive weeks in February-March 2025
Final Data Preparation	April–May 2025
Data Analysis and Final Reporting	Data analysis will occur June-August 2025. Reporting will be continuous from Notice to Commence through October 15, 2025 (FSR 14). Draft Final Report due August 1, 2025, AQRP presentations in August 2025, Final Report due August 31, 2025. Additional details on specific project reporting can be found in Section **Error! Reference source not found.**.

3. SCIENTIFIC APPROACH

3.1. SAMPLING DESIGN

UH MAQL3

The UH Mobile Air Quality Lab #3 (MAQL3) is a modified 2018 Freightliner Crew Cab straight truck with a twenty-four (24) feet box, forward observation deck, and articulating rooftop mounted 20-foot tower. Gas, aerosol, and meteorological measurements will be sampled from an inlet mounted to the end of the tower and stand ~30 feet above ground when raised. Four 15,000 BTU air conditioners will control the temperature and humidity in the lab space while electricity is provided by a 20kW onboard Tier 4 diesel generator. Instrumentation housed inside the lab space, on the observation deck, and the tower will measure ozone (O_3), nitric oxide (NO), nitrogen dioxide (NO_2), reactive nitrogen compounds (NO_Y), carbon monoxide (CO), sulfur dioxide (SO_2), meteorological measurements, photolysis rate of nitrogen dioxide (jNO_2), formaldehyde (HCHO), aerosols, and mixed layer heights.

A Handix Portable Optical Particle Spectrometer (POPS) will measure aerosol size distribution and number. This task also provides for the operation of an isoprene monitor on loan to the University of Houston from the University of Texas-Austin. Trace gas measurements of O_3, NO, nitrogen oxides (NO_X), NO_Y, CO, and SO_2 will also be collected from MAQL3. Meteorological and local condition measurements will include wind speed and direction, temperature, relative humidity, pressure, jNO_2, boundary layer height, GPS, sky conditions (all-sky camera), and forward, rear, left, and right cameras.

Figure 1. Photos of MAQL3. The upper right photo shows an example of instruments installed in the rear lab space and the lower right image shows an example of the operator stations in the cab.

Aerodyne minAML

The miniature Aerodyne Mobile Lab (minAML) provides mobile measurements with a smaller instrument footprint. Two operators can navigate narrow roadways with a focused instrument manifest. A 7 kW gas generator powers the on board equipment and a roof-top air conditioner. Inlets run through the roof out onto a boom extending forward over the hood (~2.3 m high). A sonic anemometer (2D or 3D) mounted on a sample mast measures wind speed and direction. A Hemisphere GPS (V103) compass determines the position and orientation of the vehicle.

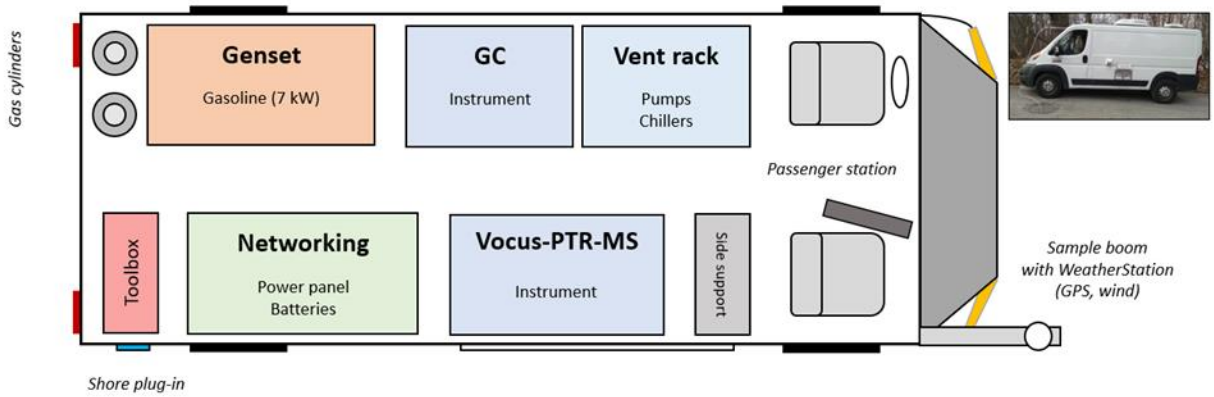

Figure 2. Schematic of an example instrument manifest in the minAML.

Typically, the commercial and research-grade atmospheric instruments deployed are fast (1–2 s response), sensitive (good signal to noise) and selective (specific to a molecule). Output data is saved to a robust archive (in the event of unscheduled shutdown) and displays in real-time on a monitor for scientists to make in-project decisions. Common instruments include the Vocus time-of-flight mass spectrometer (PTR- TOF) run in proton transfer reaction mode to quantify VOCs [Krechmer et al., 2018]. To provide speciation and quantitation for isomeric compounds (e.g. C8 aromatic species: ethyl benzene, o-, m- and p-xylenes), the Vocus PTR-TOF can switch from direct ambient sampling to gas chromatograph (GC) pre-separation sampling [Claflin et al., 2021]. During routine, automated sampling, the Vocus will measure direct samples for 3.5 hours (typical) and a GC sample for 30 minutes (typical) during a repeated 4-hour measurement cycle. During intensive sampling periods, such as when performing source mapping or plume analysis, the Vocus will be switched to manual control where the Vocus PTR-TOF remains in direct sample mode until the operator initiates a GC sample analysis, typically while the mobile lab is parked in a target plume. The Vocus system can report most classes of VOC species, such as aromatic, alkenes, biogenics (e.g. isoprene), and oxygenated, halogen- and nitrogen-containing VOCs.

3.2. GENERAL APPROACH AND MEASUREMENT PROCESSES

Texarkana RV Park which is located in the Southwest corner of Texarkana is the primary planned base location. There are sufficient 30- and 50-amp electrical connections at this facility and it is located away from many interferences (e.g. industrial sources). The location of the facility makes it a good upwind sampling location for Texarkana with a southwest wind. Measurements made from the proposed site will need to account for emissions from U.S.

Highway 59, located on the southeast edge of the property; the fast time-response instruments can separate these inputs as they will be made up of discrete brief plumes associated with individual vehicles. There is also a major paper mill located to the south of Texarkana and it is likely that this will be sampled at times from the base location. We will only be located here during the overnight periods while spending most days driving a variety of routes with the mobile labs. The routes driven will be to various potential aerosol sources as well as examining the area around C1031 (approximately 5 mi away) and driving to other upwind locations.

Under most conditions the two mobile labs will operate in unison with one following the other at a distance that minimizes the risk of sampling the exhaust of the lead vehicle. This approach is often taken while conducting intercomparisons of mobile laboratories and should be suitable for this project. Care will be taken to assure that GPS data are logged and that data system times are synchronized to a common network time server. In some scenarios such as when adjusting for actual weather and road conditions it may be useful to send the minAML ahead to determine if a route is suitable for both mobile labs.

If the opportunity presents, it may be desirable to allow the labs to separate and sample in different areas, depending on meteorology and objectives for the day, such as the MAQL3 sampling a $PM_{2.5}$ dust event while the VOC-focused minAML characterizes VOC sources. A combination of cell phone, text messaging, and CB radio communications by the passengers in the labs will likely be used while driving to coordinate the two platforms and relay measurement information. The collocated periods while stationary at the RV Park site will be used to verify comparability of overlapping measurements between the two platforms. Each group has well developed data handling procedures which result in multiple daily backups both in the field and on remote servers.

Weather permitting, the teams will plan to drive 5–6 days each week, with the remaining days allocated to instrument maintenance, calibration, preliminary data processing, and crew rest. While the duration of each driving day may vary based on the objective, the field teams are well versed in evaluating conditions and identifying objectives that can reasonably be accomplished. Initial routes will be planned to survey areas of known and likely emission sources. Some sources may be sampled at different times to determine if emissions vary throughout the day. During overnight hours, instruments will remain on to sample ambient air at the RV park, either using the standard measurement sequences as when driving surveys or with additional instrument calibrations. Overnight stationary measurements may be possible near industrial sources or at certain favorable upwind spots relative to Texarkana provided a suitable and safe location is identified.

4. SAMPLING PROCEDURES

4.1. SITE SPECIFIC FACTORS

The MAQL3 and minAML are outfitted with instrumentation that samples the local air and characterizes it for a specific chemical or class of chemicals. This instrumentation runs pseudo continuously, with a constant intake flow that is processed to produce 1-second data. Anemometers and global positioning system devices also provide rapid time response information.

Once the campaign begins, the instrumentation suite will be operated continuously, switching between pre-arranged “shore” power and the on-board generator. Approximately 3 minutes are required to re-establish quality assured data following the power switches

We plan to have shore power and a nominal base at one location (Texarkana RV Park) in the Texarkana area. We do plan to conduct stationary measurements for extended time periods away from this base and conduct mobile measurements. Prevailing and forecast meteorological conditions will dictate the movements of both mobile laboratories. For source-related work in the Texarkana area, we will determine which wind profiles work best for specific sources and plan accordingly. Prevailing wind conditions will contribute to decisions to move the mobile laboratories to facilities upwind of the Texarkana area as well. When sampling plumes upwind of the Texarkana area we will then conduct transects along the track of the plume as it progresses towards Texarkana.

The campaign will be conducted during a three-week interval. Scientists will analyze the data while in the field and regularly interact with the Project Manager and others to get feedback regarding future planning while considering overall project objectives.

4.2. SAMPLING PROCEDURE

No discreet sample collection is planned for this project as all measurements are online methods.

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5. MEASUREMENT PROCEDURES

O_3 will be measured by chemiluminescence. NO will be measured by chemiluminescence, NO_X by chemiluminescence with UV-LED NO_2 photolytic converter, and NO_Y by chemiluminescence with a heated molybdenum converter at the sample inlet. SO_2 will be measured by pulsed fluorescence while CO will be measured by off-axis cavity ring-down spectrometry. All sample lines use Teflon tubing and fittings, however some stainless steel fittings are occasionally used in some situations as appropriate. With the exception of NO_Y, all inorganic trace gases are sampled through a 47 mm Teflon filter which is nominally changed weekly. NO_Y is sampled through a dedicated inlet with a molybdenum catalytic converter inlet heated to 300°C. A combination of internal pre-reactor, catalyst, or zero air overflow methods will be used to evaluate trace gas instrument baselines as appropriate for the specific instrument measurement methods.

A Handix Portable Optical Particle Spectrometer will measure aerosol size distribution and number. A three-wavelength tricolor absorption photometer (TAP; Model 2901, Brechtel Inc., Hayward, CA) measures aerosol light absorption at wavelengths 365 (ultraviolet), 528 (green), and 652 (red) nanometers. TAP uses ten solenoid valves to cycle through eight filter spots and two reference filter spots. The light-emitting diode (LED) light source simultaneously shines through the sample and reference spots loaded with a 47-millimeter glass-fiber filter (Brechtel TAP-FIL100). The reference spot allows a measurement by difference approach in the TAP so the increase in light attenuation due to deposited particles on the sample spot is directly compared to the light attenuation of a reference spot. This allows attenuation by collected aerosol to be distinguished from attenuation by the blank filter. The TAP is set to rotate to the next filter spot when a filter spot's transmission reaches user-set value (Baylor uses 50%), and the reference channel gets altered whenever the sample spot is changed. Each of the eight sample spots is separated from the other by O-rings that clamp the filter material to prevent any inter-spot leakage. The air flow passes through the filter and into a solenoid valve controlled by the TAP Reader software.

Light scattering (σ_{sp}) will be measured using a TSI 3563 nephelometer (https://gml.noaa.gov/aero/maintenance/Neph_Ops_manual.pdf). In most integrating nephelometers, a white light source is used to illuminate the air sample, and light scattered by particles (and gases) at a particular wavelength is measured using a photomultiplier tube. In this project, a three-wavelength instrument is used. The TSI 3563 measures light scattering at three separate wavelengths simultaneously (450 Blue, 550 Green, and 700 Red). In addition, the TSI 3563 provides a separate measurement of particle back-scatter (σ_{bscat}). The instrument automatically calculates Rayleigh scattering from internally measured temperature and pressure and corrects the reported signal for those factors. Averaging time is matched to the TAPs and will be recalculated as needed.

The calibration of the ARI Aerosol Mass Spectrometer (AMS) is important for accurate quantification of particulate by chemical species. In order to minimize uncertainties in the reported mass concentrations, it is desirable that the fluctuations of the detection efficiency of the

AMS are closely monitored and properly corrected throughout the whole campaign. The parameters that capture the AMS detection efficiency are IE_{NO3-}, which is the ionization efficiency of a reference compound—Nitrate (NO_3^-), and the air beam signal (AB), which is the ion rate (Hz) detected for a major air signal, e.g. N_2^+ in this study[*Allan et al.*, 2003; *Jiménez et al.*, 2003]. While AB can be monitored continuously during instrument operation, the determination of IE_{NO3-} requires interruption of sampling to perform a calibration experiment (typically 1–2hrs). Given this restriction and the expectation (based on previous experience) that IE would not be highly variable, periodic IE_{NO3-} calibrations will be conducted during this study. Because the ratios of IE_{NO3-} to AB remains remarkably constant (r.s.d. < 1%) the continuous AB signal can be used to correct for the variations in the AMS detection efficiencies to a very good approximation.

Two other AMS parameters significantly influence the absolute values of its PM measurements: the collection efficiency (CE) and relative ionization efficiency (RIE). CE is introduced to correct for incomplete detection of nonrefractory particles, NR-PM, by the AMS, e.g., due to irregularly shaped particles that do not completely reach the vaporizer [*Jayne et al.*, 2000; *Tobias et al.*, 2000]. Although strictly speaking CE should be a function of particle size and shape, at present it is defined as the correction factor for the bulk mass concentrations, i.e., the fraction of the particle mass that is measured by the AMS. A CE value of 0.5 is assigned to sulfate, based on extensive observations from several laboratory and field tests for sulfate aerosols. The same CE value (i.e., 0.5) is applied to particles containing nitrate and ammonium, because they appear to be internally mixed with sulfate particles most of the time.

The CE value for total $NR\text{-}PM_1$ organics is estimated based on their size distributions, which often show two modes – a larger accumulation mode of ambient background particles that appears to be internally mixed with Sulfate Ion (SO_4^{2-}), NO_3^- and ammonium (NH_4^+), and a smaller ultra-fine mode that seems to be mainly emitted from combustion-related sources. A CE value of 0.5 is thus applied to the accumulation mode organics (due to the internal mixing with SO_4^{2-}) and CE for the smaller mode is assumed to be 1.0 because laboratory studies have shown close to 100 % AMS transmission for sooty combustion particles. By studying the size distributions of total organics, as well as individual organics mass fragments averaged over the whole sampling period, we have found that these two modes can be best separated at Dva = 160 nm and that the mass ratio of the smaller (Dva < 160 nm) to the larger mode (Dva > 160 nm) is roughly 2/3. The CE value of the bulk organics is therefore set at 0.7.

Relative ionization efficiency (RIE) is the ratio of the electron impact ionization efficiency of a given species to IE_{NO3}^- on a per unit mass basis. Note that IE_{NO3}^- is the IE of NO_3^- measured based on two major ions, m/z's 30 and 46, instead of all the mass fragments. RIE values of individual species representative have been determined in a range of laboratory measurements and tabulated [*Zhang et al.*, 2006].

Finally, two other key AMS parameters require calibration. The AMS volumetric sampling flow rate and the particle velocity. The sample flow rate will be determined using a Gilibrator (bubble flowmeter). The particle aerodynamic size reported by the AMS is based on measured particle velocities. The size-velocity calibration is performed using an atomizer with an Ammonium nitrate (NH4NO3) solution followed by DMA size selection in the range 60–700 nm.

minAML Measurements

The rapid measurement of Volatile Organic Compounds (VOC's) on board the minAML will be key to assist in attribution of overall enhanced particle and gas phase signals to specific sources. Vehicular, biomass burning, and industrial VOC markers will all be rapidly quantified and displayed in real time informing decisions regarding the placement of both mobile laboratories to better determine sources.

- Proton Transfer Reaction Mass Spectrometer (PTR-MS) Instrument Assessment

The PTR-MS instrument provides a measurement of a selected set of organic gases possessing proton affinities greater than water. Most non-alkane organics possessing more than 2 carbons can be detected using the PTR-MS. This instrument is located immediately behind the driver in the mobile laboratory to minimize the length of the sampling inlet.

Specific step-by-step instructions for bringing this instrument on-line and a copy of the instrument manual on are available elsewhere (see Appendix A). The description provided in this document pertains to the normal operation of the instrument. Details of the instrument have been previously published in *Krechmer et al.* [2018].

The PTR-MS parameters drift tube pressure, detection region pressure, drift tube temperature and reagent ion intensity should always be within the following specifications:

Drift tube pressure = 2.1 (± 0.05) mbar
Detection region pressure < 45 x 10^{-6} mbar
Drift tube temperature 60 (± 1) ^{o}C

The drift tube pressure and temperature are automatically controlled and maintained via a PID feedback loop.

The PTR-MS uses a tap from the main gas phase sample inlet through a short length, ~ 4 feet, of 1/4" OD PFA tubing, with a sample pump pulling at 4.5 standard liters per minute (slpm) to minimize residence time but maintain laminarity. The PTR-MS draws 0.25 slpm of this flow into the instrument for analysis and the rest is exhausted through the sample pump. The PTR-MS has three modes of operation: measure, zero, and calibrate. Zero and calibration periods are automatically actuated at pre-defined intervals using electronically controlled solenoid valves. The measure, calibrate and zero modes are fully automated.

Instrument zeros are software-controlled and scheduled to occur at a regular specified interval using an on-board zero air generator. The PTR-MS uses a 3-way solenoid valve to overflow the instrument inlet with zero air at a flow rate greater than the instrument draw (nominal 0.25 slpm).

The excess zero gas is vented via the PTR-MS sample pump, and therefore the zero (and calibrate) mode does not affect other instruments on the gas phase sample inlet.

VOC free air is produced by pulling filtered ambient air through a heated oxidation catalyst. A ¾"OD stainless steel tube packed with a 50:50 mix of Platinum and Palladium coated alumina beads is housed within a small oven that is heated to 400 ^{o}C and oxidizes any VOCs to CO_2. The instrument background is mass dependent with some ions having non-zero values. Atmospherically persistent compounds such as acetone (m/z 59) should exhibit discernable decreases in their ion intensities when the PTR-MS is sampling zero air.

Instrument calibrations are performed automatically at regular intervals (generally every hour) by serially diluting the PTR-MS multi-component calibration gas with VOC free air from the on-board zero air generator. The calibration gas is added to the zero air stream via 3-way solenoid valve, upstream of the PTR-MS inlet to allow sufficient mixing. Excess diluted calibration gas is vented to the PTR-MS sample pump, similar to zero-mode, so that the calibration procedure does not affect any of the other gas phase measurements. The flows of the calibration gas and the VOC free dilution gas are controlled via mass flow controllers. Serial dilutions are performed by mixing 2–5 ml/min of the calibration gas into a zero-gas dilution flow of 250–400 ml/min.

- <u>Gas Chromatography Instrument Assessment</u>

The Thermal Desorption Pre-Concentrator (TDPC)-GC instrument is a 2-channel GC system that provides semi-continuous quantitation of trace organic gases within the volatility ranges of each chromatograph channel [Claflin et al., 2021]. The instrument has a "high-volatility" VOC, and a "mid-volatility" VOC channel as configured for this field campaign. Each channel relies upon a two-stage adsorbent / thermal desorption pre-concentration system to provide adequate analyte for separation and analysis by the Vocus PTR-TOF.

The GC system shares a common inlet with other gas-phase instruments and is located next to the PTR-MS instrument inside the mobile laboratory to reduce the inlet length, and to allow for simpler temporal correlation with real-time VOC measurements made with the PTR-MS system.

The GC system pulls approximately 1–2 slpm of ambient air from the main inlet via 1/4" OD PFA tubing, typically less than 4 feet in length. A subset of this sample flow (100–200 Standard cubic centimeters per minute (sccm)) is directed to the GC inlet for analysis, with the rest of the flow vented. The gas sample is split to separate multibed sample tubes, which are held at a fixed temperature (typically 20 °C) during sample collection. The flow to each tube is controlled by calibrated mass flow controllers (MFCs) to provide known sample volumes. After sample collection (typical 100 sccm for 10 min), the sample tubes are forward-flushed with carrier gas to reduce the water-loading in the tubes. The tubes are then heated with a controlled temperature ramp to 300 °C in 60 seconds to transfer analyte to narrow-bore focusing traps (Markes International U-T15ATA-2S) held at 20 °C, using low flow-rate carrier gas (typically 2 sccm). The analyte is held on the focus trap until flash-heated and injected upon the respective separation column, for separation and detection. Separation and detection take 20 minutes and requires that the Vocus is off-line from ambient measurements to analyze the GC effluent.

The GC system will be used differently depending upon if the mobile lab is actively driving or stationary, either to investigate a source site or in off-hours while at the RV park. While mobile, the GC remains in the standby state and can be manually triggered by the field scientist to collect an ambient sample. This sample can then be immediately injected into the GC system and then onto the Vocus for analysis or held until the scientist identifies a time period where direct Vocus measurements can be missed.

When the mobile lab is stationary during active sampling periods, the GC and Vocus operate on a 4-hour cycle, with 3.5 hours of direct Vocus measurements and 30 min of GC-Vocus data. When the mobile lab is stationary overnight, the GC and Vocus are switched to a 10-hr cycle, with the GC collecting an ambient sample once every three hours for the first 9 hours of the time period. For the last hour of the cycle, the GC collects a zero and calibration sample (see below). The Vocus is offline from direct measurement for the full hour.

The TDPC-GC is operated in three modes: ambient sampling, cal mode and zero mode. The cal and zero modes enable internal solenoid valves to overflow the GC inlet with a mixture of calibrant gas and zero gas, or just zero gas, respectively. The calibrant used for this campaign is a gas cylinder purchased from Apel-Riemer Environmental Inc, with a mixture of 19 VOCs diluted to nominal 1 ppm in nitrogen (with one component nominal 100 ppb due to low volatility). The mixing ratios of the analytes in the gas cylinder are certified by the vendor prior to delivery, with accuracy ±5% for all species. The GC flows this calibrant gas continuously at nominally 0.5 sccm via critical orifice and is occasionally directed to the GC inlet (see above). This flow rate is controlled by the gas cylinder regulator pressure and will be checked daily via a bubble flow meter. Sample tubes must be changed routinely to maintain quantitative instrument response. For the Texarkana field campaign, sample tubes will be replaced every 7th day, to maintain <100 samples collected per tube.

The TPDC-GC system records temperatures, flows and pressures relevant to the sample collection and chromatographic analysis. The following parameters should be maintained throughout the campaign:

Sample flow rate = 100[†] sccm (± 1 sccm)
Sample tube temperature = 20 (± 1) °C during sample collection
Focus trap temperature = 20 (± 1) °C during sample focusing

[†]Sample flow rate may be adjusted during ambient sampling in rare instances, to accommodate exceptionally high or low VOC mixing ratio (e.g. near-source plume measurement). In these cases, the flow rate is controlled ± 1 sccm.

6. QUALITY METRICS (QA/QC CHECKS)

6.1. GENERAL INFORMATION

Mobile Lab Measurements

A blended cylinder of CO, SO_2, NO, and propene will be used to challenge the majority of the instrumentation aboard the MAQL3. Additional discussion and impacts on data uncertainty will be addressed in the final reports as a function of combined instrument uncertainty. The blended gas challenges in the MAQL3 will be introduced automatically with a dilution system and valves to the inlet of the sample line upstream of the filter to best represent ambient conditions and account for and/or identify potential losses in the inlet lines and filter. A combination of internal pre-reactor, catalyst, or zero air overflow methods will be used to evaluate trace gas instrument baselines as appropriate for the specific instrument measurement methods.

The frequency of upscale gas dilution challenges will be determined based on pre-deployment testing. An internal scrubber further scrubs the zero-air supply to determine background conditions.

Table 1. Procedures to Assess QA objective for AMS

Measurement Parameter	Analysis Method	Assessment Method
Organics, NO_3, SO_4, NH_4, Chl	AMS	Flow rate checked continuously by pressure and instrument air beam signal. Ion Signal to mass loading performed with classified ammonium nitrate aerosol (*nitrate equivalent loading*);

Table 2. Objectives and Acceptance Criteria for AMS

Analysis Method	Assessment	Instrument/ Parameter	Criteria Accuracy	Completeness	Precision	Corrective Action Given Failure to meet Criteria
PM focused with an aerodynamic lens and 'concentrated' by differential pumping. PM vaporized with laser absorption. Gaseous PM constituents ionized with electron impact and classified by mass to charge ration	Airbeam signal Flow rate Particle time of flight pressure regime	AMS	Calibration of Relative ionization efficiency must match.	80%	NA	Flow rate restored by cleaning the orifice. Calibration performance of collection efficiency and relative ionization efficiency evaluated. Laser re-aligned according to the established procedure in the manual.

minAML Measurements

minAML core measurement assessment notes are tabulated in tables below.

Table 3. Procedures to Assess QA objective for Additional Measurements

Measurement Parameter	Analysis Method	Assessment Method	Corrective Action
Ion count of protonated VOCs	Sample reaction with protonated water	Hourly dedicated sampling of the VOC-free air with matched humidity. Daily calibration using standards to determine instrument response.	Sensitivities for the suite of VOCs included in calibration are determined and applied to data. Adjustments to instrument tuning are made as necessary to maintain adequate sensitivity.
Speciated VOC ion counts	Gas Chromatogram with Mass Spectrometer Detector	Daily measurements of VOC-free air with matched humidity. Daily calibration standards to track retention times. Pre-campaign determination of the ion count/ppb VOC using multiple standard calibration tanks. In-field checks of the response per ppb VOC are done with the calibration chromatograms	Sensitivities for the suite of VOCs included in calibration are determined and applied to data. Adjustments to instrument tuning are made as necessary to maintain adequate sensitivity.
Wind Speed and Direction	Airmar 200WX WeatherStation Instrument	The anemometer direction is checked against a coordinated manual fan blowing on the anemometer along the four quadrants (ahead, driver, passenger, rear). Wind speed calibration is compared by looking at the GPS velocity signal during a mobile condition with light ambient wind.	The manufacturer has a compass calibration procedure which will be executed as needed. If that does not correct the issue Airmar will be replaced.
Position	Global Position System (GPS) Airmar 200WX WeatherStation Instrument	Examining the output from the GPS compared to an online source such as google maps verifies the function. All mobile ground tracks are mapped into the UTM coordinate space to put traces onto a georeferenced image of the roadway, terrain, facility boundaries	Repositioning of the GPS will be done if communication becomes unreliable. Replacement of the GPS will be done if necessary to receive accurate signals

Table 4. Objectives and Acceptance Criteria

Analysis Method	Assessment	Parameter	Criteria Accuracy	Completeness	Precision	Corrective Action Given Failure to meet Criteria
Reaction with protonated water and classified by mass to charge ratio (parent and daughter ions)	Reagent ion source voltage Ion molecule region pressure Flow rate to instrument	PTR-MS all	Response Factors should be within 15% of the running instrument performance	85%	Typically, 1-10 pptv at 1Hz, depending upon compound	Flow, reagent ion and pressure problem are corrected using procedure described in the PTRMS manual
Preconcentration via adsorbent tube, separation by gas chromatography and detection by PTR and time-of-flight mass spectrometry.	Sample flow rate check Trap temperature check Leak check of flow path	GC-PTR-ToF all	Flow ± 5%; Temperatures ± 2.5 °C;	90%	Typically 1-10 pptv at 30 min, compound specific	Flow: adjust MFC setting, leak check inlet Temperature: check TDPC cooler, heater temperature sensors, temp controller cabling Leak: inspect internal fittings, sample and focusing traps

6.1.1. Detection Limit

Detection limits will be expressed in units of concentration and reflect the smallest concentration of a compound that can be measured with a defined degree of certainty. The analytical instrument detection limit (IDL) for other parameters will be established with the application of available standards according to 40 *CFR* Part 136, Part B, where applicable.

6.1.2. Blanks / Zeros

The system contribution to the measurement results is determined by analysis of a blank or zero air (filtered air) level as part of each calibration and span check. As part of the calibration, the zero level is used along with the upscale concentrations to establish the calibration curve. As part of the span check, the zero level is used as a quality control check for monitoring zero drift. If a method is found to have a system contribution for a target pollutant at a concentration greater than three times the detection limit or greater than 10 percent of the median measured concentration for the pollutant (whichever is larger), efforts must be taken to remove the contribution. Any system contribution for a target pollutant (or for another constituent that interferes with analysis for a target pollutant) that is above the detection limit must be thoroughly characterized such that the extent of influence on the target pollutant measurement certainty is well understood. This may require an elevated frequency of blank analyses for an adequate period to characterize the contribution. A data flag will be used when concentrations in the blank sample measurements indicate a contribution to the sample measurement result that is determined to be significant relative to the quality objectives specified for the measurement.

6.2. QUALITY ASSURANCE OBJECTIVES

The following sections describe the quality assurance objectives for this project. The findings of these activities will be included in the final reports.

6.2.1. Precision

Precision is a measure of the repeatability of the results. Estimates of precision are assessed in different ways for different measurement technologies.

Precision for measurements from continuous monitors will be estimated by analysis of a test atmosphere containing the target compounds being monitored. Precision for trace gases is estimated from precision checks that are done as part of routine span checks of the monitors. This precision check consists of introducing a known concentration of the pollutant into the monitor in the concentration range required by 40 *CFR* Part 58. The resulting measured concentration is then compared to the known concentration.

6.2.2. Accuracy

Accuracy is the closeness of a measurement to a reference value and reflects elements of both bias and precision. Accuracy will be determined by evaluating measurement system responses for replicate analysis of samples containing the compounds of interest at concentrations representative of the ambient atmospheres typically being monitored during the study as outlined in 40 *CFR* 58. Note that technical system audits are not required for a Category III QAPP.

6.2.3. <u>Completeness</u>

Data completeness is calculated on the basis of the number of valid samples collected out of the total possible number of measurements. Data completeness is calculated as follows:

$$\%\ \text{Completeness} = \frac{\text{Number of valid measurements} \times 100}{\text{Total possible number of measurements}}$$

Completeness, which measures the percentage of measurements to the number of measurements. In order to meet the objectives of the project's research plan, the acceptance criteria for field measurements and laboratory completeness is 90%. The completeness of both field and laboratory will be reported.

6.3. DATA AUDITING

Technical Systems Audits are not required for this project. Audits of data quality (minimum 10%) will be performed by the data processing team and designated QA representatives of each organization using visual inspection of the data, comparison of the data to the QA/QC criteria described in this document, and comparison with other measurements, as applicable. Data that passes these examinations will be deemed acceptable. Should data not pass examination on one or more of the checks, the data will be further examined by the researchers and as appropriate may be flagged as invalid, valid, or valid but having failed a check. Once the Audit of Data Quality are completed, a report of the findings will be included in the final report.

6.4. INSTRUMENT SPECIFICS

MAQL3 Measurements

Mass flow controller signals will be recorded in DAQFactory software as well as valve states and the associated data flags to indicate non-ambient data during calibrations and instrument challenges. These signals will be used to calculate mixing ratios of test atmospheres for instrument sensitivity calculations.

A blended cylinder of CO, SO_2, NO, and propene will be used to challenge the majority of the instrumentation aboard the MAQL3. Additional discussion and impacts on data uncertainty will be addressed in the final reports as a function of combined instrument uncertainty. The blended gas challenges in the MAQL3 will be introduced automatically with a dilution system and valves to the inlet of the sample line upstream of the filter to best represent ambient conditions and account for and/or identify potential losses in the inlet lines and filter. A combination of internal pre-reactor, catalyst, or zero air overflow methods will be used to evaluate trace gas instrument baselines as appropriate for the specific instrument measurement methods.

The frequency of upscale gas dilution challenges will be determined based on pre-deployment testing. An internal scrubber further scrubs the zero air supply to determine background conditions.

7. DATA ANALYSIS, INTERPRETATION, AND MANAGEMENT

7.1. DATA REPORTING REQUIREMENTS

The data will be provided in time-stamped delimited text format. Data will include the time series (and relevant GPS information) of all parameters discussed above.

7.2. DATA VALIDATION PROCEDURES

Ambient data that have passed the QA/QC checks described above will be considered to be validated.

7.3. DATA ANALYSIS

Limited data analysis will occur under this project, however, future analysis projects may use the data to attempt to identify causes of air pollution in the location(s) sampled. This could be achieved by standard techniques such as correlation/regression. The information provided by this data will be useful in understanding pollution dynamics in this region and therefore in developing control strategies and determining whether local or regional controls may be best suited for this area.

7.4. DATA STORAGE

All data collected/generated during the course of this project will be backed up on each institution's servers, or at UH and backed up at St. Edward's University or another off-campus location and will be maintained for a minimum of 3 years after the completion of the project.

8. REPORTING

8.1. DELIVERABLES

Deliverables for this project will include a description of the specific reports to be submitted and their due dates are outlined below.

One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The Project PI will submit the reports unless that responsibility is otherwise delegated with the approval of the AQRP Project Manager.

All reports 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. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Abstract: At the beginning of the project, an Abstract will be submitted to the AQRP 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.

Abstract Due Date: August 23, 2024

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the AQRP Project Manager as a Microsoft Word 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.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	August, September, October 2024	October 31, 2024
Quarterly Report #2	November, December 2024, January 2025	January 31, 2025
Quarterly Report #3	February, March, April 2025	April 30, 2025
Quarterly Report #4	May, June, July 2025	July 31, 2025

DUE TO PROJECT MANAGER

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the AQRP Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP MTR Template found on the AQRP website. Note that MTRs will continue on the same schedule through October 2025.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start–August 31, 2024	September 10, 2024
Technical Report #2	September 1–30, 2024	October 10, 2024
Technical Report #3	October 1–31, 2024	November 10, 2024
Technical Report #4	November 1–30, 2024	December 10, 2024
Technical Report #5	December 1–31, 2024	January 10, 2025
Technical Report #6	January 1–31, 2025	February 10, 2025
Technical Report #7	February 1–28, 2025	March 10, 2025
Technical Report #8	March 1–31, 2025	April 10, 2025
Technical Report #9	April 1–30, 2025	May 10, 2025
Technical Report #10	May 1–31, 2025	June 10, 2025
Technical Report #11	June 1–30, 2025	July 10, 2025
Technical Report #12	July 1–31, 2025	August 10, 2025

DUE TO PROJECT MANAGER

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) by each institution on the project using the AQRP FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start–August 31, 2024	September 15, 2024
FSR #2	September 1–30, 2024	October 15, 2024
FSR #3	October 1–31, 2024	November 15, 2024
FSR #4	November 1–30, 2024	December 15, 2024
FSR #5	December 1–31, 2024	January 15, 2025
FSR #6	January 1–31, 2025	February 15, 2025
FSR #7	February 1–28, 2025	March 15, 2025
FSR #8	March 1–31, 2025	April 15, 2025
FSR #9	April 1–30, 2025	May 15, 2025
FSR #10	May 1–31, 2025	June 15, 2025
FSR #11	June 1–30, 2025	July 15, 2025
FSR #12	July 1–31, 2025	August 15, 2025
FSR #13	August 1–31, 2025	September 15, 2025
FSR #14	Final FSR	October 15, 2025

DUE TO GRANT MANAGER

Draft Final Report: A Draft Final Report will be submitted to the AQRP 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.

Draft Final Report Due Date: August 15, 2025

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the AQRP 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.

Final Report Due Date: August 31, 2025

Project Data: All project data including but not limited to quality assurance and quality control measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (August 31, 2025). 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 August 2025.

Presentations and Publications/Posters: All data and other information developed under this project which is included in published papers, symposia, presentations, press releases, websites and/or other publications shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

8.2. FINAL PRODUCT

The Final Report will provide a comprehensive overview of activities undertaken during the Texarkana Intensive Campaign project and any data collected and analyzed. The Final Report will highlight major activities and key findings, including the Audit of Data Quality, provide pertinent analysis, describe encountered problems and associated corrective actions, and detail relevant statistics, including data, parameter, or model completeness, accuracy, and precision.

9. REFERENCES

Allan, J. D., et al. (2003), Quantitative sampling using an Aerodyne aerosol mass spectrometer - 2. Measurements of fine particulate chemical composition in two U.K. cities, *Journal of Geophysical Research-Atmospheres*, *108*(D3), doi:10.1029/2002JD002359.

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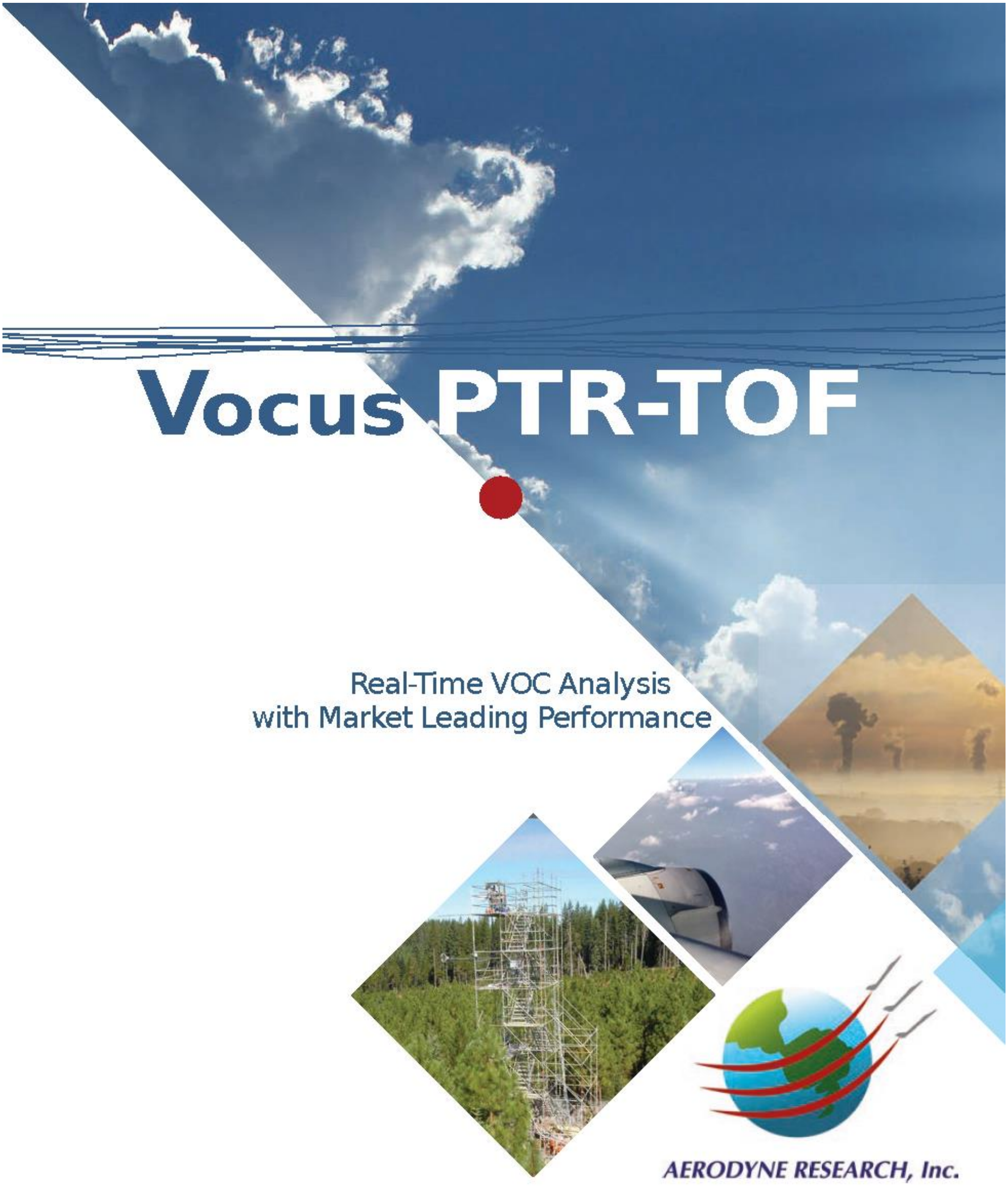
NASA, 2021. TRACER-AQ Science Plan, https://www-air.larc.nasa.gov/missions/tracer-aq/docs/TRACERAQ_SciencePlan_v1.pdf, January 2021.

10.Appendix A – Vocus PTR-TOF


Vocus PTR-TOF
Real-Time VOC Analysis
with Market Leading Performance
AERODYNE RESEARCH, Inc.

With sub-ppt limits of detection and mass resolving power up to 15000, the Vocus PTR-TOF is taking laboratory and field analysis of VOCs in exciting new directions.

Market Leading PTR-MS Performance

Ultra-Low Limits of Detection

- Proprietary Vocus reaction cell reduces wall losses and focuses product ions
- Maximize analyte signals with combination of Vocus reaction cell, ion cooling interface, and sensitive TOF mass analyzer
- Up to 10x the sensitivity of other commercial PTR-MS
- Sub-ppt limits of detection in seconds

Highest Available PTR-MS Mass Resolving Power

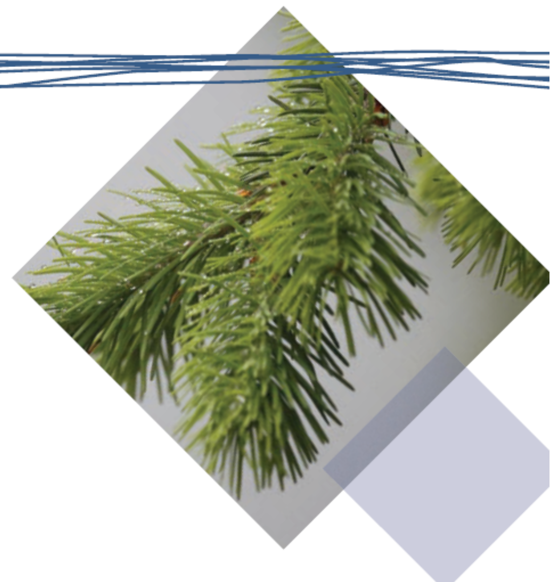
- Mass resolving power up to 15000 enables identification of isobaric compounds in complex mixtures
- Identification of analytes and confirmation of peak assignments based on exact mass and isotope patterns

Select a Model to Meet Your Needs

	Sensitivity cps/ppb benzene	**Limit of Detection (LOD)** 1-min, BTX	**Resolving Power at Specified Sensitivity**[a] M/ΔM
Vocus PTR-TOF standard	10000	< 1 ppt	5000
Vocus PTR-TOF C compact	Krechmer, J., Lopez-Hil□ker, F. et al. : Evaluation of a New Reagent-Ion Source and Focusing Ion–Molecule Reactor for Use in Proton-Transfer-Reaction Mass Spectrometry, Anal. Chem., 90(20), 12011–12018, doi:10.1021/acs.analchem.8b02641, 2018.		
Vocus PTR-TOF 2R high resolution	10000	< 1 ppt	10000

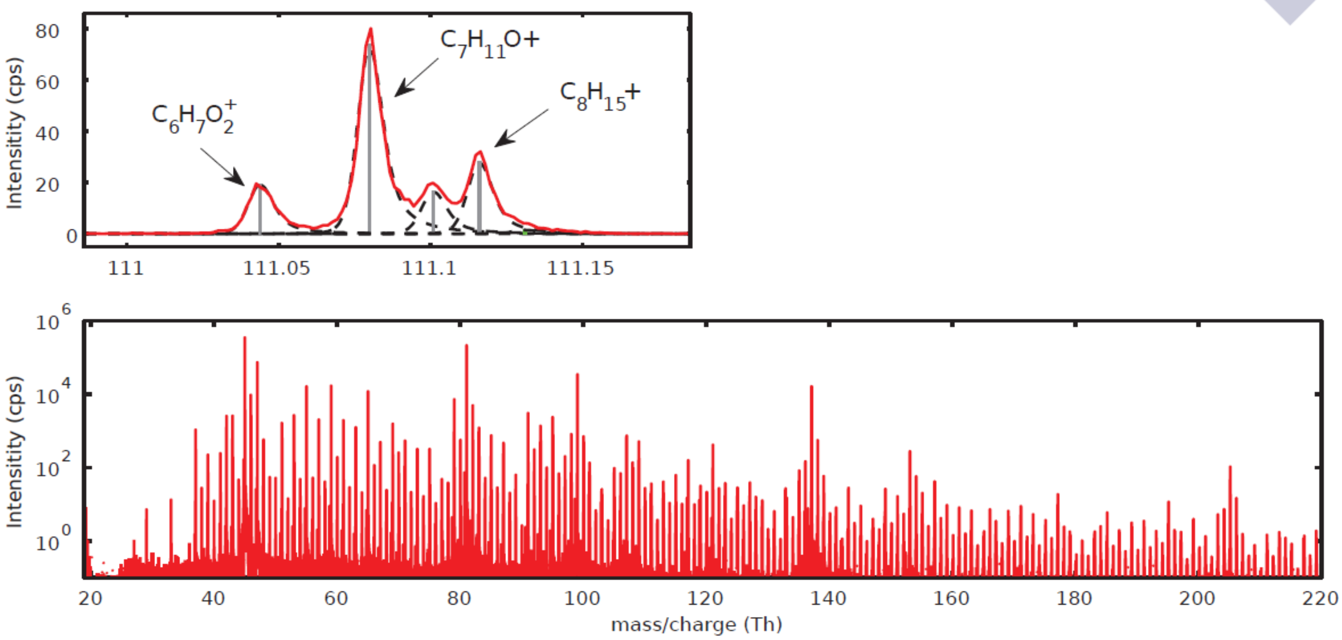
a. Each model can be operated with higher resolving power at reduced sensitivity.

Resolving Power up to 15000 with the Vocus PTR-TOF 2R



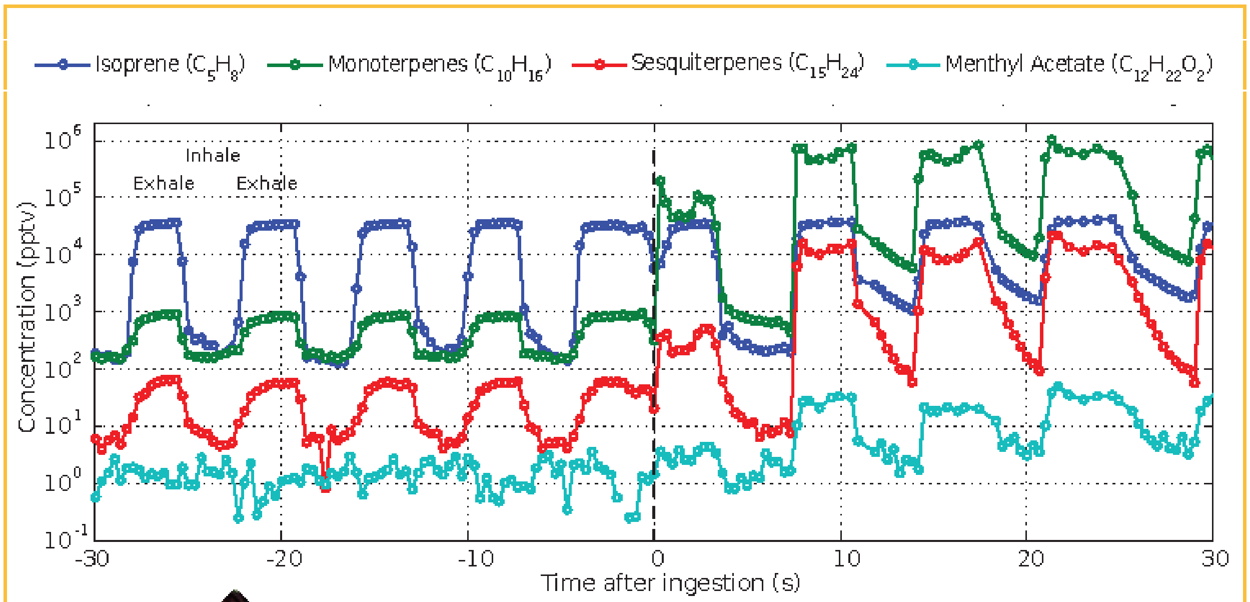
Confident analysis of complex mixtures often demands resolution of individual peaks.

This mass spectrum shows the diverse collection of biogenic VOCs that was emitted when a single pine needle was cut in lab air in front of the inlet of the Vocus PTR-TOF 2R. The inset demonstrates the capability of the 2R to separate and identify isobars.



Real-Time Monitoring of VOCs with Millisecond Time Response

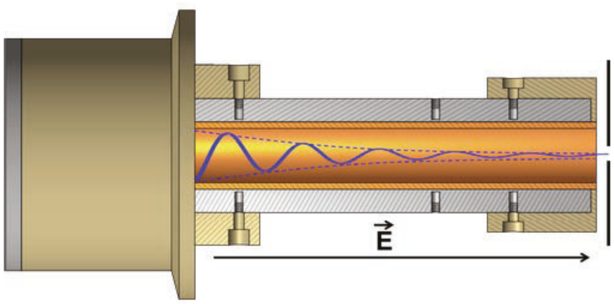
The Vocus PTR-TOF can quantify dynamic changes in even ultra-low concentration compounds.



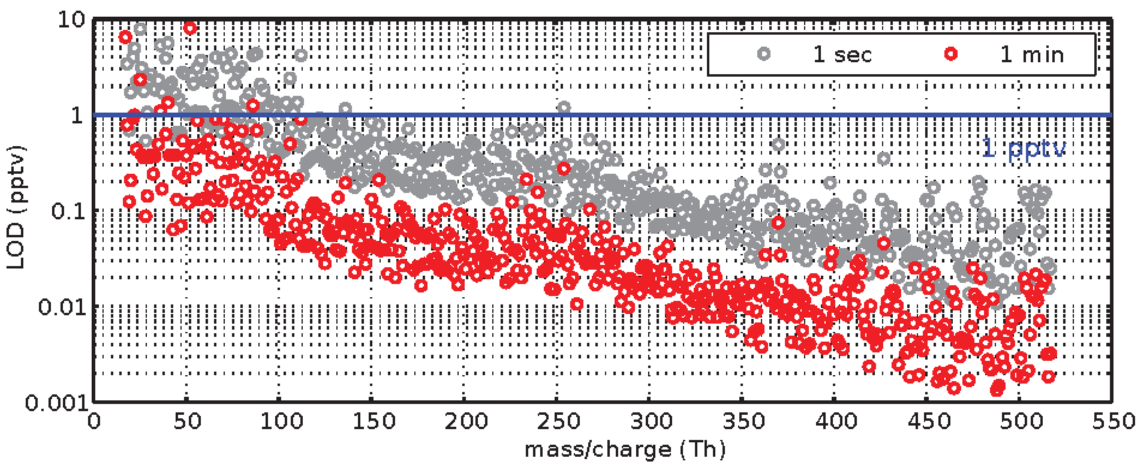
Human breath was monitored in real time at 3 Hz before and after the ingestion of a Ricola™ herb cough drop. Hundreds of compounds were present in the post-ingestion data, including monoterpenes, sesquiterpenes, and other compounds of herbal origin. A subset of detected compounds is shown in order to demonstrate the fast time response and broad dynamic range of the Vocus PTR-TOF.

Vocus™ is a Leap Forward in PTR Source Design

The RF focusing and uniform drift fields of the Vocus source enable real-time analysis of volatile organic compounds (VOCs) with unprecedented limits of detection and speed.



Sample Flow Rate	50 – 500 sccm typical 150 sccm
Operating Pressure	0.5 – 5 mbar typical 1-2 mbar
Axial Gradient	Uniform Linear Field 0-5 V/mm
Reagent Ions	$(H_2O)_nH_3O^+$, NO^+, O_2^+



Sub-ppt limits of detection in seconds

Calculated as 3 times the standard deviation of signal with ultra clean air and assuming the sensitivity of BTX.

Vocus PTR-TOF

Vocus 2R
484 x 619 x 1484
160 kg
<1200 W

AERODYNE RESEARCH, Inc.

aerodyne.com
ptr-info@aerodyne.com

11. Appendix B – Aerodyne's minAML

Mobile platforms for real-time detection and quantification of atmospheric emissions

The Aerodyne Mobile Laboratory (AML) and miniature AML (minAML) have been deployed across the world in many contexts since the 1990s: emissions (e.g., on-road, industrial), mobile mapping (e.g., community impact), and stationary photochemistry studies (e.g., urban outflow). Aerodyne has integrated instrument suites on other platforms, including research aircraft, shipping containers, and boats. Use of a mobile laboratory collecting real-time data while in motion, enables the study of many important scientific questions about the atmosphere (*Kolb et al., 2004*).

Aerodyne Mobile Laboratory (AML)

Each project on the AML deploys an instrumentation package tailored to its specific goals. A driver and scientist navigate local roads up front while an instrument specialist monitors incoming data from the cargo area (**Figure 1**). Two inlets, one dedicated to particulate matter and another for gas phase species, are ~2.8 m above ground extended over the hood. Sample air is drawn continuously at a flow rate of ~9-18 standard liters per minute through each of these two inlets with various instruments sub-sampling. Two 12.5 kW diesel generators (120/240 split phase) power the lab between 8 battery-protected circuits while mobile. Three air conditioners manage the internal heat burden and instrument exhaust vents into a pump bay underneath the floor. Typical operating protocols and sampling techniques have been described in Herndon et al., 2005.

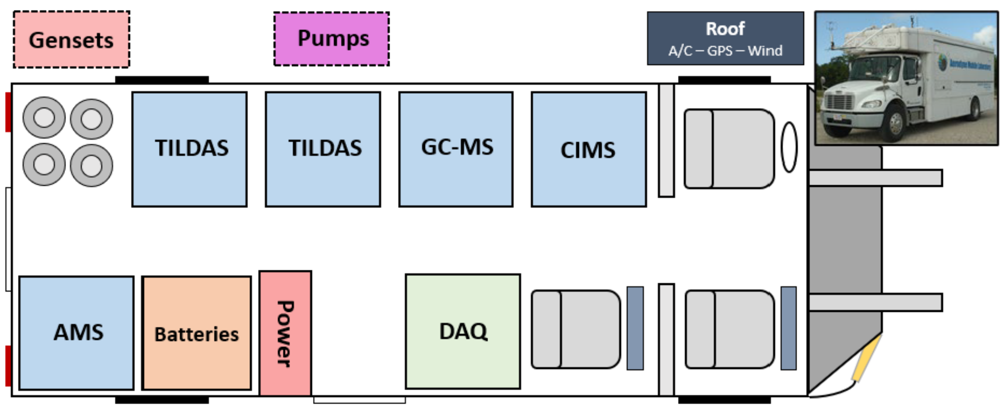


Figure 1. Schematic of an example instrument manifest in the AML. Individual studies typically alter the instrument payload according to the specific goals and the best instrument technologies available. Dashed-line boxes indicate equipment that is underneath the cargo area of the vehicle.

Miniature Aerodyne Mobile Laboratory (minAML)

A smaller version of the AML, the minAML offers the same modularity and workflow. Two operators can navigate narrow roadways with a focused instrument manifest (**Figure 2**). A 7 kW gas generator powers the on board equipment and a roof-top air conditioner. Inlets run through the roof out onto a boom over the hood (~2.3 m high).

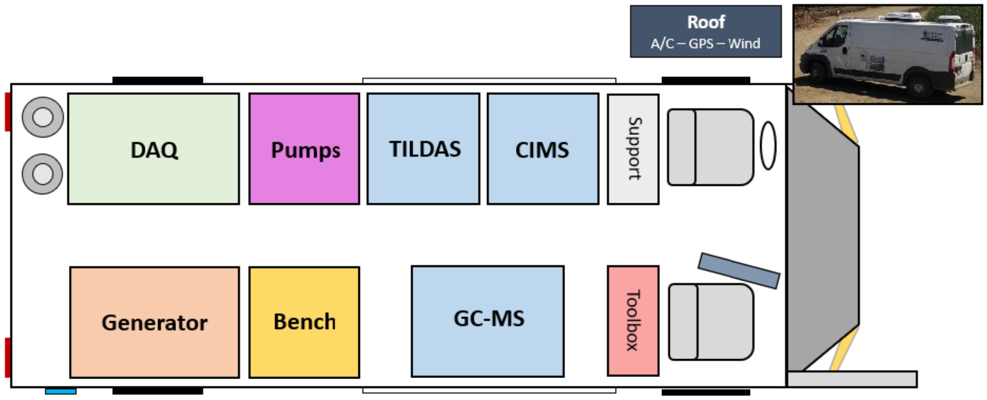


Figure 2. Schematic of an example instrument manifest in the minAML.

Typically, the commercial and research-grade instruments deployed are fast (1-2 s response), sensitive (good signal to noise) and selective (specific to a molecule). Output data saves to a robust archive (in the event of unscheduled shutdown) and displays real-time on a monitor for scientists to make in-project decisions. Common instruments include the proton transfer reaction mass spectrometer (PTR-MS) to quantify VOCs (*Krechmer et al., 2018*) and tunable infrared laser direct absorbance spectrometers (TILDAS) to quantify several small gaseous species (*McManus et al., 2015*). A sonic anemometer (2D or 3D) mounted on a sample mast measures wind speed and direction. A Hemisphere GPS (V103) compass determines position and orientation of the vehicle.

Tracer release methodology

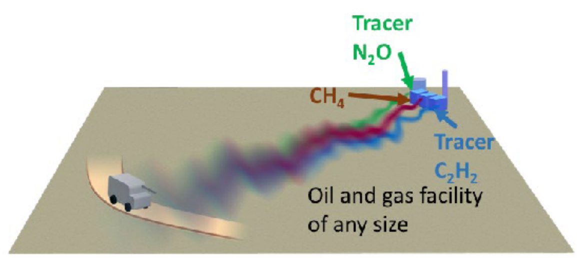


Figure 1. Field photo (left) and schematic (right) of a tracer release setup.

Tracer release has been used to quantify emissions at industrial facilities like natural gas well pads, compressor stations, and dairy farms (*Roscioli et al., 2015*). These studies rely on releasing small quantities of one or more tracer gases like nitrous oxide (N_2O) or acetylene (C_2H_2) at or near to a facility. Tracer gases co-disperse with site emissions like methane (CH_4) and are measured downwind by the mobile laboratory. The tracer release method compares the ratio of concentrations considering the known tracer release rate. This technique allows for accurate and complete facility-scale emission quantification, with typical uncertainties better than 30%.

Neighborhood pollution impact

Fast-response online measurement methods aboard the mobile laboratories enable us to map spatial gradients of emitted pollutants. **Figure 4** depicts the ground track of the AML as it quantifies 1,3-butadiene around residential areas near a ship channel in Houston, Texas. Colored by concentration of the pollutant, these transects produce a convincing picture of the upwind facility that is most likely emitting this chemical. In this example, the wind consistently comes out of the SSE. Analysis methods for converting mobile lab ground tracks into potential population exposures are described in Yacovitch et al., 2015.

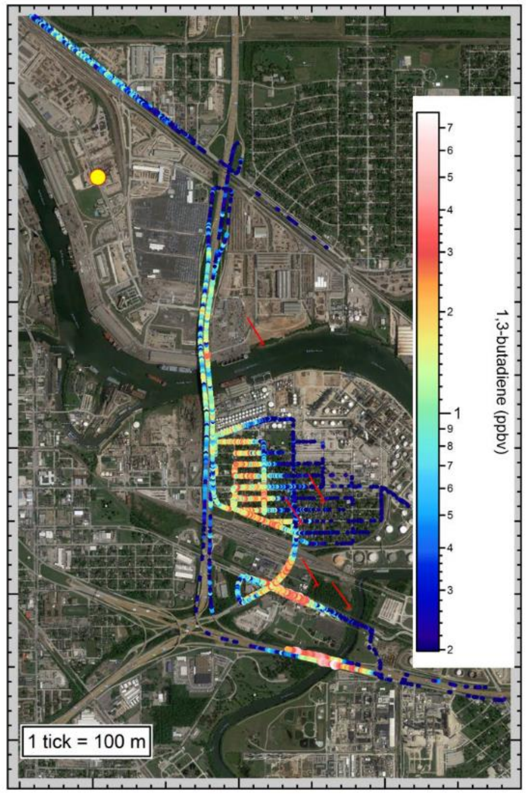


Figure 4. Concentration map of 1,3 butadiene overlaid on neighborhood street grid.

Fenceline surveys and leak detection

Operation of these mobile laboratories in a "surveillance mode" offers rapid detection and source identification of equipment leaks without emission rate quantification. The live data, wind and GPS position allow the scientist in the passenger seat to direct the driver closer and closer to a suspected leak location until it is pinpointed. Measured wind and Gaussian plume simulations are also used to determine source locations. For petrochemical facilities or refineries in particular, the chemical specificity available with the AML allows for a more complete and detailed accounting of individual VOC sources. Marker molecules and ratios between species provide insight into the type of emission being observed.

References

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Yacovitch, T. I., S. C. Herndon, J. R. Roscioli, C. Floerchinger, W. B. Knighton, and C. E. Kolb (2015), Air Pollutant Mapping with a Mobile Laboratory During the BEE-TEX Field Study, Environmental Health Insights (Supplementary File 15660), 7-13, doi:10.4137/EHI.S15660.

Scope of Work

Project 24-007
Texarkana Intensive Campaign

Prepared for:

Air Quality Research Program (AQRP)
The University of Texas at Austin

Prepared by:

James Flynn
University of Houston

Rebecca Sheesley
Sascha Usenko
Baylor University

Edward Fortner
Brian Lerner
Aerodyne Research, Inc.

September 12, 2024
Version #2

QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

Approvals

This Scope of Work was approved electronically on 2024-09-20 | 10:13:01 PDT
by Vincent M. Torres, The University of Texas at Austin

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Project Manager, Texas Air Quality Research Program

This Scope of Work was approved electronically on 2024-09-20 | 13:57:04 CDT
by Chola Regmi, Texas Commission on Environmental Quality

Signed by:
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Chola Regmi
Project Liaison, Texas Commission on Environmental Quality

Table of Contents

1 ABSTRACT

The Texarkana Texas (TX)-Arkansas (AR) metropolitan area has recently become an area of concern due to elevated fine Particulate Matter ($PM_{2.5}$) aerosol loadings. The area is forested and contains a few large paper mills which are one potential source of the PM. These paper mills are located in Texas, Arkansas, and Louisiana. There are other possible industrial sources of $PM_{2.5}$ and it is possible that the $PM_{2.5}$ is being advected into the area from sources well outside of the area. The upcoming changes to regulatorily acceptable $PM_{2.5}$ levels necessitate a better understanding of the cause of these enhanced $PM_{2.5}$ levels in the Texarkana area. A comprehensive study of the particle and gas phase chemical species associated with these $PM_{2.5}$ exceedance episodes will assist in interpreting the source of these air masses.

A three-week field deployment in Texarkana, TX during the February-March 2025 time period to examine the sources of high $PM_{2.5}$ loadings in the Texarkana area will be conducted. This study will obtain information regarding the chemical species present in these high loading events in both particle and gas phase. This information will better inform policymakers with respect to the health hazards associated with these higher aerosol loading events.

Objectives for this study include

1. Characterize selected $PM_{2.5}$ and Volatile Organic Compound (VOC) point sources in the Texarkana area.
2. Evaluate background $PM_{2.5}$ conditions in the vicinity, including upwind of the Texarkana TX-AR metropolitan area. Given the location of the metropolitan area this will likely involve measuring areas outside of the state of Texas but would not emphasize detailed emission factors for out-of-state sources.
3. Any highly local effects which might be present and impacting the measurement of $PM_{2.5}$ at the Texarkana New Boston Station (C1031) will be examined.

The University of Houston, Baylor University, and Aerodyne are nationally recognized for their experience in development and deployment of mobile air quality labs. These customizable, comprehensive, and dynamic platforms provide on-the-go monitoring and analysis of aerosol, VOCs, trace gas, boundary layer height and meteorological parameters. Texarkana's air quality is impacted by local sources, photochemical processing and transport from multiple regions. This complexity can be overcome with the deployment of mobile air quality laboratories which have several advantages in study areas such as Texarkana. These advantages include real-time monitoring, flexibility in sampling location and time, response to plumes or events (e.g., potential aerosol or precursor plumes), source characterization (e.g., upwind vs downwind), repeat measurements, and accessibility in complex environments.

2 BACKGROUND

The Texarkana TX-AR metropolitan area has recently become an area of concern due to elevated $PM_{2.5}$ aerosol loadings. The area is forested and contains a few large paper mills which are one potential source of the PM. These paper mills are located in Texas, Arkansas and Louisiana. There are other possible industrial sources of $PM_{2.5}$ and it is possible that the $PM_{2.5}$ is being advected into the area from sources well outside of the area. The upcoming changes to regulatorily acceptable $PM_{2.5}$ levels necessitate a better understanding of the cause of these enhanced $PM_{2.5}$ levels in the Texarkana area. A comprehensive study of the particle and gas phase chemical species associated with these $PM_{2.5}$ exceedance episodes will assist in interpreting the source of these air masses.

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3 OBJECTIVES

Objectives for this study include:

1. Characterize selected $PM_{2.5}$ and VOC point sources in the Texarkana area.
2. Evaluate background $PM_{2.5}$ conditions in the vicinity, including upwind of the Texarkana TX-AR metropolitan area. Given the location of the metropolitan area, this will likely involve measuring areas outside of the state of Texas but would not emphasize detailed emission factors for out of state sources.
3. Any highly local effects which might be present and impacting the measurement of $PM_{2.5}$ at the Texarkana New Boston Station (C1031) will be examined.

The University of Houston, Baylor University, and Aerodyne are nationally recognized for their experience in development and deployment of mobile air quality labs. These customizable, comprehensive, and dynamic platforms provide on-the-go monitoring and analysis of aerosol, VOCs, trace gas, boundary layer height and meteorological parameters. Texarkana's air quality is impacted by local sources, photochemical processing and transport from multiple regions. This complexity can be overcome with the deployment of mobile air quality laboratories which has several advantages in study areas such as Texarkana. These advantages include real-time monitoring, flexibility in sampling location and time, response to plumes or events (e.g., potential aerosol or precursor plumes), source characterization (e.g., upwind vs downwind), repeat measurements, and accessibility in complex environments.

4 TASK DESCRIPTIONS

The following tasks describe the work to be performed and specify the scope of the tasks, due dates, responsible organization(s), and deliverable(s) to successfully complete this project.

4.1 Develop Work Plan

A Scope of Work (this document), detailed budget and justification, and Quality Assurance Project Plan (QAPP) will be developed and delivered to the AQRP. The QAPP will be a composite of a measurement and research model development and application type of QAPP.

Due date: August 23, 2024.
Responsible organization: University of Houston with assistance from Baylor and Aerodyne
Deliverables: Approvable Work Plan

4.2 Project Preparations

Project preparations including planning, analysis of past weather conditions, available sampling routes, locations for stationing the mobile labs while not driving, vehicle and instrument maintenance, and payload integration will begin upon receipt of Notice to Commence and conclude prior to the field deployment phase.

Due date: Nominally January 31, 2025
Responsible organization: University of Houston with assistance from Baylor and Aerodyne.
Deliverables: Confirmation of plans and progress in the subsequent Monthly Technical Reports (MTR).

4.3 Field Deployment

Two mobile laboratories will be deployed, the University of Houston/Baylor Mobile Air Quality Lab #3 (MAQL3) and the miniature Aerodyne Mobile Lab (minAML) to the Texarkana, TX area for three consecutive weeks in February–March 2025. All trace gas measurements aboard the MAQL3 are 1 Hertz (Hz) and will include ozone (O_3) (chemiluminescence), nitric oxide (NO) (chemiluminescence), nitrogen oxides (NO_X) (chemiluminescence with photolytic nitrogen dioxide (NO_2) converter), reactive nitrogen compounds (NO_Y) (chemiluminescence with heated Mo inlet converter), carbon monoxide (CO) (off-axis cavity ringdown), sulfur dioxide SO_2 (pulsed fluorescence), and formaldehyde (HCHO) (Hantzch reaction). Aerosol measurements will primarily be 1 Hz when mobile and include size resolved non-refractory $PM_{2.5}$ chemical composition with a High-Resolution Time of Flight Aerosol Mass Spectrometer (HR-ToF-AMS), and $PM_{2.5}$ scattering (3λ nephelometry) and absorption (3λ absorption photometry). The HR-ToF-AMS will have a $PM_{2.5}$ lens installed which will allow for better quantification of particulate between 500nm–2.5 um improving the characterization of biomass burning and aged aerosols. Meteorological and GPS measurements will also be collected at 1 Hz and include temperature, relative humidity, pressure, wind speed and wind direction, zenith (2-π) NO_2 photolysis rate, latitude, longitude, altitude, and vehicle speed. A Vaisala ceilometer will measure boundary layer heights, and either be installed on the rear bumper as in prior deployments for TCEQ and NASA or over the cab.

The Aerodyne minAML will carry VOC focused instruments and includes the Vocus time-of-flight mass spectrometer (PTR-TOF) run in proton transfer reaction mode to quantify VOCs. To provide speciation and quantitation for isomeric compounds (e.g. C8 aromatic species: ethyl benzene, o-, m- and p-xylenes), the Vocus PTR-TOF can switch from direct ambient sampling to gas chromatograph (GC) pre-separation sampling. During routine, automated sampling, the Vocus will measure direct samples for 3.5 hours (typical) and a GC sample for 30 minutes (typical) during a repeated 4-hour measurement cycle. During intensive sampling periods, such as when performing source mapping or plume analysis, the Vocus will be switched to manual control where the Vocus PTR-TOF remains in direct sample mode until the operator initiates a GC sample analysis, typically while the mobile lab is parked in a target plume.

Due date: February–March 2025
Responsible organization: University of Houston with assistance from Baylor and Aerodyne
Deliverables: Documentation of deployment and preliminary data plots of field data in MTRs.

4.4 Final Data Preparation

Review and processing of field data will commence upon completion of the field deployment and final calibrations. Quality Assurance (QA)/ Quality Control (QC) data will be reviewed and included with the final data set.

Due date: Nominally May 31, 2025 to internal collaborators; within 30 days of project completion to AQRP.
Responsible organization: University of Houston with assistance from Baylor and Aerodyne
Deliverables: Documentation of final data processing in MTRs. Data to be delivered to AQRP within 30 days of project completion

4.5 Data analysis and final reporting

Primary data analysis will occur under this project, however, future projects may use the data to conduct more in-depth analysis and modeling of chemistry and meteorology. The primary analysis will be achieved by standard techniques such as correlation/regression. The information provided by these data will be useful in understanding pollution dynamics in this region and therefore in developing control strategies and determining whether local or regional controls may be best suited for this area.

The general statistics to be used are considered standard so little detail is provided here. Metrics to be used include averages, medians, standard deviations, diurnal profiles, and similar values. Time series will be inspected to identify commonalities, and regression analysis will be used to determine relationships between specific variables. Spatial analysis will identify areas of frequent high concentrations of pollutants and potential sources. These methods will be applied to both the output data generated from the measurements as well as to parameters derived from these measurements such as photochemical age, the ratio of NO_X to NO_Y, etc.

Aerosol data analysis will include calculation of scattering and absorption angstrom exponents to identify periods when aerosol optical properties indicate influence of dust and biomass burning above background conditions. The HR-ToF-AMS data will be analyzed using standard software developed by the HR-ToF-AMS community within Igor Pro® (https://www.wavemetrics.com/). The software allows for determination of the time series of the concentrations of inorganic $PM_{2.5}$ species, as well as that of the total organic $PM_{2.5}$ concentration. High resolution peak fitting of the AMS dataset will shed light on organic, sulfate, nitrate, chloride, and ammonium mass loadings based on the quantification of fit peaks such as Sulfur monoxide (SO) and SO_2, among others, for sulfate. High resolution fitting of AMS peaks will also be useful to determine the presence of tracers for specific sources, for example a peak fit at acetic acid ($C_2H_4O_2$+) may indicate the influence of biomass burning.

As specified in Section 7 of this Scope of Work, AQRP requires the regular and timely submission of monthly technical, monthly financial status and quarterly reports as well as an abstract at project initiation and, near the end of the project, submission of the draft final and final reports. Additionally, at least one member of the project team will attend and present at the AQRP data workshop. For each report deliverable, one report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The project's Principal Investigator (PI) (or their designee) will electronically submit each report to both the AQRP Project Manager (PM) and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. The report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

**Draft copies of any planned presentations (such as at technical conferences) or manuscripts to be submitted for publication resulting from this project will be provided

to both the AQRP PM and TCEQ liaisons per the Publication/Publicity Guidelines included in Attachment G of the subaward.**
Finally, our team will prepare and submit our final project data and associated metadata to the AQRP archive.

Due Date: The schedule for Task 4.5 Deliverables are shown in Section 7.
Responsible organization: University of Houston with assistance from Baylor and Aerodyne
Deliverables: Abstract, monthly technical reports, monthly financial status reports, quarterly reports, draft final report, final report, attendance and presentation at AQRP data workshop, submissions of presentations and manuscripts, project data and associated metadata.

5 PROJECT PARTICIPANTS AND RESPONSIBILITIES

Below is a bulleted list that summarizes the individual participants and their responsibilities.

University of Houston

- James Flynn, Project PI – Responsible for overall project management and reporting as well as providing oversight for instrument preparation and deployment. Will coordinate all team efforts as well as ensuring the field measurements and mobile labs are maintained and operated in a responsible manner.

Baylor University

- Sascha Usenko, Co-PI - Responsible for leading the AMS deployment in MAQL3 and providing operational support to the science team.
- Rebecca Sheesley, Co-PI – Responsible for leading the aerosol optical measurement collection, analysis, and interpretation of the aerosol data and the apportionment of dust and biomass burning sources.

Aerodyne Research, Inc.

- Edward Fortner, Co-PI - Responsible for leading the minAML deployment. Will assist in project planning and coordination of daily deployment plans.
- Brian Lerner, Co-PI - Responsible for VOCUS operation and VOCUS data analysis and interpretation. Will assist in project planning.

6 NOMINAL TIMELINE

Task and description	Timeline
4.1 Develop Work Plan	August 9–23, 2024
4.2 Project preparations	Receipt of Notice to Commence through the beginning of field deployment
4.3 Field Deployment	Three consecutive weeks in February–March 2025
4.4 Final Data Preparation	April–May 2025
4.5 Data Analysis and Final Reporting	Data analysis will occur June–August 2025. Reporting will be continuous from Notice to Commence through October 15, 2025 (FSR 14). Draft Final Report due August 1, 2025, AQRP presentations in August 2025, Final Report due August 31, 2025. Additional details on specific project reporting can be found in Section 7.

7 DELIVERABLES

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below.
One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The Project PI will submit the reports unless that responsibility is otherwise delegated with the approval of the AQRP Project Manager.
All reports will be written in the third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

Abstract: At the beginning of the project, an Abstract will be submitted to the AQRP 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.

Abstract Due Date: August 23, 2024

Quarterly Reports: Each Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the AQRP Project Manager as a Microsoft Word 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.

Quarterly Report Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	August, September, October 2024	October 31, 2024
Quarterly Report #2	November, December 2024, January 2025	January 31, 2025
Quarterly Report #3	February, March, April 2025	April 30, 2025
Quarterly Report #4	May, June, July 2025	July 31, 2025

DUE TO PROJECT MANAGER

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the AQRP Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP MTR Template found on the AQRP website. Note that MTRs will continue on the same schedule through October 2025.

MTR Due Dates:

Report	Period Covered	Due Date
Technical Report #1	Project Start–August 31, 2024	September 10, 2024
Technical Report #2	September 1–30, 2024	October 10, 2024
Technical Report #3	October 1–31, 2024	November 10, 2024
Technical Report #4	November 1–30, 2024	December 10, 2024
Technical Report #5	December 1–31, 2024	January 10, 2025
Technical Report #6	January 1–31, 2025	February 10, 2025
Technical Report #7	February 1–28, 2025	March 10, 2025
Technical Report #8	March 1–31, 2025	April 10, 2025
Technical Report #9	April 1–30, 2025	May 10, 2025
Technical Report #10	May 1–31, 2025	June 10, 2025
Technical Report #11	June 1–30, 2025	July 10, 2025
Technical Report #12	July 1–31, 2025	August 10, 2025

DUE TO PROJECT MANAGER

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey) by each institution on the project using the AQRP FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
FSR #1	Project Start–August 31, 2024	September 15, 2024
FSR #2	September 1–30, 2024	October 15, 2024
FSR #3	October 1–31, 2024	November 15, 2024
FSR #4	November 1–30, 2024	December 15, 2024
FSR #5	December 1–31, 2024	January 15, 2025
FSR #6	January 1–31, 2025	February 15, 2025
FSR #7	February 1–28, 2025	March 15, 2025
FSR #8	March 1–31, 2025	April 15, 2025
FSR #9	April 1–30, 2025	May 15, 2025
FSR #10	May 1–31, 2025	June 15, 2025
FSR #11	June 1–30, 2025	July 15, 2025
FSR #12	July 1–31, 2025	August 15, 2025
FSR #13	August 1–31, 2025	September 15, 2025
FSR #14	Final FSR	October 15, 2025

DUE TO GRANT MANAGER

Draft Final Report: A Draft Final Report will be submitted to the AQRP 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.

Draft Final Report Due Date: August 15, 2025

Final Report: A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the AQRP 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.

Final Report Due Date: August 31, 2025

Project Data: All project data including but not limited to quality assurance (QA) and quality control (QC) measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (August 31, 2025). 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 of August 2025.

Presentations and Publications/Posters: All data and other information developed under this project, which is included in **published papers, symposia, presentations, press releases, websites and/or other publications** shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Subaward.

8 REFERENCES

Anderson, D. C., J. Pavelec, C. Daube, S. C. Herndon, W. B. Knighton, B. M. Lerner, J. R. Roscioli, T. I. Yacovitch, and E. C. Wood (2019), Characterization of ozone production in San Antonio, Texas, using measurements of total peroxy radicals, *Atmos. Chem. Phys.*, *19*(5), 2845-2860, doi:10.5194/acp-19-2845- 2019

Claflin, M. S., Pagonis, D., Finewax, Z., Handschy, A. V., Day, D. A., Brown, W. L., Jayne, J. T., Worsnop, D. R., Jimenez, J. L., Ziemann, P. J., de Gouw, J., and Lerner, B. M.: An in situ gas chromatograph with automatic detector switching between PTR- and EI-TOF-MS: isomer-resolved measurements of indoor air, Atmos. Meas. Tech., 14, 133–152, https://doi.org/10.5194/amt-14-133-2021, 2021.

Fangzhou Guo, Alexander A.T. Bui, Benjamin C. Schulze, Subin Yoon, Sujan Shrestha, Henry W. Wallace, Yuta Sakai, Blake W. Actkinson, Matthew H. Erickson, Sergio Alvarez, Rebecca Sheesley, Sascha Usenko, James Flynn, Robert J. Griffin, Urban core-downwind differences and relationships related to ozone production in a major urban area in Texas, Atmospheric Environment, Volume 262, 2021, 118624, https://doi.org/10.1016/j.atmosenv.2021.118624.

Krechmer, J., et al. (2018), Evaluation of a New Reagent-Ion Source and Focusing Ion–Molecule Reactor for Use in Proton-Transfer-Reaction Mass Spectrometry, Anal. Chem., 90(20), 12011-12018, doi:10.1021/acs.analchem.8b02641.

Sujan Shrestha, Subin Yoon, Matthew H. Erickson, Fangzhou Guo, Manisha Mehra, Alexander A.T. Bui, Benjamin C. Schulze, Alexander Kotsakis, Conner Daube, Scott C. Herndon, Tara I. Yacovitch, Sergio Alvarez, James H. Flynn, Robert J. Griffin, George P. Cobb, Sascha Usenko, Rebecca J. Sheesley, Traffic, transport, and vegetation drive VOC concentrations in a major urban area in Texas, Science of The Total Environment, Volume 838, Part 2, 2022, 155861, https://doi.org/10.1016/j.scitotenv.2022.155861.

Budget and Budget Justification

Project 24-007
Texarkana Intensive Campaign

Prepared for:

Air Quality Research Program (AQRP)
The University of Texas at Austin

Prepared by:

James Flynn
University of Houston

Rebecca Sheesley
Sascha Usenko
Baylor University

Edward Fortner
Brian Lemer
***Aerodyne Research, Inc*.**

August 23, 2024
Version #1

QA Requirements: Audits of Data Quality: 10% Required
Report of QA Findings: Required in Final Report

NOTE: The Workplan package consists of three independent documents: Scope of Work, Quality Assurance Project Plan (QAPP), and budget and justification. Please deliver each document (as well as all subsequent documents submitted to AQRP) in Microsoft Word format.

Approvals

This Budget was approved electronically on 2024-09-20 | 12:11:44 CDT
by RoseAnna Goewey, The University of Texas at Austin

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RoseAnna Goewey
Program Manager, Texas Air Quality Research Program

This Budget was approved electronically on 2024-09-20 | 10:13:01 PDT
by Vince Torres, The University of Texas at Austin

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Vince Torres
Project Manager, Texas Air Quality Research Program

This Budget was approved electronically on 2024-09-20 | 13:57:04 CDT
by Chola Regmi, Texas Commission on Environmental Quality

Signed by:
Chola Regmi
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Chola Regmi
Project Liaison, Texas Commission on Environmental Quality

Budget and Budget Justification

Texarkana Intensive Campaign
AQRP Budget Summary

Principal Investigator: James Flynn

Project Dates: 08/01/2024 - 08/31/2025

A. SENIOR PERSONNEL: PI, Co-PI						
	FirstName LastName	**Title**	**Monthly Rate**	**Fringe Rate**	**FTE / % Effort**	**Funds Requested**
1.	James Flynn	Research Associate Profes	$8,352	25.9%	2.00	$16,703
2.			$0	0.0%	0.00	$0
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$16,703**
B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)						
1	1	Other Professionals / Postdoctoral Fellow	$4,040	39.8%	2.00	$8,080
2	1	Other Professionals / Researcher 4	$5,244	30.3%	3.50	$18,355
3	1	Other Professionals / Researcher 3	$4,633	31.9%	1.00	$4,633
4	1	Other Professionals / Research Tech Supervisor	$3,805	34.8%	3.00	$11,415
	TOTAL OTHER PERSONNEL					**$42,483**
	TOTAL SALARIES AND WAGES (A+B)					**$59,186**
C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)						
1.	Senior Personnel					**$4,323**
2.	Other Personnel					**$14,232**
	TOTAL FRINGE BENEFITS					**$18,555**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					**$77,741**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)						
a)						$0
b)						$0
c)						$0
	TOTAL EQUIPMENT					**$0**
E. TRAVEL			**Cost per Trip**	**# of Trips**		
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)		$250	2		$500
2.	Field deployment		$4,252	3		$12,756
						$13,256
F OTHER DIRECT COSTS						
1.	Materials and Supplies					$30,075
2.	Professional Services - Idependent Contractors					$0
3.	Subcontracts (contracts will be issued by UT)					
a)	Baylor University					$88,951
b)	Aerodyne					$76,519
c)						$0
d)						$0
4.	Tuition and Fees					$0
5.	Other	RV Pad Rentals				$4,348
	TOTAL OTHER DIRECT COSTS					**$199,893**
G. TOTAL DIRECT COSTS (A THROUGH F)						**$290,890**
H. TOTAL INDIRECT COSTS (MTDC)			**IDC Rate:**	15.000%		**$18,813**
I. TOTAL COSTS						**$309,703**

NOTE: *Please indicate whether you are using Modified Total Direct Costs (MTDC) or Total Direct Costs (TDC) in the calculation of Indirect Costs (IDC). You may modify this template as needed to show calculation of direct or indirect costs or other project specific budgetary needs.*

University of Houston Budget & Justification

University of Houston
Texarkana Intensive Campaign
AQRP Budget

Principal Investigator: James Flynn

Project Dates: 08/01/2024 - 08/31/2025

A. SENIOR PERSONNEL: PI, Co-PI						
	FirstName LastName	**Title**	**Monthly Rate**	**Fringe Rate**	**FTE / % Effort**	**Funds Requested**
1.	James Flynn	Research Associate Profes	$8,352	25.9%	2.00	$16,703
2.			$0	0.0%	0.00	$0
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$16,703**
B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)						
1	1	Other Professionals / Postdoctoral Fellow	$4,040	39.8%	2.00	$8,080
2	1	Other Professionals / Researcher 4	$5,244	30.3%	3.50	$18,355
3	1	Other Professionals / Researcher 3	$4,633	31.9%	1.00	$4,633
4	1	Other Professionals / Research Tech Supervisor	$3,805	34.8%	3.00	$11,415
	TOTAL OTHER PERSONNEL					**$42,483**
	TOTAL SALARIES AND WAGES (A+B)					**$59,186**
C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)						
1.	Senior Personnel					**$4,323**
2.	Other Personnel					**$14,232**
	TOTAL FRINGE BENEFITS					**$18,555**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					**$77,741**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)						
a)						$0
b)						$0
c)						$0
	TOTAL EQUIPMENT					**$0**
E. TRAVEL			**Cost per Trip**	**# of Trips**		
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)		$250	**2**		$500
2.	Field deploymnet		$4,252	**3**		$12,756
	TOTAL TRAVEL					**$13,256**
F OTHER DIRECT COSTS						
1.	Materials and Supplies					$30,075
2.	Professional Services - Idependent Contractors					$0
3.	Subcontracts (contracts will be issued by UT)					
	a)					
	b)					
	c)					$0
	d)					$0
4.	Tuition and Fees					$0
5.	Other	RV Pad Rentals				$4,348
	TOTAL OTHER DIRECT COSTS					**$34,423**
G. TOTAL DIRECT COSTS (A THROUGH F)						**$125,420**
H. TOTAL INDIRECT COSTS (MTDC)			**IDC Rate:**	**15.000%**		**$18,813**
I. TOTAL COSTS						**$144,233**

NOTE: *Please indicate whether you are using Modified Total Direct Costs (MTDC) or Total Direct Costs (TDC) in the calculation of Indirect Costs (IDC).*
You may modify this template as needed to show calculation of direct or indirect costs or other project specific budgetary needs.

A. SALARIES

Dr. James Flynn, Co-Principal Investigator, 15.4% effort over 13 months, will be responsible for the overall project management and reporting requirements. He will advise Travis Griggs, Sergio Alvarez, and Alexandra Ulinski on the preparation and operation of the MAQL3 and oversee their efforts on the subsequent data analysis. PI Flynn will also deploy to the field to help coordinate the operations and be the primary driver of the MAQL3.

Sergio Alvarez, Researcher 4, 26.9% effort over 13 months, will lead the preparation, operation, and calibration of the instruments deployed in the MAQL3. He will also lead the data processing and analysis team and will oversee the quality assurance of the data. He will assist James Flynn with the management and reporting activities.

Dr. Travis Griggs, Postdoc, 15.4% effort over 13 months, will assist with the instrument preparation and calibration prior to the deployment and operations during the campaign. He will also assist Sergio Alvarez with the data processing and analysis after the field measurements.

Alexandra Ulinski, 23% effort over 13 months, will assist with the instrument preparation, calibration, and field deployment. While in the field Alexandra will conduct the preliminary data processing for quick-look plots to inform next steps and aid in the early identification with potential instrument issues. She will also assist Sergio Alvarez with the data processing and analysis after the field measurements.

Eugenia Velasco, Researcher 2, 7.7% effort over 13 months, will assist with the various reporting requirements associated with this project as well as reviewing and ensuring proper formatting and accessibility requirements are met for the deliverables.

Total salary budget requested: $59,186.

C. FRINGE BENEFITS

The Department of Health and Human Services (DHHS) has given its approval to budget fringe at actual cost rather than a percentage of the salary. A fringe benefits calculator has been developed as a tool to assist in calculating the fringe benefits for sponsored research budgets. The calculator can be found on the University of Houston’s Division of Research Website.

Total fringe benefits budget requested: $18,555.

E. TRAVEL

Texarkana field deployment ($12,756) – We request support for field travel for three people to deploy the MALQ3 to Texarkana for three weeks. Lodging and meal expenses are based on the current GSA and TexTravel rates. Funds are also included to rotate field personnel during the deployment. Given the number of people and duration, a short-term rental may be used instead of individual hotel rooms to allow greater flexibility in meal options, however the per person-night rate would stay within set allowances.

Presentations ($500) – Support for two personnel to travel ($250 x 2) to Austin, Texas to participate in the AQRP workshop in August 2025 are also requested. Travel costs in this budget are based on sponsored research travel for previous similar trips and are calculated for domestic travel.

Total travel budget requested: $13,256.

F. OTHER DIRECT COSTS

MATERIALS AND SUPPLIES

Vehicle operations ($14,075) – We request support for the mobile lab and support vehicle fuel ($9,075). This estimate is based on recent fuel process, mileage, round trip distance between Houston and Texarkana, and anticipated amount of driving in Texarkana and the surrounding area. A support truck will carry additional supplies to and from the field as well as provide local transportation while deployed to Texarkana. An additional usage fee to support maintenance such as oil and filter changes on the truck and generator, tires, air suspension, etc. on the MAQL3 and the various subsystems of $5,000 is also included.

Instrument support ($16,000) – We request support for the preparation, installation, operation, and maintenance of the UH instruments and data systems which will be deployed in the MAQL3 in support of this campaign. Included in these costs are tubing and fittings ($2,500), calibration and consumable gases ($3,000), internet connectivity ($500), instrument maintenance items ($5,000), and a contingency amount of $5,000 to support unexpected preparation and field related expenses.

Total materials and supplies budgeted requested: $30,075.

OTHER COSTS

RV Pad Rental - UH will cover renting three RV pads ($4,347) (two for UH/MAQL3 and one for Aerodyne). UH was originally hosting the mobile labs at the UTEP monitoring site to provide space and power at no cost. The revised scope of work in the Texarkana area will require the RV pad rental to provide safe parking and access to suitable electrical connections.

Total Other Cost requested: $4,347.

SUBCONTRACT(S)

Aerodyne: Aerodyne will be a subcontractor under this project and will be contracted through UT Austin's Subaward Agreement. The costs associated for the subcontract are $76,519 for the period of 08/01/2024 through 08/31/2025. The subcontractor will be responsible for deploying the instrumented minAML and collecting VOC measurements in conjunction with the MAQL3 as described in the proposal. The subcontractor will also contribute to the project planning, analysis, reporting, and presentation.

Baylor University (BU): BU will be a subcontractor under this project and will be contracted through UT Austin's Subaward Agreement. The costs associated for the subcontract are $88,951 for the period of 08/01/2024 through 08/31/2025. The subcontractor will be responsible preparing, integrating, operating, and finalizing data from the aerosol instrumentation in the MAQL3 as described in the proposal. The subcontractor will also contribute to the project planning, analysis, reporting, and presentation.

Total subaward budget requested: $165,470

H. INDIRECT COSTS

The indirect cost rate of 15% of modified total direct costs (MTDC) is used as instructed by the AQRP's published proposal preparation instructions. Modified total direct costs shall exclude equipment, capital expenditures, charges for patient care, rental costs, tuition remission, scholarships and fellowships, participant support costs and the portion of each subaward in excess of $25,000.

Total indirect cost budget requested: $18,813.

Baylor University Budget & Justification

AQRP Budget

Principal Investigator: Dr. Rebecca Sheesley

Project Dates: 08/01/2024 to 07/31/2025

	FirstName LastName	Title	Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
A. SENIOR PERSONNEL: PI, Co-PI						
1.	Rebecca Sheesley	Professor	$15,152	29.5%	0.10	$1,515
2.	Sascha Usenko	Professor	$13,563	29.5%	0.10	$1,356
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$2,871**
B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)						
1	1	Other Professionals / Postdoctoral Fellow	$3,958	29.5%	5.00	$19,792
2	0	Other Professionals / UPDATE TITLE	$0	0.0%	0.00	$0
3	0	Graduate Student	$0	0.0%	0.00	$0
	TOTAL OTHER PERSONNEL					**$19,792**
	TOTAL SALARIES AND WAGES (A+B)					**$22,663**
C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)						
1.	Senior Personnel					**$847**
2.	Other Personnel					**$5,839**
	TOTAL FRINGE BENEFITS					**$6,686**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)					**$29,349**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)						
a)						$0
b)						$0
c)						$0
	TOTAL EQUIPMENT					**$0**
E. TRAVEL			**Cost per Trip**	**# of Trips**		
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)		$8,000	1		$8,000
2.	Foreign					$0
	TOTAL TRAVEL					**$8,000**
F OTHER DIRECT COSTS						
1.	Materials and Supplies					$40,000
2.	Professional Services - Idependent Contractors					$0
3.	Subcontracts (contracts will be issued by UT)					
	a)					$0
	b)					$0
	c)					$0
	d)					$0
4.	Tuition and Fees					$0
5.	Other					$0
	TOTAL OTHER DIRECT COSTS					**$40,000**
G. TOTAL DIRECT COSTS (A THROUGH F)						**$77,349**
H. TOTAL INDIRECT COSTS			**IDC Rate:**	15.000%		**$11,602**
I. TOTAL COSTS						**$88,951**

NOTE: *Please indicate whether you are using Modified Total Direct Costs (MTDC) or Total Direct Costs (TDC) in the calculation of Indirect Costs (IDC). You may modify this template as needed to show calculation of direct or indirect costs or other project specific budgetary needs.*

A. SALARIES

Dr. **Rebecca Sheesley, Principal Investigator, 0.77% effort,** will be responsible for oversight of aerosol optical measurements, contributions to field design and analysis of aerosol optical and composition data.

Dr. Sascha Usenko, Co-Investigator, 0.77% effort, will be responsible for oversight of aerosol composition measurements, contributions to field design and analysis of aerosol optical and composition data.

Post doctoral associate (TBD), 38.46% effort, will perform aerosol instrument preparation, assist in field deployment and data analysis.

B. FRINGE BENEFITS

The fringe benefit rates used in the proposal budget are based on the rates approved by the Department of Health and Human Services (DHHS, 5/30/2023). Fringe benefits are calculated as 29.5% of salary for faculty and staff. The rate for part-time employees is 13.6%.

Total fringe benefits budget requested: $6,686.

C. EQUIPMENT

NA

E. TRAVEL

Funds are requested for project personnel to travel to El Paso for a 3-week field campaign and 3 day travel to Houston for field deployment preparation. Travel costs in this budget are based on sponsored research travel for previous similar trips and are calculated for the domestic travel of two to take a trip to El Paso, a trip to Houston and a day trip to Austin (AQRP meeting).

Total travel budget requested: $8,000.

F. OTHER DIRECT COSTS

MATERIALS AND SUPPLIES

Supplies are calculated at $36,923 per year to cover the deployment of three aerosol instruments, HR-TOF-AMS, TAP and nephelometer, including: instrumental consumables, field supplies and consumables, office supplies and consumables, computers and computer parts, lab supplies and consumables, storage, hardware, safety, training, and instrumentation rentals. Supplies may also cover software such as but not limited to data handling, storage, acquisition, data processing, figure creation, and training.

Total materials and supplies budgeted requested: $40,000.

TUITION
NA

SUBCONTRACT(S)
NA

H. INDIRECT COSTS

The indirect cost rate of 15% of modified/total direct costs (MTDC/TDC) is used as instructed by the AQRP's published proposal preparation instructions. MTDC is calculated as the total of direct costs, less [equipment in excess of $5,000 and less tuition remission applied to GRA salary].

Total indirect cost budget requested: $11,602.

Aerodyne Budget and Justification

AQRP Budget

Principal Investigator: Dr. Edward Fortner & Dr. Brian Lerner

Project Dates: 08/01/2024 - 08/31/2025

A. SENIOR PERSONNEL: PI, Co-PI						
	FirstName LastName	**Title**	**Monthly Rate**	**Labor Overhead**	**FTE / % Effort**	**Funds Requested**
1.	Edward Fortner	Principal Investigator	$9,251	140.0%	5%	$6,351
2.	Brian Lerner	Co-Principal Investigator	$9,916	140.0%	5%	$6,465
3.			$0	0.0%	0%	$0
	TOTAL SENIOR PERSONNEL					**$12,816**
B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)						
1	1	Mr. Conner Daube / Manager of Field Measurement Servc	$7,174	140.0%	4%	$3,932
2	1	TBD / Instrument Scientst	$8,667	140.0%	4%	$4,750
3	0	Graduate Student	$0	0.0%	0%	$0
	TOTAL OTHER PERSONNEL					**$8,682**
	TOTAL SALARIES AND WAGES (A+B)					**$21,498**
C. LABOR OVERHEAD (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)						
1.	Senior Personnel					$17,942
2.	Other Personnel					$12,155
	TOTAL LABOR OVERHEAD					**$30,097**
	TOTAL SALARIES, WAGES AND LABOR OVERHEAD (A+B+C)					**$51,595**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)						
a)						$0
b)						$0
c)						$0
	TOTAL EQUIPMENT					**$0**
E. TRAVEL			**Cost per Trip**	**# of Trips**		
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)		$12,264	1		$12,264
2.	Domestic (Incl. Canada, Mexico and U.S. Possessions)		$2,679	1		$2,679
3.	Foreign					
	TOTAL TRAVEL					**$14,943**
F OTHER DIRECT COSTS						
1.	Materials and Supplies					$0
2.	Professional Services - Idependent Contractors					$0
3.	Subcontracts (contracts will be issued by UT)					
	a)					$0
	b)					$0
	c)					$0
	d)					$0
4.	Tuition and Fees					$0
5.	Other					$0
	TOTAL OTHER DIRECT COSTS					**$0**
G. TOTAL DIRECT COSTS (A THROUGH F)						**$66,538**
H. TOTAL INDIRECT COSTS			**IDC Rate:**	15.000%		**$9,981**
I. TOTAL COSTS						**$76,519**

NOTE: Please indicate whether you are using Modified Total Direct Costs (MTDC) or Total Direct Costs (TDC) in the calculation of indirect costs (IDC).

You may modify this template as needed to show calculation of direct or indirect costs or other project specific budgetary needs.

AERODYNE RESEARCH, INC.
Texarkana Intensive Campaign
AQRP Budget Justification

A/B. SALARIES for Senior and Other Personnel

Dr. Edward Fortner, Principal Investigator, 5.3% effort, will be responsible for project management, reporting, campaign planning and execution.

Dr. Brian Lerner, Co-Principal Investigator, 5% effort, will be responsible for data analysis, final data quality assurance will assist in campaign planning and execution and contribute to reports.

Mr. Conner Daube, Manager of Field Measurement Services, 4.2% effort, will be responsible for campaign planning and execution and instrument integration.

TBD, Senior Research/Instrument Scientist, 4.2% effort, will perform instrument operation and limited preliminary data analysis while assisting in campaign planning and execution.

Total salaries budget requested: $21,498.

C. LABOR OVERHEAD

Aerodyne Research, Inc. (ARI) charges 140% overhead on the direct labor portion of its grants and contracts. Labor Overhead rates cover Indirect Labor, Facility Expenses, Leave and Fringe Benefits.
Total labor overhead requested: $30,097.

E. TRAVEL

Funds are requested for a 3-week field campaign in Texarkana. Table 1 outlines the costs associated with 4 personnel travelling to Texarkana to conduct the field campaign. Table 2 outlines the costs associated with 2 personnel transporting the mobile lab to Texarkana from Billerica, MA and back including associated charges. Travel costs in this budget are based on actual costs of flights, rental cars and hotel, sponsored research travel for previous similar trips and U.S. GSA rates.

Table 1: Texarkana Field Campaign Staffing Costs. Other transportation includes costs for rental car gas.

Origin	Billerica MA		
Destination	Texarkana, TX		
Purpose			
# Persons	4		
# Days	11		
# Nights	10		
COST ITEM	ITEM UNITS	UNIT RATE	ITEM COST
Air Fare	3	600	1,800
Daily Car Rent	21	100	2,100
Daily Lodging	40	107	4,280
Daily Meals	44	59	2,596
Airport Shuttle	6	115	690
Onsite Gas for Mini AML	4,200	3.1	766
Other Transportation	210	3.1	33
Total Cost Per Trip			12,264
Number of Trips			1
Total Estimated Cost			12,264

Table 2: Round trip transportation and usage costs of the MinAML mobile lab

Origin	Billerica MA		
Destination	Texarkana, TX		
Purpose			
# Persons	2		
# Days	3		
# Nights	2		
COST ITEM	ITEM UNITS	UNIT RATE	ITEM COST
Air Fare	2	350	700
Daily Car Rent	0	100	0
Daily Lodging	6	107	642
Daily Meals	4	59	236
Airport Shuttle	2	115	230
Mini AML Fuel	2,387	3.1	871
Total Cost Per Trip			2,679
Number of Trips			1
Total Estimated Cost			2,679

Total travel budget requested: $14,943.

H. INDIRECT COSTS (General &Administration)

Aerodyne Research, Inc. (ARI) charges a 15% G&A on direct labor, overhead, equipment purchases, travel, consulting services, and other direct costs to cover B&P and IR&D, Finances and Management. Our cognizant federal auditor, the Department of Energy, annually audits costs actually incurred and determines final indirect cost application rates. The Contracting Officer at DOE's Office of Grants and Cooperative Agreements and Office of Science Consolidated Service Center is Emiela M. Bradford, Phone: 630-385-0562, emiela.bradford@science.doe.gov. Please contact Ms. Bradford to discuss indirect cost application rates and any other matters pertinent to the company's contracting relationship with the federal government. A copy of our provisional Indirect Cost Rate Agreement can be provided upon request.

Total indirect cost budget requested: $9,981.

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