Abstract

Project 24-003
Improving Emission Rates Estimates of Commercial Marine Vessels

The Texas Commission on Environmental Quality (TCEQ) relies on emission inventories to shape the State Implementation Plan (SIP), crucial for managing air pollutants such as nitrogen oxides (NO_X) and ozone (O_3). Recognizing the significance of reliable data, the team of the University of Houston (UH) and Ramboll propose this research project to address the research priority identified by the Air Quality Research Program (AQRP) to improve emission inventories for commercial marine vessels (CMV).

CMV emissions, particularly NO_X, constitute a substantial portion of coastal NO_X emissions. In the Houston-Galveston-Brazoria nonattainment area, CMVs accounted for approximately 18% of NO_X emissions in 2019, with a continued significant contribution expected for years to come. Among different vessel categories, smaller commercial vessels, notably towboats, were responsible for about 42% of CMV NO_X emissions in Texas in 2019 (TCEQ, 2023). Towboat and tugboat emissions have greater uncertainty than other CMV categories due to the lack of information on engines and the uncertainties of engine loads and operating parameters. This proposal aims to improve our understanding of commercial marine exhaust emissions, focusing on NO_X, volatile organic compounds (VOC), $PM_{2.5}$, and hydrocarbon speciation. The emphasis on smaller vessels will improve our ability to intercept their exhaust plumes.

Employing the instrumented UH research boat, our approach involves sampling emission plumes from vessels downwind of busy shipping lanes in Galveston Bay. Plumes will be identified by elevated levels of carbon dioxide (CO_2), NO_X, and other compounds. We expect to sample plumes from hundreds of towboats to meaningfully constrain the emission inventory. Leveraging real-time Automatic Identification System (AIS) transponder data, which reports vessel identification, position, speed, and draft, enhances our ability to connect measured plumes to individual vessels and ascertain engine information.

Emissions rates, derived from the field measurement data, will be compared with EPA expected values for each of the sampled and identified vessel engines. Multiple encounters with the same vessel over the sampling period will provide insights into emission variability. The analysis results have the potential to enhance the accuracy of the commercial marine emission inventory and speciated VOC reactivity. Such improvement can be integrated into various modeling frameworks, including those utilized for SIP modeling that support air quality planning efforts.

Quality Assurance Project Plan

Project 24–003

Improving Emission Rates Estimates of Commercial Marine Vessels

Prepared for:

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

Prepared by:

James Flynn
University of Houston

Chris Lindhjem
Ramboll

Jerker Samuelsson
FluxSense

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: Measurement & Secondary Data Products. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

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

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

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the Improving Emission Rates Estimates of Commercial Marine Vessels project. The Principal Investigator (PI) for the project is James Flynn and the Co-PIs are Chris Lindhjem and Jerker Samuelsson.

Electronic Approvals:

This QAPP was approved electronically on 2024-09-20 | 12:10:52 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 | 12:10:52 PDT
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Quality Assurance Project Plan Manager, Texas Air Quality Research Program

This QAPP was approved electronically on 2024-09-20 | 14:53:33 CDT
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TCEQ Liaison, Texas Commission on Environmental Quality

This QAPP was approved electronically on 2024-09-20 | 11:32:40 PDT
by James Flynn, University of Houston

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Principal Investigator, University of Houston

QAPP Distribution List

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Chris Lindhjem, Co-Investigator

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Jerker Samuelsson, Co-Investigator

1. PROJECT DESCRIPTION AND OBJECTIVES

1.1. PROCESS AND/OR ENVIRONMENTAL SYSTEM TO BE EVALUATED

The Texas Commission on Environmental Quality (TCEQ) relies on emission inventories to develop the State Implementation Plan (SIP), crucial for managing air pollutants such as nitrogen oxides (NO_X) and ozone (O_3). Recognizing the significance of reliable data, the team of the University of Houston (UH) and Ramboll propose this research project to address the research priority identified by the Air Quality Research Program (AQRP) to improve emission inventories for commercial marine vessels (CMV).

CMV emissions, particularly NO_X, constitute a substantial portion of coastal NOx emissions. In the Houston-Galveston-Brazoria nonattainment area, CMVs accounted for approximately 18% of NOx emissions in 2019, with a continued significant contribution expected for years to come. Among different vessel categories, smaller commercial vessels, notably towboats, were responsible for about 42% of CMV NOx emissions in Texas in 2019 (TCEQ, 2023). Towboat and tugboat emissions have greater uncertainty than other CMV categories due to the lack of information on engines and the uncertainties of engine loads and operating parameters. This proposal aims to improve our understanding of commercial marine exhaust emissions, focusing on NOx, volatile organic compounds (VOC), fine particulate matter ($PM_{2.5}$), and hydrocarbon speciation. The emphasis on smaller vessels will improve our ability to intercept their exhaust plumes. Although the focus of this project is to understand emissions from these smaller vessels while underway, if project resources allow and the work conducted safely, the project team may explore the logistics of sampling these vessels while stationary and running solely on auxiliary engines through discussions with the AQRP Project Manager.

1.2. PURPOSE AND OBJECTIVES

This project will sample emission plumes from vessels immediately downwind from well-defined shipping lanes in Galveston Bay. Automatic Identification System (AIS) data for the proposed monitoring location was reviewed and observed passage of ~4 towboats per hour during daylight which indicates that we can expect to sample plumes from hundreds of towboats during the study. Plumes will be identified by measuring elevated carbon dioxide (CO_2) concentrations downwind of a unique and identified vessel. Similar work has been conducted to field sample highway trucks (Bishop et al., 2022) and marine vessels (Williams et al., 2009) emissions plumes. For each plume measurement, the concentration ratio of emissions to CO_2 was converted to emissions per unit of fuel consumed using a carbon balance method. The emission rates as a function of fuel consumed were compared with that expected of engines meeting the emission standards by model year. In addition, by collecting canisters for hydrocarbons we will speciate emissions. The main tasks include:

1. Utilize the UH marine vessel sampling system for 20 days of field sampling downwind of the Galveston Bay shipping channel to capture emissions from multiple vessels each day.
2. Estimate emission rates for each vessel using field data and determine engine characteristics (model year, model, power level) for comparison with emissions standards.
3. Collect VOC canisters in plumes to identify hydrocarbon constituents more accurately.

2. ORGANIZATION AND RESPONSIBILITIES

2.1. KEY PERSONNEL

James Flynn, Project PI, University of Houston

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 boat are maintained and operated in a responsible manner.

Jerker Samuelsson, Co-PI, FluxSense

Responsible for the mobile extractive optical measurements and development of final data from the FluxSense instrumentation. Will lead the FluxSense portion of the project and oversee the installation of the instrumentation and training of UH personnel to operate, maintain, and troubleshoot as well as ensuring FluxSense personnel are available for remote support and limited field deployments during the campaign.

Chris Lindhjem, Co-PI, Ramboll

Responsible for the classification of commercial marine vessel types and the calculation of associated emission factors based on plume data provided by UH and FluxSense. Will lead Ramboll's portion of the project including reporting to UH and assisting in presentations.

Sergio Alvarez, University of Houston

Responsible for the quality assurance of data delivered by UH. Will review raw, interim, and final data developed by staff, postdocs, and students involved in the collection and processing of the data.

Jerker Samuelsson, FluxSense

Responsible for the quality assurance of data provided by FluxSense. Will review raw, interim, and final data collected during the project.

Fiona Jiang, Ramboll

Responsible for the quality assurance of calculations and work products produced by Ramboll.

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.

- Develop Work Plan – August 23, 2024.
- Project preparation and ordering - Within 60 days of receiving AQRP issued start date.
- Task 1.1: Instrument integration - To begin with Notice to Commence and completed before field deployment.
- Task 1.2: Field deployment - Approximately two months between the completion of instrument integration through April 2025.
- Task 2: Analysis and emission rate calculation - April–June 2025.
- Task 3: Project reporting and presentation - 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.

3. SCIENTIFIC APPROACH

3.1. SAMPLING DESIGN

The instrumentation package will include instrumentation for NO, NO_2, CO, CO_2, SO_2, Global Positioning System (GPS) receiver, all-in-one weather station, and a ruggedized PC with a cellular data connection. A ceilometer will also be installed on the research boat to measure the boundary layer height over the water, which is often parameterized in photochemical models and can have a significant impact on model results. An Aroma-VOC instrument will be rented and installed and operate for bulk VOC measurements. Mobile extractive Fourier Transform Infrared (FTIR) and Differential Optical Absorption Spectroscopy (DOAS) will be installed and collect measurements of 1) FTIR - total alkanes, methane, CO, CO_2, N_2O, HCHO, and acetaldehyde, and 2) DOAS - benzene, toluene, ethylbenzene, p-xylene, m-xylene, naphthalene, furfural, phenol, SO_2. Additional speciated VOC data will be sampled via canisters for offline analysis for certain plumes. Automated and crew operated cameras and the AIS information from the boat's systems will be used to document passing vessel information and identity.

For this project, the Osprey will anchor with the sample inlets oriented into the prevailing wind a safe distance outside the channel downwind of commercial traffic in an area likely to see frequent towboat operations, often several per hour, both with and without barges. While anchored, the outboard engines will be shut off to reduce fuel costs and emissions. The upper section of the shipping lane in the vicinity of the Bayport Channel and Morgans Point where the Bay narrows is a high-traffic area for towboats and the UH crew has operated extensively in this area over the last three years.

4. SAMPLING PROCEDURES

4.1. SITE SPECIFIC FACTORS

The UH research boat, an Osprey 30, has been modified to carry a tandem shock-mounted equipment rack inside an air-conditioned cabin. The research boat is a 30' offshore fishing boat which has been specially modified to house research equipment and the associated supporting infrastructure. Propulsion is provided by a pair of Suzuki 300 hp outboard engines fed by two 115-gallon fuel tanks. The estimated useful range of the research boat is 180 miles and cruises in calm conditions at speeds of 30 mph or more. Electrical power is provided by a 9kW diesel generator installed below the aft deck and fed by a dedicated 27-gallon diesel fuel tank. Online measurement sample inlets and meteorological sensors will be positioned forward of the bow, when practical, to reduce the impact of exhaust or obstructions from the research boat. Periods which are determined to have been impacted by local exhaust will be excluded from the analysis which will focus on large scale ambient features over the water. Some instrumentation, such as the FluxSense and boundary layer instruments, will be mounted to the roof of the boat or if necessary, a support structure over the rear deck of the boat.

4.2. SAMPLING PROCEDURE

VOC canister samples will be sampled on the upwind side of the research boat, such as from the side or bow. Approximately 18 canisters (16 samples plus 2 duplicates) and 2 blank VOC canisters provided by Desert Research Institute (DRI) (Reno, NV) will be used during the campaign. These canisters will be cleaned and prepared prior to shipping. Grab type samples will be collected by rapidly opening the sample valve manually once real-time instrumentation aboard the research boat indicates a plume has been encountered. The valves will be closed when no additional sample can be heard entering the canister. It is anticipated that the bulk of the samples will be collected in the second half of the field effort to allow the crew time to observe the typical plume behavior and timing in the early stages of the project. Additional sampling information can be found in Appendix A. All sampling handling procedures, including sample holding, shipping, and unique numbering of samples as required by DRI will be followed to assure that the data can be attributed to the proper plume and measurement period.

5. MEASUREMENT PROCEDURES

Online measurement sample inlets will be positioned to reduce the impact of exhaust from the sampling platform and collocated on the boat whenever practical. Periods which are determined to have been impacted by local exhaust will be excluded from the analysis which will focus on large scale ambient features over the water.

NO will be measured with a Thermo 42c-TL, while a Teledyne T500U cavity attenuated phase shift instrument will provide direct measurements of NO_2. A Teledyne T300U will be used to measure CO. A pressure- and flow-controlled Licor LI-7000 system will measure CO_2. SO_2 will be measured with a trace-level Thermo 43 series instrument. $PM_{2.5}$ measurements will be collected using a Teledyne T640 with a custom inlet system for mobile operations.

An Airmar 220WX weather transmitter will report GPS position, speed course over ground, compass heading, relative wind speed, and direction, compass corrected wind speed and direction, temperature, relative humidity, and atmospheric pressure. A Vaisala CL-51 ceilometer will augment the instrument package for boundary layer heights.

Data will be collected from these instruments using DAQFactory data acquisition software (Azeotech, Ashland, OR) or Vaisala's BL-View software in the case of the ceilometer. The data will be post-processed and averaged into a format suitable for storage and use in a database with software such as Igor Pro and MATLAB.

Extractive Fourier Transform InfraRed spectroscopy (MeFTIR) and ultraviolet DOAS (Differential Optical Absorption Spectroscopy, MeDOAS) will be used for the concentration measurements of methane, CO, CO_2, N_2O, formaldehyde, acetaldehyde, benzene, toluene, ethylbenzene, p-xylene, m-xylene, naphthalene and SO_2. MeFTIR and MeDOAS measurements are presented in enhancement values i.e. the difference from a reference level, e.g. background.

Background spectra are collected before each new measurement series and optically removed from the subsequent measurements.

6. QUALITY METRICS (QA/QC CHECKS)

6.1. GENERAL INFORMATION

Trace gas calibrations on the research boat will be performed by blending gas standards of NO, NO_2, CO, and SO_2 with zero air and feeding to the inlet system as appropriate. Provisions to carry the gas standards as well as a zero air generator will be made such that the research boat instruments can be calibrated before and after sampling trips. The CO_2 measurements will be referenced to a near-ambient, anticipated to be between 400-500 ppmv, standard at all times, and spanned with a higher standard before and after sampling trips, following guidance from research teams at NASA Langley.

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 online organic and inorganic trace gases and CO_2 will be established with the application of available standards according to the Code of Federal Regulations Title 40 (40 *CFR)* Part 136, Part B, where applicable. Other measurements will rely on laboratory results and instrument manufacturer specifications.

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.

Two VOC canisters (10% of total allotment) will be utilized as blanks to evaluate system contributions.

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. Spans will be done every day the boat goes out into Galveston Bay before and after the trip. Nominally weekly multipoint calibrations will also be performed for the inorganic trace gases and Aroma-VOC instrument. Other instruments will be challenged per manufacturer guidance. 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.
- Precision will be measured quantitatively for the PM samples utilizing field and laboratory replicate samples as well as replicate instrument injections. A minimum of 10% of the total field samples collected will be field duplicate samples.

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. Completeness

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:

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

Completeness measures the percentage of valid measurements to the total number of possible measurements. In order to meet the objectives of the project's research plan, the acceptance criteria for field measurement completeness is 90%. The completeness 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 QA personnel in Section 2.1 using visual inspection of the time-series measurement 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. Findings of the Audit of Data Quality will be included in the draft and final reports.

6.4. INSTRUMENT SPECIFICS

6.4.1. ***NO, CO, SO_2 and NO_2, measurements***

The NO, CO, and SO_2 measurements will be challenged with a dilution of calibration gas standard (nominally 150 ppm CO, 5 ppm NO, 5 ppm SO_2) in zero air using an onboard zero air generator and dilution system. These challenges will occur nominally once per week. Ambient measurements will be compared to nearby land-based measurements when it is reasonable to believe there should be agreement. The NO instrument performs a baseline measurement and applies a correction internally for each data point. For CO, the instrument uses a catalytic zero to assess and reset the baseline nominally once per hour to minimize instrument drift. Zero air baseline checks will be performed prior to sampling outings to establish the SO_2 baseline for that day.

As a direct measurement, NO_2 will be challenged using test atmospheres with multiple upscale points plus a zero to determine the sensitivity and verify the linearity of the instrument responses. NO_2 will either be generated using a titration reaction of O_3 + NO from a cylinder or by dilution of a NO_2 gas standard (nominally 5 ppm). In all cases, the gas standards will be certified.

6.4.2. ***CO_2 measurements***

The LI-7000 CO_2 analyzer can be configured in a variety of ways and provides flexibility for different installations and data needs. For this project, the CO_2 measurements will be configured in line with guidance from the NASA Langley teams who deploy the same model instrument on aircraft campaigns. In this mode, a certified cylinder gas with nominally ambient CO_2 concentrations will be flowed through the reference cell. Ambient air will flow through the sample cell and the resulting measurement will be relative to the reference gas value. A high span gas from a certified gas cylinder will be introduced to the sample cell to confirm the upscale response before and after sampling trips.

6.4.3. **Aerosol concentration *($PM_{2.5}$ mass)***

The T640 mass monitor will be zeroed before and after sampling trips by the introduction of a HEPA filter at the inlet. Leak checks, flow audits, and photomultiplier tube (PMT) checks (using Teledyne SpanDust) will be performed in accordance with the instrument operation manual.

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. VOC canister data will be provided in tabular spreadsheet format compatible with Excel.

Calculated emission rate information will be provided in terms of pollutants per unit of fuel consumed.

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

Ramboll will perform the emissions calculations using the data collected in this work. Ramboll will follow 40 *CFR*, Chapter I, Subchapter U, Part 1065, Subpart G emission calculations for engines employing the measured emissions concentrations and accepted average fuel characteristics. The emissions rates for each measurement will be reported compared to the EPA emissions to fuel consumption ratios from Table 2 in the accompanying Scope of Work using pollutant emissions concentration compared with carbon dioxide concentration. The CFR calculation is the same as that used in the study from the International Council on Clean Transport (Comer et al. 2023). NOx, VOC, and $PM_{2.5}$ emission rates will be calculated with the basic equation shown in Equation 1. This equation can be modified to include other carbon containing species such as carbon monoxide and total hydrocarbon emissions to improve accuracy, but diesel engines usually produce low carbon monoxide and hydrocarbon compared with carbon dioxide emissions resulting in a 0.1% or lower bias.

$$ER_{NOx} = ((NO_{x\ measured} - NO_{x\ background}) / (CO_{2\ measured} - CO_{2\ background})) \times FCC\ x(46\ gNO_x/12\ gC) \quad \text{Eq(1)}$$

ER_{NOx} = the NOx emission rate (g NOx/g fuel)
$NO_{x\ measured}$ = the concentration of NOx in the plume
$NO_{x\ background}$ = the background concentration of NOx
$CO_{2\ measured}$ = the concentration of CO_2 in the plume
$CO_{2\ background}$ = the background CO_2 concentration in ppm outside of the plume
FCC = fuel carbon content (usually about 0.87 g-Carbon/g-fuel for diesel fuel)

The calculations will be reviewed by multiple researchers to quality assure the results. A member of the research team who did not set up data analysis calculations will review emissions calculations tables. In addition, the Project PIs and other members of the research team will review the calculations and results. Results of findings of the Audits of Data Quality and all QA/QC procedures will be discussed in the Final Report.

7.4. MEASUREMENT COMPARISON

In addition, Ramboll will use the vessel identification to estimate the vessels' engine models and model years to provide emissions rates estimates expected by EPA (2022) to compare with the measured and calculated. We will provide the best estimate of the vessel characteristics (type, engine model, and model year) from public data such as those published by the owner\operators of the vessel, secondary sources including vessel build and repair shops or other public sites, and the US Army Corps of Engineers[1] vessel database.

Ramboll will identify the secondary data on vessels' engine model and model year collected using a checklist for quality concerns. The secondary data on vessels may have quality concerns such as being out of date, misidentified vessels, or other concerns. Ramboll will provide a description of the data source and other notes on data quality and considerations when reporting results to provide the reader context. The checklist reported for each vessel will include:

1. Identify data source decision as best estimate
2. Identify the data source (US Army Corps of Engineers Institute for Water Resources Website, and other websites that report such data including vessel builder and repair shops, or other anecdotal sources)
3. Qualitative rating, the quality of the secondary data collected.
4. Comment field on data quality.

7.5. RESULTS COMPARISONS AND EVALUATION

The calculated emission factor results from the field measurements' data analysis will be compared with EPA's published emission standards (2020) and emission factors (2022) for each vessel. The measurement methods for this project do not allow for the calculation of engine load factors. Given that a single vessel may undergo multiple samplings, we will scrutinize the results to understand the variability in field measurements. Combining this data with vessel activity information (speed, draft, etc.), we will discuss and summarize the comparison results, highlighting any significant findings and conclusions. This analysis has the potential to enhance the accuracy of the commercial marine emission inventory.

The comparison may identify differences and outlier data, so the data evaluation will use the EPA expected results (using the estimated engine model and model year) as a guide to identify data concerns. Conditions during sampling including atmospheric (wind, wave, heat or humidity), vessel operation (with/without barge, speed, draft, etc.), or other reasons will be identified, categorized, and considered whether they have affected the results. The final report will include a discussion of the summary data results along with the individual data of each vessel measurement.

7.6. 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 an off-campus location such as Baylor or St. Edward's University 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 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 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 Draft and Final Reports will provide a comprehensive overview of activities undertaken during the Improving Emission Rates Estimates of Commercial Marine Vessels project and any data collected and analyzed. The Final Report will highlight major activities and key findings, including findings from the Audits 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

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Williams, E.J., Lerner, B.M., Murphy, P.C., Herndon, S.C. and Zahniser, M.S., 2009. "Emissions of NOx, SO_2, CO, and HCHO from commercial marine shipping during Texas Air Quality Study (TexAQS) 2006." *Journal of Geophysical Research: Atmospheres*, 114(D21).

10.Appendix A – DRI VOC Canister QA/QC

1 SCOPE AND APPLICATION

This is a modified TO-15 method intended for analysis of Volatile Organic Compounds (VOC) in ambient air. VOC include the C_2-C_{12} hydrocarbons and other compounds of vapor pressures greater than 0.1 torr at 25 °C and 760 mm Hg which can be analyzed by gas chromatography flame ionization detection/mass spectrometry (GC-FID/MS). The method's minimum detection limit (MDL) is 0.01-0.05 ppb volume (ppbv). Mass spectrometry provides definitive identification of VOCs.

2 SUMMARY OF METHOD

A known volume of gaseous sample is passed through multiple traps, retaining C_2 and heavier VOCs without trapping methane, oxygen, or nitrogen. The trap containing the condensed VOC is heated to and its contents injected into a gas chromatographic capillary columns where separation of the VOCs takes place. Detection of the hydrocarbons is by mass spectrometry, and the resultant peaks are quantified and recorded on a computer system. Some hydrocarbons have such low molecular weight that they are impractical or impossible to analyze by mass spectrometry and these are separated on-line and detected by FID.

This SOP is broken up into sections. Sections 3 through 6 cover general material, while sections 7 and 11 discuss the analysis technique for the VOCs.

3 DEFINITIONS

3.1 Accuracy

The degree of agreement of the measurements with the true value of the Standard Reference Material (SRM) or SRM-traceable standard measured for hydrocarbons.

3.2 Precision

The reproducibility of measurements from the same canister under essentially the same conditions.

4 PERSONNEL REQUIREMENTS

The researcher using this procedure is expected to be familiar with basic laboratory practice and the Varian GC/MS system and controlling computers. Specific requirements for these instruments are found in the appropriate manuals.

5 FACILITIES REQUIREMENTS

No special laboratory facilities are required.

6 SAFETY REQUIREMENTS

The calibration standards, collected sample, and most laboratory reagents used in this method pose no hazard to the researcher if normal laboratory safety practices are followed. Eye and hand protections are required when using liquid nitrogen.

Adherence to the American Chemical Society (ACS) guideline regarding the safe handling of chemicals used in this method is required.

6.1 Heated Surfaces

The GC injection ports, column, column oven, and detectors are maintained at temperatures high enough to cause burns. The researcher should exercise caution to avoid contact with these surfaces.

6.2 Cryogenic Liquids. - Liquid Nitrogen

WARNING: Cryogenic fluid may cause severe frostbite. Wear eye and hand protection. Use with adequate room ventilation. Keep contact with air to a minimum to avoid buildup of liquid oxygen (see above).

7 APPARATUS AND EQUIPMENT

This section describes the instrument requirements for this method.

7.1 GC-FID/MS

The GC-FID/MS system includes a Lotus Consulting (Long Beach, CA) Ultra-Trace Toxics sample (UTTS) preconcentration system, built into a Varian 3800 gas chromatograph with flame ionization detector (FID) coupled to a Varian Saturn 2000 ion trap mass spectrometer (MS). The instrument is connected to a desktop computer with Varian Workstation 6.9 software installed for instrument control, data acquisition, and data processing.

7.1.1 Gas Chromatograph Columns

Three gas chromatographic columns are employed for resolving VOC, and a fourth is needed for balancing flows but does not connect to a detector. This allows simultaneous detection using both the FID and MS. The analysis columns are: Phenomenex Zebron ZB-1 column (15m x 0.32mm x 1µm), Agilent J&W CP Al_20_3/KCl column (25m x 0.53mm x 10µm) and Phenomenex Zebron ZB-1MS column (60m x 0.32mm x 1µm).

7.1.2 Trapping

The Lotus UTTMS (Ultra Trace Toxics Mass Spectrometer) preconcentration system consists of three traps that are for water control, CO_2 control and final focus. Mid- and heavier weight hydrocarbons are trapped on the front trap consisting of 1/8” nickel tubing packed with multiple adsorbents. Trapping is performed at 55 C and eluting is performed at 200 C. The rear traps consist of two traps: empty 0.040” ID nickel tubing for trapping light hydrocarbons and a cryo-focusing trap for mid and higher weight hydrocarbons isolated in the front trap. The cryo-focusing trap is built from 6” x 1/8” nickel tubing filled with glass beads. Trapping of both rear traps occurs at -80 C and eluting at 250 C. Light hydrocarbons, C_2-C_5, are deposited to a Phenomenex Zebron ZB-1 column (15m x 0.32mm x 1µm) plumbed to a column-switching valve in the GC oven, then to a Agilent J&W CP Al_20_3/KCl column (25m x 0.53mm x 10µm) leading to the flame ionization detector for quantitation of light hydrocarbons. The mid-range and heavier hydrocarbons, C_4-C_{12}, cryo-focused in the rear trap are deposited to a Phenomenex Zebron ZB-1MS column (60m x 0.32mm x 1µm) connected to the ion trap mass spectrometer. The GC initial temperature is 5 C held for approximately 9.5 minutes, then ramps at 3 $C.min^{-1}$ to 200 C for a total run time of 80 minutes.

7.2 Tubing and Connectors

All tubing is chromatographic-grade stainless steel. All connectors are stainless steel compression tube fittings (Swagelok^{TM} or equivalent).

7.3 Regulators for Compressed Gases

The carrier gas, helium, is controlled by a two-stage regulator mounted at the tank. All gases are ultra-high purity grade. The instrument requires He, N_2, Air, H_2 and liquid nitrogen (not high purity).

CAUTION: Due to the possibility of contamination by organic materials, only regulators with stainless steel diaphragms should be used.

8 REAGENTS/MATERIALS

All gases used to operate the GC system are high quality grade and may vary in specifications with manufacture. Instrument calibration gases are obtained from the

National Institute of Standards and Technology (NIST) and are referred to as Standard Reference Materials (SRM). Use of reagent-grade chemicals for all dilutions and standards materials is recommended.

8.1 Gases and Cryogens

The following are recommended for use with this method.

8.1.1 Helium Carrier Gas

Ultra High Purity (99.995 %), followed by a water/oxygen/hydrocarbon trap.

8.1.2 Liquid Nitrogen

Commercial grade is acceptable. The dewar should be rated at 50psi or less. Liquid nitrogen is taken from the "Liquid" outlet on the dewar and is used for cryogenic cooling of the GC oven and cryogenic focusing during sample trapping. Nitrogen gas is drawn from the "vent" outlet on the dewar. Vent gas must pass through a carrier gas filter prior to entering the GC as it is used for FID makeup gas and instrument blank gas. A 180 liter dewar will typically last for two or three days of continuous analyses. If not performing analyses, the dewar will last longer but will eventually be drained of its contents through the vent gas line or by releasing pressure.

8.1.3 Hydrogen

Ultra High Purity Grade is used as fuel gas for the FID.

8.1.4 Air

Ultra High Purity Grade is used as fuel gas for the FID.

9 ANALYSIS

9.1 Instrument Method

GC and MS settings may vary based on the target analytes, but for most cases the only changes in instrument settings are related to the desired sample volume. This is achieved by allowing the sample stream to flow through the cryogenic traps for the appropriate amount of time at a constant flow rate of 50 $ml.min^{-1}$. Typical ambient sample volumes are 300 ml, and samples with higher concentrations of analytes may be analyzed with lower volumes to avoid overloading of the instrument. Sample acquisition methods are located in the directory c:\varianws\methods. Method settings for all timed events, valves, heated zones, flows, detectors, and respective compound table are archived with each data file. Supporting material includes printouts for GC and MS settings from a sample analyzed by 300 ml injection.

9.2 Calibration.

Calibration curves are made by the molecular ion peaks of the VOC using the external calibration method. Calibration calculations use the force zero method and must be better than 0.95 r^2. Calibration sources are dependent upon project. For TO-15, use the 74 component mixture in the 0.1-10 ppb, range of concentrations, Table 1, traceable to the NIST Standard Reference Materials (Air Environmental, Inc., Denver, CO). For other projects, use the appropriate source for the compounds of interest. Up to 6 calibration levels are obtained by analyzing 25 ml, 50 ml, 100 ml, 150 ml, 200 ml, and 300 ml volumes of the same calibration standard by performing sample injections with respective methods.

The FID response is calibrated in ppbCv and MS response is calibrated using ppbv with at least three calibration levels for each compound of interest. A calibration check (using a median calibration level) is analyzed daily to check for accuracy of analyses. If the relative accuracy of measurement (defined as a percent difference from the standard value) is off by more than 30%, the instrument is recalibrated. Blanks are performed once daily. Approximately 10% of the samples should be analyzed in replicate. The replicate analyses are flagged in our database and the programs we have for data processing extract these replicates and determine a replicate precision. These are then converted into an absolute precision for each measurement which can be reported if required.

Table 1 74 Component Calibration Mixture (Cylinder CC402259)

Compound	Concentration (ppb)	Uncertainty	Compound	Concentration (ppb)	Uncertainty
Ethene	6.49	±5%	Cyclohexane	0.5	±5%
Acetylene	7.55	±5%	2-Methylhexane+2,3-Dimethylpentane	1.5	±5%
Ethane	12.29	±5%	Cyclohexene	1.79	±5%
Propene	2.51	±5%	3-Methylhexane	1	±5%
Propane	11.17	±5%	c-1,3-Dimethylcyclopentane	3.25	±5%
Propyne	5.88	±5%	1-Heptene	4.9	±5%
i-Butane	5.08	±5%	Heptane	5.07	±5%
i-Butene	3.75	±5%	2,3-Dimethyl-2-Pentene	1.17	±5%
1-Butene	2.67	±5%	Methylcyclohexane	1.01	±5%
1,3-Butadiene	2.44	±5%	2,3,4-Trimethylpentane	0.49	±5%
Butane	10.13	±5%	Toluene	2.9	±5%
t-2-Butene	1.29	±5%	2-Methylheptane	0.48	±5%
c-2-Butene	2.44	±5%	4-Methylheptane	1.26	±5%
1,2-Butadiene	5.88	±5%	3-Methylheptane	1.01	±5%
i-Pentane	7.62	±5%	Octane	0.49	±5%
1-Pentene	1.28	±5%	Ethylbenzene	0.96	±5%
2-Methyl-1-Butene	1.2	±5%	m-Xylene	1.43	±5%
Pentane	8.1	±5%	p-Xylene	0.4	±5%
Isoprene	4.99	±5%	Styrene	0.4	±5%
t-2-Pentene	0.98	±5%	o-Xylene	0.47	±5%
c-2-Pentene	2.43	±5%	Nonane	0.95	±5%
2-Methyl-2-Butene	0.99	±5%	i-Propylbenzene	0.23	±5%
2,2-Dimethylbutane	2.56	±5%	alpha-Pinene	0.36	±5%
Cyclopentene	0.96	±5%	Propylbenzene	0.22	±5%
Cyclopentane	0.99	±5%	3-Ethyltoluene	0.21	±5%
2,3-Dimethylbutane	1.82	±5%	4-Ethyltoluene	0.4	±5%
2-Methylpentane	1.02	±5%	1,3,5-Trimethylbenzene	0.6	±5%
3-Methylpentane	1.3	±5%	2-Ethyltoluene	0.49	±5%
2-Methyl-1-Pentene	0.98	±5%	1,2,4-Trimethylbenzene+tert-Butylbenzene	2.59	±5%
Hexane	3.14	±5%	Decane	0.91	±5%
t-2-Hexene	0.49	±5%	1,2,3-Trimethylbenzene	1.2	±5%
c-2-Hexene	0.99	±5%	Indan	1.21	±5%
t-1,3-Hexadiene	2.3	±5%	1,3-Diethylbenzene	0.69	±5%
Methylcyclopentane	1.11	±5%	1,4-Diethylbenzene	0.9	±5%
2,4-Dimethylpentane	1.01	±5%	Butylbenzene	0.36	±5%
Benzene	2	±5%	Undecane	0.37	±5%

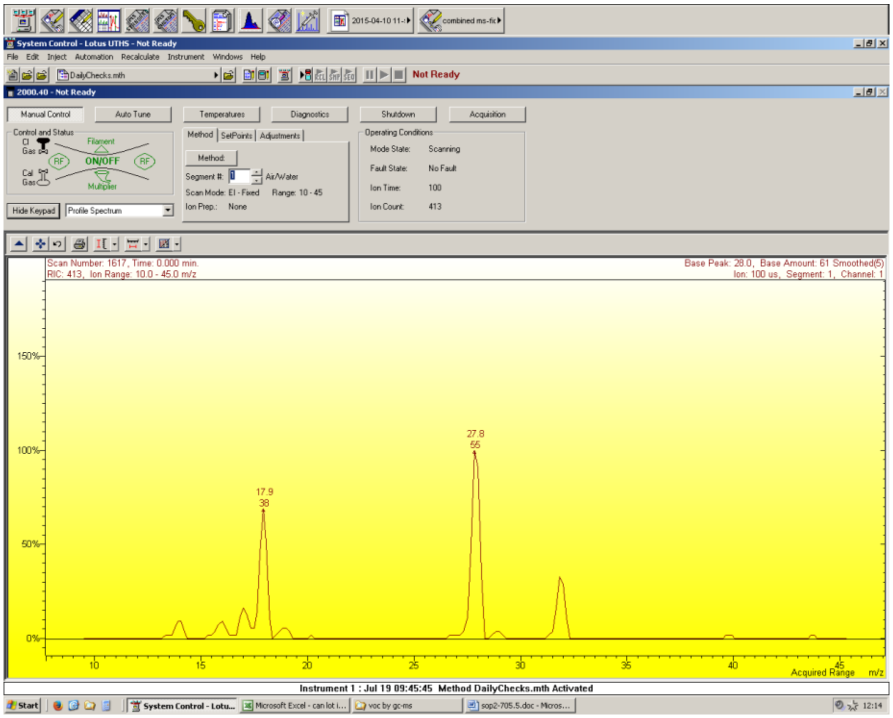
10 ANALYSIS PROCEDURES

The analysis procedure is divided into two stages: instrument preparation and sample concentration and analysis.

10.1 Preparation Stage

10.1.1 The instrument (GC/MS) preparation steps are as follows:

1) Check that the PC and GC are both on and communicating with each other. You can verify this either in System Control, or by noting the computer icon on the GC's display indicating that it has communication with the PC.
2) In System Control, activate the instrument method c:\Varianws\methods\service\dailychecks.mth and allow the system to stabilize to any changes in temperature or pressures.
3) Select the Manual control button of the 2000 window, click on the Method tab and select the segment #1 check air/water levels in the instrument (Figure 1). Turn on the MS by clicking on the ion trap ON/OFF area of the control and status picture of the trap. Levels are considered acceptable if the total ion current (TIC) is below 1000.



Segment #: 1 Air/Water
Scan Mode: EI - Fixed Range: 10 - 45
Ion Prep.: None

Mode State: Scanning
Fault State: No Fault
Ion Time: 100
Ion Count: 413

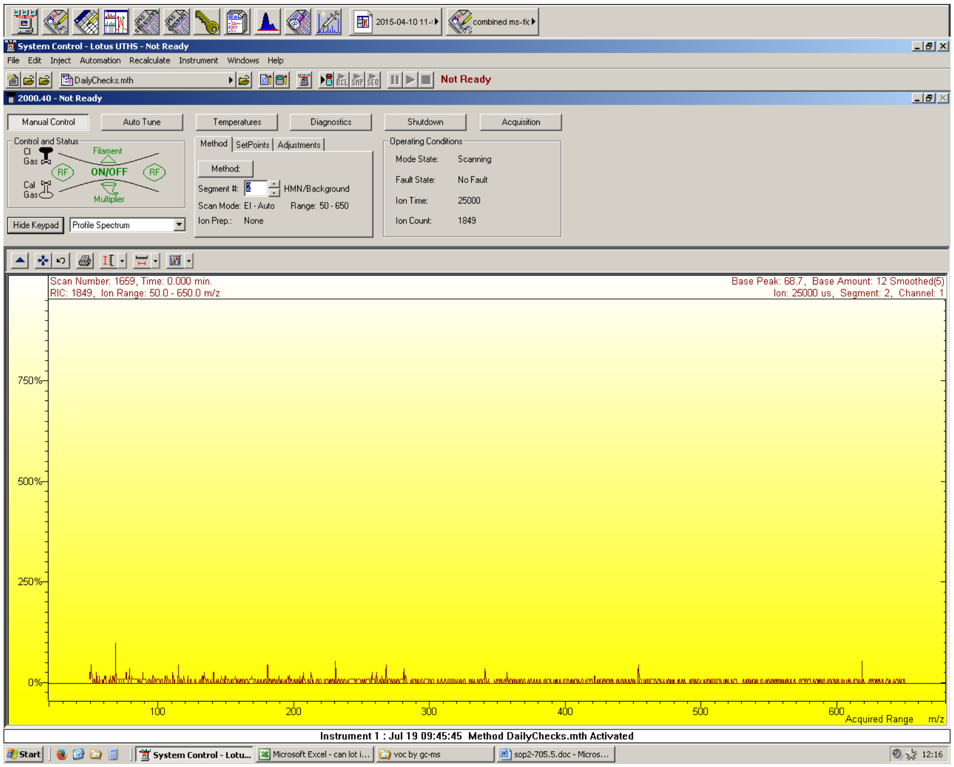
Scan Number: 1617, Time: 0.000 min.
RIC: 413, Ion Range: 10.0 - 45.0 m/z

Base Peak: 28.0, Base Amount: 61 Smoothed(5)
Ion: 100 us, Segment: 1, Channel: 1

Instrument 1 : Jul 19 09:45:45 Method DailyChecks.mth Activated

Figure 1 System Control mass spectrometer 2000 screen during Air/Water check.

4) Select the segment #2 of the MS method to check high mass noise/background (Figure 2). Levels are considered acceptable if the ionization time reaches its maximum setting of 25,000 and the TIC is less than 10,000.



Segment #: 2 HMN/Background
Scan Mode: EI - Auto Range: 50 - 650
Ion Prep.: None

Mode State: Scanning
Fault State: No Fault
Ion Time: 25000
Ion Count: 1849

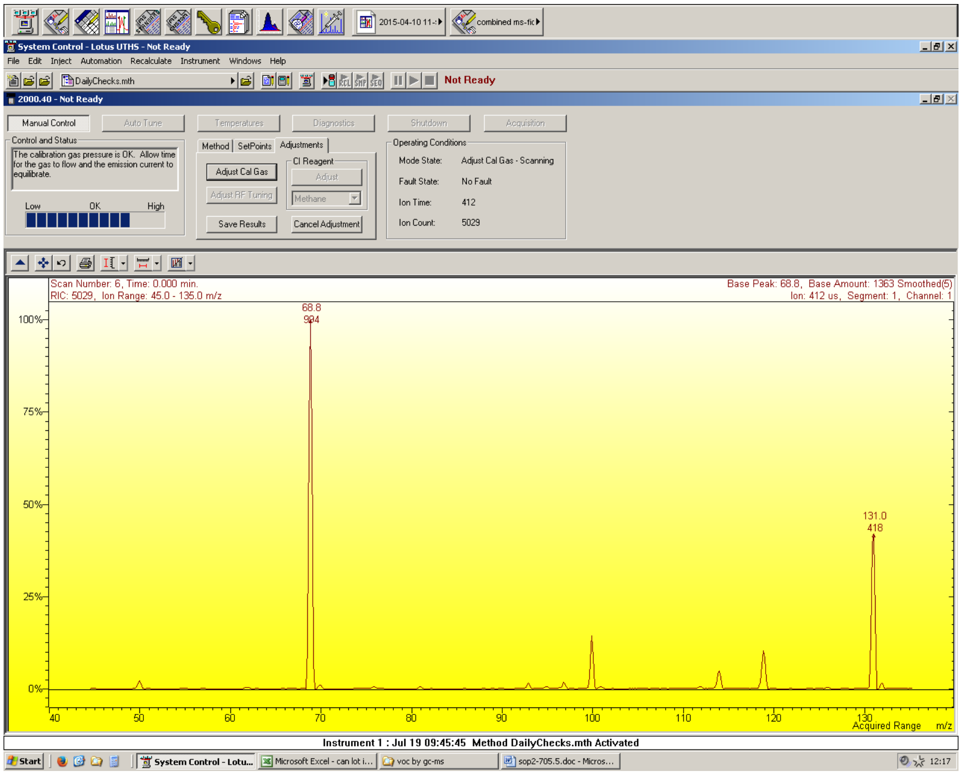
Scan Number: 1659, Time: 0.000 min.
RIC: 1849, Ion Range: 50.0 - 650.0 m/z

Base Peak: 68.7, Base Amount: 12 Smoothed(5)
Ion: 25000 us, Segment: 2, Channel: 1

Instrument 1 : Jul 19 09:45:45 Method DailyChecks.mth Activated

Figure 2 System Control mass spectrometer 2000 screen during HMN check.

5) Select the Adjustments tab and click on the Adjust Cal Gas button to check calibration gas pressure (Figure 3). Adjust the cal gas pressure by rotating the cal gas knob behind the MS front door in the direction to achieve a target ionization time of 400-500. Increasing cal gas pressure decreases the ion time, and vice versa. Click save results when finished.



The calibration gas pressure is OK. Allow time for the gas to flow and the emission current to equilibrate.

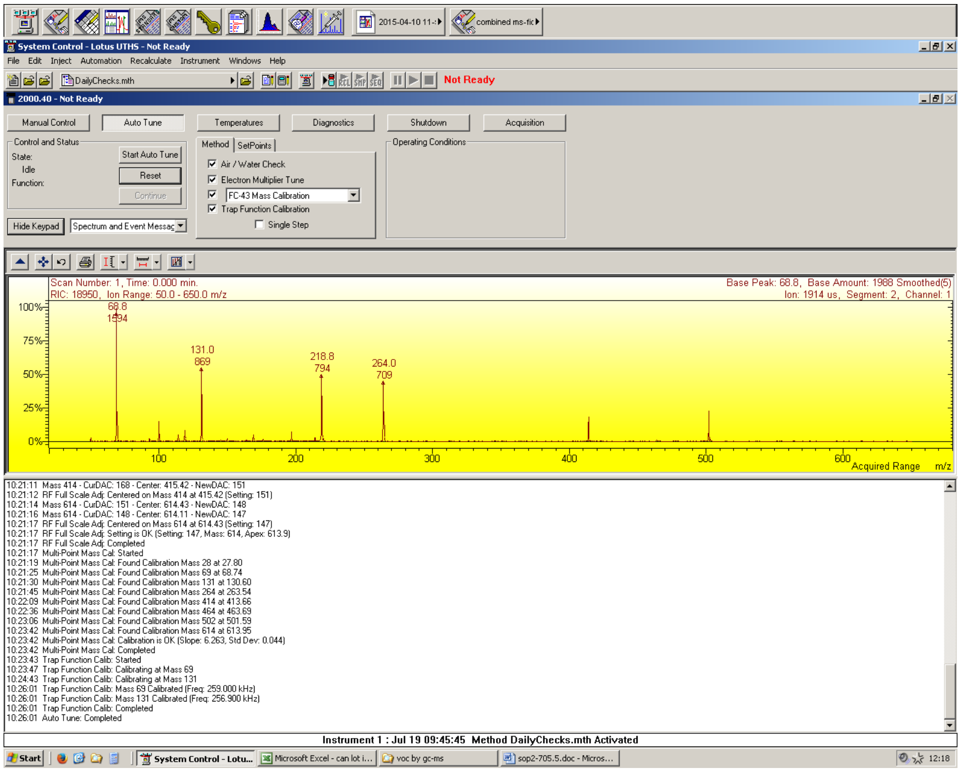
Mode State: Adjust Cal Gas - Scanning
Fault State: No Fault
Ion Time: 412
Ion Count: 5029

Scan Number: 6, Time: 0.000 min.
RIC: 5029, Ion Range: 45.0 - 135.0 m/z
Base Peak: 68.8, Base Amount: 1363 Smoothed(5)
Ion: 412 us, Segment: 1, Channel: 1

Instrument 1 : Jul 19 09:45:45 Method DailyChecks.mth Activated

Figure 3 System Control mass spectrometer 2000 screen during cal gas adjust.

6) Push the Auto Tune button and under the Method tab select all four options; Air/Water Check, Electron Multiplier Tune, FC-43 mass Calibration, and Trap Function Calibration (Figure 4). Push the Start Auto Tune button and wait for the system to finish all steps. A final electron multiplier setting of EM10^5<2000 is preferred. If it is higher, either the trap is dirty and needs to be cleaned, or the detector is aging and should be replaced.



```
10:21:11  Mass 414 - CurDAC: 168 - Center: 415.42 - NewDAC: 151
10:21:12  RF Full Scale Adj: Centered on Mass 414 at 415.42 (Setting: 151)
10:21:14  Mass 614 - CurDAC: 151 - Center: 614.43 - NewDAC: 148
10:21:16  Mass 614 - CurDAC: 148 - Center: 614.11 - NewDAC: 147
10:21:17  RF Full Scale Adj: Centered on Mass 614 at 614.43 (Setting: 147)
10:21:17  RF Full Scale Adj: Setting is OK (Setting: 147, Mass: 614, Apex: 613.9)
10:21:17  RF Full Scale Adj: Completed
10:21:17  Multi-Point Mass Cal: Started
10:21:19  Multi-Point Mass Cal: Found Calibration Mass 28 at 27.80
10:21:25  Multi-Point Mass Cal: Found Calibration Mass 69 at 68.74
10:21:30  Multi-Point Mass Cal: Found Calibration Mass 131 at 130.60
10:21:45  Multi-Point Mass Cal: Found Calibration Mass 264 at 263.54
10:22:09  Multi-Point Mass Cal: Found Calibration Mass 414 at 413.66
10:22:36  Multi-Point Mass Cal: Found Calibration Mass 464 at 463.69
10:23:06  Multi-Point Mass Cal: Found Calibration Mass 502 at 501.59
10:23:42  Multi-Point Mass Cal: Found Calibration Mass 614 at 613.95
10:23:42  Multi-Point Mass Cal: Calibration is OK (Slope: 6.263, Std Dev: 0.044)
10:23:42  Multi-Point Mass Cal: Completed
10:23:43  Trap Function Calib: Started
10:23:47  Trap Function Calib: Calibrating at Mass 69
10:24:43  Trap Function Calib: Calibrating at Mass 131
10:26:01  Trap Function Calib: Mass 69 Calibrated (Freq: 259.000 kHz)
10:26:01  Trap Function Calib: Mass 131 Calibrated (Freq: 256.900 kHz)
10:26:01  Trap Function Calib: Completed
10:26:01  Auto Tune: Completed
```

```
Instrument 1 : Jul 19 09:45:45  Method DailyChecks.mth Activated
```

Figure 4 System Control mass spectrometer 2000 screen during autotune.

7) Push the Acquisition button to leave the MS in the proper state to begin analyses.

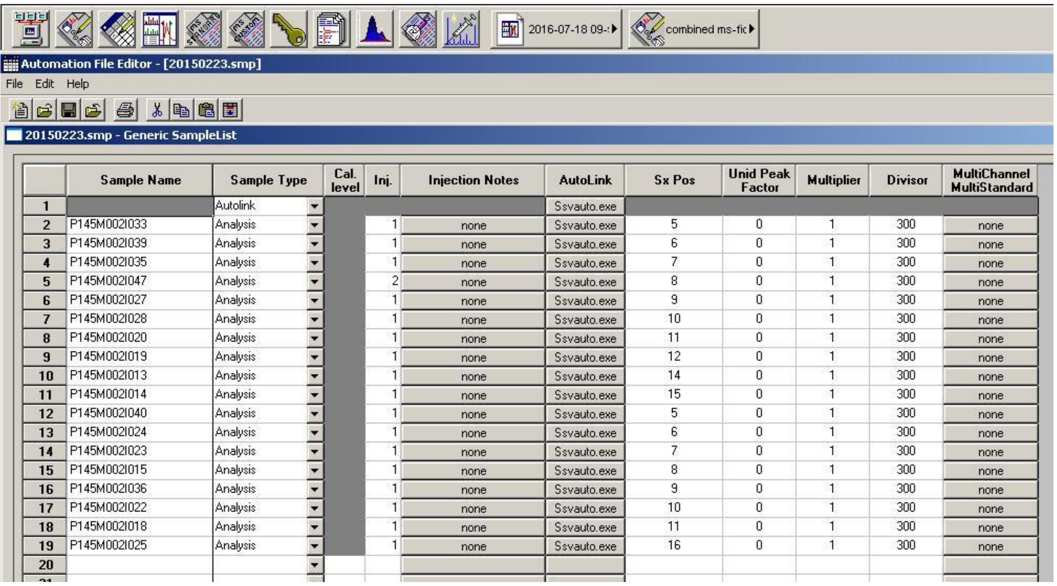
10.1.2 Create/modify sample and sequence lists to be run

1) Open the sample list for running a system blank, c:\varianws\blank.smp and press OK to select sample list section type “generic.” Change the directory in which to save data files by pressing the “Data Files” button on the bottom of the window and selecting the directory as desired. Save changes and close the file.

2) Open the sample list for running a calibration level, c:\varianws\calibration.smp and change the directory in which to save data files by pressing the “Data Files” button on the bottom of the window and selecting the directory as desired.

3) Click the Edit Automation Files icon in the Workstation toolbar and select File, New, SampleList to create a new list of samples for analysis. Choose the

directory in which to save the sample list. Press OK to select sample list section type "generic." Make "Sample Type" in first row "Autolink," under "Autolink" heading, browse for and select C:\varianws\ssvauto.exe, in Other Parameters box enter the text "-i" (without the parentheses). List each sample to be analyzed in the "Sample Name" column, with "Sample Type" Analysis selected. Leave "Inj." at 1, unless multiple injections of the same sample back to back are desired for replicates. (Approximately one in ten samples should be analyzed as replicates). Fill in "Injection Notes" if desired. In the "Sx pos" enter the sample inlet number. Inlet one is reserved for nitrogen used during blank analyses and inlet thirteen is connected to the calibration standard. Click the "Data Files" button and select the directory as desired. Save changes to the new sample list and close it. An example of a sample list is shown below in Figure 5 Example of a sample list with autolink and sample position numbers.Figure 5.



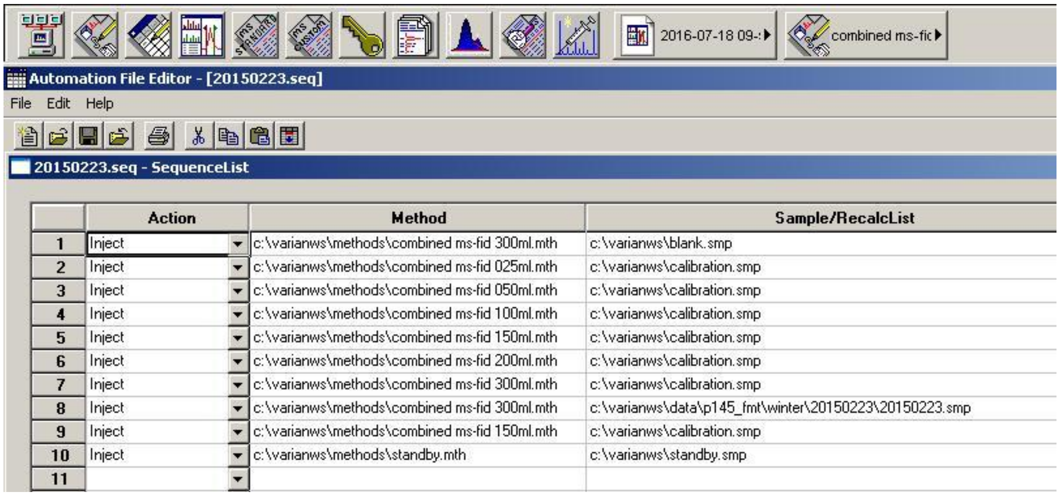
	Sample Name	Sample Type	Cal. level	Inj.	Injection Notes	AutoLink	Sx Pos	Unid Peak Factor	Multiplier	Divisor	MultiChannel MultiStandard
1		Autolink				Ssvauto.exe					
2	P145M002I033	Analysis		1	none	Ssvauto.exe	5	0	1	300	none
3	P145M002I039	Analysis		1	none	Ssvauto.exe	6	0	1	300	none
4	P145M002I035	Analysis		1	none	Ssvauto.exe	7	0	1	300	none
5	P145M002I047	Analysis		2	none	Ssvauto.exe	8	0	1	300	none
6	P145M002I027	Analysis		1	none	Ssvauto.exe	9	0	1	300	none
7	P145M002I028	Analysis		1	none	Ssvauto.exe	10	0	1	300	none
8	P145M002I020	Analysis		1	none	Ssvauto.exe	11	0	1	300	none
9	P145M002I019	Analysis		1	none	Ssvauto.exe	12	0	1	300	none
10	P145M002I013	Analysis		1	none	Ssvauto.exe	14	0	1	300	none
11	P145M002I014	Analysis		1	none	Ssvauto.exe	15	0	1	300	none
12	P145M002I040	Analysis		1	none	Ssvauto.exe	5	0	1	300	none
13	P145M002I024	Analysis		1	none	Ssvauto.exe	6	0	1	300	none
14	P145M002I023	Analysis		1	none	Ssvauto.exe	7	0	1	300	none
15	P145M002I015	Analysis		1	none	Ssvauto.exe	8	0	1	300	none
16	P145M002I036	Analysis		1	none	Ssvauto.exe	9	0	1	300	none
17	P145M002I022	Analysis		1	none	Ssvauto.exe	10	0	1	300	none
18	P145M002I018	Analysis		1	none	Ssvauto.exe	11	0	1	300	none
19	P145M002I025	Analysis		1	none	Ssvauto.exe	16	0	1	300	none
20											

S

Figure 5 Example of a sample list with autolink and sample position numbers.

4) Create a new sequence list, which is a list of sample lists to be analyzed with the respective methods. Acquisition methods are located in the directory c:\varianws\methods and are named by the sample volume needed for injection. Typically, a 300 ml injection of nitrogen blank is run first to be sure the system is purged of any background interferences that may have accumulated while in standby mode. Then, either a calibration check or full calibration sequence is

analyzed, followed by the sample set to be run, and finally a calibration check, if needed. For the last row in the sequence list, activate the c:\varianws\Standby.mth method and sample list which leaves the GC-MS with the proper settings. An example of a sequence list is shown in Figure 6 below.



	Action	Method	Sample/RecalcList
1	Inject	c:\varianws\methods\combined ms-fid 300ml.mth	c:\varianws\blank.smp
2	Inject	c:\varianws\methods\combined ms-fid 025ml.mth	c:\varianws\calibration.smp
3	Inject	c:\varianws\methods\combined ms-fid 050ml.mth	c:\varianws\calibration.smp
4	Inject	c:\varianws\methods\combined ms-fid 100ml.mth	c:\varianws\calibration.smp
5	Inject	c:\varianws\methods\combined ms-fid 150ml.mth	c:\varianws\calibration.smp
6	Inject	c:\varianws\methods\combined ms-fid 200ml.mth	c:\varianws\calibration.smp
7	Inject	c:\varianws\methods\combined ms-fid 300ml.mth	c:\varianws\calibration.smp
8	Inject	c:\varianws\methods\combined ms-fid 300ml.mth	c:\varianws\data\p145_fmt\winter\20150223\20150223.smp
9	Inject	c:\varianws\methods\combined ms-fid 150ml.mth	c:\varianws\calibration.smp
10	Inject	c:\varianws\methods\standby.mth	c:\varianws\standby.smp
11			

Figure 6 Example of sequence list of sample lists to be analyzed with respective injection methods.

10.2 Analysis

With the GC and MS both in “Ready” state, open the newly created sequence list and press the begin sequence list button. Confirm you want to start the first sample list with the respective method. The system will perform automated analyses of all sample lists in the sequence list, storing the MS and FID chromatograms acquired in the designated directories. Data acquisition methods may have compound lists in them that do not include all the desired compounds, or not have current peak assignments or calibrations. This is OK as chromatograms are typically reprocessed off-line.

11 DATA PROCESSING

11.1 Mass Spectrometry Data

11.1.1 Update data processing method

There are several steps to processing MS chromatograms once acquired. First, the compound table in the data processing method should be updated with the correct retention times and amounts for each calibration level should be confirmed to match what was actually injected. Then the updated method is used to process the calibration levels in order to update the instrument response factor for each compound. For MS chromatograms, this is done by selecting the View/Edit Methods icon in the toolbar and opening the data processing method to be used. This is typically the most recently used method that includes all the compounds of interest in the compound table. If there is no preexisting data processing method for the compounds of interest, one must be created from another data handling method, or from scratch. Refer to the instrument tutorial manuals for step-by-step instructions on this process.

In the Method directory tree on the left side of the window under the 2000 Mass Spec MS Data handling, select Compound Table. The compounds of interest appear in a table with retention times, abbreviated names, and other parameters. Below the table, press the Select Data File button and select a mid-level calibration file. In the table, double click on the Quan Ions cell for first compound. If the flag is not at the highest point of the correct peak, click on the highest point to reassign the retention time for that compound. At the bottom of the window, press the Next button and press Yes to accept the changes. Repeat for all compounds in the compound list.

11.1.2 Create a calibration recalculation list

Select the Automation File Editor icon in the Workstation toolbar. Create a new recalculation list and choose the directory to save it under, typically the same as where chromatograms are saved. Open the Windows Explorer program and highlight the calibration files, then click and drag them over the recalculation list. The chromatogram name and information populate the table automatically. Highlight the first row and press the Insert button to the right of the table. In the Sample Type cell in the new first row, select New Calib Block. In the rows below that, select Calibration for Sample Type. In the Cal level column enter the corresponding calibration level for each chromatogram. Save the recalculation list and close the window.

11.1.3 Process the calibration levels to update the calibrations in the data processing method

Select the Review/Process MS data icon in the Workstation toolbar. Find the directory with the chromatograms in the Selection pane on the left side of the window. To process the calibration levels, select the Process Data icon above the Selection Pane. In the Method File section, press the Browse button and select the updated data processing method. In the Recalc List File section, press the Browse button and select the calibration recalculation list just created. In the processing rules section, be sure the “all lines” radio button is selected. Press the Process button and wait for the program to finish integrating all chromatograms for the compounds in the compound table. When it’s finished, select the View Results icon. Scroll through all the compounds in each calibration level, checking to be sure the correct peak was identified and integrated properly. Also check that the calibration curve response factor and R^2 values are within reason ($R^2>0.95$). Save any changes made to the method and exit the View Results window.

11.1.4 Create a recalculation list for unknown samples

Select the Automation File Editor icon in the Workstation toolbar. Create a new recalculation list and choose the directory to save it under, typically the same as where chromatograms are saved. Open the Windows Explorer program and highlight the sample chromatograms to processed, then click and drag them over the recalculation list. The chromatogram name and information populate the table automatically. If the canister sample was diluted, enter the appropriate dilution factor in the multiplier box. Also, be sure to enter the sample volume (ml) in the Divisor box. This volume is controlled by the method used to analyze the sample. The software is set up to include the method name with sample volume in the actual chromatogram name. Save the new recalculation list and close the window.

11.1.5 Process the unknown samples using the updated data processing method

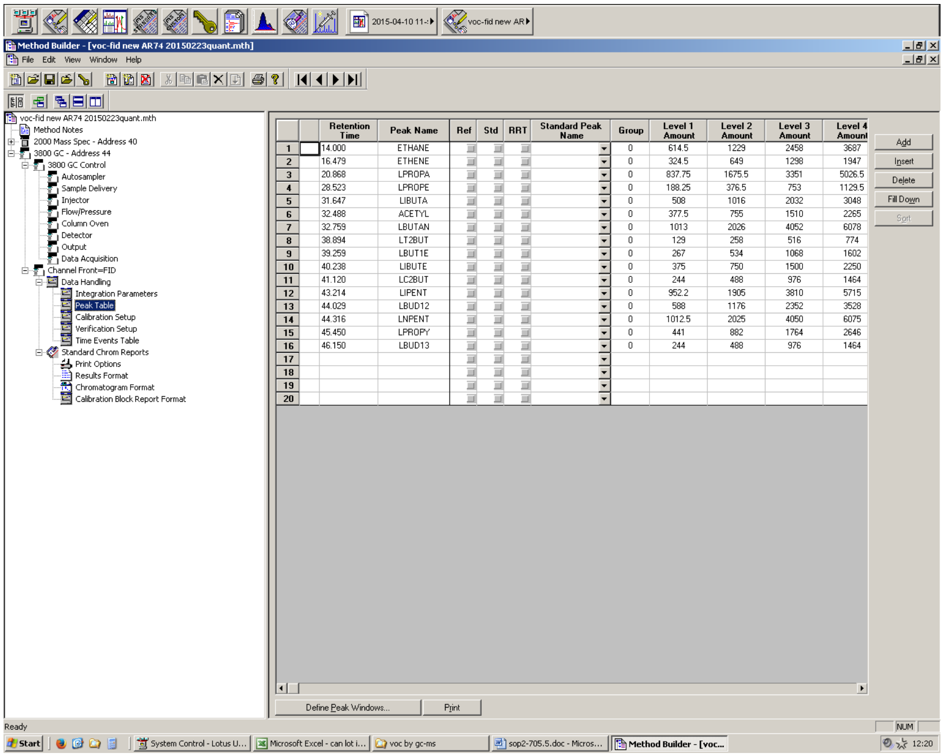
Select the Review/Process MS data icon in the Workstation toolbar. Find the directory with the chromatograms in the Selection pane on the left side of the window. To process the sample chromatograms, select the Process Data icon above the Selection Pane. In the Method File section, press the Browse button and select the calibrated data processing method. In the Recalc List File section, press the Browse button and select the sample recalculation list just created. Press the Process button and wait for the program to finish integrating all chromatograms for the compounds in the compound table. When it's finished, select the View Results icon. Scroll through each compound in each chromatogram to check that the proper peak was identified and integrated correctly. At the end of file, push the Print button and select Sample Reports then select ASCII. Save the text file in the same folder as the chromatogram, but shorten it's name to just the sample's PMI, followed by "–ms.txt." Repeat this process for all samples in the recalculation list. Select Save to preserve your Results View Changes.

The data processing method controls how the ASCII text file is structured. In order for the OLDS database to import results for each compound in the text file, the user-defined format for the text file should be in the following order; Compound Number, Retention Time, Peak Name, and Amount. This is selected in Results Format level of the Standard MS Reports section of the Channel 1=MS Data portion of 2000 Mass Spec section of the Method Directory when viewing the data processing method using Method Editor. In addition to having the proper output file structure, it is critical that the Compound ID for each analyte in the Compound Table be spelled exactly the same as the abbreviated name used for that compound in OLDS. Check with the OLDS administrator to confirm Compound ID's are correct, or new compounds need to be added to the database. Supporting material contains an example ASCII text file.

11.2 Flame Ionization Detector Data

11.2.1 Update data processing method

There are several steps to processing FID chromatograms once acquired. First, the retention times in the peak table in the data processing method should be updated with the correct retention times and amounts for each calibration level should be confirmed to match what was actually injected. Then the updated method is used to process the calibration levels in order to update the instrument response factor for each compound. For FID chromatograms, this can be done in the data processing method by clicking the Method Builder icon in the Workstation Toolbar and opening the desired data processing method file. Then, click on Peak Table under the Data Handling section of the channel for the FID in the 3800 GC Control heading (Figure 7). This is typically the most recently used method that includes all the compounds of interest in the peak table. If there is no preexisting data processing method for the compounds of interest, one must be created from another data handling method, or from scratch. Refer to the instrument tutorial manuals for step-by-step instructions on this process.



		Retention Time	Peak Name	Ref	Std	RRT	Standard Peak Name	Group	Level 1 Amount	Level 2 Amount	Level 3 Amount	Level 4 Amount
1		14.000	ETHANE	☐	☐	☐		0	614.5	1229	2458	3687
2		16.479	ETHENE	☐	☐	☐		0	324.5	649	1298	1947
3		20.868	LPROPA	☐	☐	☐		0	837.75	1675.5	3351	5026.5
4		28.523	LPROPE	☐	☐	☐		0	188.25	376.5	753	1129.5
5		31.647	LIBUTA	☐	☐	☐		0	508	1016	2032	3048
6		32.488	ACETYL	☐	☐	☐		0	377.5	755	1510	2265
7		32.759	LBUTAN	☐	☐	☐		0	1013	2026	4052	6078
8		38.894	LT2BUT	☐	☐	☐		0	129	258	516	774
9		39.259	LBUT1E	☐	☐	☐		0	267	534	1068	1602
10		40.238	LIBUTE	☐	☐	☐		0	375	750	1500	2250
11		41.120	LC2BUT	☐	☐	☐		0	244	488	976	1464
12		43.214	LIPENT	☐	☐	☐		0	952.2	1905	3810	5715
13		44.029	LBUD12	☐	☐	☐		0	588	1176	2352	3528
14		44.316	LNPENT	☐	☐	☐		0	1012.5	2025	4050	6075
15		45.450	LPROPY	☐	☐	☐		0	441	882	1764	2646
16		46.150	LBUD13	☐	☐	☐		0	244	488	976	1464
17				☐	☐	☐						
18				☐	☐	☐						
19				☐	☐	☐						
20				☐	☐	☐						

Figure 7 Method Builder screen showing peak table.

To update a compound's retention time, click on the time and type in the appropriate value. This can be observed by opening a chromatogram from a calibration level in the View/Edit Chromatograms tool from the Workstation Toolbar. Place the cursor over the peak of interest and note the retention time indicated at the bottom of the screen. Save the updated method and close Method Builder.

11.2.2 Process the chromatograms

With the View/Edit Chromatograms tool from the Workstation Toolbar, open the calibration chromatograms by selecting File, Add/Remove Chromatograms, and choosing the appropriate files and select the Open Files button. Then press the Integration List dialog button and under Sample Type select Calibration for each chromatogram. Choose the correct calibration level for each in the Cal. Level column. Be sure to select the radio button for "Clear Coefficients at the Start of List." Press the Calculate Results button and Save Changes. Close the Reintegration List dialog and check that peaks were correctly identified and integrated. If needed, adjust the peak retention time window below the chromatograms by clicking and dragging the yellow bar. Any unique integration events in the method may also be adjusted here. To check the calibration curves for each compound, click the Results drop-down menu and select View Calibration Curves. Scroll through each compound to be sure that the response factor and R^2 are within reason.

11.2.3 Process the unknown samples using the updated data processing method

Now that the data processing method has updated calibrations for each compound, open sample chromatograms a few at a time by selecting File, Add/Remove Chromatograms and choosing the appropriate files and select the Open Files button. Then press the Integration List dialog button. Confirm Sample Type is Analysis and if the canister sample was diluted, enter the appropriate dilution factor in the multiplier box. Also, be sure to enter the sample volume (ml) in the Divisor box. Press the Calculate Results button Save Changes. To view the results, click the Results drop-down menu and scroll down to the list of chromatograms. Hover over one chromatogram and when the menu appears to the right, scroll down and select Review Results Only. This opens the ASCII file containing results for that chromatogram. Click the icon to Convert Results to ASCII to automatically save the ASCII file as a text file. Repeat this process for each FID chromatogram. When finished, rename each text file to just the sample's PMI followed by "–front."

The data processing method controls how the ASCII text file is structured. In order for the OLDS database to import results for each compound in the text file, the user-defined format for the text file should be in the following order; Compound Number, Retention Time, Peak Name, and Amount. In addition to having the proper output file structure, it is critical that the Compound ID for each analyte in the Compound Table be spelled exactly the same as the abbreviated name used for that compound in OLDS. Check with the OLDS administrator to confirm Compound ID's are correct, or new compounds need to be added to the database. Supporting material contains an example ASCII text file.

11.3 Upload and Archive

Copy the chromatograms, data processing methods, sample lists, recalculation lists, and text files to a directory for the project on a shared drive to create an archived and networked backup of the processed instrument data. The shared drive should be one that is backed up daily, typically is located in I:\data\OAL-data4. Also, copy text files for the MS and FID chromatogram results for each sample to the appropriate directory in the project folder on the OAL's "H-drive". These are the files that contain results that will be incorporated into the OLDS database for data validation and reporting.

12 REFERENCE

1. U.S. EPA, *Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air*, “Compendium Method TO-15: Determination of Volatile Organic Compounds (VOCs) in Air Collected in Specially-Prepared Canisters and Analyzed by Gas Chromatograph/Mass Spectrometry (GC/MS),” EPA/625/R-96/010b

13 SUPPORTING MATERIAL

13.1 Gas Chromatograph method settings

```
**********************
3800 GC
**********************
Module Address: 44
Front Valve Oven
-----------------
Oven Power: On
Temperature: 65 C
Middle Valve Oven
-----------------
Oven Power: On
Temperature: 100 C
Rear Valve Oven
-----------------
Oven Power: On
Temperature: 150 C
Valve Table
-----------
Valve 1: Sample Valve
Initial: Off
0.01 min: On
1.00 min: On
2.00 min: On
3.00 min: On
7.00 min: Off
8.00 min: Off
9.00 min: Off
10.00 min: Off
10.50 min: Off
11.00 min: Off
13.50 min: Off
Valve 2: Sample Preconcentration Trap Valve
Initial: SPT Desorb
0.01 min: SPT Desorb
1.00 min: SPT Trap
2.00 min: SPT Trap
3.00 min: SPT Trap
7.00 min: SPT Trap
8.00 min: SPT Desorb
9.00 min: SPT Desorb
10.00 min: SPT Desorb
10.50 min: SPT Desorb
11.00 min: SPT Desorb
13.50 min: SPT Desorb
Valve 3: Event A Valve
Initial: Off
```

0.01 min: Off
1.00 min: Off
2.00 min: Off
3.00 min: Off
7.00 min: Off
8.00 min: Off
9.00 min: Off
10.00 min: Off
10.50 min: On
11.00 min: On
13.50 min: On
Valve 4: Series Bypass Valve
Initial: Series
0.01 min: Series
1.00 min: Series
2.00 min: Series
3.00 min: Series
7.00 min: Series
8.00 min: Series
9.00 min: Series
10.00 min: Bypass
10.50 min: Bypass
11.00 min: Series
13.50 min: Series
Valve 5: Sample Valve
Initial: Off
0.01 min: Off
1.00 min: Off
2.00 min: On
3.00 min: On
7.00 min: On
8.00 min: On
9.00 min: Off
10.00 min: Off
10.50 min: Off
11.00 min: Off
13.50 min: Off
Valve 6: Sample Preconcentration Trap Valve
Initial: SPT Desorb
0.01 min: SPT Desorb
1.00 min: SPT Desorb
2.00 min: SPT Desorb
3.00 min: SPT Trap
7.00 min: SPT Trap
8.00 min: SPT Trap
9.00 min: SPT Trap
10.00 min: SPT Trap
10.50 min: SPT Desorb
11.00 min: SPT Desorb
13.50 min: SPT Desorb
Valve 7: Column Selection Valve
Initial: Column 1

```
0.01 min: Column 1
1.00 min: Column 1
2.00 min: Column 1
3.00 min: Column 1
7.00 min: Column 1
8.00 min: Column 1
9.00 min: Column 1
10.00 min: Column 1
10.50 min: Column 1
11.00 min: Column 1
13.50 min: Column 2
Front Injector Type 1079
------------------------
Oven Power: On
Coolant: On
Enable Coolant at: 300 C
Coolant Timeout: 20.00 min
Temp Rate Hold Total
(C) (C/min) (min) (min)
--------------------------------
130 0 8.10 8.10
250 200 71.30 80.00
Middle Injector Type 1079
------------------------
Oven Power: On
Coolant: On
Enable Coolant at: 250 C
Coolant Timeout: 20.00 min
Temp Rate Hold Total
(C) (C/min) (min) (min)
--------------------------------
-80 0 10.10 10.10
250 200 68.25 80.00
Front Injector EFC Type 3
--------------------------
Flow Rate Hold Total
(ml/min) (ml/min/min) (min) (min)
------------------------------------
Middle Injector EFC Type 3
--------------------------
Flow Rate Hold Total
(ml/min) (ml/min/min) (min) (min)
------------------------------------
5.0 0.0 20.00 20.00
Rear Injector EFC Type 3
--------------------------
Flow Rate Hold Total
(ml/min) (ml/min/min) (min) (min)
------------------------------------
5.0 0.0 20.00 20.00
Column Oven
-----------
```

```
Coolant: On
Enable Coolant at: 100 C
Coolant Timeout: 20.00 min
Stabilization Time: 0.00 min
Temp Rate Hold Total
(C) (C/min) (min) (min)
--------------------------------
60 0.0 5.00 5.00
5 100.0 9.45 15.00
200 3.0 0.00 80.00
Front FID Detector
-------------------
Oven Power: On
Temperature: 250 C
Electronics: On
Time Constant: Fast
Time Range Autozero
(min)
-----------------------
Initial 12 yes
0.00 9 no
10.00 12 yes
Front Type 11 Detector EFC
---------------------------
Make up Flow: 23 ml/min
H2 Flow: 25 ml/min
Air Flow: 300 ml/min
Output Port A
--------------
Time Signal Attenuation
(min) Source
----------------------------
Initial Front 1
Output Port B
--------------
Time Signal Attenuation
(min) Source
----------------------------
Initial Front 1
Output Port C
--------------
Time Signal Attenuation
(min) Source
----------------------------
Initial Front 1
*********************
3800 Runlog
*********************
0.00 min: Column Oven Temperature: Setpoint 60 C
0.00 min: Column Oven Enable Coolant at: Setpoint 100 C
0.00 min: Front 1079 Injector Temperature: Setpoint 130 C
0.00 min: Front 1079 Injector Enable Coolant at: Setpoint 300 C
```

0.00 min: Front Injector EFC Type 3 Pressure:
Setpoint 13.3 psi
0.00 min: Front Injector EFC Type 3 Flow:
Setpoint 2.0 ml/min
0.00 min: Front FID Temperature: Setpoint 250 C
0.00 min: Front FID Range: Setpoint 12
0.00 min: Front FID Time Constant: Setpoint Fast
0.00 min: Front Valve Oven Temperature: Setpoint 65 C
0.00 min: Middle 1079 Injector Temperature: Setpoint -80 C
0.00 min: Middle 1079 Injector Enable Coolant at: Setpoint 250 C
0.00 min: Middle Injector EFC Type 3 Pressure:
Setpoint 10.3 psi
0.00 min: Middle Injector EFC Type 3 Flow:
Setpoint 5.0 ml/min
0.00 min: Middle Valve Oven Temperature: Setpoint 100 C
0.00 min: Rear Injector EFC Type 3 Pressure:
Setpoint 6.9 psi
0.00 min: Rear Injector EFC Type 3 Flow:
Setpoint 5.0 ml/min
0.00 min: Rear Valve Oven Temperature: Setpoint 150 C
0.00 min: Output Port A Signal Source: Setpoint Front
0.00 min: Output Port A Attenuation: Setpoint 1
0.00 min: Output Port B Signal Source: Setpoint Front
0.00 min: Output Port B Attenuation: Setpoint 1
0.00 min: Output Port C Signal Source: Setpoint Front
0.00 min: Output Port C Attenuation: Setpoint 1
0.00 min: Valve 1 Setpoint: Off
0.00 min: Valve 2 Setpoint: Off
0.00 min: Valve 3 Setpoint: Off
0.00 min: Valve 4 Setpoint: Off
0.00 min: Valve 5 Setpoint: Off
0.00 min: Valve 6 Setpoint: Off
0.00 min: Valve 7 Setpoint: Off
0.00 min: Front FID Range: Setpoint 9
0.01 min: Valve 1 Setpoint: On
1.00 min: Valve 2 Setpoint: On
2.00 min: Valve 5 Setpoint: On
3.00 min: Valve 6 Setpoint: On
5.00 min: Column Oven Temperature: Setpoint 5 C
5.00 min: Column Oven Ramp Rate: Setpoint 100.0 C/min
7.00 min: Valve 1 Setpoint: Off
8.00 min: Valve 2 Setpoint: Off
8.10 min: Front 1079 Injector Temperature: Setpoint 250 C
8.10 min: Front 1079 Injector Ramp Rate: Setpoint 200 C/min
9.00 min: Valve 5 Setpoint: Off
10.00 min: Valve 4 Setpoint: On
10.00 min: Front FID Range: Setpoint 12
10.00 min: Front FID Autozero: Setpoint yes
10.10 min: Middle 1079 Injector Temperature: Setpoint 250 C
10.10 min: Middle 1079 Injector Ramp Rate: Setpoint 200 C/min
10.50 min: Valve 3 Setpoint: On
10.50 min: Valve 6 Setpoint: Off

11.00 min: Valve 4 Setpoint: Off
13.50 min: Valve 7 Setpoint: On
15.00 min: Column Oven Temperature: Setpoint 200 C
15.00 min: Column Oven Ramp Rate: Setpoint 3.0 C/min
20.00 min: Front FID Temperature: Setpoint 250 C
20.00 min: Front Valve Oven Temperature: Setpoint 65 C
20.00 min: Middle Valve Oven Temperature: Setpoint 100 C
20.00 min: Rear Valve Oven Temperature: Setpoint 150 C

13.2 Mass Spectrometer method settings

```
MODULE ATTRIBUTES
Module: 2000.40
MS Workstation Version 6.9
Module Software Version: FF12
Module Option Keys: EI
Setpoints
Trap Temperature: 150 degrees C
Manifold Temperature: 80 degrees C
Transfer Line Temperature: 170 degrees C
Filament Number: 1
Axial Modulation Voltage: 4.0 volts
Air/Water Check
Last Checked: 2/23/2015 11:20 AM
Air Level Test Result: OK
Water Level Test Result: OK
Mass 28 Peak Width: 0.6 m/z
Mass 19 to Mass 18 Ratio: 5.4%
Total Ion Count: 921 counts
Integrator Zero Set
Last Executed: 2/23/2015 11:20 AM
Integrator Zero Set Result: OK
DAC Setpoint: 182 DACs
Average Counts: 0.5 counts
Electron Multiplier Set
10^5 Gain Last Executed: 2/23/2015 11:30 AM
10^5 Gain Value Set Result: OK
10^5 Gain Value: 2650 volts
Final Gain Value Last Changed: 2/23/2015 11:29 AM
Final Gain Value Set Result: OK
Final Gain Value: 2650 volts
RF Full Scale Adjust
Last Executed: 2/23/2015 11:30 AM
RF Full Scale Adjust Result: OK
DAC Setpoint: 147 DACs
Calibration Ion Used: 614 m/z
Mass Calibration
Last Executed: 2/23/2015 11:32 AM
Mass Calibration Method: FC-43
Mass Calibration Result: OK
Ion Mass Apex DAC Location Ion Intensity
28 174.7 39
69 431.7 2415
131 821.3 1062
264 1658.5 803
414 2603.8 271
464 2918.7 30
502 3157.7 186
614 3865.0 22
Average Calibration Slope: 6.260 DAC/m/z
Standard Deviation: 0.047
```

```
Trap Function Calibration
Last Executed: 2/23/2015 11:35 AM
Trap Function Calibration Result: OK
Mass 69 Frequency: 259.800 kHz
Mass 131 Frequency: 257.300 kHz
SIS Calibration
Last Set: No Record
SIS Calibration Set Result: INCOMPLETE
Amplitude Adjust Factor: 100%
Calibration Gas Adjust
Last Checked: 2/23/2015 11:19 AM
Cal Gas Adjust Result: OK
Ionization Time: 485 uSeconds
Total Ion Count: 4934 counts
CI Gas Adjust
Last Checked: No Record
CI Gas Adjust Result: INCOMPLETE
Reagent: Methane
Ionization Time: 0 uSeconds
Total Ion Count: 0 counts
RF Tuning Adjust
Last Checked: 10/17/2012 4:10 PM
RF Adjust Result: OK
Highest Count: 731 counts
Average Count: 332 counts
```

13.3 Example of text file of Results from MS chromatogram

p145m002i001-ms.txt p145m002i001-ms.txt

13.4 Example of text file of Results from FID chromatogram

p145m002i001-Front.TXT p145m002i001-Front.TXT

Scope of Work

Project 24-003
Improving Emission Rates Estimates of Commercial Marine Vessels

Prepared for

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

By

James Flynn
University of Houston

Chris Lindhjem
Ramboll

Jerker Samuelsson
FluxSense

September 9, 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 | 12:10:52 PDT
by Vincent M. Torres, The University of Texas at Austin

DocuSigned by:
Vincent Torres
1114EC755D0543B...

Project Manager, Texas Air Quality Research Program

This Scope of Work was approved electronically on 2024-09-20 | 14:53:33 CDT
by Cody Mclain, Texas Commission on Environmental Quality

Signed by:
Cody Mclain
C5A3703E1F0A413...

Project Liaison, Texas Commission on Environmental Quality

Table of Contents

1 ABSTRACT

The Texas Commission on Environmental Quality (TCEQ) relies on emission inventories to shape the State Implementation Plan (SIP), crucial for managing air pollutants such as nitrogen oxides (NO_X) and ozone (O_3). Recognizing the significance of reliable data, the team of the University of Houston (UH) and Ramboll propose this research project to address the research priority identified by the Air Quality Research Program (AQRP) to improve emission inventories for commercial marine vessels (CMV).

CMV emissions, particularly NO_X, constitute a substantial portion of coastal NO_X emissions. In the Houston-Galveston-Brazoria nonattainment area, CMVs accounted for approximately 18% of NO_X emissions in 2019, with a continued significant contribution expected for years to come. Among different vessel categories, smaller commercial vessels, notably towboats, were responsible for about 42% of CMV NO_X emissions in Texas in 2019 (TCEQ, 2023). Towboat and tugboat emissions have greater uncertainty than other CMV categories due to the lack of information on engines and the uncertainties of engine loads and operating parameters. This proposal aims to improve our understanding of commercial marine exhaust emissions, focusing on NO_X, volatile organic compounds (VOC), $PM_{2.5}$, and hydrocarbon speciation. The emphasis on smaller vessels will improve our ability to intercept their exhaust plumes.

Employing the instrumented UH research boat, our approach involves sampling emission plumes from vessels downwind of busy shipping lanes in Galveston Bay. Plumes will be identified by elevated levels of carbon dioxide (CO_2), NO_X, and other compounds. We expect to sample plumes from hundreds of towboats to meaningfully constrain the emission inventory. Leveraging real-time Automatic Identification System (AIS) transponder data, which reports vessel identification, position, speed, and draft, enhances our ability to connect measured plumes to individual vessels and ascertain engine information.

Emissions rates, derived from the field measurement data, will be compared with EPA expected values for each of the sampled and identified vessel engines. Multiple encounters with the same vessel over the sampling period will provide insights into emission variability. The analysis results have the potential to enhance the accuracy of the commercial marine emission inventory and speciated VOC reactivity. Such improvement can be integrated into various modeling frameworks, including those utilized for SIP modeling that support air quality planning efforts.

2 BACKGROUND

The Texas Commission on Environmental Quality (TCEQ) relies upon having accurate emission inventories to develop the Texas State Implementation Plan (SIP) for air pollutants including ozone (O_3) and fine particulate matter ($PM_{2.5}$). Improving the emission inventory for commercial marine vessels (CMV) is an AQRP research priority.

CMV emissions contribute a substantial fraction of the NO_X emission inventory for coastal areas. In the Houston-Galveston-Brazoria (HGB) nonattainment area, the CMV sector contributed 18% of NO_X emissions in 2019 according to TCEQ's HGB SIP revision (TCEQ, 2023). Worldwide, shipping NOx emissions are estimated to have risen by 3.8% from 2012 to 2018, despite new regulations, and will continue to be a substantial fraction of the coastal region NOx emissions for many years (Faber et al., 2020). Table 1 shows Texas state-wide CMV emissions in 2020 separated between larger ocean-going vessels (OGV) and smaller commercial vessels. Smaller commercial vessels, especially towboats, are identified as the primary contributors to NO_X emissions in Texas. Towboats alone were modeled to contribute 42% of CMV NOx emissions. Hence, this study will predominantly focus on improving emission estimates for towboats by measuring their emissions downwind of shipping lanes with high towboat activity in Galveston Bay but may also capture plumes from other vessel types.

Table 1. 2020 Texas CMV Emissions (tons/year) by Pollutant (Ramboll, 2021)

Vessel Category	**NO_X**	**VOC**	**CO**	**PM_{10}**	**$PM_{2.5}$**	**SO_2**
Towboats	*14,433*	*185*	*2,615*	*240*	*233*	*7*
Other Smaller Commercial	7,109	184	1,377	147	142	6
Ocean-going Vessels	12,745	614	1,449	332	306	824
All CMV	34,287	983	5,441	719	681	837

The emission factors are key inputs for emission estimates. For marine diesel engines, emission factors vary by engine category (identified by small to large engine displacements, Category 1 (C1), C2, and C3), group (propulsion or auxiliary), cylinder displacement, engine power, model year, and fuel sulfur level. Table 2 compares emission factors for NO_X and PM in different units for two common engine types (C1 and C2) used for towboat propulsion power, and larger (C3) OGV ship propulsion engines. Generally, newer engines are expected to have lower emission factors.

Researchers have found inconsistencies between measured NO_X emission rates and engine standards. Comer (2023) found that C3 ship engine NO_X emission rates did not show lower emission factors with increasing Tier levels. This proposal seeks to better characterize emissions rates of commercial marine exhaust emissions of NO_X, VOCs, and $PM_{2.5}$, and hydrocarbon speciation, especially for smaller vessels where exhaust plumes can be more easily measured from the UH research boat.

Table 2. Examples of Marine Diesel Engine Emission Rates (EPA 2022)

Model Year Standard	**Tier**	**NO_X**		**PM**		**Fuel Consumption Rate** (g/kW-hr)
		g/kW-hr	g/kg-fuel	g/kW-hr	g/kg-fuel	
Example Engine: Cat 3500 Category 1 (<5 l/cylinder) - smaller commercial vessel						
Precontrolled	0	11.0	52	0.21	0.99	213
2004	1	9.2	43	0.15	0.70	213
2007	2	6.0	28	0.20	0.94	213
2013	3	4.8	23	0.11	0.52	213
2015	4	1.3	6	0.04	0.19	213
Example Engine: EMD 710 Category 2 (11.5 l/cylinder) - smaller commercial vessel						
Precontrolled	0	13.36	63	0.21	0.99	213
2004	1	10.55	50	0.21	0.99	213
2007	2	8.33	39	0.31	1.45	213
2013	3	5.97	28	0.11	0.52	213
2015	4	1.3	6	0.03	0.14	213
Example Engine: Slow speed Category 3 - OGV						
Precontrolled	0	17	92	0.15	0.84	185
2000	I	16	86	0.15	0.84	185
2011	II	14.4	78	0.15	0.84	185
2016	III	3.4	18	0.15	0.84	185

3 OBJECTIVES

We will sample emission plumes from vessels immediately downwind from well-defined shipping lanes in Galveston Bay. Automatic Identification System (AIS) data for the proposed monitoring location was reviewed and observed passage of ~4 towboats per hour during daylight which indicates that we can expect to sample plumes from hundreds of towboats during the study. Plumes will be identified by measuring elevated carbon dioxide (CO_2) concentrations downwind of a unique and identified vessel. Similar work has been conducted to field sample highway trucks (Bishop et al., 2022) and marine vessels (Williams et al., 2009) emissions plumes. For each plume measurement, the concentration ratio of emissions to CO_2 was converted to emissions per unit of fuel consumed using a carbon balance method. The emission rates as a function of fuel consumed were compared with that expected of engines meeting the emission standards by model year. In addition, by collecting canisters for hydrocarbons we will speciate emissions. The main tasks include:

1. Utilize the UH marine vessel sampling system for 20 days of field sampling downwind of the Galveston Bay shipping channel to capture emissions from multiple vessels each day.
2. Estimate emission rates for each vessel using field data and determine engine characteristics (model year, model, power level) for comparison with emissions standards.
3. Collect VOC canisters in plumes to identify hydrocarbon constituents more accurately.

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 Ramboll and FluxSense
Deliverables: Approvable Work Plan

4.2 Project preparations and ordering

Orders for all major components, such as the T640, calibration and consumable gases, installation supplies, establish professional services contract with VOC canister laboratory, and address potential modifications to the boat to incorporate the instruments.

Due date: Within 60 days of receiving AQRP issued start date.
Responsible organization: University of Houston with assistance from FluxSense
Deliverables: Confirmation of order placement and updates of expected delivery times in the subsequent Monthly Technical Report (MTR).

4.3 Task 1.1 - Instrument integration

Assemble the sampling systems into the boat, including the data acquisition system and calibration gases. Mounting solutions for the FluxSense instrumentation will also be installed prior to the instrument's arrival so that it can quickly be mounted to the boat prior to deployment to the marina. It is likely that the FluxSense rooftop instruments will be removed prior to transport over the road for bridge and tree clearance and reinstalled at the marina. All instruments will be tested and calibrated prior to deployment, to the extent possible within the warehouses at UH.

Due date: Prior to field deployment
Responsible organization: University of Houston with assistance from FluxSense
Deliverables: Updates and documentation of completed instrument packages in MTRs.

4.4 Task 1.2 - Field Deployment

Deploy the instrumented Osprey boat to a marina with easy access to Galveston Bay for two months to perform nominally 20 days of commercial marine vessel emission sampling. Emissions of trace gases, VOCs, PM, and CO_2 will be accompanied by vessel identification data such as the Maritime Mobile Service Identity (MMSI), vessel name, photos, and other pertinent information such as the absence or presence of barges and number of barges. The Osprey will anchor with the sample inlets oriented into the prevailing wind a safe distance outside the channel downwind of commercial traffic in an area likely to see frequent towboat operations, often several per hour, both with and without barges. While anchored, the outboard engines will be shut off to reduce fuel costs and emissions. The upper section of the shipping lane in the vicinity of the Bayport Channel and Morgans Point where the Bay narrows is a high-traffic area for towboats and the UH crew has operated extensively in this area over the last three years.

Due date: Upon completion of instrument integration through April 2025
Responsible organization: University of Houston with assistance from FluxSense and guidance from Ramboll
Deliverables: Documentation of deployment and preliminary data plots of field data in MTRs.

4.5 Task 2 - Analysis and emission rate calculation

Calculate Emission Rates per Unit of Fuel Consumed

After pollutant concentrations in the exhaust plumes are sampled and measured, the concentration data can be used to calculate emission rates in the unit of grams per fuel consumed. Equation 1 shows an example of how to calculate NOx emission rate. A similar approach was used in the study from the International Council on Clean Transport (Comer et al. 2023). NOx, VOC, and $PM_{2.5}$ emissions rates will be calculated.

$$ER_{NO_x} = \frac{NO_{x\,measured} - NO_{x\,background}}{CO_{2\,measured} - CO_{2\,background}} \times \frac{46\ gNO_x\ mol^{-1}}{12\ gC\ mol^{-1}} \times FCC \qquad \text{Eq(1)}$$

ER_{NOx} = the NOx emission rate (g NOx/g fuel)
$NO_{x\ measured}$ = the concentration of NOx in the plume
$NO_{x\ background}$ = the background concentration of NOx
$CO_{2\ measured}$ = the concentration of CO_2 in the plume
$CO_{2\ background}$ = the background CO_2 concentration in ppm outside of the plume
FCC = fuel carbon content (usually about 0.87 g-Carbon/g-fuel for diesel fuel)

For each sampled vessel, we will identify vessel engine characteristics including engine model, model year, and other relevant factors, to determine NOx, VOC, and $PM_{2.5}$ emission rates expected by EPA. We will provide the best estimate of the vessel characteristics (type, engine model, and model year) from public data such as those published by the owner\operators of the vessel, secondary sources including vessel build and repair shops or other public sites, and the US Government[1] vessel database.

The calculated emission factor results from the field measurements will be compared with EPA's published emission standards (2020) and emission factors (2022) for each vessel. Given that a single vessel may undergo multiple samplings, we will scrutinize the results to understand the variability in field measurements. Combining this data with vessel activity information (speed, draft, etc.), we will discuss and summarize the comparison results, highlighting any significant findings and conclusions. This analysis has the potential to enhance the accuracy of the commercial marine emission inventory.

Characterize the Hydrocarbon Speciation

During sampling an Aroma-VOC analyzer (Kashtan et al., 2023) will provide real-time VOC information for bulk aromatics. This data, along with the other trace gas measurements, will be used by the crew to identify and periodically collect a grab sample in a VOC canister which will subsequently be analyzed for 71 compounds by the Desert Research Institute's (DRI) Organic Analytical Laboratory at the University of Nevada at Reno. DRI is highly regarded for its analytical services and is frequently used by the TCEQ, contractors, and collaborating universities for sample analysis. Up to 20 can samples are planned, with a portion reserved for quality assurance blanks. The canisters will be shipped to DRI in batches of four for analysis and results will be shared with all team members. Chain of custody forms which document the conditions, pressures, date, time, and location of the sample will be recorded so the results can be integrated with the remainder of the data set.

Due date: April – June 2025
Responsible organization: Ramboll with assistance from the University of Houston and FluxSense
Deliverables: Documentation of preliminary emissions analysis of field data in MTRs.

4.6 Task 3 - Project reporting and presentation

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 reporting 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 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

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[1] WCSC Vessel Characteristics (army.mil)

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 3 Deliverables are shown in Section 7.
Responsible organization: University of Houston with assistance from Ramboll and FluxSense
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 boat are maintained and operated in a responsible manner.

FluxSense

- Jerker Samuelsson, Co-PI – Responsible for the mobile extractive optical measurements and development of final data from the FluxSense instrumentation. Will lead the FluxSense portion of the project and oversee the installation of the instrumentation and training of UH personnel to operate, maintain, and troubleshoot as well as ensuring FluxSense personnel are available for remote support and limited field deployments during the campaign.

Ramboll

- Chris Lindhjem, Co-PI – Responsible for the classification of commercial marine vessel types and the calculation of associated emission factors based on plume data provided by UH and FluxSense. Will lead Ramboll's portion of the project including reporting to UH and assisting in presentations.

6 NOMINAL TIMELINE

Task and description	Timeline
Develop Work Plan	August 9–23, 2024
Project preparation and ordering	Within 60 days of receiving AQRP issued start date
Task 1.1 - Instrument integration	To begin with Notice to Commence and completed before field deployment.
Task 1.2 - Field deployment window	Approximately two months between the completion of instrument integration through April 2025
Task 2 - Analysis and emission rate calculation	April–June 2025
Task 3 - Project reporting and presentation	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 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 1, 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 the 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 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

Bishop, G. A.; Haugen, M. J.; McDonald, B. C.; Boies, A. M. 2022. "Utah Wintertime Measurements of Heavy-Duty Vehicle Nitrogen Oxide Emission Factors". Environ. Sci. Technol. 2022, 56, (3), 1885-1893, DOI: 10.1021/acs.est.1c06428.

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Ramboll, 2021. "2020 Texas Commercial Marine Vessel Emissions Inventory and 2011 through 2050 Trend Inventories." Prepared by Ramboll, Novato, CA; submitted to the Texas Commission on Environmental Quality, Austin, TX (July 2021).

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Williams, E.J., Lerner, B.M., Murphy, P.C., Herndon, S.C. and Zahniser, M.S., 2009. "Emissions of NOx, SO2, CO, and HCHO from commercial marine shipping during Texas Air Quality Study (TexAQS) 2006." Journal of Geophysical Research: Atmospheres, 114(D21).

Budget and Budget Justification

Project 24-003
Improving Emission Rates Estimates of Commercial Marine Vessels

Prepared for

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

By

James Flynn
University of Houston

Chris Lindhjeim
Ramboll

Jerker Samuelsson
FluxSense

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 | 13:01:21 CDT
by RoseAnna Goewey, The University of Texas at Austin

DocuSigned by:
5E69E9E496774ED...

Program Manager, Texas Air Quality Research Program

This Budget was approved electronically on 2024-09-20 | 12:10:52 PDT
by Vince Torres, The University of Texas at Austin

DocuSigned by:
1114EC755D0543B...

Project Manager, Texas Air Quality Research Program

This Budget was approved electronically on 2024-09-20 | 14:53:33 CDT
by Cody Mclain, Texas Commission on Environmental Quality

Signed by:
Cody Mclain
C5A3703E1E0A413...

Project Liaison, Texas Commission on Environmental Quality

Budget and Budget Justification

Overall budget

Improving Emission Rates Estimates of Commercial Marine Vessels
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%	0.50	$4,176
2.			$0	0.0%	0.00	$0
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$4,176**

B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)

			Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
1	1	Other Professionals / Postdoctoral Fellow	$4,040	39.8%	4.25	$17,170
2	1	Other Professionals / Researcher 3	$4,633	31.9%	1.00	$4,633
3	1	Other Professionals / Researcher 4	$5,244	30.3%	3.00	$15,733
4	1	Graduate Student	$2,100	7.0%	2.00	$4,200
		TOTAL OTHER PERSONNEL				**$41,736**
		TOTAL SALARIES AND WAGES (A+B)				**$45,912**

		Funds Requested
C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)		
1.	Senior Personnel	**$1,081**
2.	Other Personnel	**$13,373**
	TOTAL FRINGE BENEFITS	**$14,454**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)	**$60,366**
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)		
a)	*Teledyne T640 FEM PM2.5 analyzer*	$31,000
b)		$0
c)		$0
	TOTAL EQUIPMENT	**$31,000**

E. TRAVEL		Cost per Trip	# of Trips	
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)	$250	2	$500
2.	Foreign			$0
	TOTAL TRAVEL			**$500**

F OTHER DIRECT COSTS		
1.	Materials and Supplies	$36,631
2.	Professional Services - Idependent Contractors	$14,000
3.	Subcontracts (contracts will be issued by UT)	
a)	Ramboll	$47,827
b)	FluxSense	$35,000
c)		$0
d)		$0
4.	Tuition and Fees	$0
5.	Other	$0
	TOTAL OTHER DIRECT COSTS	**$133,458**

G. TOTAL DIRECT COSTS (A THROUGH F)		**$225,324**
H. TOTAL INDIRECT COSTS (MTDC)	**IDC Rate:** 15.000%	**$16,724**
I. TOTAL COSTS		**$242,048**

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

University of Houston
Improving Emission Rates Estimates of Commercial Marine Vessels
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%	0.50	$4,176
2.			$0	0.0%	0.00	$0
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$4,176**

B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)

			Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
1	1	Other Professionals / Postdoctoral Fellow	$4,040	39.8%	4.25	$17,170
2	1	Other Professionals / Researcher 3	$4,633	31.9%	1.00	$4,633
3	1	Other Professionals / Researcher 4	$5,244	30.3%	3.00	$15,733
4	1	Graduate Student	$2,100	7.0%	2.00	$4,200
		TOTAL OTHER PERSONNEL				**$41,736**
		TOTAL SALARIES AND WAGES (A+B)				**$45,912**

C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)

		Funds Requested
1.	Senior Personnel	**$1,081**
2.	Other Personnel	**$13,373**
	TOTAL FRINGE BENEFITS	**$14,454**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)	**$60,366**

D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)

		Funds Requested
a)	*Teledyne T640 FEM PM2.5 analyzer*	$31,000
b)		$0
c)		$0
	TOTAL EQUIPMENT	**$31,000**

E. TRAVEL

		Cost per Trip	# of Trips	Funds Requested
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)	$250	2	$500
2.	Foreign			$0
	TOTAL TRAVEL			**$500**

F OTHER DIRECT COSTS

		Funds Requested
1.	Materials and Supplies	$36,631
2.	Professional Services - Idependent Contractors	$14,000
3.	Subcontracts (contracts will be issued by UT)	
	a)	
	b)	$0
	c)	$0
	d)	$0
4.	Tuition and Fees	$0
5.	Other	$0
	TOTAL OTHER DIRECT COSTS	**$50,631**

			Funds Requested
G.	**TOTAL DIRECT COSTS (A THROUGH F)**		**$142,497**
H.	**TOTAL INDIRECT COSTS (MTDC)**	**IDC Rate:** 15.000%	**$16,724**
I.	**TOTAL COSTS**		**$159,221**

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

A. SALARIES

Dr. James Flynn, Co-Investigator, 3.8% effort over 13 months, will be responsible for the overall project management, execution, and reporting requirements. He will ensure the project is kept on track and objectives are met in a timely manner.

Dr. Travis Griggs, Postdoctoral Fellow, 32.7% effort over 13 months, will assist with the preparation and operation of both the instrumentation and research boat to be deployed during this project. As captain of the boat, he will have responsibility for the safe operation and continued compliance with US Coast Guard requirements. Travis will also lead the in situ data processing effort and assist with the reporting requirements.

Sergio Alvarez, Researcher 4, 23.1% effort over 13 months, will lead the instrument preparation and integration into the research boat. He will also be responsible for reviewing field and calibration data to ensure the quality is suitable for use in this project. Sergio will also backfill for the instrument operator on the boat should the primary operator be unavailable.

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.

TBN, graduate student, 15.4% effort over 13 months, will be trained by Sergio Alvarez and Travis Griggs to serve as the primary instrument operator during the two months of sampling operations aboard the research boat. They will also assist Travis with boat handling and docking procedures and with preliminary data processing.

B. FRINGE BENEFITS

The Department of Health and Human Service (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 at the University of Houston's Division of Research Website. Total fringe benefits budget requested: $14,454.

C. EQUIPMENT

We request the purchase of a Teledyne T640 FEM PM2.5 analyzer to characterize particulate matter emissions associated with exhaust plumes from commercial marine vessels. This instrument and associated installation and inlet components have a nominal lead time of 30 days after receiving the order as of August 2024 and will be purchased as soon as practicable upon receipt of Notice to Commence to ensure adequate time for installation aboard the research boat. Total equipment budget requested: $31,000.

D. OTHER DIRECT COSTS

MATERIALS AND SUPPLIES

Research boat support: We request funds to support the preparation, operation, and maintenance of the Osprey research boat during this project. Included in this request is support for marina fees for three months (three weeks prior to measurements for system and methodology refinement, two months for sampling, one week for final calibrations and removal, $1,500), launching and loading using the marina's travel lift ($1,000), fuel ($6,000 for gas and diesel), and a $5,000 usage fee to support scheduled and unscheduled maintenance, wear and tear on engines and other systems and coatings, and related incidentals.

Instrument support: We request funds to support instrument preparation, operation, and maintenance expenses incurred during this project. These include tubing and fittings ($2,500), calibration and consumable gases ($3,000), instrument usage and maintenance ($5,000), and contingency funds to support incidentals and unexpected expenses incurred during the course of the project ($4,131). We request $8,500 for the rental and use of an Aroma-VOC analyzer.

Total materials and supplies budgeted requested: $36,631

TRAVEL

Funds are requested for two project personnel to travel 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: $500.

PROFESSIONAL SERVICES – INDEPENDENT CONTRACTORS

DRI VOC canister sample analysis: Funds to support the sampling and analysis of 20 VOC canisters by the Desert Research Institute are requested. These funds include the cleaning and preparation of the canisters, shipping to and from the field, analysis, and standard reporting ($14,000). Total professional services requested: $14,000

SUBCONTRACT(S)

Ramboll will be a subcontractor under this project and will be contracted through UT Austin's Subaward Agreement. The costs associated for the subcontract are $47,827 for the period of 08/01/2024 through 08/31/2025. The subcontractor will be responsible for the conversion of the measurements collected by UH into emission rates and associating these rates with vessel specifics derived from AIS information as described in Task 2. The subcontractor will also contribute to the project planning, analysis, reporting, and presentation.

FluxSense will be a subcontractor under this project and will be contracted through UT Austin's Subaward Agreement. The costs associated for the subcontract are $35,000. FluxSense will be responsible for providing and installing a MeDOAS and a MeFTIR instrument on the boat, training UH personnel to operate the instrument, and providing troubleshooting support. If needed, FluxSense personnel will travel to the field up to 2-3 times to address troubleshooting and maintenance issues beyond the capability of the UH team. The UH team will perform the day-to-day operations of these instruments during the campaign.

Total subaward budget requested: $82,827

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: $16,724

Ramboll Budget and Justification

RAMBOLL

ENVIRONMENT
& HEALTH

AQRP 2024-25 Proposal

Proposal Title: Improving Emission Rates Estimates of Commercial Marine Vessels

Ramboll Budget and Budget Justification

Lbr Classification/Name	Loaded Hourly Labor Rate	Total	
		Hrs	Dollars
P4			
Chris Lindhjem	249.00	56	13,944
Greg Yarwood	249.00	8	1,992
P2			
Fiona Jiang	183.00	96	17,568
P1			
Alex Charn	139.00	92	12,788
Support	107.00	5	535
Labor Subtotal		257	46,827
Travel			1,000
Equipment			0
ODCs Subtotal			1,000
GRAND TOTAL		257	47,827

Ramboll's proposed budget of $47,827 is based on fully loaded rates agreed between the TCEQ and Ramboll. Dr. Chris Lindhjem will be the Co-Principal Investigator for Ramboll to provide his experience with engine emissions and marine vessel emissions inventory estimates. He will oversee the analysis of data produced during the project and how the results compare with estimates used in Texas emissions inventories. Fiona Jiang who also leads Ramboll's marine vessel with years of experience in emissions inventory work will manage the data analysis and reporting. Alex Charn will characterize the vessels' engines, analyze the plume data, and provide the emission inventory perspective. Greg Yarwood will contribute his experience with Texas air quality, modeling, emissions inventories, and comparing models with ambient measurements. A travel budget of $1000 is included for one person from Ramboll to attend a AQRP workshop in Austin, TX.

FluxSense Budget & Justification

FluxSense Inc
Improving Emission Rates Estimates of Commercial Marine Vessels
AQRP Budget Summary

Principal Investigator: Jerker Samuelsson
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.	Jerker Samuelsson	CEO and Senior PI	$8,750	25.0%	0.50	$4,375
2.			$0	0.0%	0.00	$0
3.			$0	0.0%	0.00	$0
	TOTAL SENIOR PERSONNEL					**$4,375**

B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)

	Number	Category	Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
1	2	Other Professionals / Technical Specialist	$7,900	25.0%	1.00	$7,900
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					**$7,900**

TOTAL SALARIES AND WAGES (A+B)	**$12,275**

C. FRINGE BENEFITS (AUTOMATICALLY CALCULATED BASED ON ENTERED RATES)

1.	Senior Personnel	**$1,094**
2.	Other Personnel	**$1,975**
	TOTAL FRINGE BENEFITS	**$3,069**

TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)	**$15,344**

D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING $5000)

a)	*MeFTIR and MeDOAS instrument rental*	$8,800
b)		$0
c)		$0
	TOTAL EQUIPMENT	**$8,800**

E. TRAVEL

		Cost per Trip	# of Trips	Funds Requested
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)	$1,220	3	$3,660
2.	Foreign			$0
	TOTAL TRAVEL			**$3,660**

F OTHER DIRECT COSTS

1.	Materials and Supplies	$2,631
2.	Professional Services - Independent 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	**$2,631**

G. TOTAL DIRECT COSTS (A THROUGH F)		**$30,435**
H. TOTAL INDIRECT COSTS	**IDC Rate:** 15.000%	**$4,565**
I. TOTAL COSTS		**$35,000**

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.

FLUXSENSE INC
Improving Emission Rates Estimates of Commercial Marine Vessels
AQRP Budget Justification

A. SALARIES

Jerker Samuelsson, Principal Investigator, 0.5% effort, will be responsible for managing the FluxSense efforts and provide oversight, quality assurance and expertise in data analysis.

Dr. Anthony Babore, Co-Investigator, 0.5% effort, will be responsible for instrumentation installation and training of UH personnel in maintaining the instrumentation and data analysis support.

Dr Brian Offerle, 0.5% effort, will perform data analysis.

B. FRINGE BENEFITS

Fringe benefits rates are based on FluxSense's federally negotiated rates for the appropriate employee benefits level at the time of proposal submission (25% on direct salary). Total fringe benefits budget requested: $3,069

C. EQUIPMENT

Funds are requested for the following equipment:

1. Equipment 1: The budget of $8800 for instrument rental of MeFTIR and MeDOAS instruments for the purpose of VOC, BTEX, CH4 and CO analysis in Commercial Marine Vessel plumes.

Total equipment budget requested: $8,800

D. OTHER DIRECT COSTS

MATERIALS AND SUPPLIES

Supplies are calculated at $2631 for installation and maintenance of the FTIR and DOAS instrumentations in the field campaign. Total materials and supplies budgeted requested: $2,631

TRAVEL

Funds are requested for project personnel to travel to install equipment on the monitoring boat, train UH personnel in running the instrumentation and for recurring service trips to secure/restore operations. Travel costs in this budget are based on sponsored research travel for previous similar trips and are calculated for the domestic travel of one personnel to take three trips. Total travel budget requested: $3,660

TUITION

N/A

SUBCONTRACT(S)

N/A

INDIRECT COSTS

The indirect cost rate of 15% of total direct costs TDC is used as instructed by the AQRP's published proposal preparation instructions. Total indirect cost budget requested: $4,565

RoseAnna Goewey

From:	Jocelyn Mellberg <jocelyn.mellberg@tceq.texas.gov>
Sent:	Friday, September 13, 2024 10:25 AM
To:	RoseAnna Goewey
Cc:	Torres, Vincent; Torres, Vince Aqrp; Matthew Southard; Brenda Fritz; Amber Ni; Cody Mclain
Subject:	RE: UT Austin - AQRP / 24-003 Equipment Request

Good Morning,

Thank you for your email.

TCEQ authorizes contract funds to be used to acquire the **Teledyne T640 FEM PM2.5 analyzer** equipment, valued at **$31,000**. UT remains responsible for the contract provisions regarding equipment, and ensuring subawardee compliance with Texas Grant Management Standards (TxGMS), including Equipment Property Standards. Equipment standards including:

a) Keeping the equipment and continuing to use it on the activities under the subaward or contract for as long as needed.

b) Managing the equipment until disposition takes place subject to the standards in TxGMS, including maintaining property records, conducting a physical inventory at least once every two years, developing a control system, and performing adequate maintenance to keep the equipment in good condition.

c) Seeking TCEQ approval if the equipment is used for activities unrelated to the subaward or contract activities; to provide services for a fee that is less than private companies charge for equivalent services; or as a trade-in with the proceeds to offset the cost of replacement property.

d) Obtaining written disposition instructions from TCEQ when the equipment is no longer needed for the subaward or contract, or any other authorized activity, unless the per unit fair market value of the equipment is less than $5,000 or disposition instructions have been previously provided.

Let us know if you have any questions

Thanks!

Jocelyn

From: RoseAnna Goewey <rgoewey@utexas.edu>
Sent: Friday, September 13, 2024 10:02 AM
To: Jocelyn Mellberg <jocelyn.mellberg@tceq.texas.gov>
Cc: Torres, Vincent <vmtorres@mail.utexas.edu>; Torres, Vince Aqrp <v.torres@ceer.utexas.edu>; Matthew Southard <matthew.southard@tceq.texas.gov>; Brenda Fritz <Brenda.Fritz@tceq.texas.gov>; Amber Ni <Amber.Ni@Tceq.Texas.Gov>; Cody Mclain <cody.mclain@tceq.texas.gov>
Subject: UT Austin - AQRP / 24-003 Equipment Request
Importance: High

Good Morning Jocelyn,

On behalf of The University of Texas (UT), I am submitting this formal request for approval to acquire a **Teledyne T640 FEM PM2.5 analyzer** equipment, valued at **$31,000**, as part of our ongoing project with the Texas Commission on Environmental Quality (TCEQ) Air Quality Research Program (AQRP). This equipment is essential and necessary for the work outlined in the **Project 24-003** Workplan, which will be performed by the

University of Houston (UH) under the subaward (PI: Flynn, Title: Improving Emission Rates Estimates of Commercial Marine Vessels). UH will coordinate the procurement of the equipment.

UT will remain responsible for adhering to the Texas Grant Management Standards (TxGMS), particularly the Equipment Property Standards, which include:

- Using the equipment for contract-related activities as long as it is required.
- Managing and maintaining the equipment in accordance with TxGMS standards, including property records, physical inventories, control systems, and adequate maintenance.
- Seeking TCEQ's approval if the equipment is used for non-contract activities or for services that private companies typically charge for, or as a trade-in to offset the cost of new property.
- Obtaining written disposition instructions from TCEQ when the equipment is no longer needed, unless the fair market value is less than $5,000 or other instructions have been provided.

We appreciate your attention to this matter and look forward to your approval.

Please feel free to reach out if you have any questions or need further information.
RoseAnna
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ROSEANNA GOEWEY, MBA, Program Manager
The University of Texas at Austin | Cockrell School of Engineering | Center for Energy and Environmental Resources
10100 Burnet Road | Bldg. 133 (EME), Rm. 1.318A| Mail Code: R7100 | Austin, TX 78758 | (512) 232-5040 | rgoewey@utexas.edu

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Document Pages: 79	Signatures: 9	Envelope Originator:
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Vincent Torres vmtorres@eid.utexas.edu Associate Director The University of Texas at Austin, Center for Energy & Environmental Resources Security Level: Email, Account Authentication (None)	DocuSigned by: Vincent Torres 1114EC755D0543B... Signature Adoption: Uploaded Signature Image Using IP Address: 128.62.227.73	Sent: 9/20/2024 1:00:38 PM Viewed: 9/20/2024 2:09:38 PM Signed: 9/20/2024 2:10:52 PM
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