Scope of Work

Project #22-020
Quantifying the Emissions and Spatial/Temporal Distributions of Consumer Volatile Chemical Products (VCPs) in the Greater Houston Area

Prepared for

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

By

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2022.09.12
Version #5

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.

All AQRP Reports and Documents must be Accessible. Please refer to:
https://aqrp.ceer.utexas.edu/WritingGuidance.pdf

Approvals

This Scope of Work was approved electronically on **<u>09/02/2022</u>** by Elena McDonald-Buller, The University of Texas at Austin

Elena McDonald-Buller
Project Manager, Texas Air Quality Research Program

This Scope of Work was approved electronically on **<u>09/13/2022</u>** by Bipin Sharma, Texas Commission on Environmental Quality

Bipin Sharma
Project Liaison, Texas Commission on Environmental Quality

Scope of Work

1. Background

Air pollution is the fifth largest cause of death in the world.[1] Volatile organic compounds (VOCs) can also undergo chemical reactions with atmospheric oxidants to form major atmospheric pollutants, such as photochemical ozone (O_3) and particulate matter (PM).[2, 3] Traditionally, a significant portion of the VOCs from the urban environment comes from traffic and tailpipe emissions, power plants, and residential combustion.[4] During the past few decades, as VOC emission reduction strategies have been successfully implemented, traffic related VOC emissions have decreased rapidly, leading to an increase of the relative contribution of other types of VOCs.[5] With this changing emission profile of carbonaceous compounds in urban areas, volatile chemical products (VCPs) have become one of the most significant sources of anthropogenic VOCs.[4, 6, 7]

VCPs typically consist of organic species from consumer products and business activities, including cleaning agents, printing inks, personal care products, pesticides, and coatings.[7-9] Compounds such as decamethylcyclopentasiloxane (D5-siloxane), ethanol, alkenes, and monoterpenes are major VCP emission sources in the urban environment.[6, 7] Recent studies conducted in New York City, Los Angeles, and a few European cities have shown that VCPs account for half of the petrochemical VOCs in urban areas, comparable to or exceeding the emissions of a summer forest.[10, 11] However, as VCP emission is strongly dependent on the number and type of consumer and business activities as well as population, there are significant variations in the spatial and temporal distributions and dominant species of VCPs among different cities.[8]

Currently, the emissions of VCPs from residential, commercial, institutional, and industrial sources have been included in the National Emissions Inventory (NEI) as the solvent utilization sector [4]. In Texas, VOC emissions from motor vehicles decreased from 486.4 Gg in 1996 to 70.5 Gg in 2021 based on the State Tier 1 criteria air pollutants emission trends data,[12] but VOC from solvent utilization only decreased from 321.5 Gg to 216.9 Gg in the same period. Such trend highlights an increasing relative importance of VCP in VOC emissions within the state of Texas. Even though NEI-based emission inventory demonstrates that more than 70% of the VCPs in Texas are emitted from consumer and commercial solvent use, these emission estimates might still be lower than reality.[13] For instance, McDonald et al.[11] showed that the VCP emissions at Los Angeles based on NEI might be a factor of 2-3 lower. Seltzer et al.[4] also developed a new VCP emission inventory (VCPy) based on a new modeling framework. In this framework, the emission of an organic compound from a product depends on the magnitude of the product use timescale and the evaporation timescale of the component. Emission occurs if the evaporation timescale is less than the assigned product use timescale, leading to additional increase in VCP emission. The estimated 2017 VCP emissions in Texas from the VCPy inventory is 247 Gg, almost 20% higher than the NEI estimation of 212 Gg.[4] However, there is no measurement data to verify the accuracy of either emission inventories in Texas.

Emissions of VCPs are dominated by oxygenated compounds, alkanes (such as acetone, isopropyl alcohol, propane, and isobutane), and personal care products (such as D5-siloxane and monoterpenes).[4] Even though certain oxygenated compounds are typically not highly reactive in the formation of tropospheric O_3 as indicated by their low Maximum Incremental Reactivity (MIR) values,[14] personal care products, one of the top three VCP categories of consumer products (e.g., personal care and household products, such as cleaning products and detergents), could contribute to significant O_3 formation.[15] These personal care products often contain fragrances such as monoterpenes, which can readily react with atmospheric oxidants such as OH, NO_3, and O_3 due to their double bond structure, thus having relatively short atmospheric lifetimes compared with alkanes from vehicle emissions and other types of VCPs.[10, 11] The MIR values of monoterpenes are comparable to major aromatic compounds from motor vehicles (e.g., toluene MIR = 3.97 vs. d-limonene MIR = 3.99),[14] highlight the importance of VCP in ozone formation in the urban area. Coggon et al.[10] estimated that the emission of anthropogenic monoterpene in New York City is 14.7-24.4 kg d^{-1} km^{-2}, mostly from fragranced VCPs. These high emissions rates are similar to the summertime monoterpene emissions for a typical forest in the United States.[3] In the populated urban regions, such as New York City, where O_3 formation is VOC-limited, VCPs account for more than half of the 20 ppb maximum daily average 8-h (MDA8) O_3 attributed to anthropogenic VOCs. Previous study also showed that representing the oxygenated VOCs from the VCPs (oVCPs) explicitly in photochemical mechanisms could lead to approximately 15-20% increase in peroxyacetyl nitrate (PAN) concentrations compared to simulations with oVCPs represented by hydrocarbons.[8] The higher PAN predictions could enhance the O_3 formation in downwind areas.[16, 17] Recent studies demonstrate that VCP-derived SOA contributes to half of the background SOA in Los Angeles and significantly reduces the bias of ozone and PM mass concentration.[8, 9]

As the fourth largest city in the US, with more than 7 million people in the surrounding areas, Houston has no reported ambient measurements of the VCP to our knowledge, highlighting the urgent need to update the VCP emission inventory in the Greater Houston Area validated by ambient measurements with detailed spatial and temporal resolution. The recent VCPy emission inventory also shows higher than expected VCP emissions in the Greater Houston Area,[4] further demonstrating the need to use real-world measurements to constrain the uncertainties in model parameterization. In addition, current modeling results sometimes underpredict peak O_3 concentrations on high O_3 days in Houston.[18, 19] An improved understanding of VCPs in the Houston area may also improve predictions of O_3 concentration in the Greater Houston Area, bridging the gap between modeled and measured O_3 concentration.

2. Scientific Objectives

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

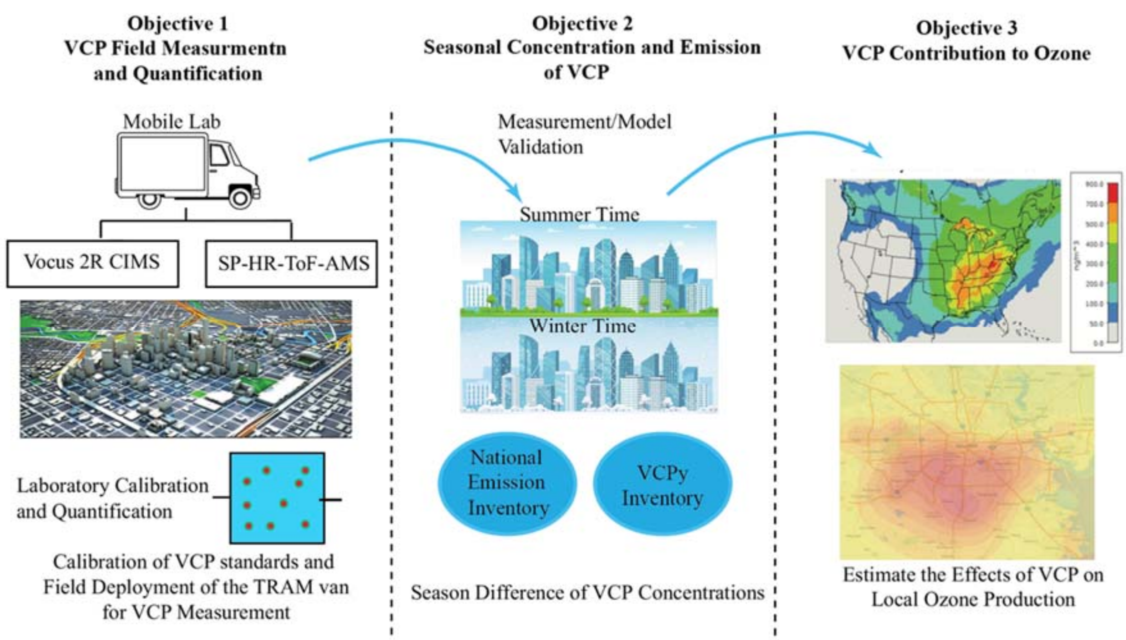

Figure 1. *Overview of our research approach and objectives that address the overarching project hypothesis*

Based on the overarching goal, we identified three major scientific objectives for this proposed research: **(1)** conduct field measurements of a broad range of VOCs, including oxygenated VOCs and monoterpenes, in the Greater Houston area using the Vocus Chemical Ionization Time-of-Flight Mass Spectrometer (Vocus CI-MS) on a mobile platform; **(2)** characterize seasonal difference of VCP concentrations in Houston; and **(3)** improve understandings of how VCP affect air quality in the Houston, including MDA8 O_3. These three scientific objectives will be described in detail in section 3.

Our proposal directly addresses the AQRP research priority areas "Improve emission inventories" and "Changing emission patterns in Texas". The proposal takes a multidimensional approach using observations from "TRACER-AQ measurement", data analysis, and modeling studies to improve understanding of "emission inventories", "changes in the emission impacts of industrial sources", and "emission impacts of population growth in areas with limited current monitoring". The results from this study will be publicly available to the scientific community.

3. Scope of Work

An overview of our approach is shown in Figure 1, which encompasses analyzing previous field measurement data and combining measurement data with detailed photochemical models and two latest sets of VCP emission estimations, i.e., the National Emissions Inventory (NEI) and VCPy.[4] The seasonality difference of VCP in the Houston area will also be understood. Lastly, the updated VCP emission inventory will be used to estimate the contribution of VCP to local ozone concentrations. The scientific research objectives will be accomplished by the following three tasks.

Task 1: Determine the spatial and temporal distribution of VCPs in the Greater Houston Area

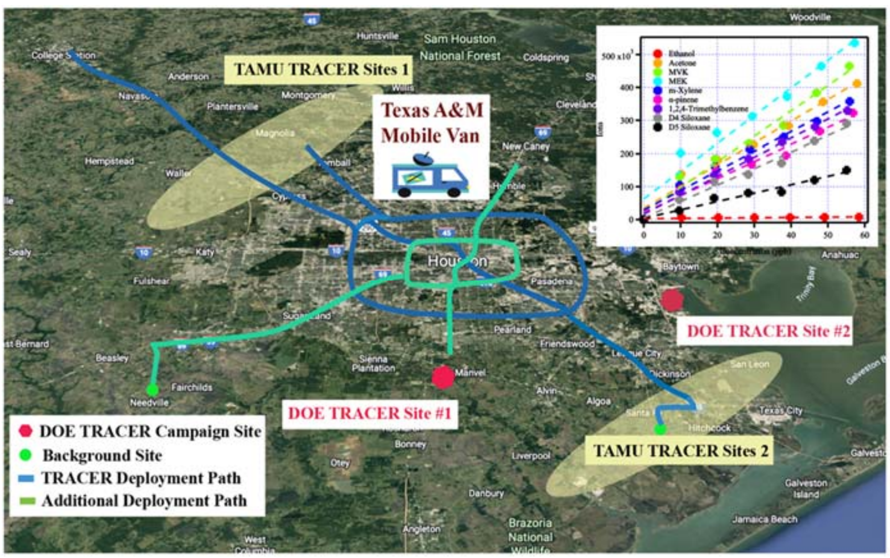

Figure 2. *Field deployment map of the Texas A&M Mobile Van. The blue line represents the deployment route during the TRACER campaign. The green line represents the additional deployment path after TRACER, to further capture VCP emissions. The green solid dots are background sites where there is limited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

PI Zhang is part of the Texas A&M TRACER team and will collect ambient gas and particle data during the TRACER Intensive Operation Period (IOP) in the summer 2022. Specifically, Texas A&M University Rapid Measurements Van (TRAM van) will be deployed to measure the urban climate and atmospheric composition across the Greater Houston Area (GHA). The TRAM van includes a Vocus 2R Chemical

Ionization Mass Spectrometer (Vocus 2R CI-MS) and Vocus Inlet for Aerosols (VIA). **Prior studies demonstrate that Vocus 2R CI-MS and VIA are capable of providing a comprehensive chemical characterization of atmospheric VCPs.**[7, 8] VIA consists of a precisely controlled heating tube that can be heated up to 250 °C. When aerosol particles pass through the VIA, the organic species will be evaporated into the gas phase and then be detected by the Vocus CI-*MS*. Having VIA is especially useful because the oxidation products of VCP-derived monoterpenes have lower volatility and can partition between the gas and particle phase.[20, 21] A combination of the regular Vocus CI-*MS* and VIA-Vocus system will be able to detect the total amount of VCPs and their oxidation products in the gas- and particle-phase. As shown in the inset of Figure 2 above, our preliminary Vocus CI-MS data show strong linearity of several key VCP compounds. Further analysis shows that the Vocus CI-MS can reach ppb to ppt detection for these VCP species after considering the stability of the baseline. We will further extend our work based on the method described by previous studies to detect two hundred major VCP species.[7, 8]

Full quantification of the monoterpenes and their oxidation products can help constrain ozone formation from the VCPs. In addition, other atmospheric relevant parameters, including the temperature, relative humidity, aerosol mass loading, and O_3, will also be recorded by the meteorological station and a Soot Particle Aerosol Mass Spectrometer (SP-AMS).

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

Before, during, and after the field study, Vocus CI-MS will be optimized and calibrated with common VCP compounds spanning a wide range of volatilities and atmospherically relevant relative humidity (RH) conditions. An enhancement ratio (ER), which is defined as Eqn. (1), can be used to calculate the contribution of VOCs from VCP sources.

$$ER = \frac{[VOC]_{in\ city} - [VOC]_{background}}{[Reference\ VOC]_{in\ city} - [Reference\ VOC]_{background}} \qquad (1)$$

The reference compounds for the traffic emission and biogenic emission are benzene and α-pinene, respectively. Eqns. (1) can be used to quantify VOCs from VCP contributions by calculating the ER value.[8] When ER value is higher than 1, there is VCP contribution in the VOC concentration. In addition, the positive matrix factorization (PMF) and multilinear engine (ME-2) methods will also be applied to both Vocus CI-MS and VIA-Vocus data to identify the VOCs from VCP sources.[22]

The combined data from the mobile van facility, the Vocus 2R CI-MS, VIA, and other mobile van measurements, including AMS, will provide crucial key information in understanding the spatial and temporal variabilities of the VCP and their oxidation products in the Greater Houston Area. These ambient-derived data will also be used as constraints to optimize the VCP emissions using a high spatial resolution regional chemical transport model, as described in Task 2.

Task 2: Characterizing the Seasonality Difference of VCP in the Houston Area

VCP emissions are highly dependent on human activities. The spatial and temporal distributions of VCPs in the Greater Houston area will likely show a strong seasonal difference during to different emission profiles and human activities between different seasons. Our study proposes to be the first to understand the seasonal difference of VCP emissions and concentrations in an urban area.

To understand the seasonal differences of VCP emissions, we plan to deploy the Texas A&M Measurement van twice during the funding period to cover both fall and winter VCP emission profiles of the Houston Area. We plan to test and condition the mobile van for the first 1-2 weeks and then measure the mobile van for 3-5 weeks each between October-November 2022 and January-February 2022. We aim to deliver 10-15 days of useful data between each deployment, so in total we should obtain 20-30 days of useful data between the whole funded periods that can capture the seasonality variation of VCP emissions in Houston. The data collected from these two time periods will be analyzed to compare the VCP composition, concentration, and spatial distributions to understand the differences of VCPs in the ambient environment between fall and wintertime in a metapolitical areas.

In addition, the seasonal difference of VCP can be used to improve model simulations. Two sets of VCP emissions from the traditional models will be compared with our field measured seasonal data. The first set of emissions will be based on the 2017 and 2020 emissions provided by US EPA, generated using the 2017 NEI data. Emissions for 2022 will be estimated using linear interpolation using 2017 and 2020 emission estimations. The second set of emissions will be based on the VCPy emission inventory from US EPA with the most recent update of the VCPy inventory.[4] We plan to use the county-level trend from recent years to estimate emissions in 2022. Detailed VOC speciation profiles to generate speciated VCPs in the VCPy inventory will be obtained from US EPA and processed using the SpecDB program from Dr. William Carter of UC Riverside.[27] Emissions from other emission sectors will be generated using the 2017 and 2020 NEI emissions, linearly interpolated to 2022. Lightning NOx emissions will be calculated inline using flash counts from the National Lightning Detection Network (NLDN).

Biogenic emissions will be generated using the latest version of the Model of Emissions of Gases and Aerosols from Nature (MEGAN) v3.2. To better represent biogenic emissions from urban vegetations, the default Leaf Area Index (LAI), total vegetation cover, and BVOC emitting tree fractions in the MEGAN input database for the urban Houston areas will be replaced by the 1-km resolution dataset developed from AQRP project 20-007. The improvements in the input data will allow a more accurate estimation of the monoterpene concentrations from biogenic sources in urban areas so that the impact of monoterpenes from VCPs can be differentiated.

Two sets of CMAQ runs will be conducted using the two sets of VCP emissions to cross-validate our seasonal VCP measurement data. Model performance statistics for O_3, NOx, and $PM_{2.5}$ will be statistically evaluated to ensure that the model captures the general feature of air pollution during the study periods. The predicted concentrations of major gaseous VCP species, including the oVOCs, isoprene, and monoterpenes, will be compared with measurements from Task 1. Gas and particle phase monoterpene tracers (pinic acid, pinonic acid, and MBTCA) will also be compared with measurements to provide further evaluation of the monoterpene emissions. In addition, VOC measurements of major hydrocarbon species at the automatic gas chromatography (auto-GC) sites throughout the Greater Houston area will also be compared with observations. The inventory that leads to better overall model performance will be selected for further improvement to assess the impacts of VCPs on O_3 and SOA, as described in Task 3.

Task 3: Assess the effects of urban VCPs on air quality, including MDA8 O_3 and monoterpene SOA.

In this study, emissions of major primary VOCs from different sources, including the oVOCs and explicit monoterpenes, will be tracked using different model species. For example, the d-limonene from personal care products and biogenic emissions will be represented by two model species, D-LIMONENE_X1 and D-LIMONENE_X2. These species will have identical chemical reactions and products, so the overall reactivity of the simulated atmosphere is not changed. By this approach, the contributions of VCPs to the ambient VOC concentrations can be directly determined.

The emissions of individual oVOCs and monoterpenes can be improved using a multilinear regression approach, as shown in Eqn. 2,

$$\boldsymbol{C}_{pred} = \alpha_1 \boldsymbol{C}_{p,1} + \alpha_2 \boldsymbol{C}_{p,2} + \cdots + \alpha_n \boldsymbol{C}_{p,n} \quad (2)$$

where $\boldsymbol{C}_{pred}$ is the improved prediction of the total concentration of the one VCP species. $\boldsymbol{C}_{p,i}$ is the predicted concentration of the VCP from the i^{th} source. n is the total number of sources explicitly tracked in the CMAQ simulation. The α values are the estimated emission adjustment factors of the VCP for different sources. The adjustment factors are determined by optimizing the objective function $\tilde{Q}$ shown in Eqn. 3,

$$\begin{aligned}\tilde{Q} &= Q_0 + \lambda Q_p \\ &= \sum_{i=1}^{N} \left(\ln C_{obs,i} - \ln C_{pred,i}\right)^2 + \lambda \sum_{j=1}^{N} \left(\ln \alpha_j\right)^2 \end{aligned} \quad (3)$$

where N is the number of available observations. The first part of the equation, Q_0, is a unique function with log-transformation to quantify the difference between predicted and observed VOC concentrations, as opposed to the sum of the squares of the residuals used in regular multilinear regression analyses. As explained in detail in our previous work,[28] the log-transformation better estimates the regression coefficients for log-normally distributed atmospheric data. In this study, the additional penalty term (Q_p) is included to constrain the adjustment factors so that they do not lead to unrealistically large changes in the estimated emissions. The L-curve method will be used to find the optimal lambda value in Eqn. 3.[29]

In addition to applying this method to one species at a time, the analysis can also include all observed VOCs simultaneously to determine the overall VOC emission adjustment factors for each source. In addition to the VOCs observed from the mobile measurements, observations of major hydrocarbon species at the automatic gas chromatography (auto-GC) sites throughout the Greater Houston area will also be included. The concentrations of the observations and predictions will be normalized so that the high and low-concentration species can both contribute to determining the emission adjustment factors. Both approaches will be explored, and an optimized emission inventory will be generated.

A final set of CMAQ simulations will be conducted to evaluate the impact of consumer VCPs on MDA8 O_3 and monoterpene SOA. Three simulations will be conducted: (1) without emissions of VCPs; (2) with VCPs emissions from other sectors but without consumer VCPs, and (3) with all VCP emissions. The difference between the cases will allow us to determine the impact of VCPs, and consumer VCPs on O_3 and SOA concentrations in the area. In addition to the brute-force approach to determine the impacts of VCPs on O_3, a source-oriented CMAQ model[30, 31] will also be applied to determine source contributions to O_3 from VCPs. The source-oriented model uses a version of lumped SAPRC mechanism, thus also serves the purpose of assessing the impact of representing the oVCP species implicitly vs. explicitly on O_3 formation. A preliminary study using the source-oriented model for east Texas was performed for September 2017, using the 2017 NEI. Figure 3 shows an example of the MDA8 O_3 source apportionment results at an urban monitor site in Houston (Houston Bayland Park). It shows that VOCs emitted from non-combustion sources (mostly solvent utilization) have high contributions to anthropogenic O_3 that are on par or higher than those from gasoline and diesel vehicles.

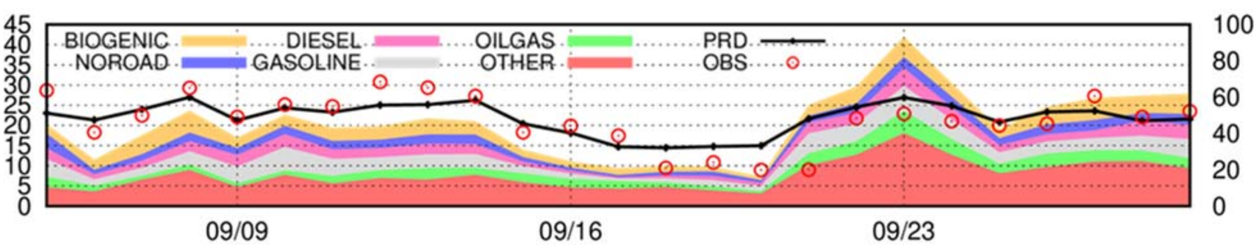

Figure 3. *Predicted MDA8 ozone (black line, right y-axis) and observations (red circles, right y-axis) at the Houston Bayland Park, both in ppb, for September 2017, alongside the contributions of different emission sectors to non-background ozone (ppb, left y-axis).*

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4. Qualification of the Research Organization and Key Personnel

Project Lead PI Dr. Zhang is an expert in atmospheric chemistry, with an extensive background in integrating Vocus 2R CI-MS, VIA-Vocus, and other chemical characterization tools for the study of the atmospheric transformation of gases organics encompassing a wide range of volatilities leading to secondary organic aerosol (SOA). He has performed laboratory and field measurements of atmospheric gases and particles, including participation in several field campaigns and led a dozen laboratory collaborations. To date, Dr. Zhang has received two collaborative federal grants as the lead or co-lead PI as well as funding from national laboratories and local entities. Dr. Zhang's extensive experience in characterizing atmospheric composition using Vocus 2R CI-MS and SP-HR-ToF-AMS during his NSF Postdoctoral Fellowship and his appointment at Texas A&M, as well as his involvement in the TRACER campaign and access to the mobile van data, make him uniquely aligned for this research to address the need for analytical methods for real-time characterization and quantification of VCP and their aerosol products in the urban environments.

Project Unfunded Collaborator Dr. Ying is an air quality expert with 20 years of experience in urban and regional air quality modeling and air pollution source apportionment. Dr. Ying's research has been supported by the US EPA, National Institutes of Health (NIH), Texas Air Research Center (TARC), Texas Transportation Institute, and the Texas Air Quality Research Program (AQRP). Dr. Ying is the key developer of the source-oriented approach for source apportionment of gaseous and particulate pollutants in regional chemical transport models. The source-oriented technique has been implemented in the Community Multiscale Air Quality (CMAQ) model and the California Institute of Technology/University of California, Davis (CIT/UCD) model. These models have been applied to study source and source-region contributions to primary and secondary gaseous and particulate pollutants in the US, Mexico, and China. Dr. Ying is also experienced in working with complex photochemical models. His research group is one of the few in the world currently implementing large semi-explicit photochemical mechanisms (such as the Master Chemical Mechanism) for ozone and secondary organic aerosol studies in regional air quality models.

5. Schedule and Deliverables

This project brings together two teams from the field of experimentalist/measurement (Zhang) with atmospheric chemistry modeling (Ying) to jointly understand an increasingly important group of species, VCP, their emission inventory, and their atmospheric implications. This proposed work takes advantage of the DOE TRACER campaign data to understand urban VCP in the Houston region. In close collaboration with Co-Lead PI Ying, Lead/Contact PI Zhang will oversee all aspects of the proposed project and analyze the field data using the Vocus 2R CI-MS and VIA. Co-Lead PI Ying will oversee the modeling of the VCP, the emission inventory refining, and integrate the seasonal field data collected by PI Zhang for model validation and improvement. Monthly meetings will be held to discuss progress/plans for ongoing and future work related to our project objectives, as outlined in our proposed timeline for meeting these objectives shown in Table 1. Full-day virtual meetings will be held once every 3 months to discuss results and outline potential publications. We expect to deliver (1) spatial and temporal distributions of VCPs in the Houston area; (2) characterize seasonal difference of VCP concentrations in Houston; (3) impacts of VCP on local air quality such as ozone; and (4) 1-3 publications related to the project objectives described above. Monthly report and quarterly report will also be submitted to AQRP. All the deliverables are listed below.

Table 1. Timetable of Proposed Work

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

Abstract
At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities and will be written for a non-technical audience.
Due Date: Ten (10) business day after notice of intent to fund

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

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

DUE TO PROJECT MANAGER

Monthly Technical Reports
Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the Monthly Technical Report Template.
Due Dates:

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

DUE TO PROJECT MANAGER

Financial Status Reports
Financial Status Reports will be submitted monthly to the AQRP Grant Manager (RoseAnna Goewey, r.goewey@ceer.utexas.edu) by each institution on the project using the FSR Template.
Due Dates:

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

DUE TO GRANT MANAGER

Draft Final Report
A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.
Due Date: August 1, 2023
Final Report
A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.
Due Date: August 31, 2023

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

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

References

1. Landrigan, P. J.; Fuller, R.; Acosta, N. J. R.; Adeyi, O.; Arnold, R.; Basu, N.; Baldé, A. B.; Bertollini, R.; Bose-O'Reilly, S.; Boufford, J. I.; Breysse, P. N.; Chiles, T.; Mahidol, C.; Coll-Seck, A. M.; Cropper, M. L.; Fobil, J.; Fuster, V.; Greenstone, M.; Haines, A.; Hanrahan, D.; Hunter, D.; Khare, M.; Krupnick, A.; Lanphear, B.; Lohani, B.; Martin, K.; Mathiasen, K. V.; McTeer, M. A.; Murray, C. J. L.; Ndahimananjara, J. D.; Perera, F.; Potočnik, J.; Preker, A. S.; Ramesh, J.; Rockström, J.; Salinas, C.; Samson, L. D.; Sandilya, K.; Sly, P. D.; Smith, K. R.; Steiner, A.; Stewart, R. B.; Suk, W. A.; van Schayck, O. C. P.; Yadama, G. N.; Yumkella, K.; Zhong, M., The Lancet Commission on pollution and health. *The Lancet* **2018,** *391* (10119), 462-512.
2. Yuan, B.; Shao, M.; de Gouw, J.; Parrish, D. D.; Lu, S.; Wang, M.; Zeng, L.; Zhang, Q.; Song, Y.; Zhang, J.; Hu, M., Volatile organic compounds (VOCs) in urban air: How chemistry affects the interpretation of positive matrix factorization (PMF) analysis. *J. Geophys. Res. (Atmos.)* **2012,** *117* (D24).
3. Guenther, A. B.; Jiang, X.; Heald, C. L.; Sakulyanontvittaya, T.; Duhl, T.; Emmons, L. K.; Wang, X., The Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1): an extended and updated framework for modeling biogenic emissions. *Geosci. Model Dev.* **2012,** *5* (6), 1471-1492.
4. Seltzer, K. M.; Pennington, E.; Rao, V.; Murphy, B. N.; Strum, M.; Isaacs, K. K.; Pye, H. O. T., Reactive organic carbon emissions from volatile chemical products. *Atmos. Chem. Phys.* **2021,** *21* (6), 5079-5100.
5. McDonald, B. C.; Gentner, D. R.; Goldstein, A. H.; Harley, R. A., Long-Term Trends in Motor Vehicle Emissions in US Urban Areas. *Environ. Sci. Technol.* **2013,** *47* (17), 10022-10031.
6. Gkatzelis, G. I.; Coggon, M. M.; McDonald, B. C.; Peischl, J.; Aikin, K. C.; Gilman, J. B.; Trainer, M.; Warneke, C., Identifying Volatile Chemical Product Tracer Compounds in US Cities. *Environ. Sci. Technol.* **2021,** *55* (1), 188-199.
7. McDonald, B. C.; de Gouw, J. A.; Gilman, J. B.; Jathar, S. H.; Akherati, A.; Cappa, C. D.; Jimenez, J. L.; Lee-Taylor, J.; Hayes, P. L.; McKeen, S. A.; Cui, Y. Y.; Kim, S.-W.; Gentner, D. R.; Isaacman-VanWertz, G.; Goldstein, A. H.; Harley, R. A.; Frost, G. J.; Roberts, J. M.; Ryerson, T. B.; Trainer, M., Volatile chemical products emerging as largest petrochemical source of urban organic emissions. *Science* **2018,** *359* (6377), 760-764.
8. Coggon, M. M.; Gkatzelis, G. I.; McDonald, B. C.; Gilman, J. B.; Schwantes, R. H.; Abuhassan, N.; Aikin, K. C.; Arend, M. F.; Berkoff, T. A.; Brown, S. S.; Campos, T. L.; Dickerson, R. R.; Gronoff, G.; Hurley, J. F.; Isaacman-VanWertz, G.; Koss, A. R.; Li, M.; McKeen, S. A.; Moshary, F.; Peischl, J.; Pospisilova, V.; Ren, X.; Wilson, A.; Wu, Y.; Trainer, M.; Warneke, C., Volatile chemical product emissions enhance ozone and modulate urban chemistry. *Proc. Natl. Acad. Sci. USA* **2021,** *118* (32), e2026653118.
9. Pennington, E. A.; Seltzer, K. M.; Murphy, B. N.; Qin, M.; Seinfeld, J. H.; Pye, H. O. T., Modeling secondary organic aerosol formation from volatile chemical products. *Atmos. Chem. Phys.* **2021,** *21* (24), 18247-18261.
10. Coggon, M. M.; Gkatzelis, G. I.; McDonald, B. C.; Gilman, J. B.; Schwantes, R. H.; Abuhassan, N.; Aikin, K. C.; Arend, M. F.; Berkoff, T. A.; Brown, S. S.; Campos, T. L.; Dickerson, R. R.; Gronoff, G.; Hurley, J. F.; Isaacman-VanWertz, G.; Koss, A. R.; Li, M.; McKeen, S. A.; Moshary, F.; Peischl, J.; Pospisilova, V.; Ren, X.; Wilson, A.; Wu, Y.; Trainer, M.; Warneke, C., Volatile chemical product emissions enhance ozone and modulate urban chemistry. **2021,** *118* (32), e2026653118.
11. McDonald, B. C.; Gouw, J. A. d.; Gilman, J. B.; Jathar, S. H.; Akherati, A.; Cappa, C. D.; Jimenez, J. L.; Lee-Taylor, J.; Hayes, P. L.; McKeen, S. A.; Cui, Y. Y.; Kim, S.-W.; Gentner, D. R.; Isaacman-

VanWertz, G.; Goldstein, A. H.; Harley, R. A.; Frost, G. J.; Roberts, J. M.; Ryerson, T. B.; Trainer, M., Volatile chemical products emerging as largest petrochemical source of urban organic emissions. **2018,** *359* (6377), 760-764.

12. Bray, C. D.; Strum, M.; Simon, H.; Riddick, L.; Kosusko, M.; Menetrez, M.; Hays, M. D.; Rao, V., An assessment of important SPECIATE profiles in the EPA emissions modeling platform and current data gaps. *Atmos. Environ.* **2019,** *207*, 93-104.
13. Lewis, A. C.; Hopkins, J. R.; Carslaw, D. C.; Hamilton, J. F.; Nelson, B. S.; Stewart, G.; Dernie, J.; Passant, N.; Murrells, T., An increasing role for solvent emissions and implications for future measurements of volatile organic compounds. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* **2020,** *378* (2183), 20190328.
14. Carter, W., Updated maximum incremental reactivity scale and hydrocarbon bin reactivities for regulatory applications. *California Air Resources Board Contract* **2010,** *1*, 07-339.
15. Yeoman, A. M.; Shaw, M.; Carslaw, N.; Murrells, T.; Passant, N.; Lewis, A. C., Simplified speciation and atmospheric volatile organic compound emission rates from non-aerosol personal care products. *Indoor Air* **2020,** *30* (3), 459-472.
16. Alvarado, M. J.; Logan, J. A.; Mao, J.; Apel, E.; Riemer, D.; Blake, D.; Cohen, R. C.; Min, K. E.; Perring, A. E.; Browne, E. C.; Wooldridge, P. J.; Diskin, G. S.; Sachse, G. W.; Fuelberg, H.; Sessions, W. R.; Harrigan, D. L.; Huey, G.; Liao, J.; Case-Hanks, A.; Jimenez, J. L.; Cubison, M. J.; Vay, S. A.; Weinheimer, A. J.; Knapp, D. J.; Montzka, D. D.; Flocke, F. M.; Pollack, I. B.; Wennberg, P. O.; Kurten, A.; Crounse, J.; Clair, J. M. S.; Wisthaler, A.; Mikoviny, T.; Yantosca, R. M.; Carouge, C. C.; Le Sager, P., Nitrogen oxides and PAN in plumes from boreal fires during ARCTAS-B and their impact on ozone: an integrated analysis of aircraft and satellite observations. *Atmos. Chem. Phys.* **2010,** *10* (20), 9739-9760.
17. Jacob, D. J.; Logan, J. A.; Gardner, G. M.; Yevich, R. M.; Spivakovsky, C. M.; Wofsy, S. C.; Sillman, S.; Prather, M. J., Factors regulating ozone over the United States and its export to the global atmosphere. *J. Geophys. Res. (Atmos.)* **1993,** *98* (D8), 14817-14826.
18. Czader, B. H.; Li, X.; Rappenglueck, B., CMAQ modeling and analysis of radicals, radical precursors, and chemical transformations. *J. Geophys. Res. (Atmos.)* **2013,** *118* (19), 11,376-11,387.
19. Sayeed, A.; Choi, Y.; Eslami, E.; Jung, J.; Lops, Y.; Salman, A. K.; Lee, J.-B.; Park, H.-J.; Choi, M.-H., A novel CMAQ-CNN hybrid model to forecast hourly surface-ozone concentrations 14 days in advance. *Scientific Reports* **2021,** *11* (1), 10891.
20. Lopez-Hilfiker, F. D.; Mohr, C.; D'Ambro, E. L.; Lutz, A.; Riedel, T. P.; Gaston, C. J.; Iyer, S.; Zhang, Z.; Gold, A.; Surratt, J. D.; Lee, B. H.; Kurten, T.; Hu, W. W.; Jimenez, J.; Hallquist, M.; Thornton, J. A., Molecular Composition and Volatility of Organic Aerosol in the Southeastern US: Implications for IEPOX Derived SOA. *Environ. Sci. Technol.* **2016,** *50* (5), 2200-2209.
21. Lopez-Hilfiker, F. D.; Pospisilova, V.; Huang, W.; Kalberer, M.; Mohr, C.; Stefenelli, G.; Thornton, J. A.; Baltensperger, U.; Prevot, A. S. H.; Slowik, J. G., An extractive electrospray ionization time-of-flight mass spectrometer (EESI-TOF) for online measurement of atmospheric aerosol particles. *Atmos. Meas. Tech.* **2019,** *12* (9), 4867-4886.
22. Buchholz, A.; Ylisirniö, A.; Huang, W.; Mohr, C.; Canagaratna, M.; Worsnop, D. R.; Schobesberger, S.; Virtanen, A., Deconvolution of FIGAERO–CIMS thermal desorption profiles using positive matrix factorisation to identify chemical and physical processes during particle evaporation. *Atmos. Chem. Phys.* **2020,** *20* (13), 7693-7716.
23. Ying, Q.; Li, J.; Kota, S. H., Significant Contributions of Isoprene to Summertime Secondary Organic Aerosol in Eastern United States. *Environmental Science and Technology* **2015,** *49* (13), 7834-7842.

24. Hu, J.; Wang, P.; Ying, Q.; Zhang, H.; Chen, J.; Ge, X.; Li, X.; Jiang, J.; Wang, S.; Zhang, J.; Zhao, Y.; Zhang, Y., Modeling biogenic and anthropogenic secondary organic aerosol in China. *Atmospheric Chemistry and Physics* **2017,** *17* (1), 77-92.
25. Zhang, J.; He, X.; Ding, X.; Yu, J. Z.; Ying, Q., Modeling Secondary Organic Aerosol Tracers and Tracer-to-SOA Ratios for Monoterpenes and Sesquiterpenes Using a Chemical Transport Model. *Environmental Science & Technology* **2022,** *56* (2), 804-813.
26. Estes, M.; Johnson, J.; Tai, P. K.; Wilson, G.; Yarwood, G., TCEQ Ozone Forecasting System. **2013**.
27. Carter, W. P. L., Development of a database for chemical mechanism assignments for volatile organic emissions. *J. Air Waste Manage. Assoc.* **2015,** *65* (10), 1171-1184.
28. Liao, K.; Park, E. S.; Zhang, J.; Cheng, L.; Ji, D.; Ying, Q.; Yu, J. Z., A multiple linear regression model with multiplicative log-normal error term for atmospheric concentration data. *Science of The Total Environment* **2021,** *767*, 144282.
29. Hansen, P. C.; O'Leary, D. P., The Use of the L-Curve in the Regularization of Discrete Ill-Posed Problems. *SIAM J. Sci. Comput.* **1993,** *14* (6), 1487-1503.
30. Wang, P.; Chen, Y.; Hu, J.; Zhang, H.; Ying, Q., Source apportionment of summertime ozone in China using a source-oriented chemical transport model. *Atmospheric Environment* **2019,** *211*, 79-90.
31. Wang, P.; Chen, Y.; Hu, J.; Zhang, H.; Ying, Q., Attribution of Tropospheric Ozone to NOx and VOC Emissions: Considering Ozone Formation in the Transition Regime. *Environmental Science and Technology* **2019,** *53* (3), 1404-1412.