FY 2024 - 2025

Project Number: 24-024

Title: Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area

Institution(s) Represented: The University of Texas at Austin (PI: Pawel K Misztal; co-PIs: Lea Hildebrandt-Ruiz, David Sullivan, Elena McDonald-Buller, Yosuke Kimura)

Lead PI: Pawel K Misztal

AQRP Project Manager: Vincent M. Torres

TCEQ Project Liaison: Celinda Vallejo-Rodriguez

Awarded Amount: $280,810.00

Abstract

The United States Environmental Protection Agency recently lowered the annual National Ambient Air Quality Standard (NAAQS) for fine particulate matter or particulate matter small than 2.5 µm in diameter ($PM_{2.5}$) from 12 to 9 µg m^{-3}. This new annual standard brings the El Paso region to near non-attainment for PM2.5, underlining the importance of understanding the composition and sources of PM2.5 and O3 in El Paso.

An improved understanding of El Paso organic aerosol and ozone is therefore essential and will directly benefit the Texas Commission on Environmental Quality (TCEQ) in guiding how to manage El Paso's air quality.

Project 24-024 will focus on improving our understanding of the contributions of volatile organic compounds (VOC) to formation of secondary organic aerosol (SOA). This work will contribute with spatiotemporal observations of SOA composition and its gas-phase organic precursors, measured by a comprehensive suite of state-of-the-science instrumentation deployed in the University of Texas electric mobile laboratory. Work will include analysis of recently collected data in El Paso, conducting novel comprehensive mobile and stationary measurements in El Paso region, and air quality modeling by the Comprehensive Air-quality Model with extensions (CAMx).

The proposed work is highly relevant to the TCEQ AQRP priority research areas, and will contribute to knowledge about the sources contributing to high PM, O3 and VOC (e.g. toluene) episodes in this region.

Quality Assurance Project Plan

Project 24-024

Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area

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David Sullivan

Elena McDonald-Buller

Yosuke Kimura

The University of Texas at Austin

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

QAPP Requirements: This QAPP requires descriptions of project description and objectives; organization and responsibilities; scientific approach; sampling and measurements procedures; model selection; model calibration; model verification; model evaluation; model documentation; quality metrics; data analysis, interpretation, and management; reporting; and references.

QA Requirements:

Technical Systems Audits - Not Required for the Project

Audits of Data Quality – 10% Required

Report of Findings – Required in Final Report

September 24, 2024

Revision : 2

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the ***Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area*** project. The Principal Investigator for the project is Pawel K Misztal and Co-PIs are Lea Hildebrand Ruiz, David Sullivan, Elena McDonald-Buller and Yosuke Kimura.

Electronic Approvals

This QAPP was approved electronically on 2024-09-26 | 20:03:40 PDT
by Project Manager Vincent M. Torres, The University of Texas at Austin.

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This QAPP was approved electronically on 2024-09-26 | 20:03:40 PDT
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This QAPP was approved electronically on 2024-09-26 | 15:57:05 CDT
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This QAPP was approved electronically on 2024-09-26 | 15:47:37 CDT
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Table of Contents

1. PROJECT DESCRIPTION AND OBJECTIVES

1.1 Process and/or environmental system to be evaluated.

The United States Environmental Protection Agency recently lowered the annual National Ambient Air Quality Standard (NAAQS) for $PM_{2.5}$ from 12 to 9 µg m^{-3} (US EPA, 2024). This new annual standard brings the El Paso region to near non-attainment for $PM_{2.5}$, underlining the importance of understanding the composition and sources of $PM_{2.5}$ in El Paso.

The Texas State Implementation Plan (SIP) includes strategies for attaining air-quality standards for ozone, fine particulate matter ($PM_{2.5}$) and regional haze. While ozone is the main concern in terms of attainment of the national ambient air quality standards (NAAQS)[1] across the state, several areas are near non-attainment for $PM_{2.5}$. Karle et al.[2] reported decline in yearly high ozone events in El Paso by a factor of two between 2000 and 2020, which was attributed to a significant fall in the vehicle crossing and reduced congestions along the US-Mexico border. Monitoring sites in El Paso, TX, have recorded $PM_{2.5}$ concentrations exceeding the daily standard (35 µg/m^3). With further tightening of annual standards for PM2.5 from 12 to 9 µg/m^3, it is possible that exceedances can be avoided with appropriate source control and abatement strategies. For example, before removal of exceptional event impacts on the PM2.5 values measured at the Chamizal monitor, the measured PM2.5 concentrations there have caused concern about maintaining attainment of the PM2.5 NAAQS[1]. No recent major air quality field campaigns focusing on particulate matter (PM), ozone (O_3) and volatile organic compounds (VOCs) have been conducted in El Paso. This is the focus of the proposed work.

Several factors are thought to contribute to the high $PM_{2.5}$ concentrations in El Paso. Mountains on either side of the Rio Grande can help to trap the air in the El Paso region. The dry climate contributes to low inversions and resulting high concentrations, especially in the colder months. Heavy truck traffic near and across the border to Mexico contributes to high emissions from motor vehicles. Local dust storms originating in Texas, New Mexico, and Mexican states affect PM concentrations in El Paso. African dust and smoke from burning vegetation in southern Mexico and Central America also contribute. Additionally, local sources from industry, transportation, and the burning of biomass (and other materials) for residential heating can also affect concentrations.[3–5]

1.2 Purpose of the project and objectives

The overarching goal of this project is to improve understanding of the sources of $PM_{2.5}$ and its gas-phase precursors in the El Paso region. The measurements taken as part of this project will include speciated measurements of PM and will be able to separate the effects of traffic, biomass burning (including wildfires), secondary species, and dust. The unique synergy could be achieved by collocating our measurements with TCEQ at Ojo de Agua Rd (CAMS1021) which is in the residential area NW of El Paso between US-Mexico border and Franklin Mountains. Existing collaboration between Dave Sullivan and TCEQ resulted in conversations to use UT trailer for auto-GC measurements. This site will provide insights into the reasons for high concentrations observed, which can include reactions of anthropogenic and biogenic pollutants to form secondary PM and ozone. Furthermore, the site would be representative for the El Paso community. This project will deploy new monitoring technologies which have high time resolution (from real-time to < 5 min) further complementing auto-GC measurements and will conduct statistical analysis on data from these new and existing monitoring activities. The proposed work is highly relevant to the TCEQ Air Quality Research Program (AQRP) priority research areas, which will be addressed by conducting "air quality field campaigns to examine the chemical and physical processes that lead to ozone and fine particulate matter formation and accumulation" The following research questions will guide the execution of the proposed work and tasks:

R1: Why does El Paso experience high concentration enhancements for toluene and other VOCs, and how are those relevant for the formation of ozone and PM2.5?

R2: What is the quantified source apportionment based on time-resolved measurements of a broad range of VOC markers along with ozone and PM2.5 bulk and speciated measurements?

R3: What is the transport of gaseous and PM pollutants from Mexico?

R4: What are the viable scenarios of meeting the regulatory new standards based on the source sensitivity analysis for the El Paso region?

1.3 Task Descriptions

Task 1: Preparation of measurement campaigns.

Meetings will be held with TCEQ staff and, as appropriate, with other researchers conducting air quality measurements in El Paso and local El Paso stakeholders, to select the optimal location and time for measurements. Efforts will be taken to minimize any inconvenience or interruption of operations if a TCEQ site is selected for temporary use. Sites currently operated by UT or UTEP may also be considered. Co-PI Sullivan is currently planning on deploying a new auto-GC aboard the UT measurement trailer as part of an already separately funded TCEQ project. Our current suggestion is that the UT electric mobile van will be used for both mobile and stationary measurements with the base and anchor point at this location.

Task 2a: Advanced statistical data analysis of O_3, speciated PM measurements, total mass of fine and coarse PM, and analysis of VOCs (O3/PM precursors) using auto-GC from all monitoring sites in the El Paso region.

Advanced statistical data analysis will be performed on speciated VOC and PM measurements and total mass of fine and coarse particulate matter concentrations measured at monitoring sites in El Paso. The purpose of these analyses will be to assess the contributions of foreign transport (which can include dust from Africa or Mexico, and smoke from southern Mexico and Central America), domestic transport, and local sources to PM2.5 in El Paso. All available data from the years 1999 – 2024 will be included in this analysis. Methods of analysis on filter-based PM2.5 data and auto-GC VOC data will include principal component analysis (PCA), positive matrix factorization (PMF), surface wind, and meso and synoptic back trajectory analysis, and other methods. Previous PCA conducted by co-PI David Sullivan on PM2.5 data collected at the Chamizal site (CAMS 41) revealed a weak factor related to fires, and PMF analysis at Guadalupe National Park also revealed a likely fire factor. Comprehensive PMF analysis conducted as part of this project, as well as combination with results from analysis of new data, could confirm a broad range of sources including the influence of fire related emissions and further quantify their contribution to PM2.5. Additional forms of data analyses that will be applied in identifying PM sources are 1) the use of surface winds to look at average concentrations as functions of wind direction, or the percent of times a value exceeds a preset threshold; 2) the examination of upper air back trajectories and how elevated concentrations of PM are related to upwind transport pathways or regions; 3) examination of PMF results with surface winds and upper air back trajectories to estimate upwind source directions or locations;[6] 4) temporal characterizations to assess seasonality, day of the week effects, and diel patterns; 5) comparisons of PM to other pollutant and source marker measurements in the El Paso area that include two automated gas chromatograph (auto-GC) systems that measure 46 hydrocarbon species from two- to twelve-carbons on an hourly time resolution.

Task 2b. Spatiotemporal modeling of air mass transport patterns and emission source contributions to concentrations of criteria pollutant and precursors and selected hazardous air pollutants (HAPs) to inform measurement design.

The Comprehensive Air Quality Model with Extensions (CAMx) will be used to investigate spatiotemporal patterns of criteria pollutants, precursors, and selected HAP concentrations and contributions from domestic and cross-border emissions sources. A 2016 CAMx platform that was developed by the TCEQ to support the 2021 Regional Haze State Implementation Plan (SIP) revision[7], which includes both ozone and particulate matter modeling will be updated and applied for this effort. McDonald-Buller and Kimura have previously used this platform to examine transboundary air pollution and the impacts of planning initiatives and regulatory policies associated with Mexico's energy sector. [8,9] CAMx v.7 will be used with meteorological fields from the Weather Research and Forecasting (WRF) Model v.3.81 over a time period spanning 15 December 2015 - 31 December 2016, which includes the model ‘spin up’ period. The CAMx horizontal grid domain is shown in Figure 1.1. The vertical grid structure includes 29 vertical layers between 34 and 18250 m AGL.

Figure 1.1. CAMx North American domain (red) with 36 km x 36 km horizontal resolution and nested CONUS domain (blue) with 12 km x 12 km horizontal resolution. (Source: https://www.tceq.texas.gov/airquality/airmod/data/rh/domain)

Several updates to the platform are planned with selection of the final model configuration to be made in consultation with TCEQ and AQRP project management. Emission inventory updates for the El Paso-Juarez region and reprocessing for the 2016 CAMx platform will be guided by the U.S. Environmental Protection Agency's (EPA's) 2022v1 emissions modeling platform to the extent feasible.[10] The flexinesting option in CAMx will be used to improve the horizontal spatial resolution over the El Paso-Juarez region from its current resolution of 12-km to $\leq$ 4-km. The Carbon Bond mechanism used for gas phase chemistry (CB6r4) will be updated to the most recent revision. CAMx simulation(s) will provide spatiotemporal concentrations of criteria pollutants and precursors as well as toluene and other HAPs of concern, for regional mapping, hotspot identification, and comparisons to existing measurements across different meteorological and emission conditions in the region. Probing tool options within CAMx, such as the Reactive Tracer (RTRAC) algorithm for explicit modeling of air toxics and Particulate Source Apportionment (PSAT), and brute force (e.g., zero-out) approaches will be considered as appropriate to characterize emission source contributions and develop concentration roses that identify these contributions by wind direction at receptors across the region to inform the measurement design.

Task 3: Intensive spatiotemporal measurements of size-resolved PM composition and concentrations (by a HR-AMS), O_3, and a large suite of volatile precursors (by the Vocus-PTRTOFMS) in two different seasons Winter 2024, Spring/Summer 2025.

The mobile measurements will be performed using the UT Austin electric mobile lab (Figure 1.2) equipped with and range of research-grade instruments (Table 5.1). The UT electric Ford E-Transit mobile lab van has a substantial battery-based power supply that allows for approximately 6 hours of uninterrupted mobile measurements given a full charge. We will use the DC charging networks, the 240 V level 2 connector at the sites (for charging overnight) as well as regional network of RV parks around the El Paso region to charge the van and the battery pack overnight. A separate rental vehicle will be used to scout routes and shuttle students who need breaks from driving. The field measurement crew will thus consist of four research personnel. *Survey tracks* are planned to scout for hotspots in O_3, black carbon, $PM_{2.5}$, and a broad range of VOC precursors and source markers. These survey drives are proposed to be conducted within a 50-mile radius of El Paso for half of the two 2-week periods, one at the beginning (Dec/January) and one at the end of campaign (May/June). Exact times and routes will be coordinated with TCEQ and the research team. Focused tracks around identified hotspots, near major pollution sources, and community receptor sites will be performed in the second week of each campaign. The electric van will also be used as a stationary measurement vehicle overnight and between the drives collocated with TCEQ or other strategic points.

Figure 1.1 Configuration of the UT electric mobile laboratory for these field measurements.

Task 4: Stationary measurements in El Paso, TX, including highly time resolved composition measurements of PM.

When not taking mobile measurements, the instrumented van will be parked at a stationary site collecting stationary data. Thus, in addition to the mobile measurements mentioned above we will also be collecting stationary measurements in El Paso during both campaign periods – ca January 2025 and May 2025. Both periods may capture the influence of fires (mostly from agricultural burning): Data from speciated $PM_{2.5}$ measurements at the Chamizal monitoring station, averaged from 2001 – 2016, show that the months with highest concentrations of potassium (a tracer for fires) are April – June, followed by November – January. Final site and time selection will be made in coordination with the TCEQ (Task 1). Instrumentation used in these stationary measurements is summarized in Table 4.1.

Task 5: Analysis of data collected during Tasks 3-4, including positive matrix factorization analysis and multivariate factor analysis to quantify the source apportionment of O_3, PM, and VOCs.

Data analysis will include positive matrix factorization (PMF) of the mass spectral data from the HR-AMS. The PMF2 algorithm (version 4.2) by P. Paatero will be used to solve the bilinear unmixing problem. PMF has proven useful in the analysis of ambient organic aerosol data, and details of the mathematical model, its application, output evaluation, and factor interpretation have been described.[20] PI Hildebrandt Ruiz has published several papers which relied on PMF to separate measured organic aerosol into different factors.[21–23] One factor commonly extracted from PMF analysis is 'biomass burning organic aerosol' which can be used to quantify the contributions of wildfires, agricultural fires, and/or residential biomass burning on particulate matter in El Paso. Data from the multi-wavelength Aethalometer can also be used for identifying the effects of biomass burning on particulate matter in El Paso: The aethalometer calculates BC mass concentration based on optical attenuation at 880 nm. The PM concentration based on optical attenuation at 370 nm is often referred to as 'UV-absorbing particulate matter' (UVPM) and is generally composed of BC and brown carbon.[24] The difference between UVPM and BC (often referred to as ΔC) indicates the presence of nonrefractory light-absorbing carbon. ΔC has demonstrated strong correlations with levoglucosan and thus has been suggested as a qualitative tracer for biomass burning.[24,25] However, recent research shows that non-woodsmoke sources such as kerosene and soft coals (e.g., lignite) can also be important contributors;[26] thus, additional measurements (such as data collected with the ACSM as part of this work) are necessary to quantify the contributions of biomass burning to PM. The analysis proposed here is similar to the work done in a current project lead by Hildebrandt Ruiz and Misztal. The ACSM has collected valuable data under much more moderate concentrations, e.g., during the ambient measurements taken by the PIs group in Conroe, TX.[23,26,27]

Task 6: Synthesis of results from tasks 2-5 to guide modeling of source impact scenarios.

The CAMx configuration developed in Task 2b will be adjusted under different scenarios based on the findings of the measurement campaign to examine the effects on modeled pollutants. This project represents the opportunity to compare data from research grade instruments producing highly time resolved particle size distributions and PM speciation data with EPA federal reference method and federal equivalent method measurements from regulatory instruments in Texas. The comparisons of these methods are expected to extend our understanding of instrument accuracy and sensitivity. More importantly, more data will be available to look at the short-term variability in speciated data not available in 24-hour filter-based methods, which will give insight into the chemistry of secondary species and clues as to source categories and individual emission sources.

2. ORGANIZATION AND RESPONSIBILITIES

2.1 Project Personnel

This project is being conducted by UT-Austin, under a grant from the Texas Air Quality Research Program. The project Co-Principal Investigators (PIs) are Drs. Pawel Misztal, Lea Hildebrandt Ruiz, David Sullivan, Elena McDonald-Buller, Yosuke Kimura. Dr. Pawel Misztal is responsible for overseeing the project execution and completion and will also take the lead on intensive spatiotemporal mobile and stationary measurements of speciated gas-phase aerosol precursors in the El Paso region in two different seasons. Dr. Lea Hildebrandt Ruiz will co-lead the study and specifically will lead speciated aerosol measurements from mobile and stationary platforms. Dr. David Sullivan will be responsible for the statistical analysis of the El Paso data that are already available. Dr. Elena McDonald-Buller and Yosuke Kimura are responsible for the modeling efforts. The Co-PIs will assume overall responsibility for the research and associated quality assurance. All Principal Investigators will contribute to the final report. The project will be overseen by AQRP Project Manager Dr. Vincent Torres and a TCEQ Project Liaisons.

The scientists working on this project and their specific responsibilities are listed below.

Dr. Pawel K Misztal is an assistant professor at UT Austin and will be the principal investigator of this project. He received a PhD in Chemistry from the University of Edinburgh in the UK and was a postdoc and research specialist in the department of Environmental Science, Policy and Management at the University of California at Berkeley from 2010 to 2018. Dr. Misztal has more than 10 years of experience measuring chemical composition of air and comprehensive air quality at different spatiotemporal scales. He led an airborne CABERNET project in California and worked with CARB to evaluate air quality models on ecosystem scale emission observations. At UT Austin, he is building a research program in novel air quality measurements and understanding factors in air quality affecting human health. He is a PI or co-PI on multiple federally funded projects including NOAA AC4, DOE IFL, HEI Energy, DHS and others. He is also a recipient of an NSF CAREER "SPIN-UP-AQ" faculty award. Above all, Dr. Misztal is strongly dedicated to Texas through collaborations to improve air quality and actively working with TCEQ colleagues, TxDOT, AQRP, AQFP, TARC and other state programs on achieving the common goals.

Dr. Lea Hildebrandt Ruiz is an associate professor at UT-Austin and will be the co-principal investigator of this project. Dr. Hildebrandt Ruiz earned degrees from the California Institute of Technology (B.S.) and Carnegie Mellon University (Ph.D.). Her research expertise lies in air quality and atmospheric chemistry, and she has published 71 peer-reviewed manuscripts in these areas. Dr. Hildebrandt Ruiz has led several projects focused on ambient measurements and detailed analysis of mass spectrometric data including positive matrix factorization analysis.

Dr. David Sullivan is a Research Associate at The University of Texas at Austin. He has been the Principal Investigator on a wide range of projects dealing with ambient air quality and meteorological monitoring, pollution source apportionment, pollution transport, air quality trends, emissions inventories, mobile air pollution monitoring, and other topics. He was previously a data analyst, team leader, and section manager at the Texas Commission on Environmental Quality, 1993 – 2005. He received his undergraduate degree in Engineering and Applied Sciences from Harvard University, and his M.S. in Operations Research and Industrial Engineering and his Ph.D. in Management Sciences and Information Systems from The University of Texas at Austin.

Dr. Elena McDonald-Buller is a Senior Research Engineer at the Center for Energy and Environmental Resources at The University of Texas at Austin with more than 25 years of experience. Her research interests include air quality modeling, energy systems, analysis of air quality measurements, emissions inventory assessment and development, and the influences of land use/land cover change and extreme weather events on air quality. She received her undergraduate degree in Civil Engineering from Michigan State University, M.S. in Environmental Engineering from the Florida Institute of Technology, and Ph.D. in Civil and Environmental Engineering from The University of Texas at Austin.

Dr. Yosuke Kimura is a Research Associate at The University of Texas at Austin. For more than twenty years, he has contributed expertise to research projects involving emissions modeling, photochemical modeling, and dispersion modeling and has had a lead role in air quality data processing, management, and visualization activities. He received his undergraduate degree in material science and M.S. in sanitary engineering from Kyoto University, Japan, and a Ph.D. in Civil Engineering from The University of Texas at Austin.

2.2 Project Schedule including main milestones

The project schedule by task is presented below. The project schedule by task is presented below. The project start date is assumed to be August 12, 2024. Technical work will not begin until authorization is received from TCEQ and AQRP. The entire project will be completed by August 31, 2025.

	2024					2025							
	A	S	O	N	D	J	F	M	A	M	J	J	A
Task 1 – Preparation of Measurements	■	■			■	■			■				
Task 2 – Pre-analysis of Data and Model		■	■	■	■	■							
Task 3 – Mobile Measurements					■	■				■			
Task 4 – Stationary Measurements					■	■				■			
Task 5 – Data processing and analysis							■	■	■	■	■		
Task 6 – Synthesis of results											■	■	■
Task R - Reporting	■	■	■	■	■	■	■	■	■	■	■	■	■

UT-Austin will prepare and submit monthly technical progress reports on the 10th of the month (or following business day) as well as quarterly reports due on October 31. January 31, 2025, April 30 and July 31, 2025. Deliverables for this project also include a draft final report due August 1, 2025 and final project report due August 31, 2025, documenting all work from Tasks 1 through 6, and a project summary presentation to AQRP anticipated to occur in August 2025. AQRP will receive an electronic copy of all data generated for this project. All reports will be in the format requested by AQRP.

3. SCIENTIFIC APPROACH

The objectives of this project are to quantify the contributions of different sources in the El Paso region to secondary aerosol formation and gas-phase aerosol precursors. We will contribute with novel spatiotemporal measurements of a broad range of volatile organic compounds and other trace gases, as well as we will provide observations of spatiotemporal changes of aerosol thanks to the state-of-the-science instrumentations. We will utilize a fully electric mobile laboratory which is capable of both mobile and stationary measurements providing unprecedented opportunity to map out sources of concern in the region. These novel observations will be analyzed in combination with existing datasets acquired by TCEQ regular monitoring and stationary trailer. Finally, air quality modeling will be integrated with measurements to provide the most accurate assessment of $PM_{2.5}$ and gaseous precursor distribution in the region.

3.1 Experimental Design

We will conduct two intensive field campaigns in winter and spring/summer providing direct spatiotemporal observations of criteria pollutants and a broad range of source markers, primary and secondary aerosol composition as a function of time and space in the El Paso region.

3.2 Measurement Approach

The mobile measurements will be performed using the UT Austin electric mobile lab (Figure 1.2) equipped with and range of research-grade instruments (Table 5.1). The UT electric Ford E-Transit mobile lab van has a substantial battery-based power supply that allows for approximately 6 hours of uninterrupted mobile measurements given a full charge.

We will use the DC charging networks, the 240 V level 2 connector at the sites (for charging overnight) as well as regional network of RV parks around the El Paso region to charge the van and the battery pack overnight. A separate rental vehicle will be used to scout routes and shuttle students who need breaks from driving. The field measurement crew will thus consist of four research personnel. Survey tracks are planned to scout for hotspots in O3, black carbon, PM2.5, and a broad range of VOC precursors and source markers.

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3.3 Air Quality Modeling

CAMx will be used for all air quality modeling simulations in this project. CAMx is a Eulerian grid model that has been approved by the EPA for regulatory applications (http://www.epa.gov/ttn/scram/photochemicalindex.htm) and is the model used by the State of Texas for ozone attainment demonstrations and air quality planning. The model has been applied extensively for both regulatory and research applications in the United States and internationally. The model and supporting documentation have been developed by ENVIRON International Corporation (https://www.camx.com). The latest version of CAMx (Version 6.10) will be used.

CAMx modeling will use a database based on a 2013 Texas ozone forecast modeling application (Johnson et al., 2013). The modeling domain covers the continental US with 36-km horizontal grid resolution and the entire Texas with 12-km resolution. A 4-km grid focusing on the Houston region will be added. The modeling period will cover the DISCOVER-AQ field campaign (August-October 2013). The meteorological conditions will be provided by a Weather Research and Forecasting (WRF) model (in hindcast mode) and the emissions inputs will be updated with the IVOC emissions developed under this study.

4. MEASUREMENT PROCEDURES

4.1 Methods Used (MEAS)

Table 4.1 summarizes the instruments used for gas- and particle phase measurements. Brief descriptions of the measurement methods are presented thereafter.

Table 4.1 Equipment in the mobile van laboratory facility.

Instrument	Compounds measured	Resolution	Comments
VOCUS 2R PTR-ToF MS	select hydrocarbons and oxygenated VOCs	1 s	unsaturated reduced and oxygenated HCs, cyclic, saturated and aromatic compounds
HR-ToF-AMS	particle bulk composition and organic aerosol atomic ratios	10 s	bulk composition: organics, sulfate, ammonium, nitrate, chloride. Measures mass spectra from which O:C and H:C ratios can be calculated
Picarro G2307	CH_4, HCHO, H_2O	1 s	Existing UT van payload
Modulair	NO_2/NO/NO_x, CO, O_3	5s	Existing equipment (QuantAQ)
Thermo	Ozone (O_3)	1 s	Existing UT van equipment (Thermo)
Thermo	H_2S, SO_2	80 s	Existing UT van payload
LI-840	CO_2, H_2O	1 s	Existing UT van payload
AE33Aethalometer	Black Carbon	1 s	Existing UT van payload
RMYoung 31000	T winds, p	1 s	Campbell Sci. (CSI) new equipment
Range finder	Flare distance and height	manual	Height of flares or stack plumes
T, RH HOBO	RH, T	1 s	UT van payload
GPS and dashcam	lat/lon/velocity	1 s	van position, CSI, new equipment

4.2 More detailed instrument descriptions

Vocus 2R Proton Transfer Reaction Time of Flight Mass Spectrometer (Vocus-PTRTOFMS): Comprehensive real-time VOC analysis by PTR-MS has led to major advances in atmospheric sciences, environmental engineering and air quality [*Park et al.*, 2013; *Li et al.*, 2020]. Given that the technology to measure chemicals at ppt levels has been developed recently over the last decade and has been precision fine-tuned only over the last few years [*Krechmer et al.*, 2018], it holds unprecedented potential in characterizing emission factors from different types of biogenic and anthropogenic sources [e.g. *Misztal et al*, 2018]. The state-of-the-art UT Vocus 2R Proton Transfer Reaction Time of Flight Mass Spectrometer (Vocus PTRTOFMS; aka the “Sniffer”) is used to monitor the real-time composition of the full VOC spectrum detectable by H_3O^+ or NH_4^+ ionization. The Vocus 2R is ultrasensitive to volatile and semivolatile compounds, owing to a highly efficient design of the ion-molecule resistive glass drift-tube reactor which can be heated up to 150 °C. With sub-ppt ($<10^{-12}$) detection limits, Vocus can detect and quantify thousands of individual VOC and SVOC ions in the ambient air at high mass and time resolution. This capability is specifically useful to understand the chemical composition of gases and aerosol from fugitive and episodic sources. The high time (<1 s) and mass resolution (15,000 m/dm) allows for air quality monitoring and evaluate changes in response to environmental or micrometeorological variables. At this low detection limit, the Vocus PTRTOFMS can quantify about 100 times more chemicals in the air than the previous generation of PTR-ToF and conventional gas chromatography instruments. Specifically advantageous in high humidity environments is that the Vocus source uses a high amount of absolute water in the reaction cell (>15 % H_2O by volume) for both the NH_4^+ and H_3O^+ reagent ions. The high absolute humidity means that changes in sample air humidity led to comparatively small humidity changes in the reactor. Thus, in contrast to other mass spectrometric instruments, the Vocus *PTR-MS* has no quantitative humidity dependence, greatly simplifying quantification of species sampled in the air where humidity can be high and change quickly. The PI has been one of the early contributors to the developments of this new technology.

Aerodyne Research High Resolution Chemical Ionization Time of Flight Mass Spectrometer (HR-ToF-CIMS). The high-resolution time-of-flight aerosol mass spectrometer (HR-AMS), manufactured by Aerodyne, Inc., quantitatively measures the size-resolved chemical composition of fine particles at high mass and time resolution. Our specific instrument has a V and W-shaped time of flight (ToF) path for higher sensitivity and higher resolution, respectively. The HR-AMS has a maximum mass spectral data acquisition rate of 100 Hz (150 Hz for size distribution data) and a mass range of 0-1000 amu. A schematic and picture of the HR-AMS are shown in Figure 4.1.

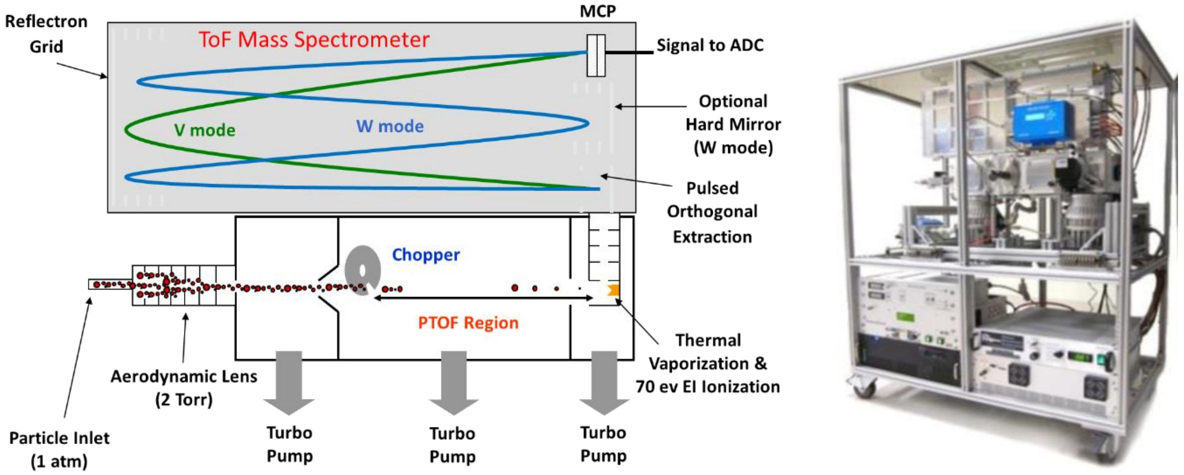


Figure 4.1. Left: HR-AMS instrument schematic. Particles are focused in an aerodynamic lens, pass through the particle-time-of-flight region (pToF) for sizing and are then vaporized. The vaporized components are ionized by electron impact and detected by a long time of flight mass spectrometer. The ToF MS has two modes: V-mode (higher sensitivity, lower resolution, shown above) and W-mode (higher resolution, lower sensitivity, not shown). Right: photo of the instrument.

After entering the inlet, particles are focused on an aerodynamic lens, pass through the particle time-of-flight region (pToF) for sizing and are then vaporized by a heated oven (at 600 °C) for detection of non-refractory components. The vaporized components are then ionized by electron ionization (EI) and detected by the time-of-flight mass spectrometer. Due to the high temperature, most components fragment and are detected as molecular fragments.

Brechtel Instruments Scanning Electric Mobility Spectrometer (SEMS). This commercially available instrument measures in the range of 0.01 μm to 2.0 μm electrical mobility diameter and consists of two main parts: a Differential Mobility Analyzer (DMA), which size-selects airborne particles based on their electric mobility, and a condensation particle counter (CPC), which counts the particles. As the DMA scans through different voltages, particles of different sizes pass through the DMA and are counted in the CPC. By scanning through different voltages, the instrument is able to provide measurements of the particle size distribution.

Quality assurance:

Quality of the HR-AMS data will be assured by conducting regular IE and RIE calibrations as mentioned above. We will also conduct co-located measurements with complementary instrumentation, specifically a scanning electrical mobility system (SEMS). The SEMS measures particle size distributions from which particle volume can be calculated. The particle volume measurements from the SEMS will be compared to particle volume measurements from the HR-AMS (converted to volume using the particle density).

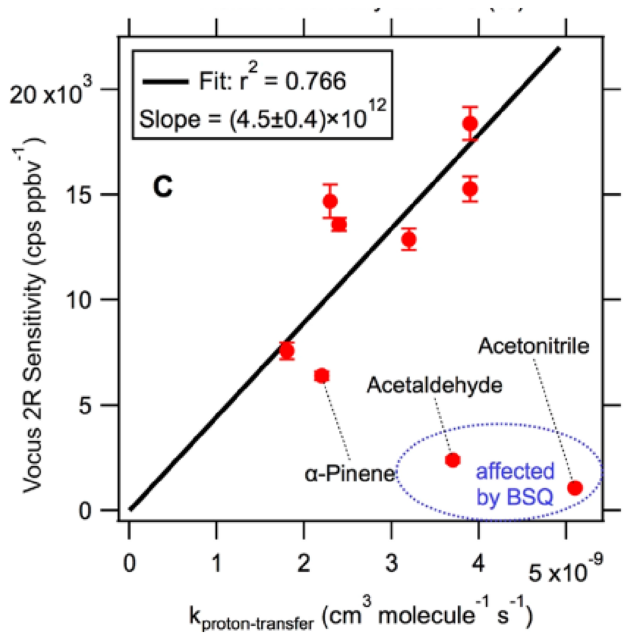
4.3 Calibration Procedures

Vocus PTR-TOF-MS

The Vocus PTR-ToF directly measures analyte concentrations in units of counts per second (CPS), which is translated into a concentration value (ppbv) through a calibration process outlined in this guide. More information on quantitation using Tofwerk software can be found at the Tofwerk website and on quantitation with the Vocus specifically can be found at the Aerodyne website. A user should review the material on these pages and some of the literature referenced on the Aerodyne webpage before calibrating data.

The primary methods used to calibrate Vocus data are the “explicit calibration with gas-phase standards in a tank or cylinder” and “estimated calibration with rate coefficients” methods that are described on the Aerodyne web page https://aerodyne.com/gas-phase-analyzers/vocus/. The calibration gas cylinders we possess cover VOCs with a range of chemical structures but only represent a small fraction of VOCs that may be detected during measurements. Therefore, the former procedure will be useful for some compounds, but most analytes will be analyzed through the latter procedure. This entails constructing a plot of calibrant proton transfer rate vs Vocus sensitivity, as shown in the plot below, for each calibrant that is analyzed from gas calibration cylinder.

The value “cps $ppbv^{-1}$” that is plotted on the y-axis is the cps value measured by the Vocus divided by the ppbv value of that analyte over a given measurement period, as calculated based on the gas concentration in the cylinder and the dilution ratio with zero air. The slope value calculated from this plot can be used to estimate the concentration of other analytes based on the proton transfer reaction rate constant (k_{ptr}) of that molecule. A database for some previously measured proton transfer reaction rate constants is kept in the supplemental data for the publication “A Library of Proton-Transfer Reactions of H_3O^+ Ions Used for Trace Gas Detection” (link; doi: 10.1007/s13361-019-02209-3). The proton transfer reaction rate for molecules of known composition but unknown structure can be estimated through methods outlined in the publication “Calculation of the sensitivity of proton-transfer-reaction mass spectrometry (PTR-MS) for organic trace gases using molecular properties” (link; doi 10.1016/j.ijms.2017.04.006).



In this project, the Vocus will be calibrated before and after each mobile measurement and regularly during the stationary measurements. Compounds of interest will be explicitly calibrated and the remaining compounds using the proton transfer reaction theory

HR-TOF-AMS

As recommended by the instrument manufacturer, the ionization efficiency (IE) of nitrate and the relative ionization efficiencies (RIE) of sulfate and ammonium in the HR-AMS will be calibrated every 1-2 weeks, and at a minimum at the beginning and end of each mobile measurement campaign. For this calibration, ammonium sulfate and ammonium nitrate particles are generated using an aerosol generation system. A differential mobility analyzer (DMA) is then used to size-select 300nm particles, which are then supplied to the HR-AMS and a condensation particle counter (CPC). A comparison of the mass measured by the HR-AMS and the CPC is used to calibrate the HR-AMS response to nitrate, ammonium and sulfate. For organics, an RIE of 1.4 is used as suggested.

Other instrument calibrations may be conducted as needed including a lens alignment, flow calibration or sizing calibration. These are not routine calibrations but may become necessary if, for example, the instrument lens shifts during transport, instrument maintenance requires a full vent of the system, etc.

SEMS

The SEMS will be operated with a 2-min time resolution. Particle sizing will be confirmed using polystyrene latex spheres, using the procedures recommended by the manufacturer. The plumbing delay between the DMA and the CPC will be measured before this set of experiments is started, as recommended by the manufacturer.

Other instruments

Other instruments will be regularly calibrated according to the SOPs established in Misztal and Hildebrandt Ruiz labs.

5. AIR QUALITY MODELING PROCEDURES

5.1 Model Selection

The primary objectives of the air quality modeling task are to investigate spatiotemporal patterns and domestic and cross-border emission source contributions to concentrations of criteria pollutant and precursors and selected hazardous air pollutants (HAPs) to inform measurement design. This study will adapt a Comprehensive Air Quality Model with Extensions (CAMx) platform originally developed by the Texas Commission on Environmental Quality (TCEQ) to support the 2021 Regional Haze State Implementation Plan (SIP) revision[1,2] for all air quality modeling simulations. CAMx is an open-source Eulerian photochemical grid modeling system for gas and particulate air pollution that has been applied across a range of spatial and temporal scales to support air quality research and regulatory assessments throughout the world.[3] It has been applied extensively in research and regulatory applications, including the development of SIPs, for the state of Texas. Drs. McDonald-Buller and Kimura have previous experience adapting the TCEQ CAMx platform to examine the impacts of emissions estimates and federal initiatives for Mexico's energy sector on transboundary air pollution to Texas and US border states for project sponsored by the National Science Foundations (NSF)[4,5]. The platform includes both ozone and particulate matter modeling, and its time period spans an entire year to capture meteorological conditions across different seasons, both of which are requirements for this study focused on El Paso-Juarez.

5.2 Model Configuration and Emissions Data Updates

CAMx v.7 will be used with meteorological fields from the Weather Research and Forecasting (WRF) Model v.3.81 for a time period spanning 15 December 2015 - 31 December 2016, which includes the approximately two-week model initial ‘spin up’ period. The CAMx horizontal grid domain is shown in Figure 1.1. The outer North American domain has 36 km x 36 km horizontal resolution and nested CONUS domain, which includes the El Paso-Juarez region, has 12 km x 12 km spatial resolution. For this study, the flexi-nesting option in CAMx will be used to create an additional innermost nested grid with a horizontal resolution of $\leq$ 4 km to improve the spatial resolution over El Paso-Juarez. The vertical grid structure includes 29 vertical layers between 34 and 18250 m AGL. Boundary and initial conditions are based on the GEOS-Chem global chemistry model version 11-02rc. Dry deposition is modeled using the Wesely scheme. Carbon Bond version 6 revision 4 (CB6r4) has been applied as the gas-phase chemical mechanism and will be updated to a more recent version for this study. The CF2 (coarse-fine) scheme with the SOAP2.2 module for secondary organic aerosol chemistry/partitioning and ISORROPIA for partitioning of inorganic aerosol constituents are used as the aerosol chemistry options.

Anthropogenic and fire emissions inputs for the TCEQ CAMx platform were based on the US Environmental Protections Agency's (EPA's) 2016v1 emissions modeling platform developed from the National Emissions Inventory Collaborative; biogenic emission inputs were based on modeling by the TCEQ using the Biogenic Emissions Information System (BEIS).[2] For this study, anthropogenic emissions for El-Paso-Juarez will be updated, guided by the EPA's 2022v1 emissions modeling platform[6] that includes estimates for the United States, Mexico, and Canada.

5.3 Air Quality Simulations

A simulation will be conducted using the final CAMx configuration described above to provide spatiotemporal concentrations of pollutants for regional mapping, hotspot identification, and comparisons to existing measurements in the region. Probing tool options within CAMx and brute force (e.g., zero-out) approaches will be considered as appropriate to characterize emission source contributions and develop concentration roses that identify source contributions by wind direction at receptors in the region to inform design of the intensive measurement campaign. As appropriate to the findings of the measurement campaign, a limited number of CAMx simulations with adjusted emissions scenarios could be conducted to examine the effects on pollutant concentrations.

5.4 Model Calibration

Maps of CAMx simulated percentile concentrations (50th, 75th, 90th, 95th, 99th, maximum) will be developed for the El Paso-Juarez region. Comparisons of CAMx simulated concentrations for the updated model configuration and measurements at Continuous Ambient Monitoring Stations (CAMS) will be made using box and whisker plots, as the emissions and meteorological input data to CAMx are not coincident in time. An objective is to identify discrepancies that may suggest areas where focused mobile sampling could be beneficial. For any CAMx simulations with adjusted emissions scenarios, regional maps of CAMx simulated percentile concentrations will be repeated for El Paso-Juarez, along with metrics at specific receptors of interest.

5.5 Model Verification

The magnitude and temporal trends of emissions for modeled pollutants across source categories will be summarized for the El Paso-Juarez region. Emission source locations will be overlayed on Google Earth maps to examine consistency with existing infrastructure and land use/land cover. Tile plots will be used to examine spatial patterns of pollutant emissions. As part of the quality assurance process (Audits of Data Quality), Dr. McDonald-Buller and Dr. Kimura will independently review at least 10% of emissions data extracted from EPA databases as well as the emissions processing methodology and input for CAMx for efforts conducted by each other. The emission inventory analyses will be reviewed with the study measurement team and AQRP and TCEQ project management to ensure that the spatial extent of the El Paso-Juarez CAMx grid domain encompasses all emission sources of significance and to support initial design of the field campaign.

CAMx simulated pollutant concentrations will be processed and analyzed using tile plots and other visualization approaches to examine spatiotemporal patterns and ensure the results are reasonable. At least 10% of the CAMx output and processed data for analyses will be independently checked by Dr. McDonald-Buller as one of the Audits of Data Quality.

5.6 Model Evaluation

CAMx simulated pollutant concentrations will be evaluated using measurements at Continuous Ambient Monitoring Stations (CAMS) for one or more years to be determined by Dr. McDonald-Buller and Dr. Kimura in collaboration with Dr. Sullivan, who will be conducting advanced statistical data analysis on pollutant measurements in El Paso. Because the emissions and meteorological input data to CAMx are not coincident in time. evaluation of the model will be made using box and whiskers plots and associated statistical metrics (e.g., minimum, lower quartile,median, upper quartile, maximum).

5.7 Model Documentation

AQRP monthly technical reports and draft and final project reports will document, as appropriate throughout the project, the CAMx configuration, emissions source locations, magnitudes, and temporal trends, and analyses of simulated pollutant concentrations and measurement intercomparisons.

6. QUALITY METRICS

6.1 QC Checks for Measurements

Vocus PTR-TOF-MS

Quality control is performed at all the stages of data acquisition and analysis. During mobile measurements, an “embarkation checklist” is used to make sure that the SOPs and instruments are working correctly. Apart from the calibrations before and after the drive, response time is derived at the inlet by an acetone test where a ppb level acetone is spiked and the time to observe signal response is derived. Leak tests are also performed to ensure that the instruments are sampling the ambient air. Finally, during the measurements, signals are previewed to immediately recognize potential issues.

SEMS

Particle sizing will be confirmed using polystyrene latex spheres, using the procedures recommended by the manufacturer. The sizing will be checked before and after this set of experiments is performed.

ACSM

The instrument response to nitrate will be measured every two weeks to test and account for changes. Variation in the collection efficiency will be observed and accounted for using total concentration data from the SEMS.

HR-ToF-AMS

The instrument will be calibrated as described above and the operation of the instrument will be monitored for any abnormalities to take immediate corrective action (e.g., restarting software acquisition).

Audits of Data Quality

The Quality Control Checks described above are part of the Audits of Data Quality that will be performed at the frequency indicated. Findings from all of the Audits of Data Quality will be included in the draft and final reports.

7. REPORTING

7.1 Deliverables from each Project Participant

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. PI Dr. Misztal will submit the reports but will be assisted by Dr. Hildebrandt Ruiz and other project participants in preparing the reports. 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 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 2 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 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

Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY24-25 MTR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
Technical Report #1	August 1 - 31, 2024	October 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 - 28, 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

Financial Status Reports

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.

Due Dates:

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

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, 2025

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, 2025

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 2025. The selected date will be updated.

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.

9. REFERENCES

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Scope of Work

Project 24-024

Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area

Pawel K Misztal
Lea Hildebrand Ruiz
David Sullivan
Elena McDonald-Buller
Yosuke Kimura

The University of Texas at Austin

Revision : 2

September 24, 2024

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 2024-09-26 | 20:03:40 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 2024-09-26 | 15:57:05 CDT
by Celinda Vallejo-Rodriguez, Texas Commission on Environmental Quality

Signed by:
Celinda Vallejo-Rodriguez
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Celinda Vallejo-Rodriguez

Project Liaison, Texas Commission on Environmental Quality

Table of Contents

1. STATEMENT OF WORK

1.1 Introduction

This document provides the work plan for the Texas Air Quality Research Program (AQRP) project 24-024 “Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area”. Work will be completed by August 31, 2025. The project Co-Investigators are Drs. Pawel K. Misztal, Lea Hildebrandt Ruiz, David Sullivan, Elena McDonald-Buller and Yosuke Kimura of the University of Texas at Austin (UT or UT-Austin). The UT-Austin team will conduct novel and spatially resolved air quality measurements using gas-phase and aerosol-phase state-of-the-science instrumentation. In addition, the modeling analysis will be conducted and integrated with measurements to provide wider and deeper understanding of air pollution sources and criteria pollutants in the El Paso region.

The United States Environmental Protection Agency recently lowered the annual National Ambient Air Quality Standard (NAAQS) for fine particulate matter or particulate matter small than 2.5 µm in diameter ($PM_{2.5}$) from 12 to 9 µg m^{-3} (US EPA, 2024). This new annual standard brings the El Paso region to near non-attainment for $PM_{2.5}$, underlining the importance of understanding the composition and sources of $PM_{2.5}$ and O_3 in El Paso.

The Texas State Implementation Plan (SIP) includes strategies for attaining air-quality standards for ozone (O_3), $PM_{2.5}$ and regional haze. While O_3 is the main concern in terms of attainment of the national ambient air quality standards (NAAQS)[1] across the state, several areas are near non-attainment for $PM_{2.5}$. Karle et al.[2] reported decline in yearly high ozone events in El Paso by a factor of two between 2000 and 2020, which was attributed to a significant fall in the number of vehicles crossing and reduced congestion along the US-Mexico border. Monitoring sites in El Paso, TX, have recorded $PM_{2.5}$ concentrations exceeding the daily standard (35 μg/m^3). With further tightening of annual standards for $PM_{2.5}$ from 12 to 9 μg/m^3, it is possible that exceedances can be avoided with appropriate source control and abatement strategies. For example, before removal of exceptional event impacts on the $PM_{2.5}$ values measured at the Chamizal monitor, the measured $PM_{2.5}$ concentrations there have caused concern about maintaining attainment of the $PM_{2.5}$ NAAQS[1]. No recent major air quality field campaigns focusing on PM, O_3 and volatile organic compounds (VOCs) have been conducted in El Paso. This field study is the focus of the proposed work. Several factors are thought to contribute to the high $PM_{2.5}$ concentrations in El Paso. Mountains on either side of the Rio Grande can help to trap the air in the El Paso region. The dry climate contributes to low inversions and resulting high concentrations, especially during the colder months. Heavy truck traffic near and across the border to Mexico contributes to high emissions from motor vehicles. Local dust storms originating in Texas, New Mexico, and Mexican states affect particulate matter (PM) concentrations in El Paso. African dust and smoke from burning vegetation in southern Mexico and Central America also contribute. Additionally, local sources from industry, transportation, and the burning of biomass (and other materials) for residential heating can also affect concentrations.[3–5] Figure 1 shows monthly average concentrations of $PM_{2.5}$ measured at 4 monitoring sites in the El Paso area in 2020, 2021 and 2022. The Ascarate Park site is very near a major highway and next to the Mexican border. It could therefore be influenced by traffic emissions, transport of pollution from Mexico, local sources or other sources or processes including dust events. Monthly averages from 2015 show that concentrations measured at Ascarate Park are at the border line of new $PM_{2.5}$ standards. Overall, the highest concentrations are seen in the winter months, with a secondary peak in the spring. The measurements taken as part of this project will include speciated measurements of PM and will be able to separate the effects of traffic, biomass burning

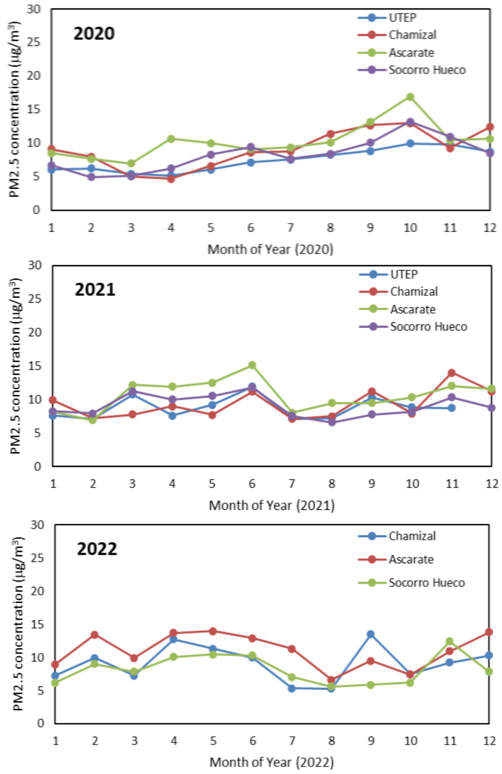

Figure 1. Monthly average $PM_{2.5}$ concentrations measured at 4 different monitoring stations in El Paso, TX.

(including wildfires), secondary species, and dust. A unique synergy could be achieved by collocating our measurements with TCEQ at Ojo de Agua Rd (CAMS1021) which is in the residential area, NW of El Paso between the US-Mexico border and the Franklin Mountains. Existing collaboration between Dave Sullivan and TCEQ resulted in the decision to use UT trailer for auto-GC measurements. Measurements at this site will provide insights into the reasons for high concentrations observed, which can include reactions of anthropogenic and biogenic pollutants to form secondary PM and ozone. Furthermore, the site would be representative of the El Paso community. This project will deploy new monitoring technologies which have high time resolution (from real-time to < 5 min) further complementing auto-GC measurements and will conduct statistical analysis on data from these new and existing monitoring activities. The proposed work is highly relevant to the TCEQ AQRP priority research areas, which will be addressed by conducting “air quality field campaigns to examine the chemical and physical processes that lead to ozone and fine particulate matter formation and accumulation” The following research questions will guide the execution of the proposed work and tasks:

R1: Why does El Paso experience high concentration enhancements for toluene and other VOCs, and how are those relevant for the formation of ozone and $PM_{2.5}$?

R2: What is the quantified source apportionment based on time-resolved measurements of a broad range of VOC markers along with ozone and $PM_{2.5}$ bulk and speciated measurements?

R3: What is the transport of gaseous and PM pollutants from Mexico?

R4: What are the viable scenarios of meeting the new regulatory standards based on the source sensitivity analysis for the El Paso region?

1.2 Task Descriptions

Task 1: Preparation of measurement campaigns.

Meetings will be held with TCEQ staff and, as appropriate, with other researchers conducting air quality measurements in El Paso and local El Paso stakeholders, to select the optimal location and time for measurements. Efforts will be taken to minimize any inconvenience or interruption of operations if a TCEQ site is selected for temporary use. Sites currently operated by UT or the University of Texas at El Paso (UTEP) may also be considered. Co-PI Sullivan is currently planning on deploying a new auto-GC aboard the UT measurement trailer as part of an already separately funded TCEQ project. Our current suggestion is that the UT electric mobile van will be used for both mobile and stationary measurements with the base and anchor point at this location.

Task 2a: Advanced statistical data analysis of O_3, speciated PM measurements, total mass of fine and coarse PM, and analysis of VOCs (O_3 and PM precursors) using auto-GC from all monitoring sites in the El Paso region.

Advanced statistical data analysis will be performed on speciated VOC and PM measurements, and total mass of fine and coarse particulate matter concentrations measured at monitoring sites in El Paso. The purpose of these analyses will be to assess the contributions of foreign transport (which can include dust from Africa or Mexico, and smoke from southern Mexico and Central America), domestic transport, and local sources to $PM_{2.5}$ in El Paso. All available data from the years 1999 – 2024 will be included in this analysis. Methods of analysis on filter-based $PM_{2.5}$ data and auto-GC VOC data will include principal component analysis (PCA), positive matrix factorization (PMF), surface wind, and meso and synoptic back trajectory analysis, and other methods. Previous PCA conducted by co-PI David Sullivan on $PM_{2.5}$ data collected at the Chamizal site (CAMS 41) revealed a weak factor related to fires, and PMF analysis at Guadalupe National Park also revealed a likely fire factor. Comprehensive PMF analysis conducted as part of this project, combined with results from analysis of new data, could confirm a broad range of sources including the influence of fire related emissions and further quantify their contribution to $PM_{2.5}$. Additional forms of data analyses that will be applied in identifying PM sources are 1) the use of surface winds to look at average concentrations as functions of wind direction, or the percent of times a value exceeds a preset threshold; 2) the examination of upper air back trajectories and how elevated concentrations of PM are related to upwind transport pathways or regions; 3) examination of PMF results with surface winds and upper air back trajectories to estimate upwind source directions or locations;[6] 4) temporal characterizations to assess seasonality, day of the week effects, and diel patterns; 5) comparisons of PM to other pollutant and source marker measurements in the El Paso area that include two automated gas chromatograph (auto-GC) systems that measure 46 hydrocarbon species from two- to twelve-carbons on an hourly time resolution.

Task 2b. Spatiotemporal modeling of air mass transport patterns and emission source contributions to concentrations of criteria pollutant and precursors and selected hazardous air pollutants (HAPs) to inform measurement design.

The Comprehensive Air Quality Model with Extensions (CAMx) will be used to investigate spatiotemporal patterns of criteria pollutants, precursors, and selected HAP concentrations and contributions from domestic and cross-border emissions sources. A 2016 CAMx platform that was developed by the TCEQ to support the 2021 Regional Haze State Implementation Plan (SIP) revision[7], which includes both ozone and particulate matter modeling will be updated and applied for this effort. McDonald-Buller and Kimura have previously used this platform to examine transboundary air pollution and the impacts of planning initiatives and regulatory policies associated with Mexico's energy sector. [8,9] CAMx v.7 will be used with meteorological fields from the Weather Research and Forecasting (WRF) Model v.3.81 over a time period spanning 15 December 2015 - 31 December 2016, which includes the model ‘spin up’ period.

The CAMx horizontal grid domain is shown in Figure 2. The vertical grid structure includes 29 vertical layers between 34 and 18250 m AGL.

Figure 2. CAMx North American domain (red) with 36 km x 36 km horizontal resolution and nested CONUS domain (blue) with 12 km x 12 km horizontal resolution. (Source: https://www.tceq.texas.gov/airquality/airmod/data/rh/domain)

Several updates to the platform are planned with selection of the final model configuration to be made in consultation with TCEQ and AQRP project management. Emission inventory updates for the El Paso-Juarez region and reprocessing for the 2016 CAMx platform will be guided by the U.S. Environmental Protection Agency's (EPA's) 2022v1 emissions modeling platform to the extent feasible.[10] The flexi-nesting option in CAMx will be used to improve the horizontal spatial resolution over the El Paso-Juarez region from its current resolution of 12-km to ≤ 4-km. The Carbon Bond mechanism used for gas phase chemistry (CB6r4) will be updated to the most recent revision. CAMx simulation(s) will provide spatiotemporal concentrations of criteria pollutants and precursors as well as toluene and other HAPs of concern, for regional mapping, hotspot identification, and comparisons to existing measurements across different meteorological and emission conditions in the region. Probing tool options within CAMx, such as the Reactive Tracer (RTRAC) algorithm for explicit modeling of air toxics and Particulate Source Apportionment (PSAT), and brute force (e.g., zero-out) approaches will be considered as appropriate to characterize emission source contributions and develop concentration roses that identify these contributions by wind direction at receptors across the region to inform the measurement design.

Task 3: Intensive spatiotemporal measurements of size-resolved PM composition and concentrations (by an HR-TOF-AMS), O_3, and a large suite of volatile precursors (by the Vocus-PTRTOFMS) in two different seasons Winter 2024, Spring/Summer 2025.

The mobile measurements will be performed using the UT Austin electric mobile lab (Table 1) equipped with and range of research-grade instruments (Figure 1).

Table 1. Payload of the UT Mobile Lab

Instrument	Compounds measured	Resolution	Comments
VOCUS 2R PTR-ToF MS	select hydrocarbons and oxygenated VOCs	1 s	unsaturated reduced and oxygenated HCs, cyclic, saturated and aromatic compounds
HR-ToF-AMS	particle bulk composition and organic aerosol atomic ratios	10 s	bulk composition: organics, sulfate, ammonium, nitrate, chloride. Measures mass spectra from which O:C and H:C ratios can be calculated
Picarro G2307	CH_4, HCHO, H_2O	1 s	Existing UT van payload
Modulair	NO_2/NO/NO_x, CO, O_3	5s	Existing equipment (QuantAQ)
Thermo	Ozone (O_3)	1 s	Existing UT van equipment (Thermo)
Thermo	H_2S, SO_2	80 s	Existing UT van payload
LI-840	CO_2, H_2O	1 s	Existing UT van payload
AE33Aethalometer	Black Carbon	1 s	Existing UT van payload
RMYoung 31000	T winds, p	1 s	Campbell Sci. (CSI) new equipment
Range finder	Flare distance and height	manual	Height of flares or stack plumes
T, RH HOBO	RH, T	1 s	UT van payload
GPS and dashcam	lat/lon/velocity	1 s	van position, CSI, new equipment

The UT electric Ford E-Transit mobile lab van has a substantial battery-based power supply that allows for approximately 6 hours of uninterrupted mobile measurements given a full charge. We will use the DC charging networks, the 240 V level 2 connector at the sites (for charging overnight) as well as regional network of RV parks around the El Paso region to charge the van and the battery pack overnight. A separate rental vehicle will be used to scout routes and shuttle students who need breaks from driving. The field measurement crew will thus consist of four research personnel. *Survey tracks* are planned to scout for hotspots in O_3, black carbon, $PM_{2.5}$, and a broad range of VOC precursors and source markers. These survey drives are proposed to be conducted within a 50-mile radius of El Paso for half of the two 2-week periods, one at the beginning (Dec/January) and one at the end of campaign (May/June). Exact times and routes will be coordinated with TCEQ and the research team. Focused tracks around identified hotspots, near major pollution sources, and community receptor sites will be performed in the second week of each campaign. The electric van will also be used as a stationary measurement vehicle overnight and between the drives collocated with TCEQ or other strategic points.

Figure 1. Configuration of the UT electric mobile laboratory for these field measurements.

Task 4: Stationary measurements in El Paso, TX, including highly time resolved composition measurements of PM.

When not taking mobile measurements, the instrumented van will be parked at a stationary site collecting stationary data. Thus, in addition to the mobile measurements mentioned above we will also be collecting stationary measurements in El Paso during both campaign periods – ca January 2025 and May 2025. Both periods may capture the influence of fires (mostly from agricultural burning). Data from speciated $PM_{2.5}$ measurements at the Chamizal monitoring station, averaged from 2001 – 2016, show that the months with highest concentrations of potassium (a tracer for fires) are April – June, followed by November – January. Final site and time selection will be made in coordination with the TCEQ (Task 1). Instrumentation used in these stationary measurements is summarized in Table 1 above.

Task 5: Analysis of data collected during Tasks 3-4, including positive matrix factorization analysis and multivariate factor analysis to quantify the source apportionment of O_3, PM, and VOCs.

Data analysis will include positive matrix factorization (PMF) of the mass spectral data from the HR-TOF-AMS. The PMF2 algorithm (version 4.2) by P. Paatero will be used to solve the bilinear unmixing problem. PMF has proven useful in the analysis of ambient organic aerosol data, and details of the mathematical model, its application, output evaluation, and factor interpretation have been described.[20] PI Hildebrandt Ruiz has published several papers which relied on PMF to separate measured organic aerosol into different factors.[21–23] One factor commonly extracted from PMF analysis is ‘biomass burning organic aerosol’ which can be used to quantify the contributions of wildfires, agricultural fires, and/or residential biomass burning on particulate matter in El Paso. Data from the multi-wavelength Aethalometer can also be used for identifying the effects of biomass burning on particulate matter in El Paso: The aethalometer calculates BC mass concentration based on optical attenuation at 880 nm. The PM concentration based on optical attenuation at 370 nm is often referred to as 'UV-absorbing particulate matter' (UVPM) and is generally composed of BC and brown carbon.[24] The difference between UVPM and BC (often referred to as ΔC) indicates the presence of nonrefractory light-absorbing carbon. ΔC has demonstrated strong correlations with levoglucosan and thus has been suggested as a qualitative tracer for biomass burning.[24,25] However, recent research shows that non-woodsmoke sources such as kerosene and soft coals (e.g., lignite) can also be important contributors;[26] thus, additional measurements, such as data collected with the high resolution time-of-flight aerosol mass spectrometry (HR-TOF-AMS) as part of this work, are necessary to quantify the contributions of biomass burning to PM. The analysis proposed here is similar to the work done in a current project lead by Hildebrandt Ruiz and Misztal. The similar instrument, aerosol chemical speciation monitor (ACSM), has collected valuable data under much more moderate concentrations, e.g., during the ambient measurements taken by the PIs group in Conroe, TX.[23,26,27]

Task 6: Synthesis of results from tasks 2-5 to guide modeling of source impact scenarios.

The CAMx configuration developed in Task 2b will be adjusted under different scenarios based on the findings of the measurement campaign to examine the effects on modeled pollutants. This project represents the opportunity to compare data from research grade instruments producing highly time resolved particle size distributions and PM speciation data with EPA federal reference method and federal equivalent method measurements from regulatory instruments in Texas. The comparisons of these methods are expected to extend our understanding of instrument accuracy and sensitivity. More importantly, more data will be available to look at the short-term variability in speciated data not available in 24-hour filter-based methods, which will give insight into the chemistry of secondary species and clues as to source categories and individual emission sources.

2. TIMELINE

The project schedule by task is presented below. The project schedule by task is presented below. The project start date is assumed to be August 12, 2024. Technical work will not begin until authorization is received from TCEQ and AQRP. The entire project will be completed by August 31, 2025.

	2024					2025							
	A	S	O	N	D	J	F	M	A	M	J	J	A
Task 1 – Preparation of Measurements	■	■			■	■			■				
Task 2 – Pre-analysis of Data and Model		■	■	■	■	■							
Task 3 – Mobile Measurements					■	■				■			
Task 4 – Stationary Measurements					■	■				■			
Task 5 – Data processing and analysis							■	■	■	■	■		
Task 6 – Synthesis of results											■	■	■
Task R - Reporting	■	■	■	■	■	■	■	■	■	■	■	■	■

UT-Austin will prepare and submit monthly technical progress reports on the 10th of the month (or following business day) as well as quarterly reports due on October 31. January 31, 2025, April 30 and July 31, 2025. Deliverables for this project also include a draft final report due August 1, 2025 and final project report due August 31, 2025, documenting all work from Tasks 1 through 6, and a project summary presentation to AQRP anticipated to occur in August 2025. AQRP will receive an electronic copy of all data generated for this project. All reports will be in the format requested by AQRP.

3. PROJECT ORGANIZATION AND RESPONSIBILITIES

This project is being conducted by UT-Austin, under a grant from the Texas Air Quality Research Program. The project Co-Principal Investigators (PIs) are Drs. Pawel Misztal, Lea Hildebrandt Ruiz, David Sullivan, Elena McDonald-Buller, Yosuke Kimura. Dr. Pawel Misztal is responsible for overseeing the project execution and completion and will also take the lead on intensive spatiotemporal mobile and stationary measurements of speciated gas-phase aerosol precursors in the El Paso region in two different seasons. Dr. Lea Hildebrandt Ruiz will co-lead the study and specifically will lead speciated aerosol measurements. Dr. David Sullivan will be responsible for the statistical analysis of the El Paso data that are already available. Dr. Elena McDonald-Buller and Dr. Yosuke Kimura are responsible for the modeling efforts. The Co-PIs will assume overall responsibility for the research and associated quality assurance. All Principal Investigators will contribute to the final report. The project will be overseen by AQRP Project Manager Vincent M. Torres and TCEQ Project Liaisons.

The scientists working on this project and their specific responsibilities are listed below.

Dr. Pawel K Misztal is an assistant professor at UT Austin and will be the principal investigator of this project. He received a PhD in Chemistry from the University of Edinburgh in the UK and was a postdoc and research specialist in the department of Environmental Science, Policy and Management at the University of California at Berkeley from 2010 to 2018. Dr. Misztal has more than 10 years of experience measuring chemical composition of air and comprehensive air quality at different spatiotemporal scales. He led an airborne California Airborne BVOC Emission Re- search in Natural Ecosystem Transects (CABERNET) project in California and worked with the California Air Resources Board (CARB) to evaluate air quality models on ecosystem scale emission observations. At UT Austin, he is building a research program in novel air quality measurements and understanding factors in air quality affecting human health. He is a PI or co-PI on multiple federally funded projects including National Oceanic & Atmospheric Administration (NOAA) Atmospheric Chemistry, Carbon Cycle and Climate (AC4), US Department of Energy Integrated Field Laboratories (DOE IFL), Heath Effects Institute Energy (HEI Energy), US Department of Homeland Security (DHS) and others. He is also a recipient of a National Science Foundation (NSF) “CAREER: SPatiotemporal INvestigation of Urban Pollution and Air Quality (SPIN-UP-AQ)” faculty award. Above all, Dr. Misztal is strongly dedicated to Texas through collaborations to improve air quality and actively working with TCEQ colleagues, TxDOT, AQRP, AQFP, TARC and other state programs on achieving the common goals.

Dr. Lea Hildebrandt Ruiz is an associate professor at UT-Austin and will be the co-principal investigator of this project. Dr. Hildebrandt Ruiz earned degrees from the California Institute of Technology (B.S.) and Carnegie Mellon University (Ph.D.). Her research expertise lies in air quality and atmospheric chemistry, and she has published 71 peer-reviewed manuscripts in these areas. Dr. Hildebrandt Ruiz has led several projects focused on ambient measurements and detailed analysis of mass spectrometric data including positive matrix factorization analysis.

Dr. David Sullivan is a Research Associate at The University of Texas at Austin. He has been the Principal Investigator on a wide range of projects dealing with ambient air quality and meteorological monitoring, pollution source apportionment, pollution transport, air quality trends, emissions inventories, mobile air pollution monitoring, and other topics. He was previously a data analyst, team leader, and section manager at the Texas Commission on

Environmental Quality, 1993 – 2005. He received his undergraduate degree in Engineering and Applied Sciences from Harvard University, and his M.S. in Operations Research and Industrial Engineering and his Ph.D. in Management Sciences and Information Systems from The University of Texas at Austin.

Dr. Elena McDonald-Buller is a Senior Research Engineer at the Center for Energy and Environmental Resources at The University of Texas at Austin with more than 25 years of experience. Her research interests include air quality modeling, energy systems, analysis of air quality measurements, emissions inventory assessment and development, and the influences of land use/land cover change and extreme weather events on air quality. She received her undergraduate degree in Civil Engineering from Michigan State University, M.S. in Environmental Engineering from the Florida Institute of Technology, and Ph.D. in Civil and Environmental Engineering from The University of Texas at Austin.

Dr. Yosuke Kimura is a Research Associate at The University of Texas at Austin. For more than twenty years, he has contributed expertise to research projects involving emissions modeling, photochemical modeling, and dispersion modeling and has had a lead role in air quality data processing, management, and visualization activities. He received his undergraduate degree in material science and M.S. in sanitary engineering from Kyoto University, Japan, and a Ph.D. in Civil Engineering from The University of Texas at Austin.

4. 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. PI Dr. Misztal will submit the reports but will be assisted by Dr. Hildebrandt Ruiz and other project participants in preparing the reports. 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 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 2 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 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

Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP MTR Template found on the AQRP website.

Due Dates:

Report	Period Covered	Due Date
Technical Report #1	August 1 - 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 - 28, 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

Financial Status Reports

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.

Due Dates:

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

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, 2025

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, 2025

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 2025. The selected date will be updated.

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.

5. REFERENCES

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Budget and Budget Justification

Project #24-024

Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area

Prepared for

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

By

Pawel K Misztal
Lea Hildebrand Ruiz
David Sullivan
Elena McDonald-Buller
Yosuke Kimura

09/24/2024
Version #2

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

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by RoseAnna Goewey, The University of Texas at Austin

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Program Manager, Texas Air Quality Research Program

This Budget was approved electronically on 2024-09-26 | 20:03:40 PDT
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Vincent Torres
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Project Manager, Texas Air Quality Research Program

This Budget was approved electronically on 2024-09-26 | 15:57:05 CDT
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Project Liaison, Texas Commission on Environmental Quality

Budget and Budget Justification

The University of Texas at Austin

Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area

AQRP Budget

Principal Investigator: **Pawel Misztal**

Project Dates: **09/01/2024 - 08/31/2025**

A. SENIOR PERSONNEL: PI, Co-PI

	FirstName LastName	Title	Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
1.	Pawel Misztal	PI	$13,974	27.0%	1.00	$13,974
2.	Lea Hildebrandt Ruiz	coPI	$16,762	27.0%	1.00	$16,762
3.	Elena McDonald Buller	coPI	$17,582	27.0%	1.00	$17,582
4.	David Sullivan	coPI	$12,528	6.4%	1.00	$12,528
	TOTAL SENIOR PERSONNEL					**$60,845**

B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)

			Monthly Rate	Fringe Rate	FTE / % Effort	Funds Requested
1	2	Other Professionals / Researchers	$7,179	27.0%	1.80	$12,922
2	1	Other Professionals / Research Coordinator	$3,346	6.4%	1.00	$3,346
3	2	Graduate Student	$2,904	15.4%	24.00	$69,696
		TOTAL OTHER PERSONNEL				**$85,964**

TOTAL SALARIES AND WAGES (A+B)	**$146,809**

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

1.	Senior Personnel	**$13,847**
2.	Other Personnel	**$14,436**
	TOTAL FRINGE BENEFITS	**$28,284**
	TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)	**$175,093**

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

a)		$0
b)		$0
c)		$0
	TOTAL EQUIPMENT	**$0**

E. TRAVEL

		Cost per Trip	# of Trips	
1.	Domestic (Incl. Canada, Mexico and U.S. Possessions)	$1,000	**20**	$20,000
2.	Foreign			$0
	TOTAL TRAVEL			**$20,000**

F OTHER DIRECT COSTS

1.	Materials and Supplies	$9,750
2.	Professional Services - Independent Contractors (Ramboll) Loaded Hourly Labor Rate=$214; 50 hours)	$10,700
3.	Subcontracts (contracts will be issued by UT)	
a)		$0
b)		$0
c)		$0
d)		$0
4.	Tuition and Fees	$26,260
5.	Other: Service center	$2,380
	TOTAL OTHER DIRECT COSTS	**$49,090**

G. TOTAL DIRECT COSTS (A THROUGH F)		**$244,183**
H. TOTAL INDIRECT COSTS	**IDC Rate:** 15.000%	**$36,627**
I. TOTAL COSTS		**$280,810**

Total Budget: $280,810

A. SALARIES

Dr. Pawel Misztal, Principal Investigator, 1 month of 100% effort, will be responsible for supervising the mobile measurements, assisting with the stationary measurements, co-advising the graduate research assistants, for overall quality assurance, communicating with AQRP and TCEQ colleagues, and reporting.

Dr. Lea Hildebrandt Ruiz, Co-Investigator, 1 month of 100% effort, will be responsible for supervising the stationary measurements, assisting with mobile measurements, co-advising the graduate research assistants, and assisting the PI with quality assurance, communication and reporting.

Dr. Elena McDonald-Buller, Co-Investigator, 1 months of 100% effort, will be responsible for the air quality modeling efforts and assisting the PI with quality assurance, communication, and reporting.

Dr. David Sullivan, Co-Investigator, 1 month at 100% effort, will be responsible for interpretation of the auto-GC VOC data and PM data collected in the El Paso area. He will also advise the project team on measurement and modeling activities based on his extensive experience in El Paso.

Dr. Yosuke Kimura, Research Associate, 1.39 months at 100% effort, will conduct CAMx model simulations and lead the technical implementation of the model configuration updates and input data pre-processing, as well as post-processing and visualization of model output.

TBA, Postdoctoral Fellow, 0.5 month of 100% effort, will assist with measurements during the intensive measurement periods.

Dori Eubank, Research Program Coordinator, 0.5 month at 100% effort, will help with monthly financial reports and other administrative tasks related to the project.

TBA, Graduate Research Assistant (GRA), 12 months of 100% effort, will be responsible for stationary measurements and will assist with mobile measurements, and analysis of data from both measurement platforms.

TBA, Graduate Research Assistant (GRA), 12 months of 100% effort, will be responsible for mobile measurements and will assist with stationary measurements, and analysis of data from both measurement platforms.

B. FRINGE BENEFITS

Fringe benefits rates are based on University of Texas at Austin federally negotiated rates for the appropriate employee benefits level at the time of proposal submission. Total fringe benefits budget requested: $28,284.

C. EQUIPMENT

none

D. OTHER DIRECT COSTS

MATERIALS AND SUPPLIES

Supplies are calculated at $9,750 per year for consumables necessary for routine work of the instruments including sampling tubing, Swagelok fittings, mass flow controllers, field accessories, compressed gases, adding electricity to the site, fencing, and other materials and supplies for the field campaign preparation and execution. Total materials and supplies budgeted requested: $12,130.

TRAVEL

Funds are requested for project personnel to travel to El Paso. Trips are envisioned for GRAs and other personnel to attend intensive field campaigns including transport, accommodation and per diem costs. $18,000 is estimated for supporting two intensive mobile and stationary field campaigns, calculated as: 4 (persons) * 150 (accommodation daily rate + per diem) * 30 days. Travel costs in this budget are based on sponsored research travel for previous similar trips. The average costs of a rental car, flights and fuel (and electric charging for the mobile lab) is estimated at $2,000. In total, $20,000 is requested for field travel purposes.

SERVICE CENTER

Funds are requested for usage of the air quality instrumentation service center. Service center funds are used to purchase instrument consumables, replacement parts and insurance, and they also account for depreciation of instruments. The service center rate for each piece of equipment has been approved by the University (UT Austin). The $2380 requested correspond to 20 days of mobile measurements.

CONTRACTORS

Ramboll will provide additional support to Dr. Kimura for implementation of the CAMx configuration updates and input data pre-processing, as well as post-processing and visualization of model output. $10,700 is allocated, including 50 hours for Dr. Ling Huang at a fully loaded hourly labor rate of $214.

TUITION

The University requires tuition remission to be budgeted for all GRAs working on sponsored projects. The [in-state/resident] tuition rate at the University of Texas at Austin for the FY $13,130 year is $625 per semester credit hours. Total tuition budget requested: $26,260.

INDIRECT COSTS

The indirect cost rate of 15% of modified/total direct costs (MTDC/TDC) is used as instructed by the AQRP's published proposal preparation instructions. MTDC is calculated as the total of direct costs, less [equipment in excess of $5,000 and less tuition remission applied to GRA salary]. Total indirect cost budget requested: $36,627.

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