FY 2026 - 2027

Project Number: 26-030

**Title: Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed**

**Institution(s) Represented:** The University of Texas at Austin (PI: Pawel K. Misztal; Co-PIs: Lea Hildebrandt Ruiz, David W. Sullivan, Elena C. McDonald-Buller)

**Lead PI:** Pawel K. Misztal

**AQRP Project Manager:** Erin Tullos

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**Awarded Amount:** $247,132.00

## Abstract

El Paso County is designated as marginal nonattainment for the 2015 ozone National Ambient Air Quality Standards (NAAQS), and the 2024 tightening of the annual $PM_{2.5}$ standard from 12 to 9 μg/m$^3$ has placed the region closer to $PM_{2.5}$ nonattainment. The El Paso-Juárez metropolitan area is one of the largest binational communities in North America, with air quality challenges arising from complex terrain, transboundary transport from Mexico, and diverse emission sources. AQRP Project 24-024, completed in August 2025, produced the most comprehensive air quality dataset collected in El Paso since the 1996 Paso del Norte Ozone Study, using an electric mobile laboratory equipped with a Vocus PTR-ToF-MS, an HR-TOF-AMS, and an aethalometer, complemented by a Comprehensive Air Quality Model with Extensions (CAMx) photochemical modeling platform for the 2022 base year. Initial extended analyses of these datasets, including ozone reactivity potential mapping and aerosol source apportionment, were presented to the Texas Commission on Environmental Quality (TCEQ) at the May 2026 State Implementation Plan Informational Meeting.

Project 26-030 will conduct advanced analyses of these existing datasets across five tasks. Ozone formation potential will be calculated under three independent frameworks (mass-based, molecular weight-based, and OH reactivity-weighted maximum incremental reactivity) using the El Paso-specific SAPRC-11 ELPTX scenario. Ozone sensitivity regimes will be mapped across the airshed using complementary indicator ratios and cross-validated against the existing CAMx simulations. Source apportionment will integrate Project 24-024 mobile Vocus and HR-TOF-AMS data with long-term TCEQ auto-GC records (2011 through 2025) and offline $PM_{2.5}$ filter samples, applying combined Vocus-AMS Positive Matrix Factorization (PMF), reactivity-weighted PMF, and roadway-influence stratification. Existing CAMx Reactive Tracer outputs will be reanalyzed to characterize domestic and international emission source contributions to toluene at five El Paso monitoring sites.

The project will deliver spatially resolved priority VOC rankings for ozone reduction, ozone sensitivity regime classifications with TCEQ-validated indicator ratios, an integrated VOC and PM source apportionment that elucidates sources of ozone and aerosol precursors, and refined toluene source attribution to support binational air quality coordination. Although El Paso is not currently in serious ozone nonattainment, the methodological framework developed under this project is directly transferable to serious and severe nonattainment areas in Texas and will support Houston-Galveston-Brazoria, Dallas-Fort Worth, and Bexar County regulatory analyses.

# Quality Assurance Project Plan

## Project 26-030

## Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed

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The University of Texas at Austin has prepared this Quality Assurance Project Plan (QAPP) following the Environmental Protection Agency (EPA) guidelines for a Quality Assurance (QA) Category III Project: Requirement for Secondary Data 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 includes descriptions of project description and objectives; organization and responsibilities; scientific approach; data sources, processing, and analysis procedures; quality metrics; data interpretation, integration, 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

Revision: 2

June 19, 2026

## Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed project. The Principal Investigator for the project is Pawel K. Misztal and Co-PIs are Lea Hildebrandt Ruiz, David W. Sullivan, and Elena C. McDonald-Buller.

Electronic Approvals

**This QAPP was approved electronically on** 2026-06-26 | 09:10:28 CDT

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## Acronyms and Abbreviations

AE-33: Aethalometer (model AE-33)
AMS: Aerosol Mass Spectrometer
AQRP: Texas Air Quality Research Program
auto-GC: Automated Gas Chromatograph
BBOA: Biomass Burning Organic Aerosol
BC: Black Carbon
BTEX: Benzene, Toluene, Ethylbenzene, and Xylenes
CAMS: Continuous Ambient Monitoring Station
CAMx: Comprehensive Air Quality Model with Extensions
CO: Carbon Monoxide
COA: Cooking Organic Aerosol
CoEP: City of El Paso
CPF: Conditional Probability Function
DFW: Dallas-Fort Worth
DQO: Data Quality Objective
EBIR: Equal Benefit Incremental Reactivity
ELPTX: El Paso, Texas (MIR scenario)
EPA: United States Environmental Protection Agency
FNR: Formaldehyde-to-Nitrogen Dioxide Ratio
HAP: Hazardous Air Pollutant
HCHO: Formaldehyde
HDV: Heavy-Duty Vehicle
HGB: Houston-Galveston-Brazoria
HNO3: Nitric Acid
HOA: Hydrocarbon-like Organic Aerosol
HR-TOF-AMS: High-Resolution Time-of-Flight Aerosol Mass Spectrometer
HYSPLIT: Hybrid Single-Particle Lagrangian Integrated Trajectory model
IUPAC: International Union of Pure and Applied Chemistry
JAC: Joint Advisory Committee for Air Quality Improvement
JPL: Jet Propulsion Laboratory
LDV: Light-Duty Vehicle
ME-2: Multilinear Engine (version 2)
MIR: Maximum Incremental Reactivity

NAAQS: National Ambient Air Quality Standard
NO2: Nitrogen Dioxide
NOx: Nitrogen Oxides
NOy: Total Reactive Nitrogen
NR-PM1: Non-Refractory Submicron Particulate Matter
NRMRL: National Risk Management Research Laboratory
O3: Ozone
OFP: Ozone Formation Potential
OH: Hydroxyl Radical
OOA: Oxygenated Organic Aerosol
ORP: Ozone Reaction Potential
P(O3): Ozone Production Rate
PM: Particulate Matter
PM1: Particulate Matter with aerodynamic diameter ≤ 1 µm
PM2.5: Particulate Matter with aerodynamic diameter ≤ 2.5 µm
PMF: Positive Matrix Factorization
PTR-ToF-MS: Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer
QA/QC: Quality Assurance / Quality Control
QAPP: Quality Assurance Project Plan
RTRAC: Reactive Tracer Probing Tool
SAPRC: Statewide Air Pollution Research Center (chemical mechanism)
SIP: State Implementation Plan
SOA: Secondary Organic Aerosol
SOW: Scope of Work
TCEQ: Texas Commission on Environmental Quality
TEMPO: Tropospheric Emissions: Monitoring of Pollution
TROPOMI: Tropospheric Monitoring Instrument
UTEP: The University of Texas at El Paso
VCP: Volatile Chemical Product
VOC: Volatile Organic Compound

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# 1. PROJECT DESCRIPTION AND OBJECTIVES

## 1.1 Process and Environmental System to be Evaluated

The El Paso metropolitan area experiences distinctive air quality challenges as a major urban area in West Texas and a binational border crossing site with Ciudad Juárez, Mexico, with diverse emission sources and complex terrain. Several ambient monitoring sites in El Paso have daily maximum eight-hour average ozone design values that exceed the level of the National Ambient Air Quality Standard (NAAQS), and the EPA tightened the annual NAAQS for fine particulate matter ($PM_{2.5}$) from 12 to 9 $\mu g/m^3$ in 2024, placing El Paso closer to nonattainment. Although El Paso is not currently in serious nonattainment for ozone, the analytical methods developed under this project are directly transferable to serious and severe nonattainment areas in Texas.

Previous analyses have indicated that transboundary pollutant transport from Juárez, as well as domestic urban, industrial, and natural sources, can significantly impact El Paso air quality (Park et al., 2020; Karle et al., 2021). Air quality challenges in El Paso are shared by Juárez, where measurements at ambient monitors across the border have exceeded Mexico federal standards for ozone and $PM_{2.5}$. Addressing these issues requires apportionment of emission sources, separation of local, regional, and international contributions, and identification of chemical precursors that drive secondary formation of pollutants such as ozone and secondary organic aerosol in the El Paso-Juárez airshed.

AQRP Project 24-024, completed in August 2025, deployed a fully electric mobile laboratory equipped with a Vocus PTR-ToF-MS, an HR-TOF-AMS, an aethalometer, and supporting analyzers in two intensive campaigns during winter 2024/2025 and late spring/early summer 2025. The project also developed a Comprehensive Air Quality Model with Extensions (CAMx) photochemical modeling platform for El Paso-Juárez for the 2022 base year, including Reactive Tracer (RTRAC) source attribution for toluene at four monitoring sites. Project 24-024 conducted initial source apportionment analyses described in the Final Report Sections 2.1.3 and 4.2.4. The current project (26-030) will conduct advanced analyses of these existing datasets to extract additional value for SIP development and regulatory decision-making.

Preliminary results from initial extended analyses were presented at the May 2026 TCEQ State Implementation Plan (SIP) Informational Meeting, attended by approximately 100 TCEQ staff. These preliminary findings, documented in detail in the Scope of Work, demonstrate that the analytical workflows are operational. Key preliminary results include mass-based ozone reactivity potential (ORP) calculated using the Carter and Heo (2012) SAPRC-11 ELPTX scenario, identifying the central El Paso, Bridge of the Americas, and Chamizal corridor as the dominant reactive VOC source region; a 4-factor PMF on AMS organic aerosol resolving HOA, COA, BBOA, and OOA factors; and a complementary 6-factor PMF on offline $PM_{2.5}$ filter samples resolving inorganic and dust factors not captured by the AMS PM1 analysis. Project 26-030 will extend each of these preliminary analyses (the mass-based ORP, the AMS organic PMF, and the offline $PM_{2.5}$ PMF) through the multi-formulation OFP analysis (Task 1), the multi-indicator sensitivity ratio analysis (Task 2), the combined Vocus-AMS PMF and reactivity-weighted PMF (Task 3), and the CAMx RTRAC reanalysis (Task 4), with synthesis and multi-framework reconciliation in Task 5, as described in Section 1.3 and summarized in the analytical workflow figure of the Scope of Work.

## 1.2 Purpose of the Project and Objectives

The overarching goal of this project is to provide TCEQ with advanced analytical products derived from the comprehensive Project 24-024 datasets, focused on ozone formation chemistry, VOC sensitivity regimes, source apportionment, and integration of observations with photochemical

modeling. The project deploys no new field measurements; all activities are reanalysis and integration of existing data.

The following research questions guide the execution of the proposed work:

**R1:** What is the spatial and temporal distribution of ozone formation potential across the El Paso region under multiple reactivity frameworks (mass-based and molecular weight-based MIR, OH reactivity-weighted, and EBIR), and which VOC species contribute most to ozone production in different locations and seasons?

**R2:** How do ozone sensitivity regimes (VOC-limited versus NOx-limited) vary spatially across the El Paso-Juárez airshed when evaluated through multiple complementary indicator ratios (VOC/NO2, VOC/NOx, O3/NOx, O3/NOy, O3/NOz, satellite HCHO/NO2), and which ratios yield results consistent with photochemical modeling?

**R3:** What are the combined gas-particle source apportionment results, integrating VOCs (from Vocus and auto-GC) and PM (HR-TOF-AMS and offline filter PMF), that elucidate the sources of ozone and aerosol precursors?

**R4:** What are the relative contributions of domestic versus international (Mexican) emission sources to elevated toluene concentrations across the five monitoring sites in El Paso, and how do the fingerprints of these sources differ?

## 1.3 Task Descriptions

### 1.3.1 Task 1: Comprehensive Ozone Formation Potential Analysis

Ozone formation potential will be calculated for VOC species measured by the Vocus PTR-ToF-MS and the auto-GC network using four complementary frameworks: mass-based MIR (Carter and Heo, 2012; Carter, 2010; Venecek et al., 2018), molecular weight-based MIR, OH reactivity-weighted MIR, and Equal Benefit Incremental Reactivity (EBIR). The MIR scale represents incremental reactivity under the high-NOx conditions most conducive to ozone formation and is appropriate for VOC-limited regimes such as the El Paso urban core, whereas the EBIR scale represents the lower-NOx condition at which VOC and NOx control yield equal ozone benefit and is therefore appropriate for the transitional and NOx-limited regimes mapped in Task 2. Rankings of priority VOCs will be compared across the four frameworks; MIR-based rankings are applied where Task 2 indicates VOC-limited conditions and EBIR-based rankings where Task 2 indicates transitional or NOx-limited conditions, with divergences reported explicitly. Spatial maps will be generated from mobile transects, and diurnal and seasonal patterns will be analyzed extending the temporal analyses presented in Project 24-024 Final Report Section 4.2.2. PI Misztal will lead this task.

### 1.3.2 Task 2: VOC Sensitivity Regime Mapping and Multi-Indicator Analysis.

Ozone sensitivity regimes will be mapped using multiple complementary indicators: VOC/NO2, VOC/NOx, O3/NOx, O3/NOy, O3/NOz, and satellite-derived HCHO/NO2 (FNR) from TROPOMI and TEMPO. Regime-classification thresholds for each indicator are summarized in Table 4.5-1 (Section 4.5). Indicator results will be compared with the CAMx simulations developed under Project 24-024, using instantaneous ozone production rates P(O3) from the CAMx Process Analysis tool applied to the 2022 base year, to identify which observational diagnostics are most reliable for the El Paso region. The procedure is detailed in Section 3.4. PI Misztal will lead this task.

### 1.3.3 Task 3: Advanced Source Apportionment of VOCs and PM.

Advanced source apportionment will integrate the Project 24-024 Vocus and HR-TOF-AMS data with long-term auto-GC records (2011-2025) from UTEP, Chamizal, and Delta Drive. Methods include constrained PMF on combined gas-particle (Vocus + AMS) matrices, Conditional Probability Function analysis, HYSPLIT back-trajectory clustering, and a reactivity-weighted PMF analysis. Day-night and roadway-stratified analyses will distinguish on-road traffic influence. Co-PIs Sullivan and Hildebrandt Ruiz will co-lead with PI Misztal.

### 1.3.4 Task 4: Domestic and International Source Contributions for Toluene.

Extended analysis of the existing 2022 base year CAMx simulations with the RTRAC probing tool completed under Project 24-024 will be used to quantify domestic and international source sector contributions to toluene at all five monitoring sites (Chamizal, Delta Drive, Womble, Socorro Hueco, UTEP). Observed toluene pollution roses at these sites will be developed to complement this analysis. An integrated analysis will also be conducted with data collected by the UT Austin Vocus PTR-ToF-MS and onboard meteorological instrumentation during the AQRP 24-024. Co-PI McDonald-Buller and Dr. Kimura will lead this task.

### 1.3.5 Task 5: Synthesis.

The final task will synthesize results from all analyses. Spatial maps of local sensitivity regimes will be developed, indicating areas of VOC sensitivity (urban core) versus areas of NOx sensitivity (suburban areas). Emission source categories and VOC species will be ranked by their contribution to ozone and $PM_{2.5}$ concentrations. The analyses will also identify remaining data gaps and priority measurements for future monitoring to support ongoing air quality research. Peer-reviewed manuscripts and presentation materials will be prepared for AQRP, TCEQ, and the broader scientific community to disseminate research findings.

# 2. ORGANIZATION AND RESPONSIBILITIES

## 2.1 Project Personnel

This project is being conducted by The University of Texas at Austin under a grant from the Texas Air Quality Research Program. The project Principal Investigator is Dr. Pawel K. Misztal and the Co-Principal Investigators are Drs. Lea Hildebrandt Ruiz, David W. Sullivan, and Elena C. McDonald-Buller. The project will be overseen by AQRP Project Manager Dr. Erin Tullos and TCEQ Project Liaison Erik Gribbin (with Tanzina Akther as backup). Dr. David Allen serves as the AQRP QAPP Manager for Project 26-030.

**Dr. Pawel K. Misztal** is an Associate Professor (Cockrell Family Fellow) at UT Austin and is the Principal Investigator. He has more than 15 years of experience studying chemical composition of air using advanced mass spectrometry techniques, including the Vocus PTR-ToF-MS deployed in Project 24-024. He led Project 24-024 and has detailed knowledge of the comprehensive Vocus datasets collected during that campaign. He will oversee project coordination and lead the OFP analysis (Task 1) and the sensitivity regime mapping (Task 2).

**Dr. Lea Hildebrandt Ruiz** is an Associate Professor at UT Austin (Professor effective Aug 2026) and is a Co-Principal Investigator. Her research expertise lies in air quality and atmospheric chemistry, with extensive experience in PMF and ME-2 analysis of aerosol mass spectrometric data. She will co-lead Task 3 (Advanced Source Apportionment), with focus on the HR-TOF-AMS PMF analysis and the combined Vocus-AMS PMF integration.

**Dr. David W. Sullivan** is a Research Associate at UT Austin and is a Co-Principal Investigator with unique expertise in El Paso VOC monitoring. He has operated auto-GCs in El Paso since 2011 and has analyzed speciated VOC data from multiple TCEQ monitoring stations including

Chamizal (CAMS 41), Delta Drive, and the UTEP site. He will co-lead Task 3, with responsibility for integration of long-term auto-GC records and multi-site PMF.

**Dr. Elena C. McDonald-Buller** is a Senior Research Engineer at UT Austin with more than 25 years of experience in air quality modeling and emissions characterization. She is a Co-Principal Investigator and will lead Task 4 (Domestic and International Source Contributions for Toluene) and contribute to Task 5.

**Dr. Yosuke Kimura** is a Research Associate at UT Austin with more than 20 years of experience with emissions and photochemical modeling. He will perform extended analysis of the existing CAMx simulations with the RTRAC probing tool as well as observations at the TCEQ and UTEP sites completed under Project 24-024. He will contribute to the integration of these results with data collected by the UT Vocus PTR-ToF-MS.

**Dr. Chun-Ying Chao** is a Postdoctoral Fellow who will assist with PMF analyses of HR-TOF-AMS data and conduct PMF analysis of the combined Vocus-AMS datasets.

**Two Graduate Research Assistants (Daniel Sung and Shihao Zhai)** will perform data analysis across Tasks 1 through 5.

## 2.2 Project Schedule and Main Milestones

The project start date is August 1, 2026. Technical work will not begin until authorization is received from TCEQ and AQRP. The entire project will be completed by August 31, 2027. The Draft Final Report will be submitted by August 1, 2027 (30 days before project end), and the Final Report by August 31, 2027. The detailed task schedule is included in the Scope of Work document.

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. Deliverables include a draft final report and a final project report documenting all work from Tasks 1 through 5, and a project summary presentation to AQRP. AQRP will receive an electronic copy of all data generated for this project.

# 3. SCIENTIFIC APPROACH

## 3.1 Overall Approach

This project conducts advanced analyses of existing datasets collected under AQRP Project 24-024 and integrates those datasets with long-term auto-GC records from TCEQ monitoring sites in El Paso. No new field measurements will be conducted. The scientific approach therefore differs from a traditional measurement campaign QAPP and emphasizes (1) data quality screening of the existing inputs, (2) analytical procedures for OFP calculations, sensitivity ratio analysis, and source apportionment, (3) cross-validation across instrument platforms and analytical frameworks, and (4) reproducibility and documentation of code, model parameters, and intermediate products.

## 3.2 Data Sources and Datasets

The project will use the following datasets, all of which were generated under prior AQRP-funded work or are publicly accessible TCEQ datasets:

- **Vocus PTR-ToF-MS data** from the UT Austin electric mobile laboratory deployed in El Paso during the winter 2024/2025 and late spring/early summer 2025 campaigns of Project 24-024, including mobile transects and stationary deployments at the UTEP site.

- **HR-TOF-AMS data** from the UT Austin mobile laboratory and stationary deployments during Project 24-024.
- **Aethalometer (AE33) data** for black and brown carbon from the Project 24-024 mobile lab.
- **Criteria pollutants and meteorology** ($O_3$, NO, $NO_2$, CO, $SO_2$, $H_2S$, T, RH, wind speed, wind direction, GPS) from the Project 24-024 mobile lab instrument suite.
- **Long-term auto-GC speciated VOC data** from the TCEQ Chamizal (CAMS 41) and Delta Drive sites operated and analyzed by Co-PI Sullivan since 2011, and from the UTEP site auto-GC operated under Project 24-024 in 2024/2025. These auto-GC data are also accessible through the TCEQ public archive; for this project they are used in the processed and quality-controlled form maintained by Co-PI Sullivan, which is the more current version. No data are accessed through non-public channels.
- **TCEQ ambient monitoring data** ($O_3$, NOx, $PM_{2.5}$, toluene, meteorology) for El Paso CAMS sites obtained from the TCEQ public archive.
- **CAMx photochemical model output** from the 2022 base year El Paso-Juárez platform developed under Project 24-024, including predicted toluene concentrations and source contributions using the RTRAC probing tool at the four previously analyzed sites and at the UTEP site (extended under this project).
- **Satellite column observations** of HCHO and NO2 from TROPOMI (Sentinel-5P) and TEMPO (geostationary) for the El Paso domain across the relevant time periods.
- **MIR and EBIR coefficient databases** from Carter (2010), the Carter and Heo (2012) SAPRC-11 ELPTX scenario, and Venecek et al. (2018), for the OFP calculations.
- **OH bimolecular reaction rate constants** from JPL Publication 19-5 (Burkholder et al., 2020) and the IUPAC Subcommittee evaluations.
- **Regime threshold values** from Sillman (1995, 1999), Duncan et al. (2010), Jin et al. (2017), and Wan et al. (2024).
- **Photochemical age inference parameters** from de Gouw et al. (2005) and Yuan et al. (2012).

## 3.3 Analytical Approach for OFP (Task 1)

Four independent OFP frameworks will be applied. The mass-based formulation calculates OFP_i = C_i * MIR_i for each species i, with C_i in µg/$m^3$ and MIR_i in g $O_3$ per g VOC, yielding µg $O_3$/$m^3$. The molecular weight-based formulation rescales each species contribution as OFP_i = C_i * MIR_i * M_O3 / M_i, with $M_{O_3}$ = 48 g/mol, yielding the same µg $O_3$/$m^3$ units but reweighting lower molecular weight species upward and higher molecular weight species downward. The OH reactivity-weighted formulation ranks species by C_i * k_OH,i * MIR_i, where k_OH,i is the OH rate constant of species i drawn according to a documented source hierarchy. OH rate constants are taken primarily from the critically evaluated recommendations of JPL Publication 19-5 (Burkholder et al., 2020) and the IUPAC Subcommittee evaluations, which provide single recommended values with stated uncertainties. For species not covered by those evaluations, values are taken from the NIST Chemical Kinetics Database, selecting the most recent peer-reviewed determination. Where no measured value is available from any of these sources, k_OH,i is estimated using the structure-activity relationship of Kwok and Atkinson (1995). The source and selection for each species are documented, and the k_OH uncertainty is propagated through the OFP uncertainty analysis. The reactivity-weighted metric captures the contribution of each species to instantaneous ozone precursor reactivity and yields rankings that closely track absolute

consumed-VOC rankings for moderate atmospheric aging without requiring knowledge of OH concentration, which was not measured in Project 24-024. For selected near-source mobile transects where co-emitted aromatic tracer pairs (for example, m,p-xylene paired with benzene) can be used to constrain photochemical age, the OH exposure $\tau\_OH = \int[OH]\,dt$ will be inferred from the deviation of the observed tracer ratio from its emission ratio (de Gouw et al., 2005; Yuan et al., 2012), and an absolute consumed-VOC OFP will additionally be calculated for cross-validation of the reactivity-weighted rankings. A fourth framework applies the Equal Benefit Incremental Reactivity (EBIR) scale (Carter, 2010; Venecek et al., 2018), which represents the lower-NOx condition at which VOC and NOx control yield equal ozone benefit and is therefore appropriate for the transitional and NOx-limited regimes mapped in Task 2; MIR-based rankings are applied in VOC-limited areas and EBIR-based rankings in transitional and NOx-limited areas, with divergences reported explicitly. All frameworks will be applied to the same species list and the resulting priority rankings will be compared in side-by-side tables. Sensitivity of the rankings to the choice of MIR vintage (Carter 2010 versus Venecek 2018) will be evaluated for the highest-ranked species under each framework.

Isoprene and other high-reactivity species are represented with their own species-specific coefficients (MIR, EBIR, and k_OH) rather than averaged values, so their reactivity is captured directly. Because a small number of high-reactivity species can dominate a reactivity-weighted ranking, the priority lists will be recomputed with and without the high-reactivity biogenic species (isoprene and monoterpenes) to quantify their influence and demonstrate ranking robustness. The MIR and EBIR metrics from the Carter SAPRC framework represent incremental ozone formed per unit VOC under full photochemical conditions and are not OH-loss-only measures, so the primary ranking does not assume OH is the sole sink. The OH reactivity-weighted framework, which uses k_OH, is one of four complementary frameworks and serves as a cross-check. Isoprene is removed predominantly by OH under typical daytime conditions and is largely represented by the OH-weighted metric, whereas the monoterpenes and other reactive alkenes have appreciable $O_3$ and nighttime $NO_3$ sinks, so OH-only weighting underestimates their total reactivity; this limitation will be stated in the Final Report, and where the data support it a total-oxidant (OH plus $O_3$) reactivity will be reported for the affected species.3.4 Analytical Approach for Sensitivity Regime Mapping (Task 2)

Six complementary indicators will be calculated where/when available: VOC/$NO_2$, VOC/NOx, $O_3$/NOx, $O_3$/NOy, $O_3$/NOz, and satellite HCHO/$NO_2$. The Table 4.5-1 thresholds are applied to whichever ratios are available at a given location and time. $O_3$/NOy is derived where total reactive nitrogen is measured (e.g., the Chamizal NCore/PAMS site) and from CAMx elsewhere, consistent with the NOy speciation produced under Project 24-024. $O_3$/NOz (NOz = NOy - NOx) is the observation-based reactive-nitrogen indicator where $HNO_3$ is not measured; $O_3$/$HNO_3$ could optionally be derived from the CAMx output as a cross-check. All surface ratios are computed from observed atmospheric concentrations at the TCEQ CAMS sites and from the Project 24-024 mobile and stationary platforms, not from emission rates, and the satellite FNR is an observed column ratio from the TROPOMI and TEMPO retrievals. For each indicator, threshold values for VOC-limited, transitional, and NOx-limited regimes will be drawn from Wan et al. (2024), Sillman (1995), and subsequent literature, with explicit documentation of the chosen thresholds in the Final Report. Indicator maps will be generated at the same spatial resolution and aggregated to the same time bins for direct comparison. Agreement among indicators will be quantified using a voting scheme and a continuous-scale agreement metric. Under the voting scheme, each observation location is independently assigned a regime classification (VOC-limited, transitional, or NOx-limited) by each available indicator, and the majority assignment is reported together with the vote count (for example, five of six indicators VOC-limited). The continuous-scale metric is the standard deviation across the available classifications mapped to numerical values (minus one for VOC-limited, zero for transitional, and plus one for NOx-limited); locations with a standard

deviation below 0.3 are reported as high-agreement, and locations above 0.6 are reported as low-agreement and identified for further review. The CAMx simulations from Project 24-024 will serve as a comparison benchmark, and the indicator that best matches the CAMx-based regime classification will be identified as the recommended observational diagnostic for the El Paso region.

In addition, the CAMx Process Analysis tool will be applied to the existing 2022 base year simulation to extract instantaneous ozone production rates P(O3) at grid cells co-located with the surface monitoring sites and along representative mobile transect segments. Observed indicator ratios at each location will then be compared against the modeled P(O3) to provide a quantitative basis for ranking which observational diagnostics are most predictive of ozone formation in the El Paso domain. At each observation location the indicator value is compared against the thresholds in Table 4.5-1; the values below the lower bound are classified VOC-limited, above the upper bound NOx-limited, and intermediate values transitional, following the convention that lower indicator values correspond to VOC-limited conditions. The observation-based regimes and the regimes implied by the CAMx P(O3) are compared, with agreement increasing confidence and divergence identifying either observational limitations or locations where the model or emission inventory may warrant further evaluation.

## 3.5 Source Apportionment Approach (Task 3)

### 3.5.1 Conventional PMF on Ambient Concentrations

Positive Matrix Factorization (PMF) takes a matrix of species concentrations measured over time and decomposes it into a smaller number of factors, each representing a chemical source profile and its associated time series (Paatero and Tapper, 1994; Norris et al., 2014). Conventional PMF on ambient concentrations means applying this decomposition directly to the measured mixing ratios, in contrast to the reactivity-weighted formulation described in Section 3.5.3. PMF analyses will be performed using the PMF evaluation tool for unconstrained runs and the SoFi Pro implementation of ME-2 (Canonaco et al., 2013) for constrained runs. Both of these tools use the same underlying math from Paatero et al. (1999). The Vocus and HR-TOF-AMS data will be analyzed individually and as combined matrices. The auto-GC dataset will be analyzed separately at each site using site-specific multi-year records and then jointly across the UTEP, Chamizal, and Delta Drive sites for multi-site PMF.

### 3.5.2 Combined Vocus-AMS PMF

Combined PMF will be performed by concatenating the Vocus and HR-TOF-AMS input matrices following the approach of Slowik et al. (2010), with appropriate scaling and uncertainty weighting between the gas-phase and particle-phase blocks. Combined PMF is expected to identify additional source factors that cannot be resolved from either dataset alone (Simon et al., 2025).

### 3.5.3 Consumed-VOC PMF

The reactivity-weighted matrix is constructed under both MIR and EBIR weights, so that the source-to-ozone attribution is available for both the VOC-limited urban core and the transitional and NOx-limited suburban areas identified in Task 2. A parallel PMF analysis will be performed on a reactivity-weighted matrix rather than on ambient concentrations. Each Vocus species in the input matrix will be scaled by $k_{OH,i} * MIR_i$ (the product of its OH rate constant and maximum incremental reactivity), so that the resulting factors represent source contributions to instantaneous ozone precursor reactivity rather than to ambient mixing ratios. A parallel reactivity-weighted matrix scales each species by $k_{OH,i}$ times $EBIR_i$, giving the regime-appropriate

attribution for transitional and NOx-limited areas. For an air parcel with shared OH exposure across species, this weighting yields source rankings that closely track those from absolute consumed-VOC PMF, without requiring knowledge of OH concentration. Reactivity-weighted PMF factors will be compared with the conventional ambient PMF factors to identify whether source rankings shift when reactivity is considered.

### 3.5.4 Roadway-Influence Stratification for Mobile Data

To distinguish on-road traffic influence in the mobile measurements, three complementary approaches will be applied. (1) Road-class stratification: mobile observations will be tagged using GPS coordinates joined with the OpenStreetMap road network classification (interstate, principal arterial, minor arterial, residential, off-road) and PMF and OFP results will be reported by road class. (2) Diagnostic tracers: black carbon (AE33), NO and NO2, and CO from the mobile lab will serve as fresh on-road traffic indicators. Vocus aromatic ratios (benzene/toluene, toluene/m,p-xylene) and HR-TOF-AMS hydrocarbon-like organic aerosol mass fraction will be used to identify time intervals dominated by tailpipe plumes. (3) On-road plume filtering: short-duration spikes (less than 60 seconds) coincident with elevated NO and black carbon will be masked from the source apportionment input matrix to produce parallel near-roadway and regional analyses. The two analyses are then subtracted to estimate on-road versus background source contributions across the mobile transect domain.

### 3.5.5 Directionality and Transport Analysis

For stationary deployments, Conditional Probability Function (CPF) analysis will resolve source directionality by coupling PMF factor contributions with local wind data. HYSPLIT back-trajectory analysis with cluster analysis (Draxler and Hess, 1998) will characterize regional transport pathways, and Concentration-Weighted Trajectory analysis applied to PMF factor time series will identify the influence of transboundary air masses from Mexico.

Source apportionment in this project is conducted entirely through PMF-based methods (conventional PMF, combined Vocus-AMS PMF, reactivity-weighted PMF, and the complementary offline $PM_{2.5}$ filter PMF conducted by Co-PI Sullivan). PMF derives source profiles empirically from the data rather than assuming fixed emission ratios, so the resulting factor profiles reflect the composition of the air mass as sampled, including the cumulative effect of in-transit photochemical aging.

## 3.6 Toluene CAMx RTRAC Reanalysis Approach (Task 4)

This task applies the existing 2022 base year CAMx and RTRAC simulations completed under Project 24-024. The previously generated RTRAC source attribution at four monitoring sites (Chamizal, Delta Drive, Womble, Socorro Hueco) will be extended to a fifth site (UTEP) using the same RTRAC output. Box-and-whisker plots of annual interquartile ranges and percentile concentrations of modeled and observed toluene concentrations will be developed for the UTEP site. Domestic and international emission source sector contributions by wind direction will be characterized for the mean and top 10% of RTRAC-predicted toluene concentrations, allowing comparisons of relative contributions of domestic and international sources during prevailing wind conditions. Toluene pollution roses for observed concentrations at each stationary monitoring site will be developed. Mobile Vocus measurements collected near the five monitoring sites during the Project 24-024 field campaigns will be integrated with the model predictions and stationary site observations to provide further support for the characterization of toluene concentrations by wind direction, spatial patterns, and source contributions.

## 3.7 Reconciliation of Multi-Framework Results

Because Task 1 evaluates ozone formation potential under four frameworks, Task 2 evaluates sensitivity regimes under six indicators, and Task 3 evaluates source apportionment under both conventional and reactivity-weighted PMF, the project applies explicit decision rules to reconcile results across frameworks before drawing conclusions.

For OFP rankings, where all four frameworks (mass-based MIR, molecular weight-based MIR, OH reactivity-weighted, and EBIR) agree on a species' membership in the top quartile of contributors, the assignment is reported as high confidence. Where the frameworks disagree, the regime-appropriate framework determines the ranking, namely MIR for the VOC-limited urban core and EBIR for the transitional and NOx-limited suburban areas identified in the Task 2 maps, and the framework dependence is reported explicitly.

For sensitivity regimes, the high-agreement and transitional classifications produced by the Section 3.4 voting scheme are carried forward and reconciled here with the Task 1 and Task 3 results without reapplying the indicator vote.For source apportionment, the conventional and reactivity-weighted PMF solutions are reported in parallel. Sources whose rankings differ substantially between the two solutions are identified as those whose ozone relevance is disproportionate to their ambient mass contribution.

Conclusions in the Final Report are drawn only from results that converge across frameworks. Divergent results are reported as caveats together with the framework dependence and regime context. This reconciliation step corresponds to Task 5 in the analytical workflow figure of the Scope of Work.

# 4. DATA PROCESSING AND ANALYSIS PROCEDURES

## 4.1 Vocus PTR-ToF-MS Data Processing

Raw Vocus mass spectral data collected under Project 24-024 were processed using PTRwid (Holzinger, 2015) and Tofware (Stark et al., 2015). For Project 26-030, the existing processed time series will be used as the primary input. Data quality screening rejected periods of instrument malfunction, including periods when time-of-flight voltages were not at setpoint, periods of inlet pressure instability, periods of failed calibration checks, and the start and end of mobile drives during instrument warm-up and shut-down. Background concentrations measured with the VocusAir catalyst were subtracted, and concentrations referenced to the daily calibration runs with certified standard gases (Apel-Riemer, Inc.). Stated measurement uncertainty for explicitly calibrated species is 10%; for species derived from proton transfer rate coefficient fits, the uncertainty is 30%. Detection limits for the Project 24-024 instrument operation are tabulated in the Project 24-024 Final Report and will be reused for this analysis. For OFP and PMF input, species with signal-to-noise ratios below 0.5 will be removed from the PMF input matrix entirely, and species with ratios between 0.5 and 2.0 will be retained but assigned higher uncertainty values, which reduces their influence on the PMF solution proportionally.

## 4.2 HR-TOF-AMS Data Processing

HR-TOF-AMS data collected under Project 24-024 were processed in Igor Pro 9.05 (Wavemetrics, Inc.) using the standard HR-AMS data analysis toolkit Squirrel version 1.26G. For Project 26-030, the dataset will also be analyzed using the highresolution data analysis toolkit Pika. This will result in updated time series of organics, sulfate, ammonium, nitrate, and chloride, which will be used in this project, and in high resolution mass spectral data, which will be used in PMF analysis in this project. Periods of instrument malfunction or flow instability are removed

from the dataset during quality control screening and are not used in any subsequent analysis. . Ionization efficiency calibrations and relative ionization efficiency calibrations conducted before and after each Project 24-024 deployment will be applied as documented in the Project 24-024 records.

## 4.3 Auto-GC Data Processing

Auto-GC data from the TCEQ Chamizal and Delta Drive sites and from the UTEP site (Project 24-024) have been processed and quality-controlled by Co-PI Sullivan following the established procedures used in his prior AQRP and TCEQ work (Park et al., 2020; Sullivan and Holdren, 2022, 2023). Hourly speciated VOC data for benzene, toluene, ethylbenzene, m,p-xylene, o-xylene, and additional aliphatic and aromatic species will be used. Cross-validation between Vocus and auto-GC measurements will be performed for overlapping species during the temporal collocation period at the UTEP site established under Project 24-024.

## 4.4 OFP Calculation Procedures

Mass-based OFP will be calculated as $OFP_i = C_i * MIR_i$, where $C_i$ is the mass concentration in $\mu g/m^3$ and $MIR_i$ is the maximum incremental reactivity coefficient in g $O_3$ per g VOC, yielding OFP in $\mu g\ O_3/m^3$. The primary MIR set will be the Carter and Heo (2012) SAPRC-11 reactivity scale using the El Paso, Texas (ELPTX) scenario, which reflects El Paso-specific NOx levels, temperature, and background VOC composition; this scenario was applied successfully to the Project 24-024 mobile dataset in the preliminary analysis presented at the May 2026 TCEQ SIM. Sensitivity tests will use Carter (2010) SAPRC-07 and Venecek et al. (2018) updated MIR values to assess robustness to the choice of MIR vintage. As in the preliminary analysis, OFP will be evaluated under two scenarios: matched compounds only, and a geometric-mean fill in which unmatched Vocus species are assigned the geometric mean MIR of the matched set. Molecular weight-based OFP will be calculated as $OFP_i = C_i * MIR_i * M_{O_3} / M_i$, where $M_i$ is the species molecular weight and $M_{O_3}$ = 48 g/mol is the molecular weight of ozone. Both formulations yield units of $\mu g\ O_3/m^3$, with the molecular weight-based version rescaling each species contribution by $M_{O_3} / M_i$ so that lower molecular weight species (e.g., acetaldehyde, methanethiol, isoprene) carry proportionally more weight than in the mass-based formulation. OH reactivity-weighted OFP will be calculated as $OFP_{react,i} = C_i * k_{OH,i} * MIR_i$, where $k_{OH,i}$ is the OH rate constant of species i drawn according to a documented source hierarchy. OH rate constants are taken primarily from the critically evaluated recommendations of JPL Publication 19-5 (Burkholder et al., 2020) and the IUPAC Subcommittee evaluations, which provide single recommended values with stated uncertainties. For species not covered by those evaluations, values are taken from the NIST Chemical Kinetics Database, selecting the most recent peer-reviewed determination. Where no measured value is available from any of these sources, $k_{OH,i}$ is estimated using the structure-activity relationship of Kwok and Atkinson (1995). This metric ranks species by their contribution to instantaneous ozone precursor reactivity and does not require knowledge of OH concentration; for an air parcel with shared OH exposure across species, the reactivity-weighted ranking closely tracks the absolute consumed-VOC ranking.

For selected near-source mobile transects where photochemical age can be inferred from co-emitted aromatic tracer pairs (for example, m,p-xylene paired with benzene), the OH exposure $\tau_{OH} = \int[OH]\,dt$ will be estimated from the deviation of the observed tracer ratio from its emission ratio following de Gouw et al. (2005) and Yuan et al. (2012), and an absolute consumed-VOC OFP will then be computed at those locations as $OFP_{consumed,i} = C_i * (\exp(k_{OH,i} * \tau_{OH}) - 1) * MIR_i$ for cross-validation of the reactivity-weighted rankings.

EBIR-based OFP will be calculated as $OFP_{EBIR,i} = C_i * EBIR_i$, where $EBIR_i$ is the Equal Benefit Incremental Reactivity coefficient for species i (Carter, 2010; Venecek et al., 2018),

expressed in g $O_3$ per g VOC and yielding the same units as the mass-based formulation. EBIR rankings are reported for the transitional and NOx-limited areas identified in Task 2 and MIR rankings for the VOC-limited urban core; where the two rankings diverge for a given species, both are reported with the regime context.

Total OFP at each location and time bin will be the sum of the species-level contributions, and species-level percentage contributions will be computed for ranking purposes. All calculations and intermediate products will be implemented in version-controlled Python and Matlab scripts archived to the project repository.

## 4.5 Sensitivity Indicator Calculation Procedures

VOC/NO2 and VOC/NOx ratios will use the sum of measured speciated VOCs (or the sum weighted by OH reactivity, calculated as sum of C_i * k_OH,i) divided by $NO_2$ or NOx in mixing-ratio units. $O_3$/NOx, $O_3$/NOy, and $O_3$/NOz are computed as concentration ratios; NOy is taken from measurements where available and from CAMx otherwise. Satellite FNR (HCHO column / NO2 column) will be computed from TROPOMI Level-2 retrievals (KNMI/SRON algorithm for HCHO and DOMINO/QA4ECV for NO2) and from TEMPO Level-2 retrievals where available. Cloud-screened, quality-flagged satellite pixels will be aggregated to a 0.05° by 0.05° grid for direct overlay with the surface indicator maps. Threshold values for regime classification will follow Wan et al. (2024) for FNR and Sillman (1995) and subsequent updates for surface ratios. Choice of thresholds will be explicitly documented in the Final Report. All surface ratios are computed from observed atmospheric concentrations at the TCEQ CAMS sites and from the Project 24-024 mobile and stationary platforms, not from emission rates, and the satellite FNR is an observed column ratio from the TROPOMI and TEMPO retrievals.

Threshold values for regime classification are observation-based and are drawn from the peer-reviewed literature (Table 4.5-1). Where regionally validated thresholds are available for Texas urban areas they are preferred (for example, Wan et al. (2024) supersedes the generic FNR threshold for the El Paso domain); otherwise the most recent peer-reviewed urban recommendation is selected and its uncertainty range is propagated through the OFP and sensitivity uncertainty analysis. Threshold sensitivity will be tested by repeating the regime classification at plus or minus 20 percent of each threshold value, and classifications that are robust to this perturbation are reported with high confidence. The chosen thresholds will be documented in the Final Report.

***Table 4.5-1.*** *Photochemical regime indicators and transition values*

| Indicator | VOC-limited | Transitional | NOx-limited | Source |
|---|---|---|---|---|
| VOC/NOx (ppbC/ppb) [a] | < 5 | 5 to 15 | > 15 | EPA PAMS 2018; Sullivan 2022 (El Paso) |
| HCHO/NO2 [b] | < 1 | 1 to 2 | > 2 | Duncan et al. 2010 |
| O3/NOy [c] | < 4 | 4 to 6 | > 6 | Sillman and He 2002 |
| O3/NOz [c] | < 7 | ~7 | > 7 | Sillman 1995 |
| VOC/NO2, O3/NOx [d] | - | - | - | - |

[a] Morning ppbC/ppb ratio; Sullivan (2022) finds El Paso near 6 to 7 [b] Satellite column ratio; Texas transition near 1.6 (Wan et al. 2024). [c] Computed where total reactive nitrogen is measured (e.g. Chamizal). [d] Reported thresholds vary widely, so the El Paso values will be set by the CAMx calibration. All values are preliminary and region-dependent and will be calibrated against the CAMx Process Analysis.

## 4.6 PMF Procedures

PMF analyses will follow the procedures and conventions described in Ulbrich et al. (2009) for unconstrained runs and in Paatero (1999) and Canonaco et al. (2013) for constrained ME-2 runs implemented through the SoFi Pro toolkit. Software versions and exact parameter settings used for each analysis will be reported in the Monthly Technical Reports and the Final Report.

The base PMF runs will target a Q/Qexpected ratio close to unity, indicating that the model residuals are consistent with the assigned uncertainties. Multiple PMF runs from random starting seeds will be performed to confirm convergence to the same solution. Bootstrap analysis will assess the statistical stability of the factor solutions. Solutions will be evaluated across a range of factor numbers, and rotational ambiguity will be examined using the Rotational Forcing Parameter (FPEAK). Where constrained PMF (ME-2) is applied, the sensitivity of results to the constraint strength will be tested systematically. Factor profiles will be compared against published reference spectra where available and known tracer ratios for source categories.

## 4.7 CAMx RTRAC Reanalysis Procedures

This task uses output files from the existing 2022 base year CAMx simulations with the RTRAC probing tool completed under Project 24-024. Output processing will use the established workflows from Project 24-024, which will include extraction of hourly toluene concentrations at the five monitoring sites, calculation of the annual mean and top 10% concentrations, classification by wind direction, and aggregation by source sector as tagged in RTRAC. Box-and-whisker plots of annual modeled and observed interquartile ranges and percentile concentrations at the UTEP monitoring site will be generated using the same methodology used in the Project 24-024 Final Report Section 5.3.3. Toluene pollution roses will be developed that show the magnitude and associated wind direction frequency of observed concentrations at each of five stationary monitoring sites for comparisons with CAMx predictions. An integrated analysis will examine these results with those from the Vocus PTR-ToF-MS. Visualization tools, such as contour maps, will be used to ensure spatiotemporal patterns of model predictions and observations are reasonable.

## 4.8 Data Archiving and Reproducibility

All processed datasets, PMF input and output matrices, OFP and sensitivity ratio products, and CAMx RTRAC analysis outputs will be archived to a project repository maintained by UT Austin. Archived materials include MD5-hashed data manifests, version-controlled Python and R scripts, and intermediate diagnostic plots. Repository access will be provided to AQRP and TCEQ. Final datasets will be delivered within 30 days of project completion in formats consistent with the Project 24-024 data delivery.

# 5. QUALITY METRICS

## 5.1 Data Quality Screening

All input datasets will be subjected to systematic data quality screening before use in the analyses. For the Vocus and HR-TOF-AMS data, the screening criteria already applied during Project 24-024 will be reused, with expanded analyses by the Project 26-030 analysis team. For the auto-GC data, Co-PI Sullivan will apply his established screening procedures. For TCEQ CAMS data, only validated AQS records will be used. For satellite data, only quality-flagged, cloud-screened pixels meeting the standard retrieval quality flags will be used. The CAMx output will include

predictions evaluated against ambient measurements for Project 24-024, along with new results evaluated similarly at the UTEP site for Project 26-030.

## 5.2 Cross-Validation Between Instrument Platforms

Cross-validation between Vocus PTR-ToF-MS and auto-GC measurements will be performed for overlapping species during the temporal collocation periods at the UTEP site established under Project 24-024. Slope, intercept, R-squared, and residual statistics will be reported for benzene, toluene, ethylbenzene, m,p-xylene, o-xylene, and additional species available from both instruments. Discrepancies of greater than the combined uncertainty of the stated Vocus uncertainty (30% for non-explicitly-calibrated species) and the stated auto-GC uncertainty (20%) will be investigated and documented. Cross-validation between HR-TOF-AMS organic mass and $PM_{2.5}$ monitor mass will use the existing collocation data, with appropriate accounting for the AMS $PM_1$ versus monitor $PM_{2.5}$ size cut difference.

## 5.3 Audits of Data Quality

At least 10% of all data products generated under this project will be independently reviewed as part of the Audits of Data Quality requirement. The audit scope includes: OFP calculations under each of the three frameworks (Task 1); sensitivity ratio calculations and threshold classifications (Task 2); PMF input matrices, model parameter settings, and factor assignments (Task 3); and CAMx RTRAC output extractions and aggregations (Task 4).For OFP calculations, Co-PI Hildebrandt Ruiz or Postdoctoral Fellow Dr. Chao will independently recompute at least 10% of the OFP values using an independent code implementation. For sensitivity ratios, Co-PI Sullivan will independently recompute at least 10% of the indicator values for selected sites and time periods. For PMF analyses, the Co-PI not leading the specific PMF run will independently verify a subset of the input data, the model parameters, and the factor assignments. For the CAMx RTRAC reanalysis, at least 10% of the CAMx output and processed data for analyses will be independently checked by Drs. McDonald-Buller and Kimura. Discrepancies between a primary analysis and its audit that exceed the acceptance thresholds in Section 5.7 trigger the following resolution process. First, both analysts jointly re-examine the input data quality and the processing parameters. Second, if the discrepancy persists, the analysis is escalated to PI Misztal for review and decision. Third, any discrepancy that remains unresolved is reported in the Final Report as a caveat with both results presented.

Findings from all Audits of Data Quality will be summarized in a section of the Draft Final Report and the Final Report.

## 5.4 PMF Quality Control

### 5.4.1 Model Calibration

The PMF input matrix will be calibrated by constructing an associated uncertainty matrix that combines instrument-specific Poisson counting error, calibration uncertainty, and a minimum uncertainty floor. Species with signal-to-noise ratios below 0.5 will be removed from the PMF input matrix entirely, and species with ratios between 0.5 and 2.0 will be retained but assigned higher uncertainty values, which reduces their influence on the PMF solution proportionally. Below-detection-limit values will be replaced with one half of the detection limit and assigned an uncertainty equal to five sixths of the detection limit. The base PMF runs will target a Q/Qexpected ratio close to unity.

### 5.4.2 Model Verification

Verification will confirm that the selected solution is mathematically valid and reproducible. Residual distributions will be examined for each species and time point to confirm they are approximately normal with mean near zero. Multiple PMF runs from random starting seeds will be performed to confirm convergence to the same solution. For each analysis, at least 10% of the PMF input data matrix will be independently verified against the original instrument time series by a Co-PI not involved in the initial data processing. Bootstrap analysis with at least 100 resampled runs will assess the statistical stability of the factor solutions.

### 5.4.3 Model Evaluation

Solutions will be evaluated across a range of factor numbers, and rotational ambiguity will be examined using the Rotational Forcing Parameter (FPEAK). Factor profiles will be compared against published reference spectra and known tracer ratios for source categories (Bhandari et al., 2022a; Patel et al., 2020; Slowik et al., 2010; Simon et al., 2025; Stockwell et al., 2021). Where constrained PMF (ME-2) is applied, the sensitivity of results to the constraint strength (a-value) will be tested systematically. The diurnal profile of the PMF factors will be plotted, and the uncertainty range of these factors will be calculated based on the standard deviation of data from multiple days. A valid PMF factor must satisfy four criteria: (1) a physically interpretable composition, that is, a recognizable source profile with known marker species in expected ratios; (2) bootstrap stability of at least 80 percent; (3) a contribution of at least 5 percent of total measured mass; and (4) residuals that are approximately normally distributed with a mean near zero. Factors are rejected if they represent noise (high residual structure), single-event outliers, or mathematical artifacts (negative loadings or unphysical correlations). Ambiguous cases, such as mixed signatures or factors that split at higher factor counts, are reported with both candidate solutions and the rationale for the preferred choice (Patel et al., 2020; Bhandari et al., 2022a).

### 5.4.4 Documentation

Software versions, parameter settings, input matrix dimensions, exclusion lists, weighting choices, factor count, FPEAK values, a-values for constrained runs, bootstrap settings, and Q/Qexpected values will be documented for each PMF analysis. All input matrices, output factor profiles and time series, and intermediate diagnostic plots will be archived to the project repository.

## 5.5 Uncertainty Propagation

Uncertainty in the OFP analyses combines: (1) measurement uncertainty in $C_i$ (10% for explicitly calibrated species, 30% for non-explicitly-calibrated species; 20% for auto-GC species); (2) MIR uncertainty drawn from the literature ranges in Carter (2010) and Venecek et al. (2018); (3) for the OH reactivity-weighted metric, additional uncertainty from $k_{OH,i}$ (typically 10 to 30% per IUPAC evaluations); and (4) for the absolute consumed-VOC sensitivity check, additional uncertainty from the inferred OH exposure $\tau_{OH}$ (typically a factor of 2 to 3 from photochemical-age methods). Total uncertainty will be propagated by Monte Carlo simulation, and reported as 1-sigma confidence intervals on species-level OFP and on the cumulative ranking. Uncertainty in the sensitivity ratio analyses combines measurement uncertainty in the numerator and denominator species, propagated in quadrature in log-space (because the indicators are ratios). Uncertainty in PMF factor contributions will be characterized by the bootstrap analysis described in Section 5.4. Uncertainty in the CAMx RTRAC outputs is inherent to the underlying simulations from Project 24-024 and will be carried forward without modification.

## 5.6 Software and Reproducibility

All custom analytical code developed under this project will be implemented in version-controlled Python, Igor, and Matlab scripts archived to a UT Austin GitLab repository accessible to AQRP and TCEQ on request. The repository will include: input data manifests with MD5 hashes, exact software versions and library dependencies, executable scripts that reproduce all reported tables and figures from the input data, and intermediate output products. CAMx RTRAC output processing will use the same software stack used in Project 24-024 for consistency.

## 5.7 Data Quality Objectives

Quantitative acceptance criteria are defined for the principal data products. Products that fail these criteria are reported with explicit caveats.

(a) Inter-instrument agreement (Vocus versus auto-GC) for benzene, toluene, and xylenes during the UTEP collocation period: regression slope between 0.70 and 1.30, coefficient of determination R-squared of at least 0.85, and mean bias within plus or minus 30 percent.

(b) PMF factor retention: Q over Q-expected between 0.8 and 1.2; bootstrap factor stability of at least 80 percent; and rotational ambiguity confirmed through the FPEAK test within plus or minus 0.5.

(c) For the comparison of the existing CAMx toluene simulation against the Project 24-024 observations, agreement metrics (correlation, normalized mean bias, and normalized mean error) are computed and reported as model-evaluation diagnostics rather than as pass-or-fail acceptance criteria. Because the 2022 base-year simulation and the 2024 to 2025 observations differ in time period and spatial representativeness (grid-cell average versus point or transect measurement), systematic differences are expected and are interpreted as candidate indicators of emission-inventory or model-representation differences (Task 2), not as a quality failure of either dataset.

# 6. REPORTING

## 6.1 Deliverables from Each Project Participant

AQRP requires certain reports to be submitted on a timely basis and at regular intervals. PI Dr. Misztal will submit the reports but will be assisted by Co-PIs and other project participants. 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 will be followed.

**Abstract:** An Abstract will be submitted to the Project Manager for use on the AQRP website, providing a brief non-technical description of the planned project activities. Due Date: Ten (10) business days after notice of intent to fund.

**Quarterly Reports:** Quarterly Reports will provide a summary of project status. Submitted as Word documents, not exceeding 2 pages, text only. Due Dates: To be determined based on project start date.

**Technical Reports:** Monthly Technical Reports will be submitted to the Project Manager and TCEQ Liaison as a Word document using the AQRP MTR Template. Due Dates: Monthly, on the 10th of each month (or following business day).

**Financial Status Reports:** Submitted monthly to the AQRP Grant Manager using the AQRP FSR Template. Due Dates: Monthly, on the 10th of each month (or following business day).

**Draft Final Report:** A Draft Final Report including an Executive Summary will be submitted to the Project Manager and the TCEQ Liaison, following State of Texas accessibility requirements. Due Date: August 1, 2027 (30 days before project end).

**Final Report:** A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted. Due Date: August 31, 2027.

**Project Data:** All project data including QA/QC data, processed datasets, source profiles, PMF input and output matrices, OFP and sensitivity ratio products, and CAMx RTRAC analysis outputs will be submitted to the AQRP Project Manager within 30 days of project completion in a format allowing AQRP, TCEQ, or other outside parties to use the information.

**AQRP Workshop:** A representative from the project will present at the AQRP Workshop on a date to be determined.

**Stakeholder Presentation:** Key findings will be presented to TCEQ Border Affairs and the Joint Advisory Committee for Air Quality Improvement to support binational air quality coordination.

**Presentations and Publications:** All data and other information developed under this project that is included in published papers, symposia, presentations, press releases, websites, and other publications will be handled per the Publication and Publicity Guidelines included in the Subaward Agreement. Draft manuscripts, presentations, and press materials will be submitted to the AQRP Project Manager and the TCEQ Project Liaison at least 30 days prior to submission for review and approval. AQRP and TCEQ will be acknowledged in resulting publications, and final published versions will be provided to AQRP for archiving.

## 7. TIMELINE

The project schedule by task is presented in Scope of Work Sect. 3. The project start date is August 1, 2026. Technical work will not begin until authorization is received from TCEQ and AQRP. The entire project will be completed by August 31, 2027. The Draft Final Report will be submitted by August 1, 2027 (30 days before project end) and the Final Report by August 31, 2027.

## 8. REFERENCES

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**AQRP Project 26-030 Work Plan**

**Scope of Work**

**Project 26-030**

**CAMx**

# Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed

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Revision: 2

June 19, 2026

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** 2026-06-27 | 04:37:06 CDT

Signed by:
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Erin Tullos, Project Manager, Texas Air Quality Research Program

**This Scope of Work was approved electronically on** 2026-06-29 | 16:09:55 CDT

Signed by:
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Erik Gribbin, Project Liaison, Texas Commission on Environmental Quality

**This Scope of Work was approved electronically on** 2026-06-26 | 09:13:15 CDT

Signed by:
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Pawel K. Misztal, Principal Investigator, The University of Texas at Austin

## Acronyms and Abbreviations

AE-33: Aethalometer (model AE-33)
AMS: Aerosol Mass Spectrometer
AQRP: Texas Air Quality Research Program
auto-GC: Automated Gas Chromatograph
BBOA: Biomass Burning Organic Aerosol
BC: Black Carbon
BTEX: Benzene, Toluene, Ethylbenzene, and Xylenes
CAMS: Continuous Ambient Monitoring Station
CAMx: Comprehensive Air Quality Model with Extensions
CO: Carbon Monoxide
COA: Cooking Organic Aerosol
CoEP: City of El Paso
CPF: Conditional Probability Function
DFW: Dallas-Fort Worth
EBIR: Equal Benefit Incremental Reactivity
ELPTX: El Paso, Texas (MIR scenario)
FNR: Formaldehyde-to-Nitrogen Dioxide Ratio
GRA: Graduate Research Assistant
HAP: Hazardous Air Pollutant
HCHO: Formaldehyde
HDV: Heavy-Duty Vehicle
HGB: Houston-Galveston-Brazoria
HNO3: Nitric Acid
HOA: Hydrocarbon-like Organic Aerosol
HR-TOF-AMS: High-Resolution Time-of-Flight Aerosol Mass Spectrometer
HYSPLIT: Hybrid Single-Particle Lagrangian Integrated Trajectory model
IUPAC: International Union of Pure and Applied Chemistry
JAC: Joint Advisory Committee for Air Quality Improvement
JPL: Jet Propulsion Laboratory
LDV: Light-Duty Vehicle
MIR: Maximum Incremental Reactivity
NAAQS: National Ambient Air Quality Standard
NO2: Nitrogen Dioxide

NOx: Nitrogen Oxides

NOy: Total Reactive Nitrogen

NR-PM1: Non-Refractory Submicron Particulate Matter

O3: Ozone

OFP: Ozone Formation Potential

OH: Hydroxyl Radical

OOA: Oxygenated Organic Aerosol

ORP: Ozone Reaction Potential

PM: Particulate Matter

PM1: Particulate Matter with aerodynamic diameter ≤ 1 μm

PM2.5: Particulate Matter with aerodynamic diameter ≤ 2.5 μm

PMF: Positive Matrix Factorization

PTR-ToF-MS: Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer

QAPP: Quality Assurance Project Plan

RTRAC: Reactive Tracer Probing Tool

SAPRC: Statewide Air Pollution Research Center (chemical mechanism)

SIP: State Implementation Plan

SOA: Secondary Organic Aerosol

SOW: Scope of Work

TCEQ: Texas Commission on Environmental Quality

TEMPO: Tropospheric Emissions: Monitoring of Pollution

TROPOMI: Tropospheric Monitoring Instrument

UTEP: The University of Texas at El Paso

VCP: Volatile Chemical Product

VOC: Volatile Organic Compound

**Glossary of analytical terms**

Framework: a conceptual basis for ranking ozone formation potential (mass-based MIR, molecular weight-based MIR, OH reactivity-weighted, and EBIR).

Method: a specific computational technique (for example, PMF, HYSPLIT, or CAMx Process Analysis).

Analysis, or Task: a named product within this Scope of Work (Tasks 1 through 5).

# Table of Contents

# STATEMENT OF WORK

## 1. Introduction

This document provides the work plan for the Texas Air Quality Research Program (AQRP) project 26-030, “Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed”. Work will be completed by August 31, 2027. The project Principal Investigator is Dr. Pawel K. Misztal and the Co-Principal Investigators are Drs. Lea Hildebrandt Ruiz, David W. Sullivan, and Elena C. McDonald-Buller of The University of Texas at Austin. The team will conduct advanced analyses of the comprehensive datasets collected under AQRP Project 24-024 (Misztal et al., 2025) to extract additional value for State Implementation Plan (SIP) development, focusing on ozone formation chemistry, VOC sensitivity regimes, particulate matter source apportionment, and integration of observations with photochemical modeling.

The Texas SIP includes strategies for attaining air quality standards for ozone, fine particulate matter ($PM_{2.5}$), and regional haze. El Paso County was designated as marginal nonattainment for the 2015 ozone National Ambient Air Quality Standard (NAAQS), and with the tightening of the $PM_{2.5}$ annual standard from 12 to 9 $\mu g/m^3$, the region faces increasing pressure to understand and reduce air pollution sources. Although El Paso is not currently in serious ozone nonattainment, the analytical methods developed in this project are directly transferable to serious and severe nonattainment areas in Texas, and the methodological framework will benefit Houston-Galveston-Brazoria, Dallas-Fort Worth, and Bexar County air quality assessments. The El Paso-Juárez metropolitan area also represents one of the largest binational communities in North America, with unique air quality challenges arising from its complex geography, climate, transboundary transport, and diverse emission sources.

AQRP Project 24-024, “Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area,” completed in August 2025, represented the most comprehensive air quality field campaign conducted in El Paso since the 1996 Paso del Norte Ozone Study. The project deployed extensive stationary and mobile measurement capabilities including: (1) Vocus PTR-ToF-MS measuring over 200 VOC species with 1-second time resolution; (2) High Resolution Time-of-Flight Aerosol Mass Spectrometer (HR-TOF-AMS) measuring bulk chemical composition and detailed mass spectra of non-refractory PM1 (NR-PM1); (3) Multi-wavelength aethalometer (AE33) for black and brown carbon; (4) Auto-GC measurements of speciated hydrocarbons at The University of Texas at El Paso (UTEP) site (operated under Project 24-024) and at the Chamizal (CAMS 41) and Delta Drive sites operated by TCEQ and analyzed by co-PI Sullivan (Figure 1); and (5) Comprehensive meteorological parameters and criteria pollutants ($O_3$, $NO_2$, CO). Project 24-024 also developed a Comprehensive Air Quality Model with Extensions (CAMx) platform for El Paso-Juárez for the 2022 base year, including Reactive Tracer (RTRAC) source attribution for toluene.

The five monitoring sites referenced throughout this work plan are distributed across the El Paso-Juarez airshed (Figure 1). Chamizal (CAMS 41; EPA 48-141-0044), approximately 0.5 km north of the U.S.-Mexico border, is a long-term TCEQ auto-GC site and one of the longer-running speciated VOC records in Texas. The El Paso Delta site (CAMS 1011; EPA 48-141-1011), at 6700 Delta Drive approximately 1.3 km from the border, is an auto-GC VOC site reestablished by The University of Texas at Austin in 2017, with the speciated hydrocarbon measurements operated and analyzed by Co-PI Sullivan. The UTEP site, established under Project 24-024 on the University of Texas at El Paso campus approximately 1.1 km from the border, housed a UT Austin auto-GC operated by Co-PI Sullivan with collocation of the Vocus PTR-ToF-MS during 2024 and 2025. Womble (EPA 48-141-0047) and Socorro Hueco (CAMS 49) provide canister VOC measurements, each approximately 2.7 km from the border, with Socorro Hueco the

easternmost of the five sites. The CAMx RTRAC source attribution under Project 24-024 was conducted at four of these sites (Chamizal, Delta Drive, Womble, and Socorro Hueco); Project 26-030 extends that analysis to the fifth site (UTEP).

While Project 24-024 successfully collected this unprecedented dataset and conducted initial source apportionment analyses, opportunities remain to extract additional value through advanced analyses specifically targeting ozone formation chemistry under multiple reactivity frameworks, VOC sensitivity regimes evaluated through complementary indicator ratios, particulate matter source apportionment using reactivity-weighted and combined gas-particle approaches, and model-observation integration. This proposed project addresses these needs directly and responds to specific TCEQ feedback received during the 26-030 review.

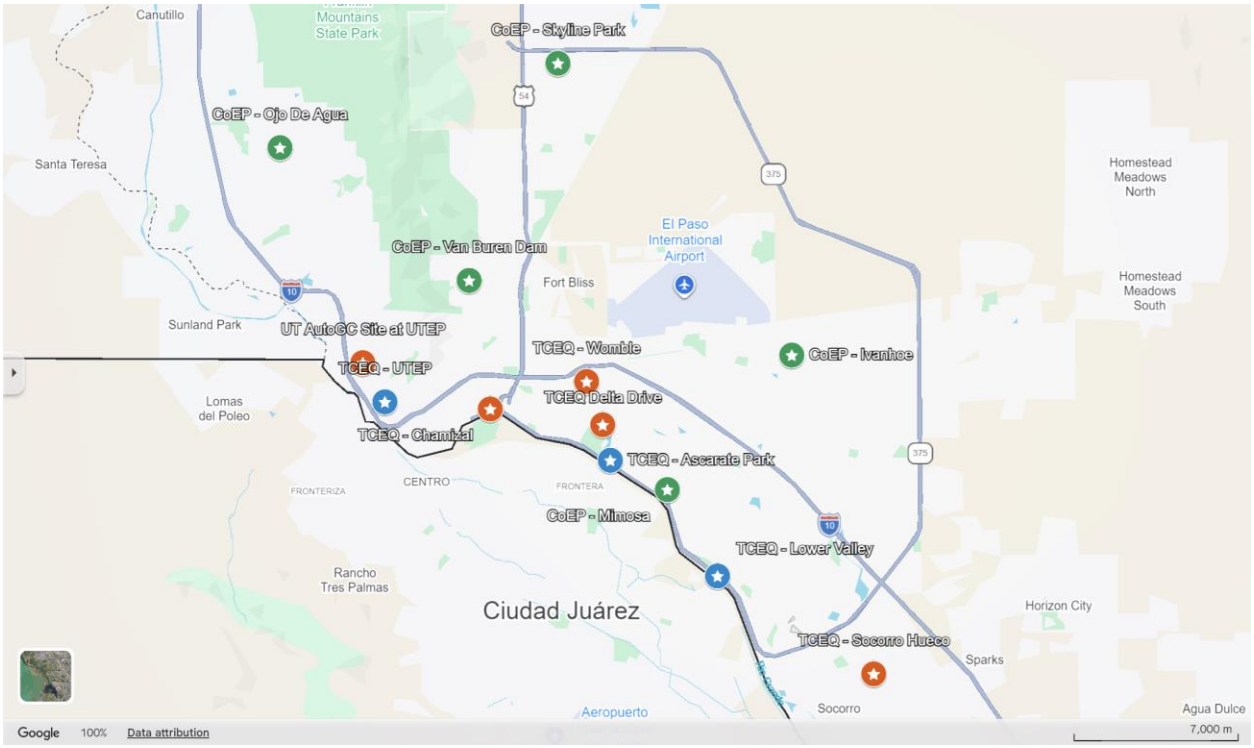


***Figure 1.*** *Locations of monitoring stations. In orange the monitoring stations of focus are highlighted with the remaining TCEQ stations in blue and City of El Paso (CoEP) stations in green.*

### 1.1 Scientific Motivation

Understanding the ozone formation regime is critical for developing effective emission reduction strategies. The ozone formation potential (OFP) of VOCs can be quantified using Maximum Incremental Reactivity (MIR) scales, which represent the incremental amount of ozone formed per unit mass of VOC emitted under conditions most conducive to ozone formation. The MIR scale was originally developed by Carter (1994) using the SAPRC chemical mechanism and has since been updated to SAPRC-07 (Carter, 2010) and evaluated for contemporary conditions by Venecek et al. (2018). Recent studies using formaldehyde-to-NO2 ratios from satellite (OMI, TROPOMI) and ground-based observations have indicated that El Paso exhibits spatially variable ozone sensitivity (Wan et al., 2024). The University of Houston study “Ozone-NOx-VOC Sensitivity in Texas Urban Areas” found that the main urban core of El Paso experiences VOC-limited or transitional conditions, while suburban and surrounding areas tend to be NOx-limited. This finding has profound implications for air quality management because in VOC-limited regimes, NOx reductions may counterintuitively increase ozone levels due to reduced NOx

titration, whereas targeted VOC reductions focusing on high-reactivity compounds would be more effective.

The comprehensive Vocus PTR-ToF-MS dataset from Project 24-024, combined with long-term auto-GC records from TCEQ monitoring sites (analyzed by Co-PI Sullivan since 2011), provides an unprecedented opportunity to calculate OFP for individual VOC species, identify the key compounds contributing most to ozone production, and map the spatial distribution of ozone sensitivity. Toluene is a Hazardous Air Pollutant (HAP) and an ozone and PM precursor. Previous work by Seila et al. (2001) reported toluene as the most abundant VOC at the Campbell site (15 ppb) during the 1996 campaign, with even higher concentrations (31 ppb) measured in Juárez. Project 24-024 mobile and stationary observations show substantially lower average concentrations (680 ppt in winter, 250 ppt in summer), representing an approximately 5 to 10-fold improvement over three decades, yet episodic maxima still reached 25 to 37 ppb during specific events documented in the Project 24-024 Final Report Section 5.3.3. Furthermore, measured average toluene concentrations between 2021 and 2024 at Chamizal and Delta Drive were the second and fifth highest, respectively, among 42 auto-GC sites in Texas. These findings for indicate ongoing domestic and international sources of toluene requiring characterization.

### 1.2 Leveraging Long-Term Auto-GC Datasets

A unique strength of this project is the integration of Project 24-024 intensive campaign data with the extensive long-term VOC monitoring record maintained in El Paso. Co-PI Sullivan has operated and analyzed auto-GC data from multiple TCEQ and City of El Paso (CoEP) monitoring stations since 2011. The Chamizal site (CAMS 41) has been collecting speciated VOC data via auto-GC since the late 1990s, making it one of the longest-running auto-GC monitoring sites in Texas. During Project 24-024, a UT Austin trailer was used to house an auto-GC operated by Co-PI Sullivan at the new UTEP site, which operated for almost the entire year with temporary collocation with the Vocus PTR-ToF-MS. This long-term and recent record enables: (1) trend analysis showing multi-decadal changes in VOC composition and concentrations; (2) assessment of seasonal and interannual variability to contextualize the Project 24-024 campaign period; (3) cross-validation between Vocus PTR-ToF-MS and GC measurements for common species (benzene, toluene, xylenes, other aromatics); and (4) multi-site spatial analysis using simultaneous measurements at UTEP, Chamizal, and Delta Drive.

Long-term trend analysis is conducted separately at each fixed monitoring site. The Chamizal and Delta Drive sites each have multi-year continuous records that yield internally consistent multi-decadal trends. Comparisons that include the UTEP site, established under Project 24-024, are presented as concurrent post-2024 comparisons only, and not as a single multi-decadal trend across all three sites.

### 1.3 Preliminary Findings from Initial Extended Analyses

Following completion of Project 24-024, the team has begun extended analyses of the collected datasets. Preliminary findings were presented at the May 2026 Texas Commission on Environmental Quality State Implementation Plan Informational Meeting (SIM), attended by approximately 100 TCEQ staff. These results, summarized below, motivate the more comprehensive analyses proposed under Project 26-030 and demonstrate that the analytical workflows are operational.

Preliminary mass-based ozone reactivity potential (ORP) was calculated for the mobile Vocus dataset using the Carter and Heo (2012) SAPRC-11 maximum incremental reactivity scale with the El Paso, Texas (ELPTX) scenario, which reflects El Paso-specific NOx levels, temperature, and background VOC composition. ORP was evaluated at each 10-second mobile time step under two scenarios: matched compounds only (48 winter, 41 summer matched compounds,

covering 84.1% and 86.4% of total VOC mass respectively) which is a conservative lower bound ORP estimate, and a geometric-mean fill in which unmatched compounds receive the geometric-mean MIR of the matched set. The geometric-mean fill scenario additionally assigns the geometric mean MIR of the matched set to detected Vocus species not present in the SAPRC-11 table, providing an upper-bound ORP estimate. Reporting both brackets the true ORP and indicates the sensitivity of the result to MIR coverage. The highest ORP values cluster along the central El Paso, Bridge of the Americas, and Chamizal corridor in both seasons (Figure 2), identifying the urban core adjacent to the border as the dominant reactive VOC source region.

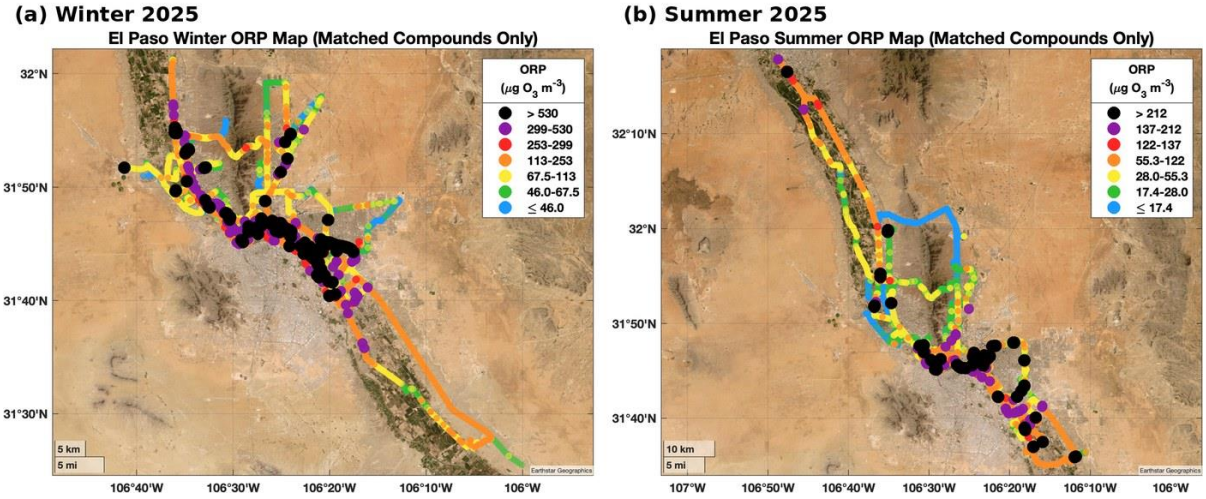


***Figure 2.*** *Preliminary mass-based ozone reactivity potential (ORP) maps from Project 24-024 mobile observations using the SAPRC-11 ELPTX maximum incremental reactivity scale (Carter and Heo, 2012). (a) Winter 2025 and (b) summer 2025, both showing the matched-compounds-only scenario (48 winter, 41 summer compounds; 84-86% VOC mass coverage). The same downtown and border corridor dominates in both seasons; summer magnitudes are roughly one-third of winter, reflecting deeper boundary layer mixing. Project 26-030 will extend this analysis with molecular weight-based and OH reactivity-weighted formulations and will compare priority rankings across the four frameworks (mass-based MIR, molecular weight-based MIR, OH reactivity-weighted, and EBIR).*

Preliminary PMF analyses on the HR-TOF-AMS data collected in the winter as part of Project 24-024 resolved a four-factor solution for organic aerosol comprising hydrocarbon-like organic aerosol (HOA, traffic-related), cooking-related organic aerosol (COA), biomass burning organic aerosol (BBOA), and oxygenated organic aerosol (OOA, secondary aged organic aerosol). Factor contributions track changes in air mass between northeastern and southeastern wind regimes (Figure 3), demonstrating the source attribution capability that Project 26-030 will extend to combined Vocus-AMS PMF and reactivity-weighted PMF (Task 3).

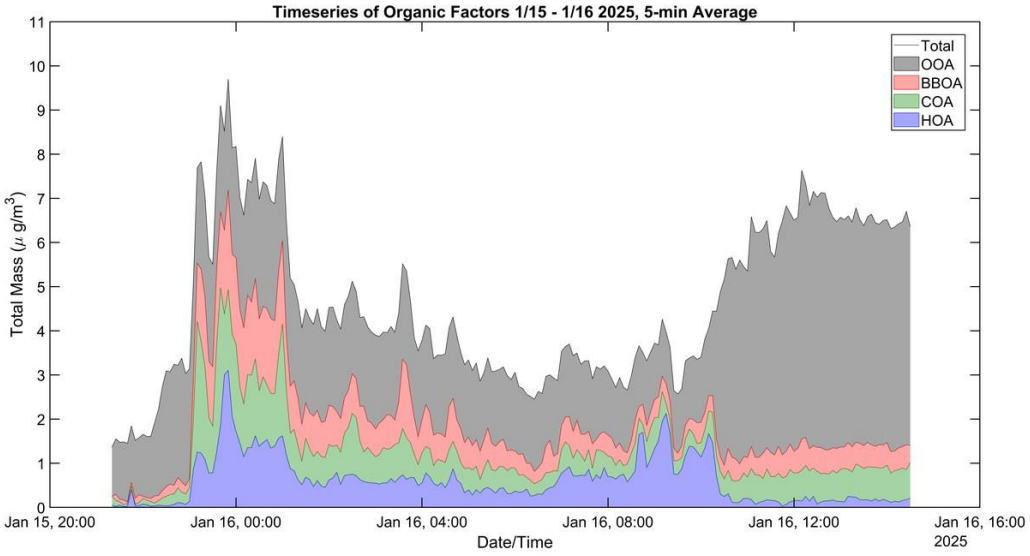


***Figure 3.*** *Preliminary 4-factor PMF on HR-TOF-AMS organic aerosol from Project 24-024 (winter campaign, 15-16 January 2025). Factor contributions (HOA, COA, BBOA, OOA) shift in response to air mass changes between northeastern and southeastern wind regimes. Project 26-030 will extend this analysis with combined Vocus-AMS PMF, reactivity-weighted PMF, and integration with offline $PM_{2.5}$ filter PMF (see Task 3 and Figure 3).*

Project 24-024 toluene observations from the Vocus PTR-ToF-MS show good preliminary spatiotemporal correspondence with the CAMx 2022 base year simulations developed for the El Paso-Juárez airshed. This positive comparison motivates the systematic five-site CAMx RTRAC analysis proposed in Task 4. Co-PI Sullivan has additionally conducted a complementary 6-factor PMF on offline $PM_{2.5}$ filter samples from the campaign that resolves inorganic and dust factors not captured by the AMS PM1 organics analysis (Figure 3 in Task 3 below).

### 1.4 Research Questions

The following research questions will guide the execution of the proposed work:

**R1:** What is the spatial and temporal distribution of ozone formation potential across the El Paso region under mass-based, molecular weight-based, and OH reactivity-weighted MIR formulations and Equal Benefit Incremental Reactivity (EBIR) formulations, and which specific VOC compounds contribute most to ozone production in different locations and seasons?

**R2:** How do ozone sensitivity regimes (VOC-limited versus NOx-limited) vary spatially across the El Paso-Juárez airshed when evaluated through multiple complementary indicator ratios (VOC/NO2, VOC/NOx, O3/NOx, O3/NOy, O3/NOz, satellite HCHO/NO2), and which ratios yield results consistent with photochemical modeling?

**R3:** What are the combined gas-particle source apportionment results, integrating VOCs (from Vocus and auto-GC) and PM (HR-TOF-AMS and offline filter PMF), that elucidate the sources of ozone and aerosol precursors?

**R4:** What are the relative contributions of domestic versus international (Mexican) emission sources to elevated toluene concentrations across the five monitoring sites in El Paso, and how do the fingerprints (chemical and temporal) of these sources differ?

## 2. Task Descriptions

The analytical workflow for Project 26-030 is summarized in Figure 4, which shows the input datasets, the analytical methods organized by task, and the deliverable products.

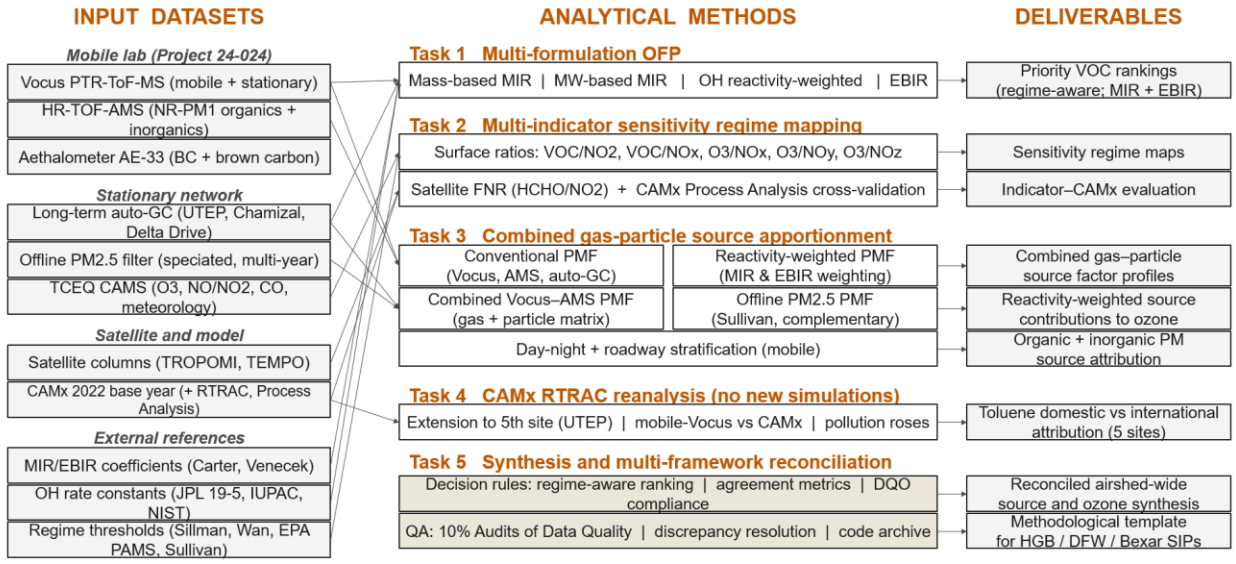


Figure 4. Analytical Workflow for AQRP project 26-030.

### 2.1 Task 1: Comprehensive Ozone Formation Potential Analysis

This task will calculate ozone formation potential for VOC species measured by the Vocus PTR-ToF-MS and the auto-GC network, using four complementary frameworks to provide a robust assessment of priority compounds for emission reduction. PI Misztal will lead this task, supported by Postdoctoral Fellow Dr. Chao and Graduate Research Assistant Daniel Sung. In this work a priority VOC is defined as a species whose product of ambient concentration and reactivity, under one of the OFP frameworks, places it among the top contributors to total OFP. Species are reported as priority if they cumulatively account for 90 percent of total OFP (a Pareto cutoff) under at least one of the four frameworks.

**Mass-based MIR approach.** For each measurement location and time period, OFP will be calculated as OFP_i = C_i * MIR_i, where C_i is the mass concentration of species i (µg/m$^3$) and MIR_i is its Maximum Incremental Reactivity coefficient (g $O_3$ per g VOC). The primary MIR set will be the Carter and Heo (2012) SAPRC-11 reactivity scale using the El Paso, Texas (ELPTX) scenario, which reflects El Paso-specific NOx levels, temperature, and background VOC composition and was applied successfully to the Project 24-024 mobile dataset in the preliminary analysis (Figure 1). Sensitivity tests will compare priority rankings against Carter (2010) SAPRC-07 and Venecek et al. (2018) updated MIR values to assess robustness to the choice of MIR vintage. As in the preliminary analysis, OFP will be evaluated under two scenarios: matched compounds only, and a geometric-mean fill in which unmatched Vocus species are assigned the geometric mean MIR of the Carter et al. MIR inventory. This approach is the standard regulatory formulation and ranks VOC species by ozone-forming mass potential.

**Molecular weight-based MIR approach.** To evaluate sensitivity of priority rankings to the choice of metric, OFP will additionally be calculated as OFP_i = C_i * MIR_i * M_O3 / M_i, where C_i is the mass concentration in µg/m$^3$, M_i is the molecular weight of species i, and M_O3 = 48 g/mol is the molecular weight of ozone. This formulation yields units of µg O3/m$^3$ (the same as the mass-based formulation) but rescales each species contribution by M_O3 / M_i, so that lower molecular

weight species carry proportionally more weight than in the mass-based formulation. Rankings of priority VOCs will be compared between the two formulations, with particular attention to whether higher molecular weight aromatic and oxygenated species (for example, C9 and C10 aromatics, monoterpenes, and Texanol) shift in relative importance compared with lower molecular weight species (for example, acetaldehyde, methanethiol, isoprene, and ethanol). This shifts the priority ranking toward fast-reacting low-MW species (formaldehyde, ethene, propene, acetaldehyde) and away from heavier aromatics and oxygenates (monoterpenes, C9-C10 aromatics), which dominate the mass-based ranking. The MW-based formulation is most appropriate when ozone formation is driven by the number of reactive carbon atoms rather than total VOC mass, and provides a useful cross-check on whether reduction priorities are sensitive to the metric choice.

Where rankings shift substantially between formulations, the affected species are reported as framework-sensitive priorities, meaning that whether they warrant emission-control attention depends on whether the regulatory goal is mass reduction (favoring the mass-based formulation) or reactive-carbon reduction (favoring the molecular weight-based formulation). This framework dependence is reported explicitly in the priority list rather than collapsed into a single ranking.

**OH reactivity-weighted approach.** As a third independent framework, OFP will be evaluated using OH reactivity weighting, in which each species is ranked by the product $C_i * k_{OH,i} * MIR_i$, where $k_{OH,i}$ is the rate constant for reaction with the OH radical. This metric captures the contribution of each species to instantaneous ozone precursor reactivity and yields species rankings that closely track absolute consumed-VOC rankings for moderate atmospheric aging without requiring knowledge of OH concentration, which was not measured in Project 24-024. OH rate constants $k_{OH,i}$ will be drawn primarily from the critically evaluated recommendations of JPL Publication 19-5 (Burkholder et al., 2020) and the IUPAC Subcommittee evaluations, which provide single recommended values with stated uncertainties. For species not covered by those evaluations, values will be taken from the NIST Chemical Kinetics Database, selecting the most recent peer-reviewed determination, and where no measured value is available from any of these sources, $k_{OH,i}$ will be estimated using the structure-activity relationship of Kwok and Atkinson (1995). This framework is particularly important for short-lived alkenes and biogenic VOCs whose ambient mixing ratios underestimate their integrated contribution to ozone formation. For selected near-source mobile transects where co-emitted urban aromatic tracers (for example, m,p-xylene paired with benzene) can be used to infer photochemical age, the OH exposure $\tau_{OH} = \int[OH]\,dt$ will be estimated from the deviation of the observed tracer ratio from its emission ratio following de Gouw et al. (2005) and Yuan et al. (2012), and an absolute consumed-VOC OFP will additionally be computed for cross-validation of the reactivity-weighted rankings.

**Equal Benefit Incremental Reactivity (EBIR) approach.** As a fourth framework, OFP will be evaluated using the Equal Benefit Incremental Reactivity scale of Carter (2010), updated where available following Venecek et al. (2018). Whereas the MIR scale represents incremental reactivity under the high-NOx conditions most conducive to ozone formation, and is therefore appropriate for VOC-limited regimes such as the El Paso urban core, the EBIR scale represents the lower-NOx condition at which VOC and NOx control yield equal ozone benefit, and is therefore more representative of the transitional and NOx-limited regimes identified in the suburban and surrounding areas in Task 2. Because Task 2 maps spatially varying sensitivity regimes across the airshed, reporting both MIR-based and EBIR-based rankings provides a regime-appropriate priority list for each area: MIR rankings are applied where Task 2 indicates VOC-limited conditions, and EBIR rankings where Task 2 indicates transitional or NOx-limited conditions. Where the MIR and EBIR rankings disagree, both are reported together with the local regime context from Task 2.

Spatial maps of OFP under all four frameworks will be generated from the mobile transects, building on the toluene mobile maps presented in Project 24-024 Final Report Section 4.2.1, to

identify hotspot areas and concentration gradients across the El Paso-Juárez airshed. Diurnal and seasonal patterns in OFP composition will be analyzed by comparing winter versus summer campaigns and weekday versus weekend periods, extending the temporal analyses presented in Project 24-024 Final Report Section 4.2.2. OFP patterns observed at stationary TCEQ sites will be compared with those from mobile measurements, integrating auto-GC data from UTEP, Chamizal, and Delta Drive to provide cross-platform validation.

Isoprene and other high-reactivity species are represented with their own species-specific coefficients (MIR, EBIR, and k_OH) rather than averaged values, so their reactivity is captured directly. Because a small number of high-reactivity species can dominate a reactivity-weighted ranking, the priority lists will be recomputed with and without the high-reactivity biogenic species (isoprene and monoterpenes) to quantify their influence and demonstrate ranking robustness. The MIR and EBIR metrics from the Carter SAPRC framework represent incremental ozone formed per unit VOC under full photochemical conditions and are not OH-loss-only measures, so the primary ranking does not assume OH is the sole sink. The OH reactivity-weighted framework, which uses k_OH, is one of four complementary frameworks and serves as a cross-check. Isoprene is removed predominantly by OH under typical daytime conditions and is largely represented by the OH-weighted metric, whereas the monoterpenes and other reactive alkenes have appreciable $O_3$ and nighttime $NO_3$ sinks, so OH-only weighting underestimates their total reactivity; this limitation will be stated in the Final Report, and where the data support it a total-oxidant (OH plus $O_3$) reactivity will be reported for the affected species.Special attention will be given to aromatic compounds including toluene and xylenes, which contribute significantly to ozone formation. Toluene exhibited episodic enhancements reaching 25 to 37 ppb during specific events documented in Project 24-024 Final Report Section 5.3.3, despite average concentrations being much lower than observed in 1996 (Seila et al., 2001). The analysis will also consider oxygenated VOCs including acetaldehyde, acetone, methylglyoxal, and other carbonyls, which can have high MIR values. Results will be presented as ranked contribution plots showing which VOC classes and individual species account for the majority of ozone formation potential across different areas of the region under each of the four OFP frameworks, with side-by-side comparison tables to identify species whose ranking is robust to framework choice and those whose ranking is sensitive to it.

### 2.2 Task 2: VOC Sensitivity Regime Mapping and Multi-Indicator Analysis

Building on recent work showing spatially variable ozone regimes in Texas urban areas (Wan et al., 2024), this task will determine and map the ozone sensitivity regimes across the El Paso region using multiple complementary indicators rather than relying on a single ratio. PI Misztal will lead this task, supported by Daniel Sung, Graduate Research Assistant.

Surface indicator ratios will be calculated from co-located ground-based measurements collected during Project 24-024 and from the long-term TCEQ monitoring network. The following ratios will be evaluated:

- **VOC/$NO_2$ ratio.** Calculated using the sum of speciated VOCs from the auto-GC and Vocus measurements, with established threshold values calibrated for Texas urban areas (Wan et al., 2024).
- **VOC/NOx ratio.** Provides a complementary view that uses the chemically active NOx pool rather than NO2 alone.
- **O3/NOx ratio.** Diagnoses the photochemical maturity of an air parcel and the relative balance of ozone production to fresh NOx emissions.

- **$O_3$/NOy ratio.** Where NOy is measured, or taken from CAMx otherwise, this ratio integrates the cumulative ozone produced per unit reactive nitrogen processed and is less sensitive to local titration than $O_3$/NOx.
- **$O_3$/NOz ratio.** Following Sillman (1995), this ratio relates ozone to the processed reactive nitrogen pool and indicates VOC-limited versus NOx-limited regimes. It is computed where total reactive nitrogen is measured and from CAMx otherwise, and is treated as exploratory since its El Paso transition value will be set by the CAMx calibration.
- **Satellite HCHO/$NO_2$ ratio (FNR).** Derived from TROPOMI and TEMPO column observations to provide broader spatial context beyond ground-based measurements.

Each indicator will be mapped spatially across the airshed and compared with the others to identify regions where the indicators agree and where they diverge. Agreement among multiple indicators provides increased confidence in the assigned regime. The set of indicator results will then be cross-compared with the CAMx simulations developed under Project 24-024 to identify which indicator ratios produce regime classifications most consistent with the modeling, providing a recommendation to TCEQ on which observational diagnostics are most reliable for future SIP and exceptional event analyses in the El Paso region.

Beyond producing the indicator maps, this task yields three products. First, a regime agreement map showing where the six indicators agree (high-confidence regime assignment) and where they diverge (locations needing further investigation). Second, a recommendation to TCEQ on which indicator ratios are most reliable under El Paso conditions, identified as the indicator that best reproduces the CAMx-based regime classification. Third, identification of locations where the observational indicators agree on a regime but CAMx disagrees, which identifies candidate areas where the model may misrepresent local chemistry or emissions and which warrant model evaluation and emission-inventory refinement. To establish a quantitative link between the observed ratios and the modeled ozone chemistry, the CAMx Process Analysis tool will be applied to the existing 2022 base year simulation to extract instantaneous ozone production rates P(O3) at each indicator location. The same six-indicator comparison can be applied to the Houston-Galveston-Brazoria, Dallas-Fort Worth, and Bexar County areas using their existing CAMS networks and CAMx platforms, with the El Paso analysis serving as the methodological template.

Weekend-weekday differences in ozone and precursor concentrations will be analyzed as an independent regime indicator, extending the temporal analysis presented in Project 24-024 Final Report Section 4.2.2. The output will include detailed maps showing where VOC reductions versus NOx reductions would be most effective for ozone mitigation, directly addressing Research Question R2. This analysis directly responds to TCEQ feedback requesting identification of sensitivity areas given the VOC-limited regime observed in the El Paso urban core, and provides a methodological template applicable to serious nonattainment areas in Texas.

### 2.3 Task 3: Advanced Source Apportionment of VOCs and PM

While Project 24-024 conducted initial source apportionment analyses, described in the Final Report Sections 2.1.3 and 4.2.4, this task will apply more advanced multivariate statistical methods to the comprehensive datasets and will integrate the results with long-term auto-GC records. Co-PIs Sullivan and Hildebrandt Ruiz will co-lead this task with PI Misztal, supported by Postdoctoral Fellow Dr. Chao and Graduate Research Assistants, Shihao Zhai and Daniel Sung.

Co-PI Sullivan brings extensive experience with auto-GC data analysis from multiple TCEQ and AQRP monitoring stations in El Paso (Park et al., 2020; Sullivan and Holdren, 2022, 2023). He has conducted PMF analyses on multi-year auto-GC datasets, providing unique insights into long-term source trends and seasonal patterns that will inform interpretation of the intensive campaign

data. Co-PI Hildebrandt Ruiz brings established expertise in PMF and ME-2 analysis of aerosol mass spectrometric data (Bhandari et al., 2020, 2022a, 2022b; Patel et al., 2020, 2021).

Project 24-024 Vocus data will be integrated with long-term auto-GC records (2011-2025) from UTEP, Chamizal, and Delta Drive to identify temporal trends, source changes, and the representativeness of campaign measurements across long-term stationary and mobile platforms. Cross-validation between PTR-ToF-MS and GC measurements will be performed for overlapping species, including BTEX, other aromatics, and selected aliphatic hydrocarbons. Multi-site PMF analysis using simultaneous measurements from the TCEQ auto-GC network will identify spatially varying source contributions across the airshed.

Detailed positive matrix factorization analysis of HR-TOF-AMS data collected during Project 24-024 will evaluate sources and formation pathways of NR-PM1. First, we will finalize PMF analysis conducted on HR-AMS data collected in the winter. Then we will conduct and finalize PMF analysis on data collected in the two summer campaigns. Next, we will conduct PMF analysis on Vocus data only. Finally, we will conduct combined PMF analysis integrating VOC data from the Vocus with NR-PM1 data from the HR-TOF-AMS for enhanced source identification of both VOCs and PM1, following the approach demonstrated in Slowik et al. (2010) and Simon et al. (2025).

**Reactivity-weighted PMF.** Conventional PMF on ambient VOC concentrations apportions the measured species pool, but does not directly reflect the contribution of each source to ozone formation, because PMF treats all species equivalently and does not account for the differential reactivity of co-emitted compounds. Building on the OH reactivity-weighted framework introduced in Task 1, a parallel PMF analysis will be performed on a reactivity-weighted matrix in which each Vocus species is scaled by k_OH,i * MIR_i (the product of its OH rate constant and maximum incremental reactivity). The reactivity-weighted matrix is constructed under both MIR and EBIR weights, so that the source-to-ozone attribution is available for both the VOC-limited urban core and the transitional and NOx-limited suburban areas mapped in Task 2. The resulting factors represent source contributions to instantaneous ozone precursor reactivity rather than to ambient mixing ratios, and for an air parcel with shared OH exposure across species the reactivity-weighted source rankings closely track those from absolute consumed-VOC PMF without requiring knowledge of OH concentration. The reactivity-weighted PMF factors will be compared with the conventional ambient PMF factors to identify whether (a) the same source factors emerge with similar relative contributions, indicating that the conventional analysis is robust for ozone-relevant interpretation, or (b) the rankings shift, indicating that certain sources contribute disproportionately to ozone formation relative to their ambient concentration share. This complementary analysis directly responds to TCEQ reviewer feedback and provides TCEQ with a source apportionment product targeted at ozone precursor management.

**Day-night and roadway-influence stratification.** Due to different oxidation regimes and the high reactivity of alkenes, day and night source apportionment will be compared using long-term GC data, mobile and stationary Vocus data, and long-term offline $PM_{2.5}$ and mobile/stationary HR-TOF-AMS data. To distinguish the influence of roadway emissions in the mobile measurements (responding directly to TCEQ reviewer feedback), three complementary approaches will be applied: (1) road-class stratification, in which mobile data are tagged using GPS and the road network classification (interstate, principal arterial, minor arterial, residential) and PMF and OFP results are compared across road classes; (2) collocated diagnostic tracers, in which black carbon (AE33), NO/NO2, and CO from the mobile lab are used as fresh on-road traffic indicators, and Vocus aromatic ratios (for example, benzene/toluene and toluene/xylene) and HR-TOF-AMS hydrocarbon-like organic aerosol mass fraction are used to identify time intervals dominated by tailpipe plumes; and (3) on-road plume filtering, in which short-duration spikes (less than 60 seconds) coincident with elevated NO and black carbon are masked from the source apportionment input matrix to produce a near-roadway analysis and a regional analysis side by

side. The two analyses are then differenced to estimate the on-road versus background source contributions across the mobile transect domain.

**Integration with offline $PM_{2.5}$ filter PMF.** Co-PI Sullivan has conducted a complementary 6-factor PMF on offline $PM_{2.5}$ filter samples collected during Project 24-024 (Figure 5) that resolves inorganic and dust source factors not captured by the AMS PM1 analysis. The factor proportions are: crustal material (30.8%), motor vehicles split between light-duty (15.4%) and heavy-duty (13.0%), fires (24.7%), ammonium sulfate (12.4%), and ammonium nitrate (3.7%). Project 26-030 will integrate these offline $PM_{2.5}$ results with the AMS PM1 organic factors and with the Vocus VOC factors to produce a unified source apportionment that spans both organic and inorganic PM, both submicron and $PM_{2.5}$ size ranges, and the gas-particle linkage. Cross-comparison of the AMS HOA and BBOA factors against the offline motor vehicle and fires factors will provide an independent verification of source identification across analytical platforms.

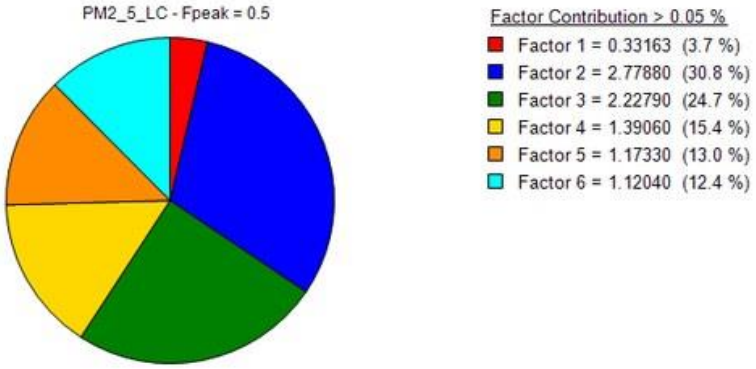


***Figure 5.*** *Preliminary 6-factor PMF on offline $PM_{2.5}$ filter samples from Project 24-024, complementary to the AMS PM1 organic PMF (Figure 2). Factor 1 = ammonium nitrate (3.7%), Factor 2 = crustal material (30.8%), Factor 3 = fires (24.7%), Factor 4 = light-duty motor vehicles (15.4%), Factor 5 = heavy-duty motor vehicles (13.0%), Factor 6 = ammonium sulfate (12.4%). The offline analysis resolves inorganic and dust factors that AMS PM1 cannot capture. Project 26-030 will integrate offline $PM_{2.5}$ PMF with AMS PM1 PMF and Vocus VOC PMF for a unified source picture across phases and size ranges.*

Source categories to be quantified include mobile sources (gasoline and diesel vehicles, with light-duty/heavy-duty separation as supported by the offline PMF), industrial emissions, solvent use and volatile chemical products (VCPs), biomass burning (including agricultural fires), secondary organic aerosol formation, and crustal/dust contributions. The analysis will build on the initial source apportionment results in Project 24-024 Final Report Sections 2.1.3 and 4.2.4 and on the preliminary AMS organics PMF (Figure 2) and offline $PM_{2.5}$ PMF (Figure 3) presented at the May 2026 TCEQ SIM, and extend them with the long-term context provided by the auto-GC record.

### 2.4 Task 4: Examining Domestic and International Emission Source Contributions

AQRP Project 24-024 examined interannual trends in measured toluene concentrations at TCEQ auto-GC sites (Chamizal and Delta Drive) and canister sampling sites (Womble and Socorro Hueco), as well as predicted spatial patterns of toluene concentrations across El Paso and Municipio de Juárez using CAMx. Co-PI McDonald-Buller and Dr. Kimura will lead this task. No new CAMx simulations will be conducted; this task focuses on extended analysis of the 2022 base year simulations completed under Project 24-024.

The CAMx RTRAC probing tool was used in Project 24-024 to examine emission source contributions to the top 10% of predicted toluene concentrations by wind direction at El Paso monitoring sites for the 2022 base year. Common to the four sites previously analyzed were contributions by Mexican on-road, nonpoint, and point source emissions. Delta Drive and particularly Womble had complex variations in emission sources with wind direction, with sources in El Paso in addition to sources from Mexico predicted to contribute to elevated toluene concentrations.UTEP

Additional analyses proposed in this task include evaluations of the existing CAMx predictions against the stationary and mobile measurements made during AQRP 24-024. A third auto-GC was installed at UTEP by Co-PI Sullivan that measured hourly toluene concentrations in 2024. Following the approach of AQRP 24-024, box and whisker plots showing the distributions of annual interquartile ranges and percentile concentrations of modeled and observed toluene concentrations will be developed for the UTEP site.

Domestic and international emission source sector contributions by wind direction for the top 10% of RTRAC-predicted toluene concentrations will be characterized at the UTEP location, as was done for the four TCEQ monitoring locations under AQRP 24-024. The previous analyses will also be extended to examine predicted emissions source sector contributions at all five ambient monitoring locations to mean concentrations to determine whether differences exist in the relative contributions of domestic and international emission sources with prevailing wind patterns for the 2022 base year. Toluene pollution roses showing the magnitude and associated wind direction frequency of observed concentrations at each stationary monitoring site will be developed to complement this analysis.

The proposed task will also integrate data collected by the UT Austin Vocus PTR-ToF-MS and onboard meteorological instrumentation during the AQRP 24-024 field campaigns, around the five TCEQ and monitoring sites. These data will characterize measured toluene concentrations by wind direction, spatial patterns, and source contributions for cross-comparison with observations and model predictions described above.

Both El Paso and Municipio de Juárez face challenges with meeting their respective federal ozone standards. The comprehensive analyses incorporating different toluene measurement approaches and modeling with the CAMx RTRAC probing tool in this task will inform evaluations of mitigation strategies that could potentially be accomplished domestically as well as those that would likely require greater binational coordination for reducing toluene emissions in El Paso.

### 2.5 Task 5: Synthesis

The final task will synthesize results from all analyses. Spatial maps of local sensitivity regimes will be developed, indicating areas of VOC sensitivity (urban core) versus areas of NOx sensitivity (suburban areas). Emission source categories and VOC species will be ranked by their contribution to ozone and $PM_{2.5}$ concentrations. The analyses will also identify remaining data gaps and priority measurements for future monitoring to support ongoing air quality research. Peer-reviewed manuscripts and presentation materials will be prepared for AQRP, TCEQ, and the broader scientific community to disseminate research findings.

All Principal Investigators will contribute to the synthesis. Although the immediate analytical focus is the El Paso-Juárez airshed, the methodological framework (multi-formulation OFP, multi-indicator sensitivity analysis, reactivity-weighted PMF, day-night and roadway-stratified source apportionment, and CAMx RTRAC source attribution) is directly transferable to serious nonattainment areas in Texas, and the Final Report will document this transferability for use by TCEQ in support of analyses in other counties. The methodology developed in this project is designed to transfer directly to other Texas nonattainment areas. Four elements are transferable.

First, the multi-indicator sensitivity ratio framework, cross-validated against CAMx Process Analysis, applies to any Texas nonattainment area with CAMS monitoring and CAMx coverage. Second, the multi-formulation ozone formation potential procedure, with its regime-aware ranking rule (MIR for VOC-limited areas and EBIR for NOx-limited areas), provides priority rankings appropriate to the local chemical regime. Third, the combined gas-particle Positive Matrix Factorization, integrating Vocus, HR-TOF-AMS, and offline filter measurements, resolves source factors that span both phases. Fourth, the day-night and roadway-stratified source apportionment supports interpretation of mobile measurements. The multi-framework reconciliation procedure described in Task 5 is itself part of the transferable framework. The Final Report will document each step of the procedure so that the analyses in other counties can adopt it directly, using their existing CAMS networks and CAMx platforms. This output corresponds to the methodological template deliverable shown in the analytical workflow figure.

Rankings that emerge from competing frameworks and methods are reconciled using the decision rules documented in QAPP Section 3.7. Where all four OFP frameworks agree on a species' top-quartile membership, the species is reported as a high-confidence priority. Where the frameworks disagree, the regime-appropriate framework determines the ranking, namely MIR for VOC-limited areas and EBIR for transitional and NOx-limited areas, with the framework dependence noted explicitly. For source apportionment, the conventional and reactivity-weighted PMF solutions are reported in parallel, and sources whose rankings differ substantially between them are identified as those whose ozone relevance is disproportionate to their ambient mass contribution.

### 2.6 Binational Coordination and Stakeholder Engagement

The El Paso-Juárez airshed is one of the largest binational metropolitan areas in North America, spanning Texas, New Mexico, and Chihuahua, Mexico. Effective air quality management in this region requires coordination across international boundaries. Building on the foundation established under Project 24-024, the research team will continue working with TCEQ Border Affairs to facilitate binational data sharing and collaboration. TCEQ Border Affairs Manager Eddie Moderow has connected the project team with key binational liaisons including Dr. Mayra Chavez, who serves as binational liaison of the Joint Advisory Committee for Air Quality Improvement, and Jose Luis Palacios, who serves as binational liaison of the Binational Air Quality Fund and an appointed member of the Administrative Unit. The project team also presented preliminary findings from initial extended analyses of Project 24-024 datasets at the May 2026 TCEQ State Implementation Plan Informational Meeting, which was attended by approximately 100 TCEQ staff (Figures 1 through 3). Project 26-030 results, particularly the multi-formulation OFP analysis, multi-indicator sensitivity regime mapping, integrated source apportionment, and toluene CAMx RTRAC findings, will be shared through the same TCEQ channels and through the established binational liaisons to support coordinated air quality research on both sides of the border.

## 3. TIMELINE

The project schedule by task is presented below. The project start date is August 1, 2026. Technical work will not begin until authorization is received from TCEQ and AQRP. The entire project will be completed by August 31, 2027. The Draft Final Report will be submitted by August 1, 2027 (30 days before project end) and the Final Report by August 31, 2027.

| | M1 | M2 | M3 | M4 | M5 | M6 | M7 | M8 | M9 | M10 | M11 | M12 | M13 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Task 1 – Ozone | X | X | X | X | | | | | | | | | |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Formation Potential | | | | | | | | | | | | | |
| Task 2 – Sensitivity Regime Mapping | | X | X | X | X | X | | | | | | | |
| Task 3 – Source Apportionment | | | X | X | X | X | X | X | X | | | | |
| Task 4 – Toluene CAMx RTRAC Analysis | | | | X | X | X | X | X | X | X | | | |
| Task 5 – Synthesis | | | | | | | | | X | X | X | X | X |
| Reporting (DFR / FR) | | | | | | | | | | | | X | X |

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. Deliverables for this project also include a draft final report and a final project report documenting all work from Tasks 1 through 5, and a project summary presentation to AQRP. AQRP will receive an electronic copy of all data generated for this project. All reports will be in the format requested by AQRP.

## 4. PROJECT ORGANIZATION AND RESPONSIBILITIES

This project is being conducted by The University of Texas at Austin under a grant from the Texas Air Quality Research Program. The project Principal Investigator is Dr. Pawel K. Misztal and the Co-Principal Investigators are Drs. Lea Hildebrandt Ruiz, David W. Sullivan, and Elena C. McDonald-Buller. Dr. Misztal is responsible for overseeing project execution and completion and will lead the OFP analysis (Task 1) and sensitivity regime mapping (Task 2). Dr. Hildebrandt Ruiz will co-lead Task 3 with focus on advanced source apportionment of HR-TOF-AMS and combined Vocus-AMS datasets. Dr. Sullivan will co-lead Task 3 with responsibility for integration of long-term auto-GC records and multi-site PMF. Dr. McDonald-Buller will lead Task 4 (toluene domestic and international source contributions) and contribute to Task 5. The project will be overseen by AQRP Project Manager Dr. Erin Tullos and TCEQ Project Liaison Erik Gribbin (with Tanzina Akther as backup). Quality assurance oversight will be provided by AQRP QAPP Manager Dr. David Allen and TCEQ QAPP Manager Mark Muldoon.

Internal project communication will follow a tiered structure. Co-Investigators will hold biweekly video conferences to coordinate analysis priorities, data integration tasks, and manuscript planning. Analytical results, processed datasets, code, and metadata will be shared among team members through a secure cloud-based repository maintained by UT Austin. Monthly Technical Reports submitted to the AQRP Project Manager and TCEQ Liaison on the 10th of each month,

together with quarterly reports, will provide formal documentation of project progress, preliminary results, and any deviations from the planned scope of work. AQRP and TCEQ representatives are welcome to participate in the biweekly coordination meetings at any point during the project.

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

**Dr. Pawel K. Misztal** is an Associate Professor (Cockrell Family Fellow) at UT Austin and is the Principal Investigator. He has more than 15 years of experience measuring chemical composition of air using mass spectrometry, including the Vocus PTR-ToF-MS deployed in Project 24-024. He led Project 24-024 and has detailed knowledge of the comprehensive Vocus datasets collected during that campaign. He is PI or Co-PI on multiple federally funded projects including NSF CAREER, NOAA AC4, and DOE awards. He will oversee all project activities and lead the OFP analysis (Task 1) and sensitivity regime mapping (Task 2).

**Dr. Lea Hildebrandt Ruiz** is an Associate Professor at UT Austin and is a Co-Principal Investigator. She has published extensively on PMF and ME-2 analysis of aerosol mass spectrometric data including HR-TOF-AMS measurements. Her expertise in multivariate statistical methods for source apportionment will be critical for the enhanced PMF analyses in Task 3. She has participated in numerous air quality field campaigns and has extensive experience interpreting source apportionment results in the context of emission inventories.

**Dr. David W. Sullivan** is a Research Associate at UT Austin and is a Co-Principal Investigator with unique expertise in El Paso VOC monitoring. He has operated auto-GCs in El Paso since 2011 and has conducted comprehensive analyses of speciated VOC data from multiple TCEQ monitoring stations including Chamizal (CAMS 41) and Delta Drive, as well as the new UTEP site established under Project 24-024. His work includes multi-year PMF analyses of auto-GC data to identify source trends and seasonal patterns. His long-term perspective on El Paso air quality trends is invaluable for contextualizing the Project 24-024 campaign results. He will co-lead Task 3.

**Dr. Elena C. McDonald-Buller** is a Senior Research Engineer at UT Austin with more than 25 years of experience in air quality modeling and emissions characterization. She is a Co-Principal Investigator and has extensive experience examining transboundary air pollution from Mexico using photochemical modeling and has conducted numerous model-observation comparison studies for Texas regulatory applications. She will lead Task 4 and contribute to Task 5.

**Dr. Yosuke Kimura** is a Research Associate at UT Austin with more than 20 years of experience with emissions and photochemical modeling. He will perform extended analysis of the existing CAMx simulations with the RTRAC probing tool as well as observations at the TCEQ and UTEP sites completed under Project 24-024. He will contribute to the integration of these results with data collected by the UT Vocus PTR-ToF-MS.

**Dr. Chun-Ying Chao** is a Postdoctoral Fellow at UT Austin who will conduct PMF analyses of the combined Vocus and HR-TOF-AMS dataset. **Two Graduate Research Assistants (Daniel Sung and Shihao Zhai)** will perform data analysis across Tasks 1 through 5, including OFP calculations, sensitivity regime mapping, source apportionment analyses, model-observation comparisons, and preparation of figures for reports and manuscripts.

**Ms. Dori Eubank,** Research Program Coordinator, will assist with monthly financial reports and other administrative tasks related to the project, including data management coordination, report preparation, and scheduling between research team members.

## 5. 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 is outlined below. PI Dr. Misztal will submit the reports but will be assisted by Co-PIs and other project participants in preparing them. 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 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 days 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 document. 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:** To be determined based on project start date.

Technical Reports

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

**Due Dates:** Monthly, on the 10th of each month (or following business day).

Financial Status Reports

Financial Status Reports will be submitted monthly to the AQRP Grant Manager by UT Austin using the AQRP FSR Template found on the AQRP website.

**Due Dates:** Monthly, on the 10th of each month (or following business day).

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, 2027 (30 days before project end).

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.

**Due Date:** August 31, 2027.

Project Data

All project data including but not limited to QA/QC data, processed datasets, source profiles, PMF input and output matrices, OFP and sensitivity ratio products, and toluene RTRAC analysis outputs 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, TCEQ, or other outside parties to utilize the information.

AQRP Workshop

A representative from the project will present at the AQRP Workshop on a date to be determined.

Stakeholder Presentation

Key findings will be presented to TCEQ Border Affairs and the Joint Advisory Committee for Air Quality Improvement to support binational air quality coordination.

Presentations and Publications

All data and other information developed under this project that is included in published papers, symposia, presentations, press releases, websites, and other publications will be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication and Publicity Guidelines included in the Subaward Agreement.

## 6. REFERENCES

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# The University of Texas at Austin

## Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juarez Airshed
## AQRP Budget

**Principal Investigator:** Pawel Misztal

**Project Dates:** 08/01/2026 - 08/31/2027

**A. SENIOR PERSONNEL: PI, Co-PI**

| | FirstName LastName | Title | Monthly Rate | Fringe Rate | FTE / % Effort | Funds Requested |
|---|---|---|---|---|---|---|
| 1. | Pawel Misztal | PI | $15,747 | 32.7% | 1.00 | $15,747 |
| 2. | Lea Hildebrandt Ruiz | coPI | $18,260 | 32.7% | 1.00 | $18,260 |
| 3. | Elena McDonald Buller | coPI | $17,582 | 2.7% | 1.00 | $17,582 |
| 4. | David Sullivan | coPI | $12,528 | 2.7% | 1.00 | $12,528 |
| | **TOTAL SENIOR PERSONNEL** | | | | | **$64,116** |

**B. OTHER PERSONNEL (SHOW NUMBERS IN BOXES)**

| | | | | | | |
|---|---|---|---|---|---|---|
| 1 | 2 | Other Professionals / Researchers | $7,179 | 32.7% | 1.00 | $14,358 |
| 2 | 1 | Other Professionals / Research Coordinator | $6,080 | 2.7% | 1.00 | $6,080 |
| 3 | 2 | Graduate Student | $3,103 | 15.0% | 12.00 | $74,472 |
| | | **TOTAL OTHER PERSONNEL** | | | | **$94,910** |
| | | **TOTAL SALARIES AND WAGES (A+B)** | | | | **$159,026** |

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

| | | |
|---|---|---|
| 1. | Senior Personnel | **$11,933** |
| 2. | Other Personnel | **$16,030** |
| | **TOTAL FRINGE BENEFITS** | **$27,963** |
| | **TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)** | **$186,990** |

**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 | **2** | $2,000 |
| 2. | Foreign | | | $0 |
| | **TOTAL TRAVEL** | | | **$2,000** |

**F OTHER DIRECT COSTS**

| | | |
|---|---|---|
| 1. | Materials and Supplies | $3,073 |
| 2. | Professional Services - Idependent Contractors | $0 |
| 3. | Subcontracts (contracts will be issued by UT) | |
| a) | | $0 |
| b) | | $0 |
| c) | | $0 |
| d) | | $0 |
| 4. | Tuition and Fees | $26,260 |
| 5. | Other | $0 |
| | **TOTAL OTHER DIRECT COSTS** | **$29,333** |

| | | | |
|---|---|---|---|
| **G.** | **TOTAL DIRECT COSTS (A THROUGH F)** | | **$218,323** |
| **H.** | **TOTAL INDIRECT COSTS** | **IDC Rate: 15.000%** | **$28,809** |
| **I.** | **TOTAL COSTS** | | **$247,132** |

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

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

# Budget Justification and Budget

**Project #26-030**
**CAMx**
**Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed**

Prepared for

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

Pawel K. Misztal
Lea Hildebrandt Ruiz
David W. Sullivan
Elena C. McDonald-Buller

## Approvals

### This Budget was approved electronically

DocuSigned by:
5E69E9F496774FD...

2026-06-26 | 09:02:57 CDT

RoseAnna Goewey — Date
Program Manager, Texas Air Quality Research Program

### This Budget was approved electronically

Signed by:
E61A0F36522D43C...

2026-06-27 | 04:37:06 CDT

Erin Tullos — Date
Project Manager, Texas Air Quality Research Program

### This Budget was approved electronically

Signed by:
11CC6848504C4ED...

2026-06-29 | 16:09:55 CDT

Erik Gribbon — Date
Project Liaison, Texas Commission on Environmental Quality

# Budget Justification

Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juarez Airshed

The University of Texas at Austin

Project Period: August 1, 2026 - August 31, 2027

**Total Budget: $247,132**

## A. SALARIES

**Dr. Pawel Misztal, Principal Investigator, 1 month of 100% effort,** will provide overall scientific leadership and project management. He will oversee all project activities and lead Task 1 (Comprehensive Ozone Formation Potential Analysis) and Task 2 (VOC Sensitivity Regime Mapping and Analysis). Dr. Misztal has detailed knowledge of the comprehensive Vocus PTR-ToF-MS datasets collected during Project 24-024 and will ensure integration of the advanced analyses with the original campaign findings.

**Dr. Lea Hildebrandt Ruiz, Co-Investigator, 1 month of 100% effort,** will co-lead Task 3 (Advanced Source Apportionment of VOCs and PM) with her expertise in positive matrix factorization (PMF) and ME-2 analysis of aerosol mass spectrometric data. She will direct the detailed PMF analysis of HR-TOF-AMS data and the combined PMF analysis integrating Vocus VOC data with NR-PM1 data for enhanced source identification.

**Dr. Elena McDonald-Buller, Co-Investigator, 1 month of 100% effort,** will lead Task 4 (Examining Domestic and International Emission Source Contributions) and contribute to Task 5. She will oversee the extended analysis of CAMx/RTRAC modeling output from Project 24-024 for toluene source attribution.

**Dr. David Sullivan, Co-Investigator, 1 month of 100% effort,** will co-lead Task 3 with his unique expertise in El Paso VOC monitoring. He has operated auto-GCs in El Paso since 2011 and will integrate Project 24-024 Vocus data with long-term auto-GC records from UTEP, Chamizal (CAMS 41), and Delta Drive.

**Dr. Yosuke Kimura, Research Associate, 1 month of 100% effort,** will perform extended analysis of the existing CAMx simulations with the RTRAC probing tool as well as observations at the TCEQ and UTEP sites completed under Project 24-024. He will contribute to the integration of these results with data collected by the UT Vocus PTR-ToF-MS.

**Dr. Chun-Ying Chao, Postdoctoral Fellow, 1 month of 100% effort,** will conduct PMF and CMB analyses of aerosol mass spectrometer data and assist with VOC data processing and OFP calculations (Tasks 1-3).

**Dori Eubank, Research Program Coordinator, 1 month at 100% effort,** will help with monthly financial reports and other administrative tasks related to the project, including data management, quality assurance, report preparation, and coordination between research team members.

**Daniel Sung, Graduate Research Assistant (GRA), 12 months of 100% effort,** will perform data analysis and contribute to Tasks 1-3, including OFP calculations, sensitivity regime mapping, and source apportionment analyses.

**Shihao Zhai, Graduate Research Assistant (GRA), 12 months of 100% effort,** will perform data analysis and contribute to Tasks 3-5, including PMF analysis, model-observation comparisons, and preparation of figures for reports and manuscripts.

**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: $27,963.

**C. Equipment**

*none*

**D. Other Direct Costs**

**MATERIALS AND SUPPLIES**

Supplies are calculated at $3,073 for computational resources, data storage, software licenses for statistical analysis (including PMF and ME-2 software), and publication costs for peer-reviewed manuscripts. Total materials and supplies budget requested: $3,073.

**TRAVEL**

Funds are requested for project personnel to travel to El Paso for coordination meetings with TCEQ staff and to present findings at the AQRP Workshop. Travel costs are calculated for 2 domestic trips at $1,000 per trip, covering airfare, lodging, and per diem. Total travel budget requested: $2,000.

**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 FY2027 is $625 per semester credit hour. 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: $28,809.