

AQRP Monthly Technical Report

PROJECT TITLE	Novel Observations and Quantified Source Apportionment of Ozone, Particulate Matter and Contributing Precursors in the El Paso Area	PROJECT #	24-024
PROJECT PARTICIPANTS	Pawel Misztal, Lea Hildebrandt-Ruiz, David Sullivan, Elena McDonald-Buller, Yosuke Kimura	DATE SUBMITTED	5/10/2025
REPORTING PERIOD	From: 4/1/2025 To: 4/30/2025	REPORT #	7

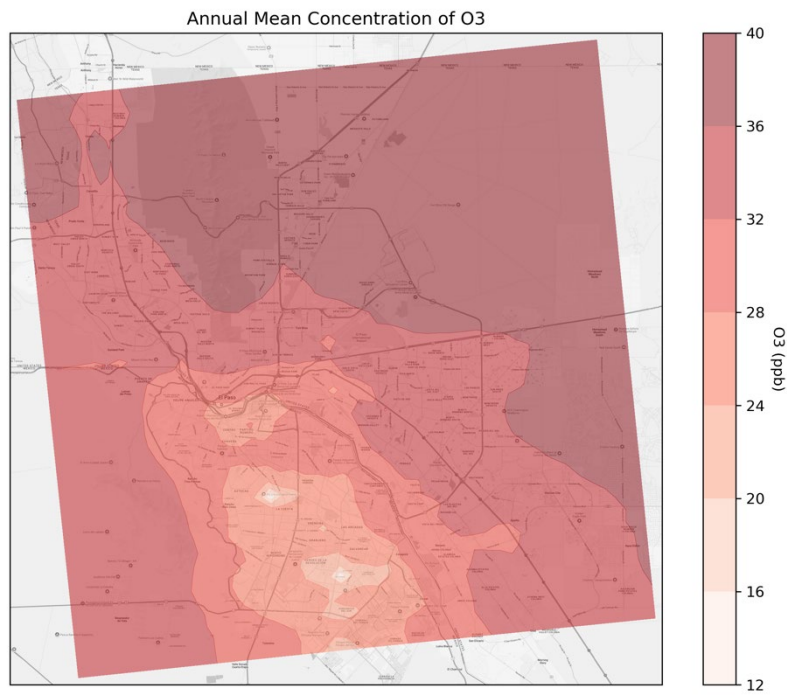
A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task for reporting period

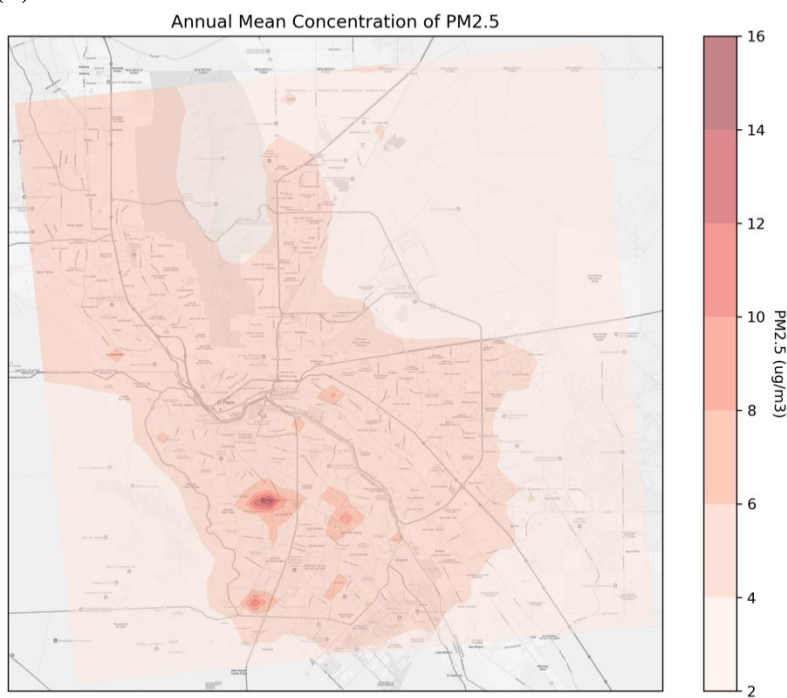
Task 2b: The El Paso-Juarez Comprehensive Air Quality Model with Extensions (CAMx) 2022 basecase simulation was completed in April. Initial contour maps of simulated annual mean and 95th percentile concentrations by grid cell of ozone (O₃), fine particulate matter (PM_{2.5}), nitrogen oxides (NO_x), carbon monoxide (CO), sulfur dioxide (SO₂), and the Carbon Bond 6 (CB6) lumped TOL species (representing toluene and other monoalkyl aromatics) are shown in Figures 1 and 2. Similar maps showing 75th percentile and maximum concentrations can be found at <https://utexas.box.com/s/13e0bw9a0ymx2a16eayo3tiw6bfl7n4x>. Quality assurance activities have been ongoing. Data collection for comparing CAMx simulated O₃ and PM_{2.5} concentrations with ambient observations was initiated for sites within El Paso (Texas Commission on Environmental Quality (TCEQ) network) and within the Juarez and Chihuahua municipalities (El Instituto Nacional de Ecología y Cambio Climático (INECC)). Ambient O₃ observations are available at six El Paso sites: Ojo de Aqua, Skyline Park, Ivanhoe, El Paso Chamizal, Ascarate Park SE, and Socorro Hueco, and four sites in Mexico: Planta de Tratamiento de Aguas Residuales Norte and Instituto de Ingeniería y Tecnología in Juarez and Centro and Sur in Chihuahua. PM_{2.5} observations are available at four of these sites: El Paso Chamizal, Ascarate Park SE, Juarez Instituto de Ingeniería y Tecnología, and Chihuahua Sur.

A Reactive Tracer (RTRAC) algorithm in CAMx was configured to examine emission source contributions to toluene and ethylene oxide concentrations in El Paso-Juarez. The modeling team processed explicit toluene and ethylene oxide emissions for the 2022 base year from the U.S. Environmental Protection Agency's (EPA) modeling platform using SMOKE. Emission source "tags" for toluene are shown in Table 1. For some source categories such as U.S. fires and area and point sources in Mexico, the CB6 lumped TOL species was used as a surrogate when explicit toluene (TOLU) emissions were not readily available. The simulation will begin at the Texas Advanced Computing Center (TACC) during the next week.

(a) O₃

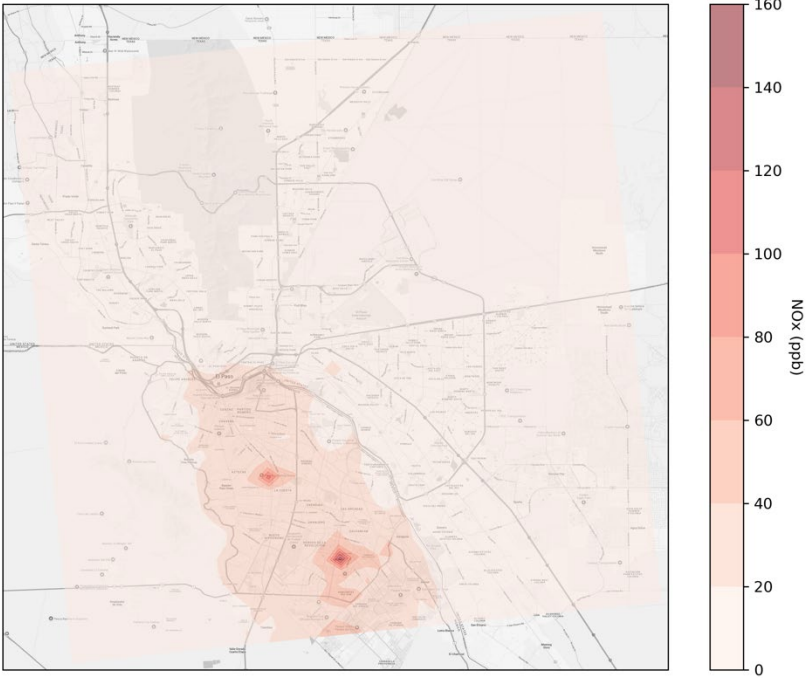


(b) PM_{2.5}



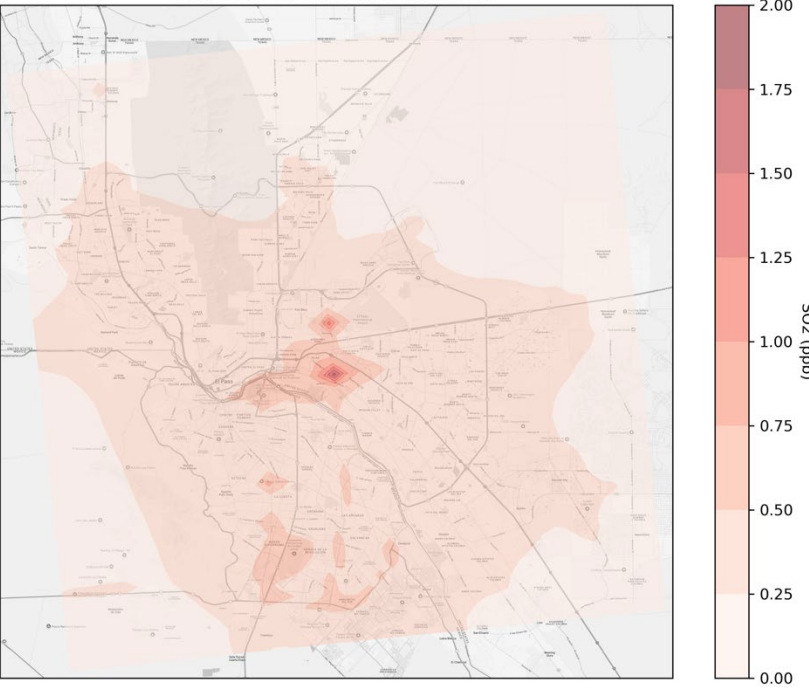
(c) NO_x

Annual Mean Concentration of NOx

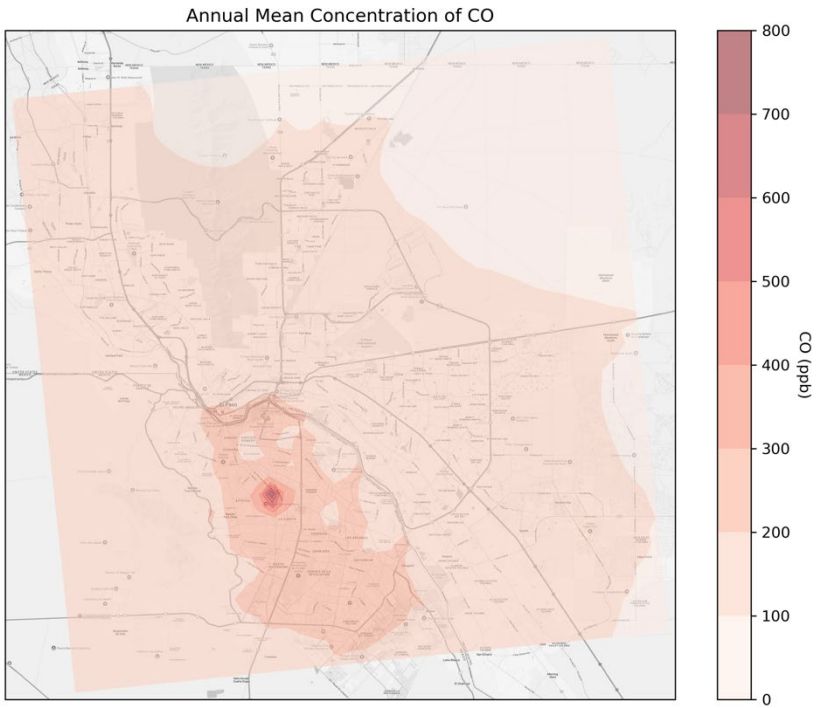


(d) SO₂

Annual Mean Concentration of SO2



(e) CO



(f) CB6 TOL

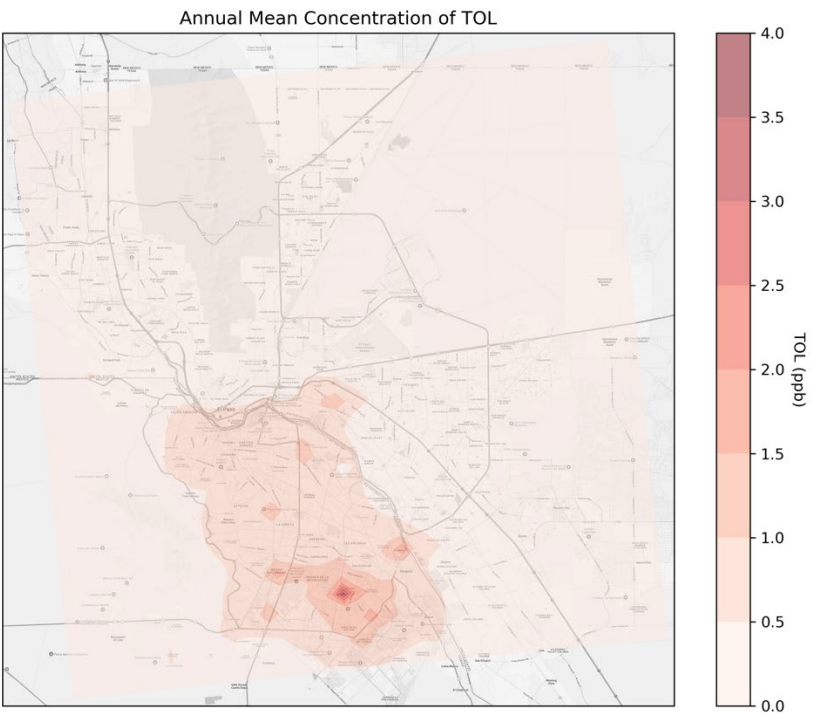
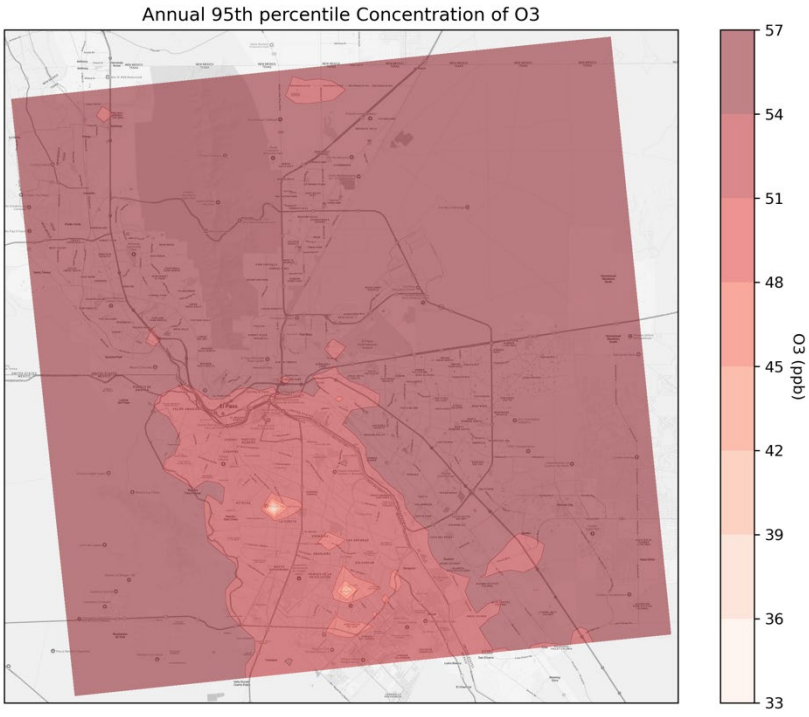
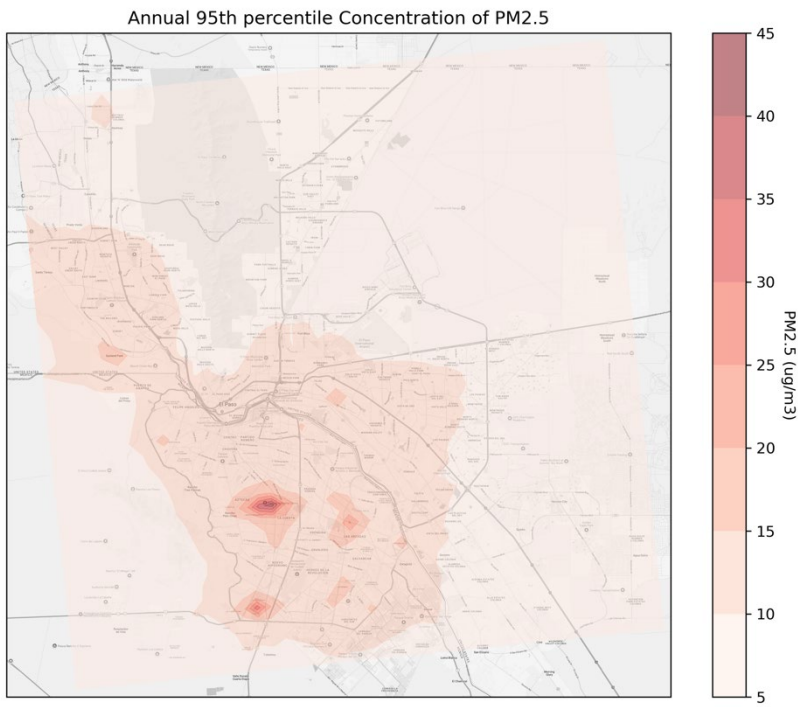


Figure 1. CAMx basecase simulated mean concentrations of (a) ozone, (b) PM_{2.5}, (c) NO_x, (d) SO₂, (e) CO, and (f) CB6 TOL species during 2022 in the El Paso-Juarez domain. Note differences in scales between plots.

(a) O₃

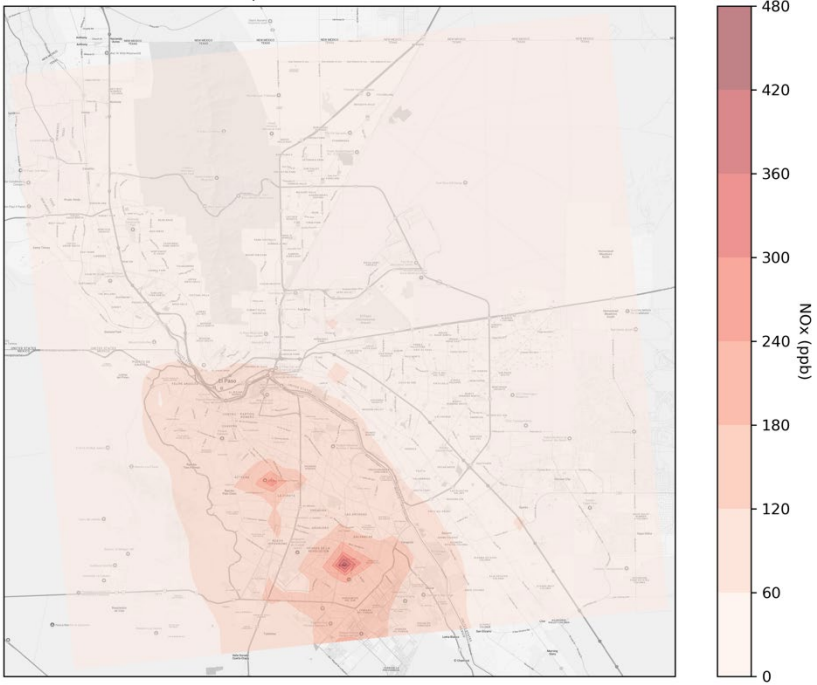


(b) PM_{2.5}



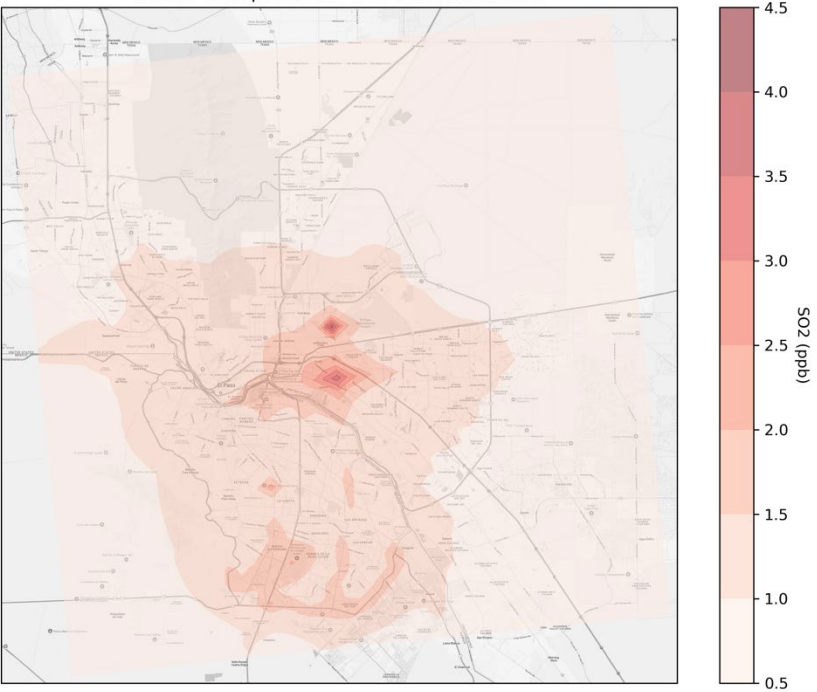
(c) NO_x

Annual 95th percentile Concentration of NO_x

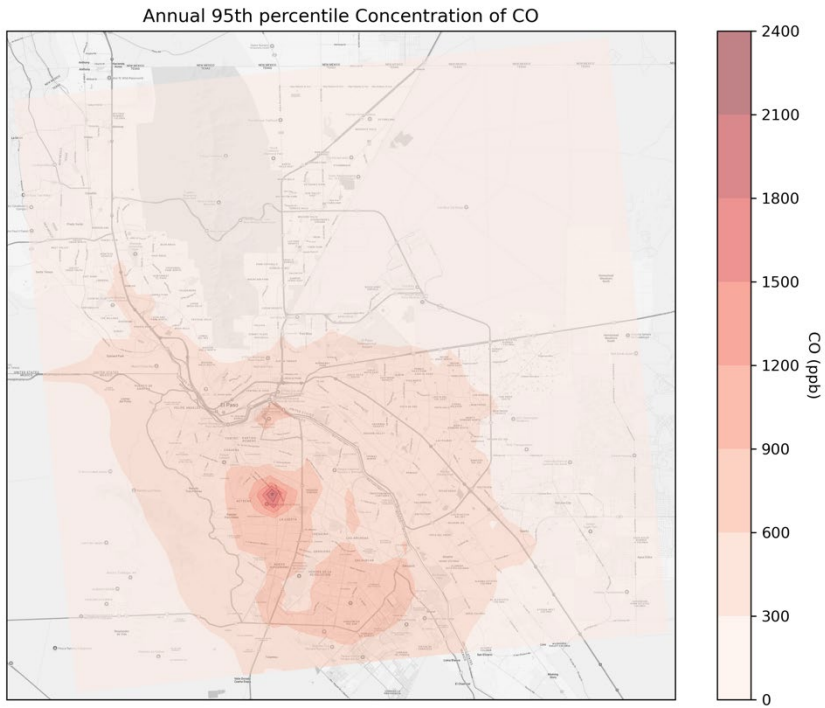


(d) SO₂

Annual 95th percentile Concentration of SO₂



(e) CO



(f) CB6 TOL

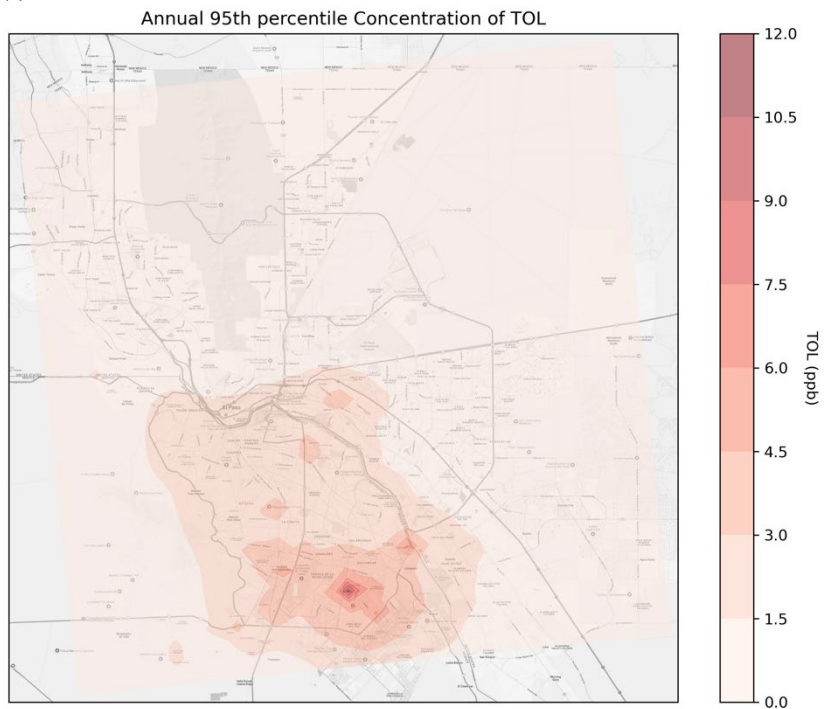


Figure 2. CAMx basecase simulated 95th percentile concentrations of (a) ozone, (b) PM_{2.5}, (c) NO_x, (d) SO₂, (e) CO, and (f) CB6 TOL species during 2022 in the El Paso-Juarez domain. Note differences in scales between plots.

Table 1. RTRAC emission source tagging for toluene.

Emission Sector ID	Description	Low Level or Elevated Source	RTRAC Grouping (NA = Source does not have toluene emissions)	Explicit Toluene (TOLU) or CB6 TOL Surrogate
afdust	Area fugitive dust	Low	NA	NA
airports	Aircraft and ground support equipment	Low	Nonroad	TOLU
livestock	Livestock	Low	NA	NA
nonpt	All other nonpoint	Low	Area	TOLU
nonroad	Nonroad	Low	Nonroad	TOLU
np_oilgas	Nonpoint source oil and gas	Low	Oil and Gas	TOLU
np_solvents	Solvents	Low	Solvent	TOLU
onroad_area	Onroad	Low	Onroad	TOLU
openburn	Open burning	Low	Area	TOLU
ptagfire	Agricultural fires	Elevated	Fire	TOL
ptfire-rx	Prescribed fires	Elevated	Fire	TOL
ptfire-wild	Wildfires	Elevated	Fire	TOL
pt_oilgas	Point source oil and gas	Elevated	Oil and Gas	TOLU
ptegu	Electric Generating Units (EGU)	Elevated	EGU	TOLU
ptnonipm	All other non-EGU point	Elevated	NEGU	TOLU
rail	Locomotives	Low	Nonroad	TOLU
rwc	Residential Wood Combustion	Low	Area	TOLU
fertilizer	Fertilizer	Low	NA	TOLU
beis4	Biogenic	Low	NA	TOLU
cmv_c1c2	Commercial Marine Vessels	Low	NA	NA
cmv_c3	Commercial Marine Vessels	Low	NA	NA
canmex_ag	(Mexico) Agriculture	Low	NA	TOLU
canmex_area	(Mexico) Nonpoint	Low	Mexico Area	TOL
canmex_point	(Mexico) Point	Elevated	Mexico Point	TOL
mexico_onroad	(Mexico) Onroad	Low	Mexico Onroad	TOLU

Task 3: Activities in April continued focusing on large data processing including data analysis from the High-Resolution Time of Flight Aerosol Mass Spectrometer (HR-TOF-AMS) and Vocus Proton Transfer Reaction Time of Flight Mass Spectrometer (Vocus-PTRTOFMS).

Preliminary particle data have been analyzed. Combined with the GPS data, spatial distributions of non-refractory PM₁ were generated during all mobile measurement periods between 1/6/2025 and 1/18/2025. To observe diurnal variation of the PM in the area, timeseries of PM concentrations were also generated for all stationary measurements during the same time. Figures 3 – 5 show examples of the results from HR-TOF-AMS.

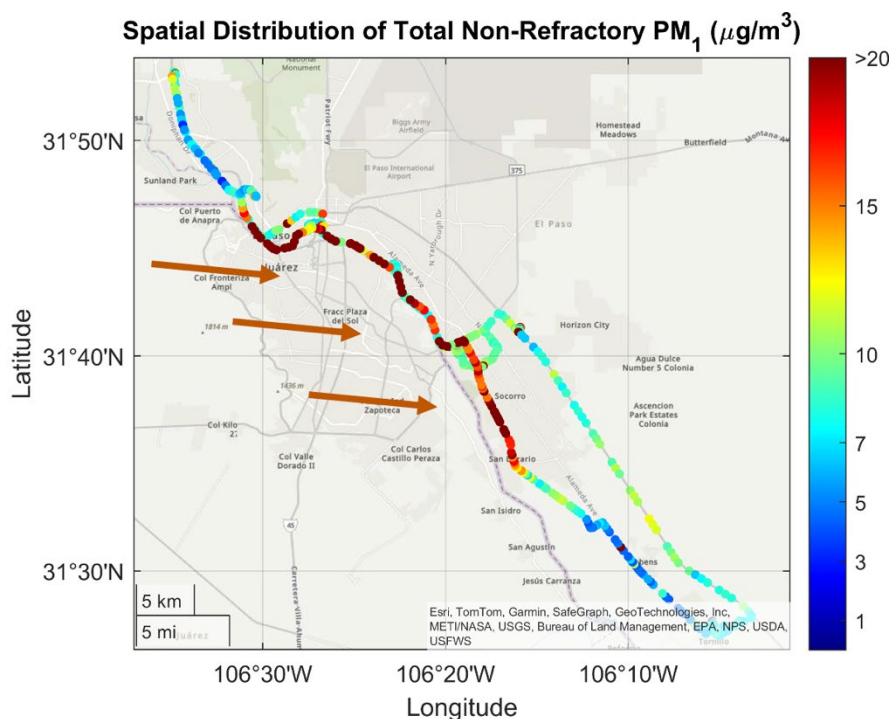


Figure 3: Spatial Distribution of Total Non-Refractory PM₁, 1/10/2025

We observed elevated PM concentrations near the US-Mexican border, with wind coming from the west. Figure 3 above shows an overview of a mobile measurement track performed on 1/10/2025, between 14:07 and 21:15 (local time). The wind direction during this time varied from W, NW and WSW direction (indicated by the burnt orange arrows on the figure), with speeds between 3 mph to 14 mph (hourly average). We noticed that while driving near the highway that borders Mexico, Figure 1 shows enhancement of total PM₁ to over 20 µg/m³. In addition, during this high concentration period, most of the PM₁ detected were organic aerosols (not shown here) with concentrations between 14 – 16 µg/m³. We also observed a slight increase of inorganic aerosol during the same high concentration period.

We noticed elevated PM concentrations overnight, suggesting there could be a strong diurnal variation of PM in the area. Figures 4 and 5 below show stationary measurement results of different PM₁ species from two different nights. From Figure 4, we observed that both organic and inorganic aerosol concentration increase starting around midnight on 1/9/2025. The PM concentrations peaked at around noon with a total of over 30 µg/m³ and then started to decrease. Figure 5 shows similar trends where we saw a sharp increase in both organic and inorganic PM around 3 AM on 1/13/2025. The PM concentration continued to increase, reaching its peak of over 30 µg/m³ around noon, before decreasing again. One reason for higher nighttime PM concentrations is a lower planetary boundary layer height (which leads to less mixing in the atmosphere); however, this does not explain the sharp increase we observed on 1/13. Further analysis including wind direction, wind speed, as well as source apportionment, is needed to determine the possible causes of these elevated PM level periods at night.

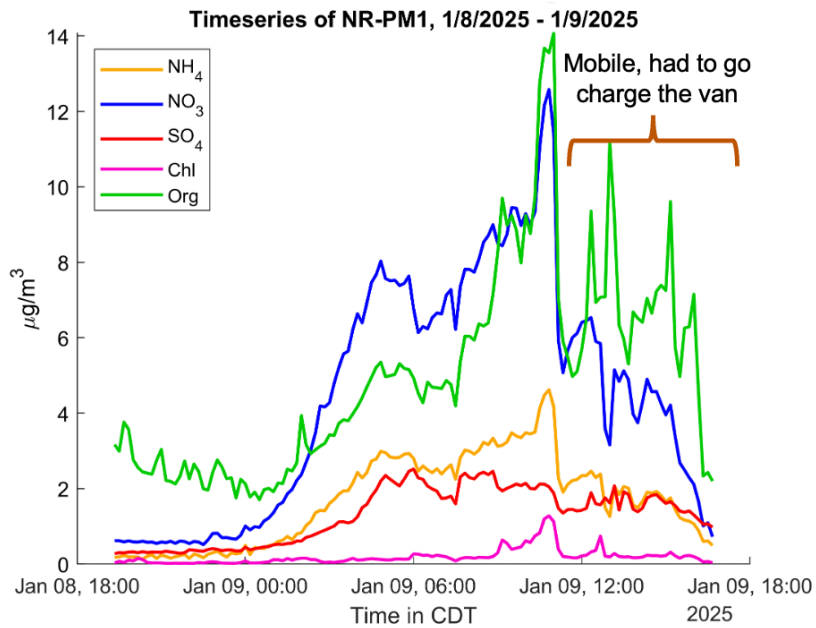


Figure 4: Timeseries of different PM species detected during stationary measurement 1/8/2025 – 1/9/2025.

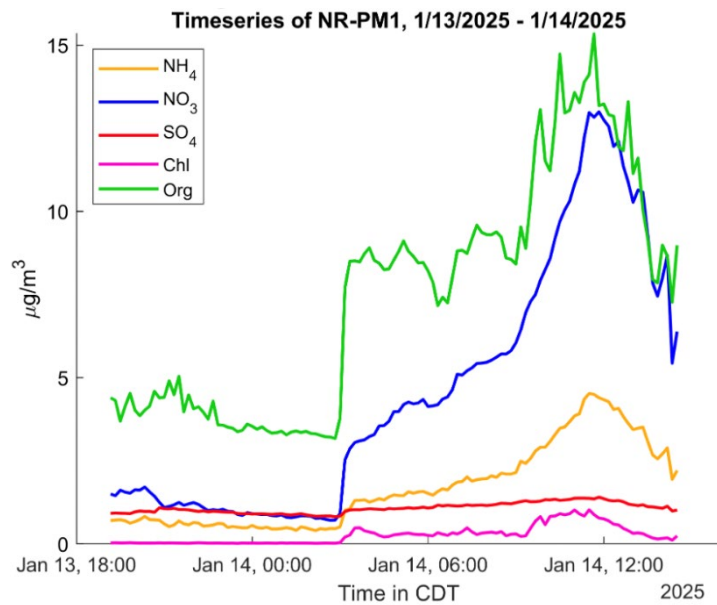


Figure 5: Timeseries of different PM species detected during stationary measurement 1/13/2025 – 1/14/2025.

Preliminary multivariate factor analysis was conducted on mobile comprehensive VOC data from the Vocus-PTRTOFMS and revealed 8 distinct factors which grouped compounds by covariance similarities (Figure 6). Out of 1524 detected ions, 683 VOCs were fed to the factor analysis to aid in source apportionment of individual and groups of VOCs. For instance, the factor tentatively attributed to “Gasoline and Petrochemical” comprised high loadings of toluene, benzene, C8 – C10 aromatics and other related VOCs. It was distributed across El Paso with different localized enhancements in the north and central El Paso. The “Combustion” factor was represented by furanoids, aromatics and nitrogen containing compounds such as C_7H_7NO consistent with benzamide. This factor’s hotspot was localized around the burning house. The factor attributed to “Cooking and VCPs” grouped long-chain fatty acids such as $C_{16}H_{30}O_2$ and long-chain hydrocarbons used in volatile chemical products (VCPs). This factor was spatially expressed close to restaurants and fast-food facilities as well near residences. The “Siloxane factor” was characterized by $C_8H_{24}Si_4O_4$ (D4), $C_{10}H_{30}Si_5O_5$ (D5) and other volatile cyclic siloxanes widely used as lubricants and in personal care products (PCPs). In contrast to primary VOCs directly emitted from different sources, a group of oxygenated VOCs (OVOCs) was represented by “OVOC” Factor which was less localized than other factors indicating mixing across the city. This factor seemed more sensitive to time of day and meteorological conditions affecting photochemical processes. Further data analysis will confirm source apportionment of PM1 SOA and other markers which will be combined with the wind direction analysis to separate El Paso contributions from those of Juarez.

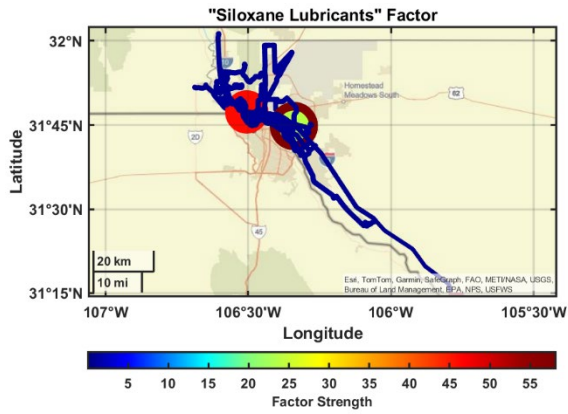
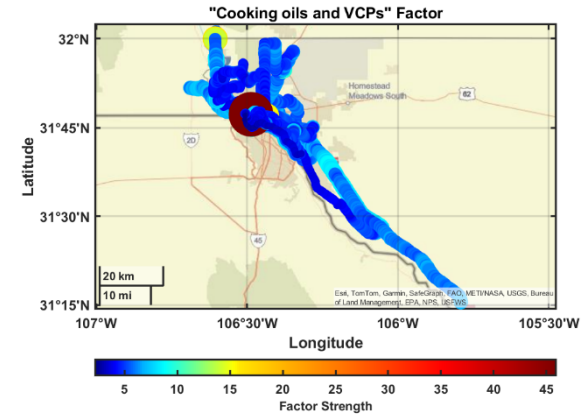
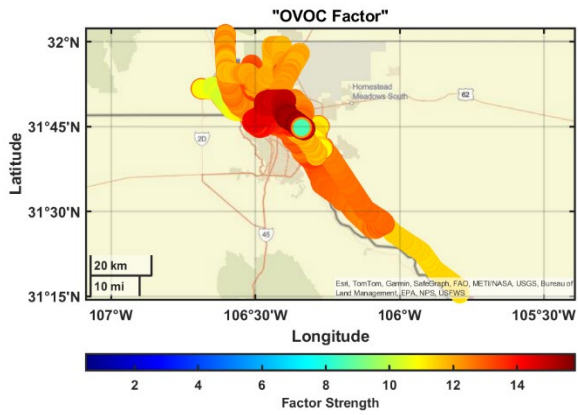
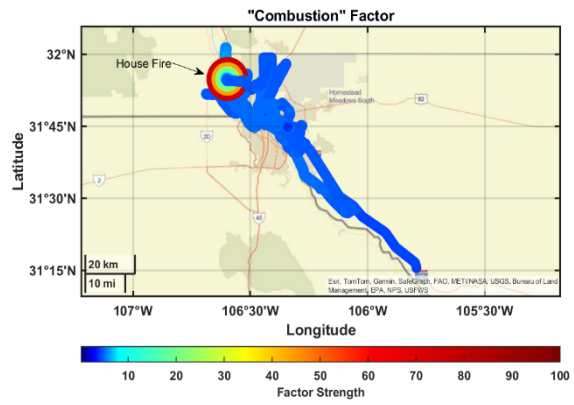
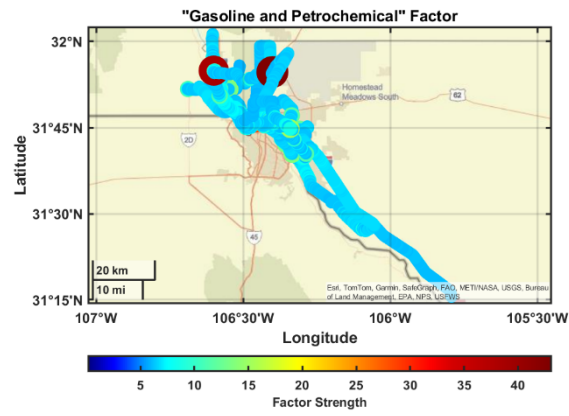


Figure 6. Spatial maps of dominant preliminary factors to help source apportionment analysis.

Preliminary Analysis

No

Data Collected

No

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments

None

Goals and Anticipated Issues for the Succeeding Reporting Period

The modeling team expects the RTRAC simulation for toluene and ethylene oxide to be completed. These results will be used for contour plots of CAMx simulated percentile concentrations of these compounds. Emission source contributions (Table 1) to CAMx simulated peak (~top 10%) concentrations will be developed at geographic locations of interest. Time series will be developed to evaluate CAMx simulated versus measured O₃, PM_{2.5}, and toluene concentrations.

The measurement team has been working on the preparations for the next campaign. The UTEP site is now fully powered and equipped to support stationary measurements. The next deployment is scheduled for May 12 – 21 (mobile phase) and June 4 – 8 (stationary phase), which will provide complementary seasonal data for comparison with the winter campaign. The data from both campaigns will be holistically integrated after the second campaign is conducted and consistently processed.

Detailed Analysis of the Progress of the Task Order to Date

None

Do you have any publications related to this project currently under development? If so, please provide a working title, and the journals you plan to submit to.

Yes No

Do you have any publications related to this project currently under review by a journal? If so, what is the working title and the journal name? Have you sent a copy of the article to your AQRP Project Manager and your TCEQ Liaison?

Yes No

Do you have any bibliographic publications (ie: publications that cite the project) related to this project that have been published? If so, please list the reference information. List all items for the lifetime of the project.

Yes No

Do you have any presentations related to this project currently under development? If so, please provide working title, and the conference you plan to present it (this does not include presentations for the AQRP Workshop).

Yes No

Do you have any presentations related to this project that have been published? If so, please list reference information. List all items for the lifetime of the project.

Yes No

Have any personnel changes occurred that were not listed in the original proposal? If so, please include a detailed description of the personnel change(s) below.

Yes No

Are any delays expected in the progress of the research? If so, please include a detailed description of the potential delay below.

Yes No

Describe any possible concerns/issues (technical or non-technical) that AQRP should be made aware of.

Are you anticipating using all the available funds allocated to this project by the end date? If not, why and approximately what is the amount to be returned?

Yes No

Submitted to AQRP by
Pawel Misztal