# 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** | 3/10/2025 |
| **REPORTING PERIOD** | **From:** 2/1/2025<br>**To:** 2/28/2025 | **REPORT #** | 5 |

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:** Activities during February included the following:

- An annual three dimensional Comprehensive Air Quality Model with Extensions (3-D CAMx) simulation based on the U.S. Environmental Protection Agency's (EPA's) Office of Air Quality Planning and Standards (OAQPS) 2022 modeling platform (https://registry.opendata.aws/epa-2022-modeling-platform/) was completed. This simulation required nearly one month of computational time at the Texas Advanced Computing Center (TACC). Boundary and initial conditions for the El Paso-Juarez were extracted for the El Paso-Juarez 12-km domain shown in Figure 1.

- All gridded emissions in binary format, meteorological fields, geographic data, ozone column, and photolysis rates from the EPA modeling platform were “windowed” to match the El Paso-Juarez 12-km domain. We note that EPA by-sector emissions files were provided in Community Multiscale Air Quality (CMAQ) Network Common Data Form (NetCDF) format. Dr. Kimura streamlined the cmaq2camx tool to convert these files to the CAMx NetCDF format which were then “windowed” to the extent of the 12-km El Paso-Juarez domain.

- Flexi-nests for the 4-km and 1-km domains (Figure 1) were defined in the CAMx configuration.

- Emissions for three categories, fertilizer, biogenics, and fugitive dust, were regridded from the EPA 2022 modeling platform for the El Paso-Juarez 4-km and 1-km nested domains. These emission files were converted from CMAQ to CAMx NetCDF files.

- Emissions for all other gridded source categories previously processed via spatial surrogates for the El Paso 4-km and 1-km nested domains were also converted from

CMAQ to CAMx NetCDF format. No changes were required for point source emissions within the El Paso-Juarez domain.

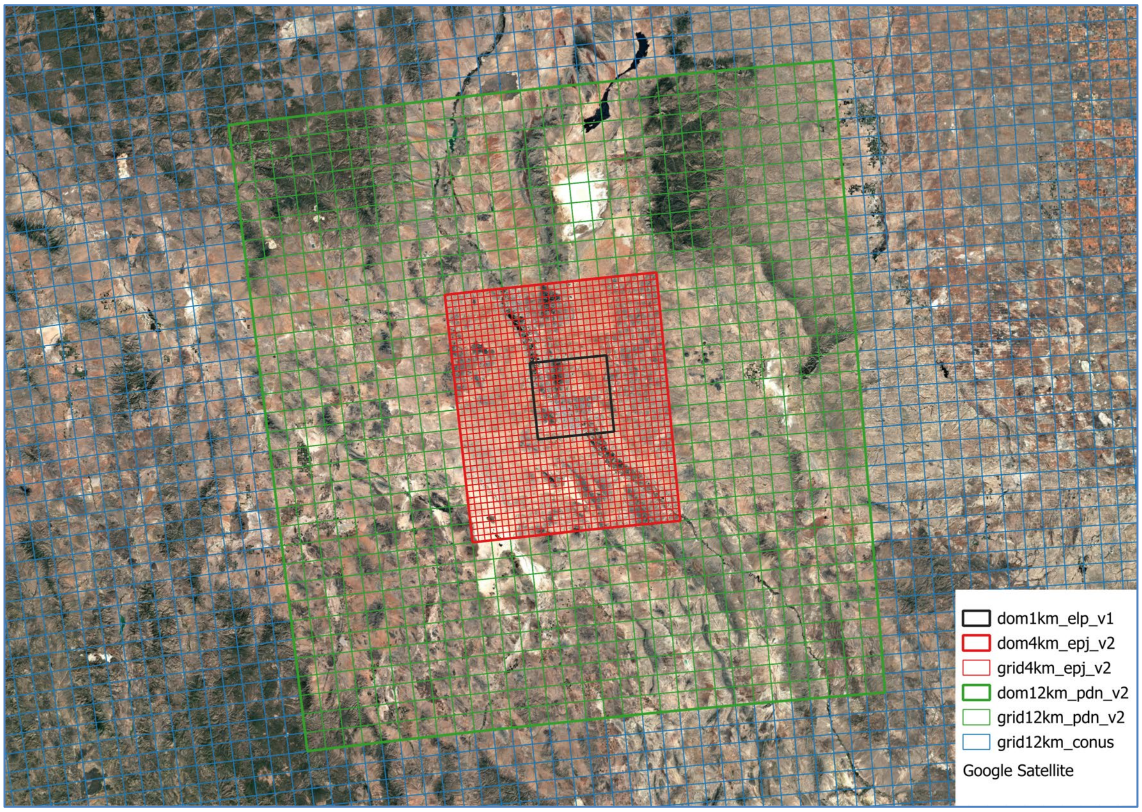



**Figure 1.** 12-km West Texas domain (green) with 4-km nested domain (red) and 1-km El Paso-Juarez innermost domain (black). The 12-km West Texas domain was windowed from the existing 12-km Continental United States (CONUS) grid of the EPA OAQPS 2022 modeling platform (blue).

**Task 3:** Activities in February continued focusing on large data processing and among others included:

Pre-processing of the entire Vocus-PTR-TOF (Vocus Proton-Transfer-Reaction Time-of-Flight Mass Spectrometer) dataset using PTRwid routine (Holzinger, 2015). To maximize efficiency, the raw Hierarchical Data Format version 5 (HDF5) data from the Vocus were uploaded to the Box and synchronized on the 128 GB workstation with Interactive Data Language (IDL).

- The PTRwid routine yielded 1525 ions in the unified mass list. The mass defect plot (Figure 2) shows the richness of chemical space, with homologous series of alkanes, carbonyls, acids, hydroxyacids, aromatics, and nitrogen containing compounds.

- As a second step, postprocessing using Matlab routine is currently ongoing. The number of volatile organic compound (VOC) ions will be reduced by removing primary ions, water clusters and compounds below abundance threshold to exclude ions close to detection limit (<900 parts per quadrillion (ppq); $10^{-15}$). The mass assignment presented in Figure 2 was automated using Matlab program to yield the closest-match formula with the measured exact monoisotopic protonated mass. Further work will verify and complement these assignments which, except for a few representatives, lack compounds containing silicon, sulfur, halogenated compounds, and other exotic compounds which need to be manually (or semi-manually) complemented.

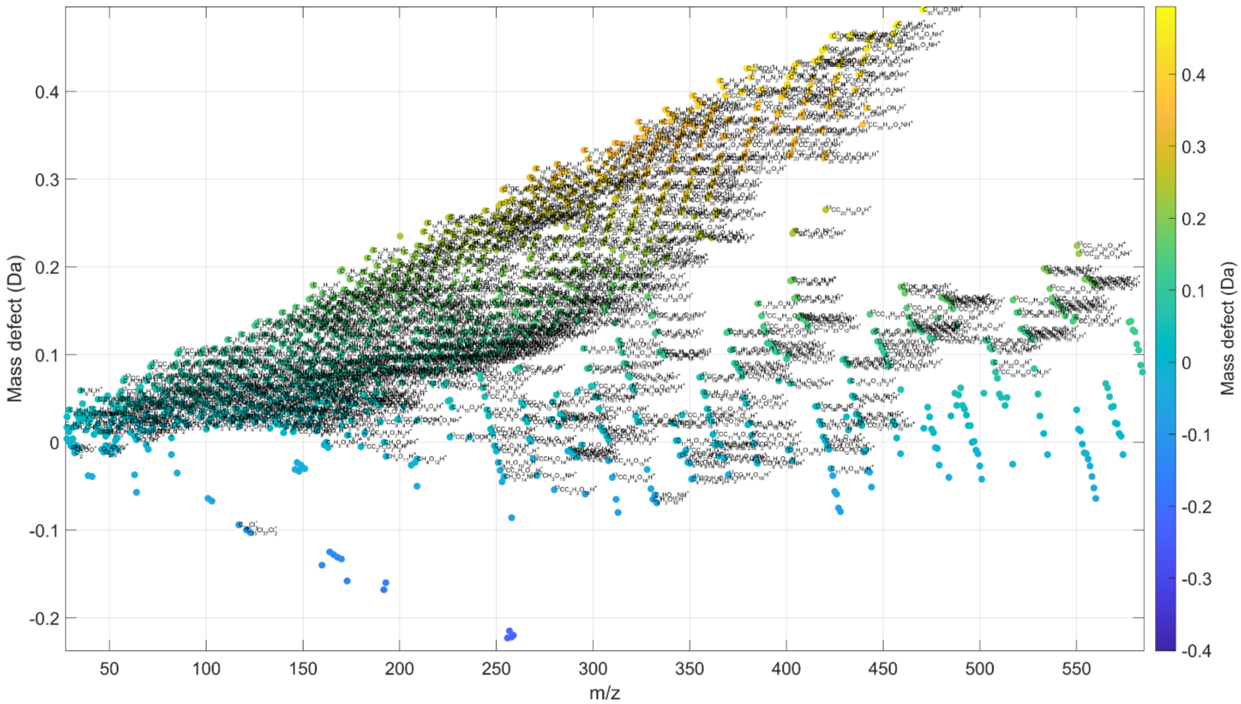



**Figure 2.** Mass defect plot for the unified mass list with more than 1500 ions detected in the El Paso Winter Campaign (the identified formulas are preliminary).

- Preliminary findings reveal hotspots for different gas and particle-phase pollutants from various source types and industries. For example, ethylene oxide enhancements were encountered downwind of sterilization facilities in the area, as well as elevated aromatics levels near a local refinery. Traffic emissions, mostly from diesel engines, contributed to sudden, significant spikes in organic aerosol levels near major roads (not shown due to ongoing data analysis). Figure 3 shows the time series of non-refractory particulate matter with a diameter of 1 micron or smaller (NR-$PM_1$) (measured by the high resolution aerosol mass spectromenter (HR-AMS)) when the van was driving near a house fire in El Paso, Texas.

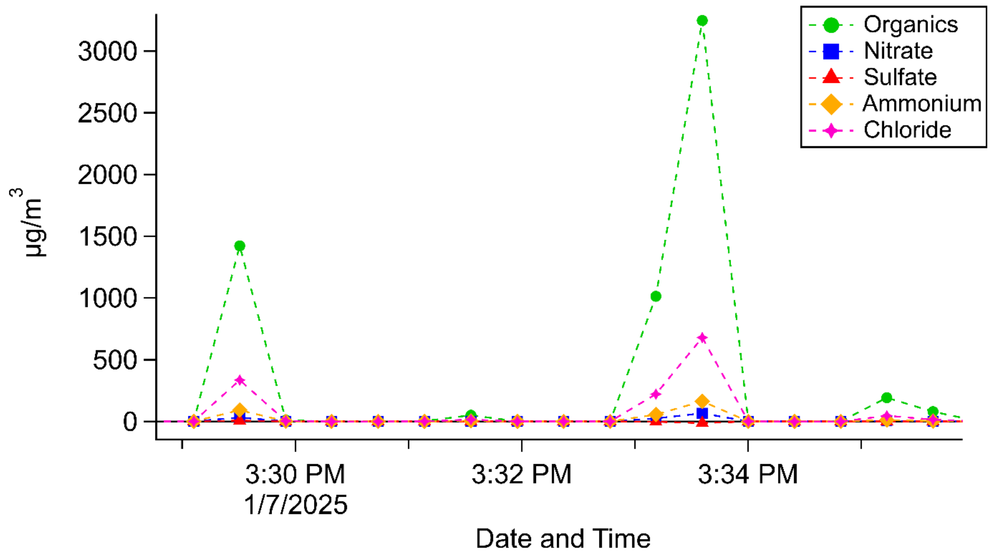



**Figure 3.** Timeseries of NR-PM$_1$ near a house fire, 1/7/2025

At around 3:29 pm, the van made its initial entry into the fire plume, where we see the immediate elevation of organic aerosols to almost 1500 µg/m$^3$. Between 3:30 pm and 3:32 pm, the driving team then decided to circle around the plume, attempting to get closer to the house fire. Around 3:33 pm, the mobile van made its second entry into the smoke plume, where we see NR-PM$_1$ organics increased to above 3000 µg/m$^3$. Additionally, in both plume capture periods, we saw elevation of chloride aerosols up to around 500 µg/m$^3$. These plumes were coinciding with plumes observed by the Vocus (preview data shown in previous MTR). The data analysis for this project is ongoing and will focus on source markers and combined VOC and particulate matter (PM) source apportionment.

- Mobile data from the QuantAQ Modulair-Gas monitor were also analyzed and the preliminary maps with observed carbon monoxide and PM$_{2.5}$ are shown in Figure 4. The largest enhancements in PM$_{2.5}$ were often correlated with carbon monoxide (CO) enhancements indicating the combustion processes are likely responsible for much of primary PM$_{2.5}$ in the region. Prominent hotspots were observed along the US – Mexico border, near active burning and other combustion sources such as cooking and motor vehicles. Further multivariate analysis using VOCs and speciated PM$_1$ will quantitatively apportion the primary and secondary particles along with VOC precursors.

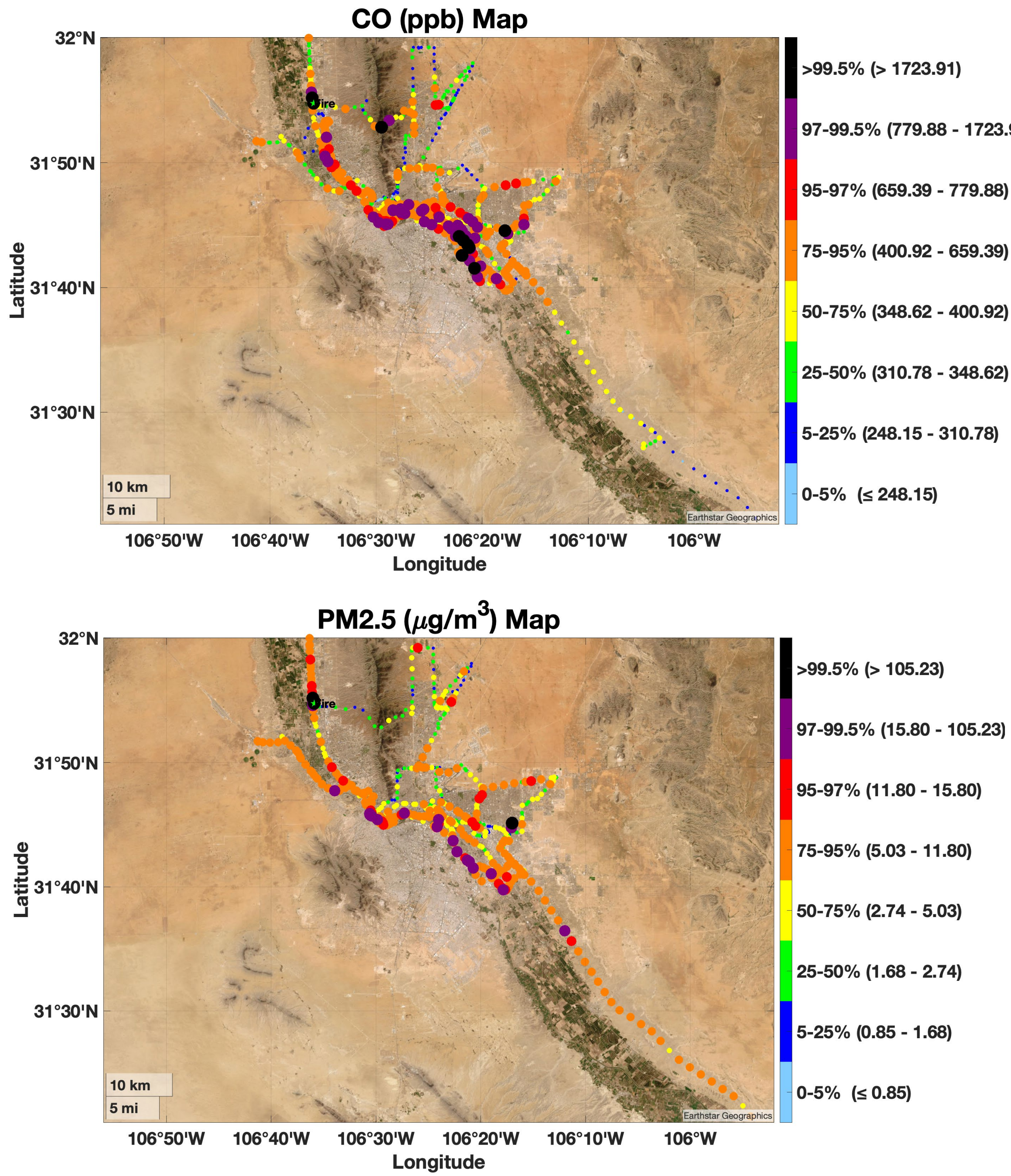



**Figure 4.** Preliminary maps for example tracers measured by QuantAQ, carbon monoxide (top panel) and $PM_{2.5}$ (bottom panel). The color scale corresponds to percentile ranges (with absolute value ranges in parentheses).

**Preliminary Analysis**
Yes

**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 that the El Paso-Juarez CAMx basecase simulation should be completed. Quality assurance assessments and comparisons with ambient measurements in the region should be initiated.
The observation team expects more preliminary data to be included in the next MTR.
The quality control of compound identification, calibrations and source apportionments will be conducted and the progress included in the next MTR. Further efforts are focused on the integrated analysis of VOC and PM data in the context of inventories and modeling data. The modeling results have been useful reference and further observation-modeling integrations are planned.
The UTEP site is now fully connected and powered. The second intensive field campaign in El Paso is currently tentatively planned for the second half of May.

**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?**

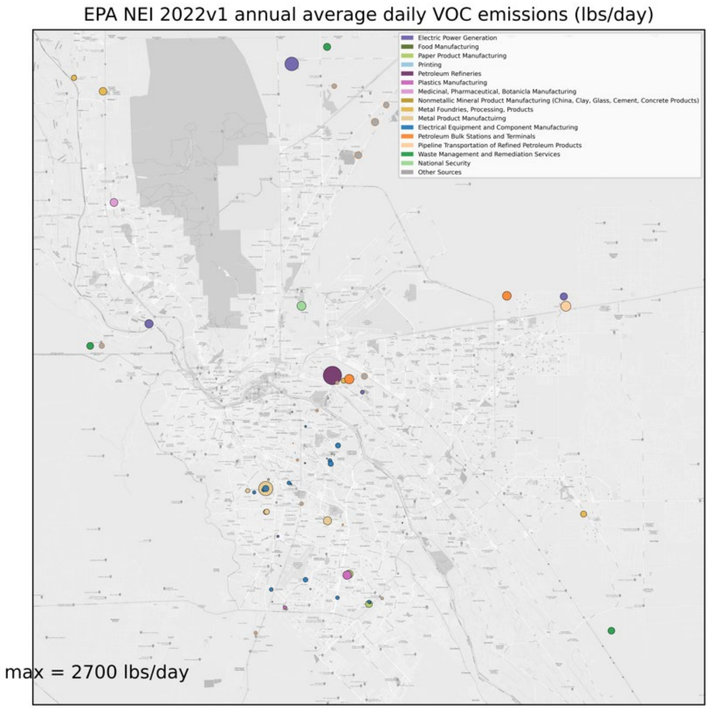
☒ **Yes** ☐ **No**

---

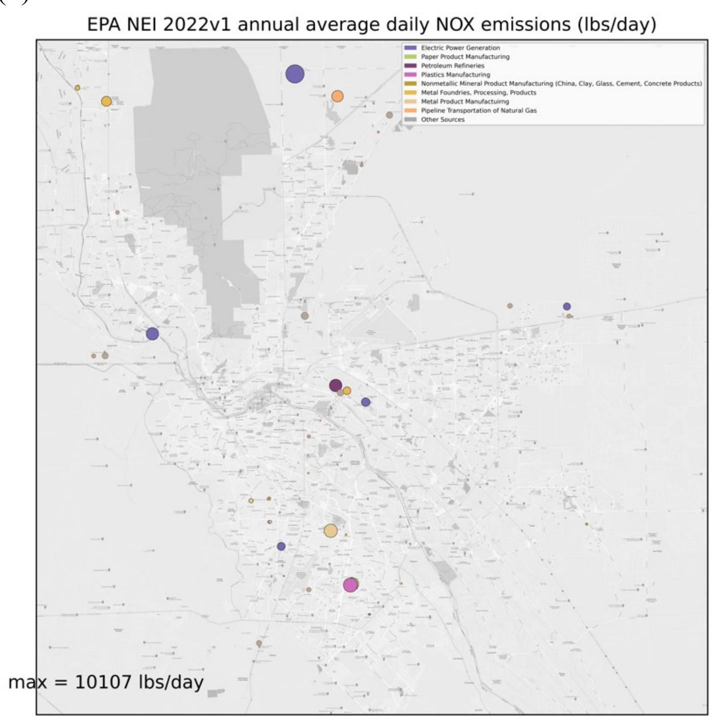
Submitted to AQRP by
Pawel Misztal

**Appendix Figure 1. Point Source Emissions by Industry Type for the El Paso-Juarez 4-km CAMx Domain**

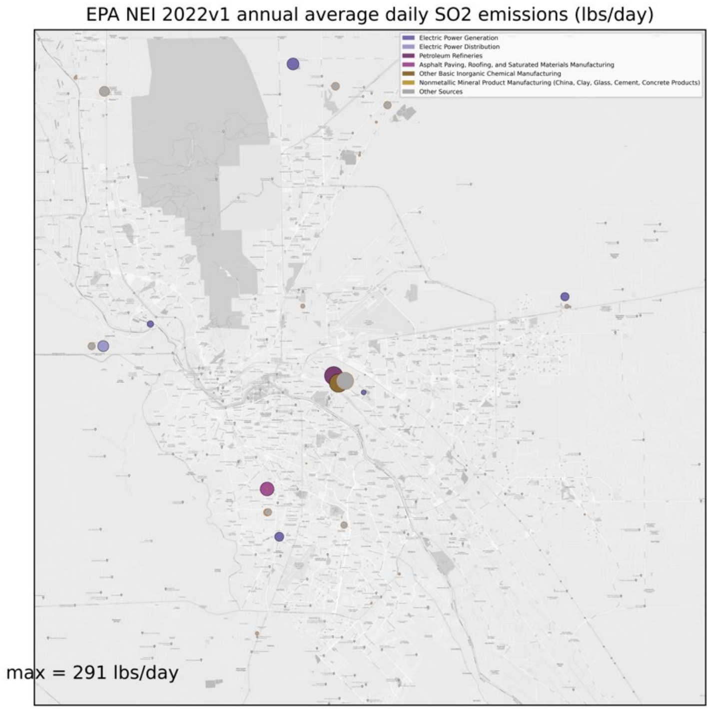
(a) VOC



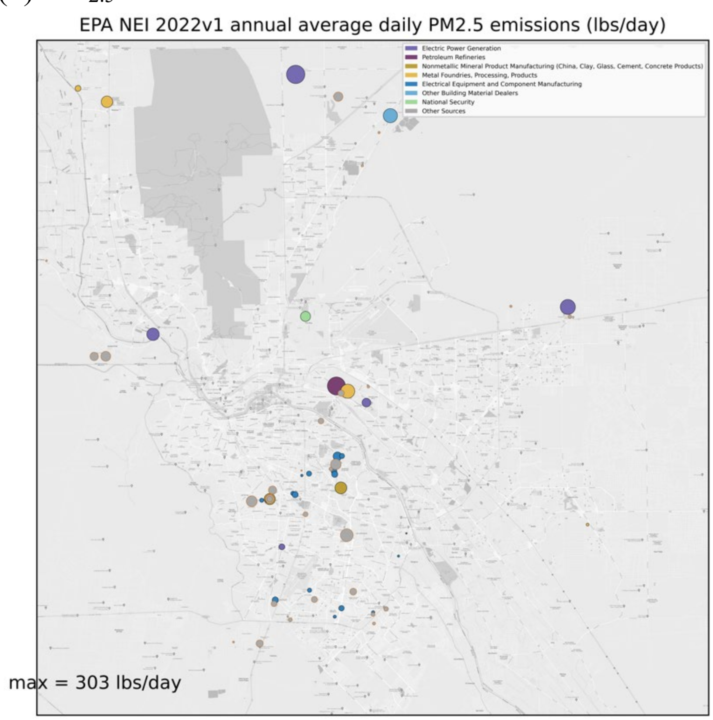

(b) NOx



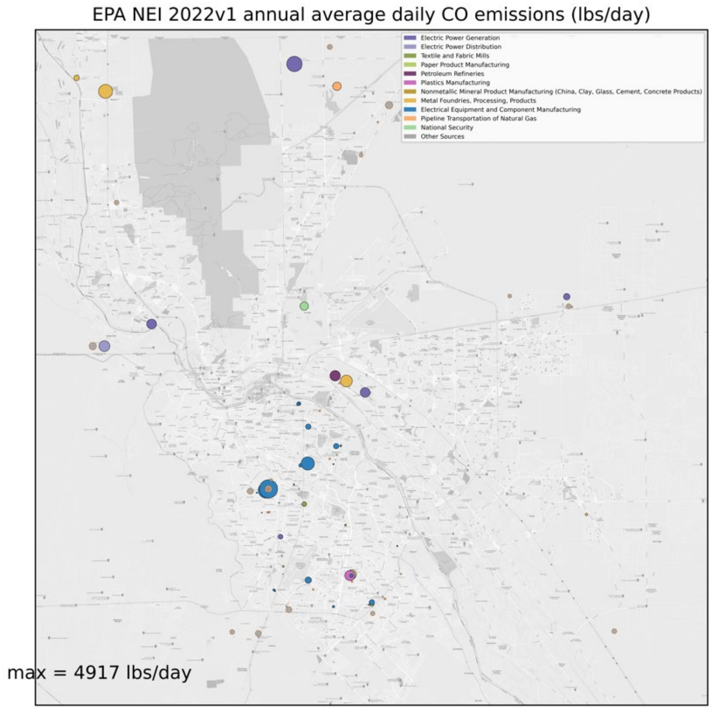
(c) $SO_2$


EPA NEI 2022v1 annual average daily SO2 emissions (lbs/day)
Electric Power Generation
Electric Power Distribution
Petroleum Refineries
Asphalt Paving, Roofing, and Saturated Materials Manufacturing
Other Basic Inorganic Chemical Manufacturing
Nonmetallic Mineral Product Manufacturing (China, Clay, Glass, Cement, Concrete Products)
Other Sources
max = 291 lbs/day

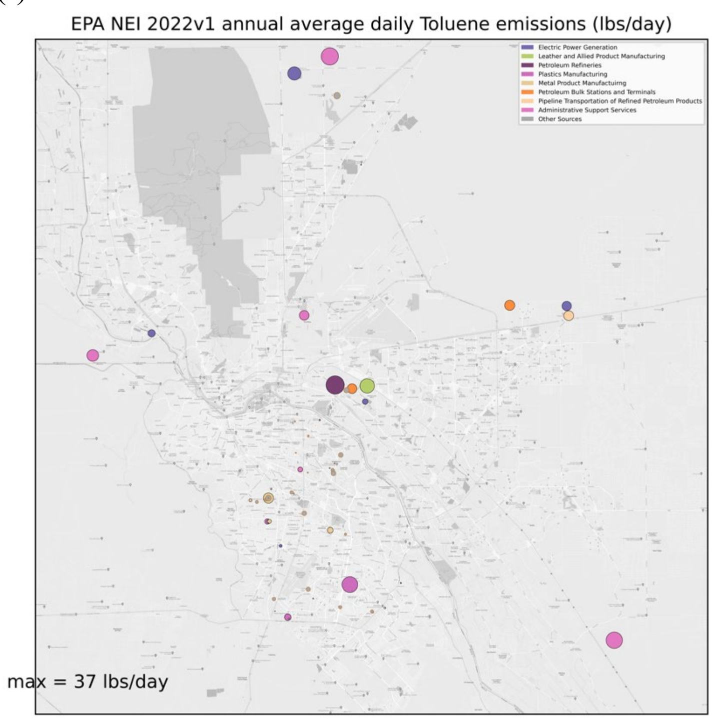
(d) $PM_{2.5}$


EPA NEI 2022v1 annual average daily PM2.5 emissions (lbs/day)
Electric Power Generation
Petroleum Refineries
Nonmetallic Mineral Product Manufacturing (China, Clay, Glass, Cement, Concrete Products)
Metal Foundries, Processing, Products
Electrical Equipment and Component Manufacturing
Other Building Material Dealers
National Security
Other Sources
max = 303 lbs/day

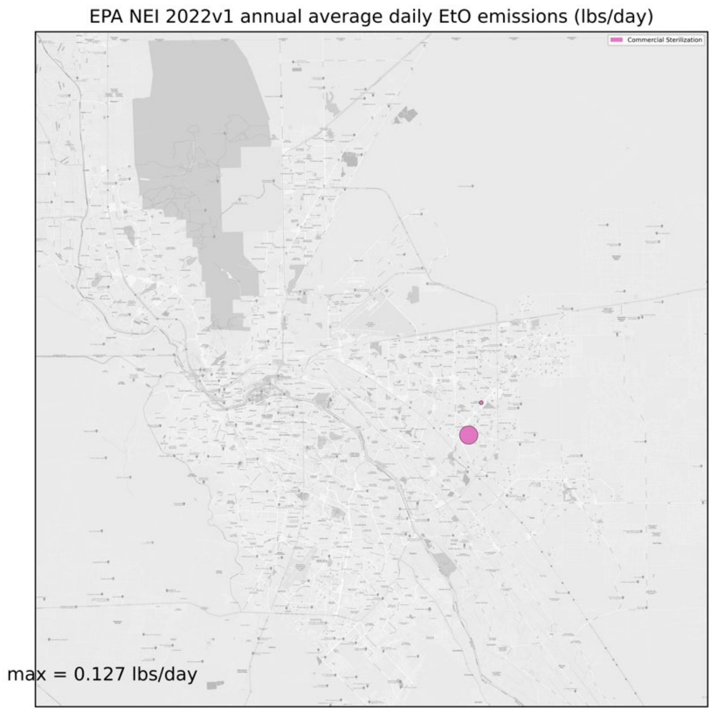
(e) CO




(f) Toluene



(g) Ethylene Oxide




**Appendix Figure 1.** Point Source Emissions by Industry Type for the El Paso-Juarez 4-km CAMx Domain