

26 AUGUST 2025

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

Pawel Misztal (PI), Lea Hildebrandt Ruiz (Co-PI), David Sullivan (Co-PI)  
Center for Energy and Environmental Resources (CEER)  
The University of Texas at Austin

Elena McDonald-Buller (Co-PI), Yosuke Kimura  
Center for Energy and Environmental Systems Analysis (CEESA)  
The University of Texas at Austin

Ling Huang, Chris Emery  
Ramboll

Contributing UT Austin students and postdocs: Daniel Sung, Shihao Zhai, Evelyn Deveraux, Chun-Ying Chao, Kacper Przykaza, Kyle Druckman



# Presentation Outline



- Gas-phase Observations (Pawel Misztal)



- PM Observations (Lea Hildebrandt Ruiz)



- CAMx Modeling (Elena McDonald-Buller)

# Campaign overview

## Winter Campaign

January 4 – 18, 2025

1,484 "data km" driven, 1,111,962 1 s datapoints x 1630 VOC ions detected

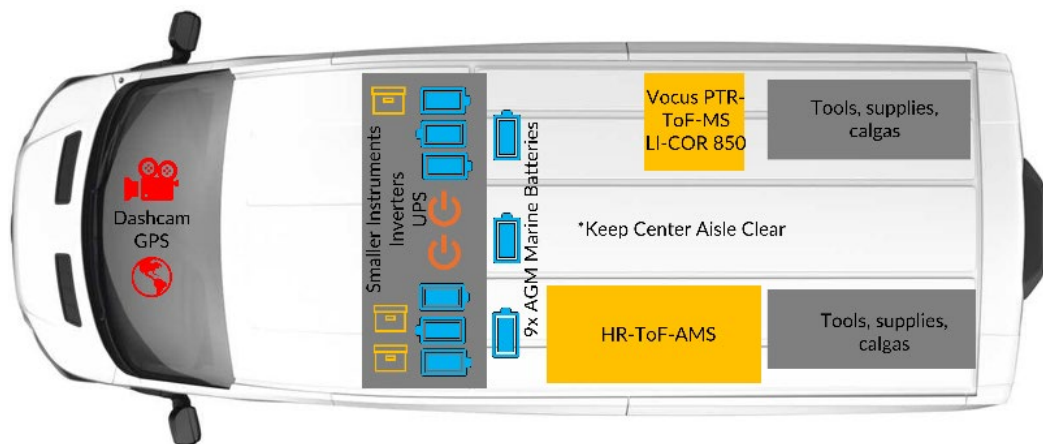
280 VOC ions above 1 pptv threshold

## Summer Campaign

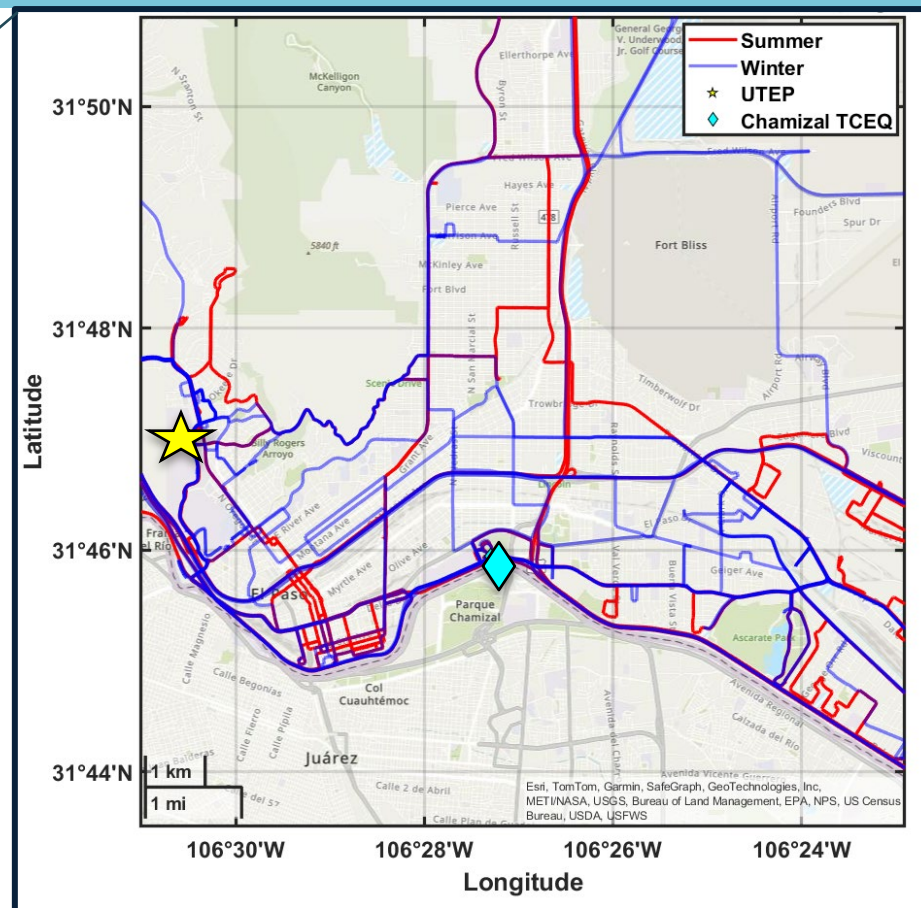
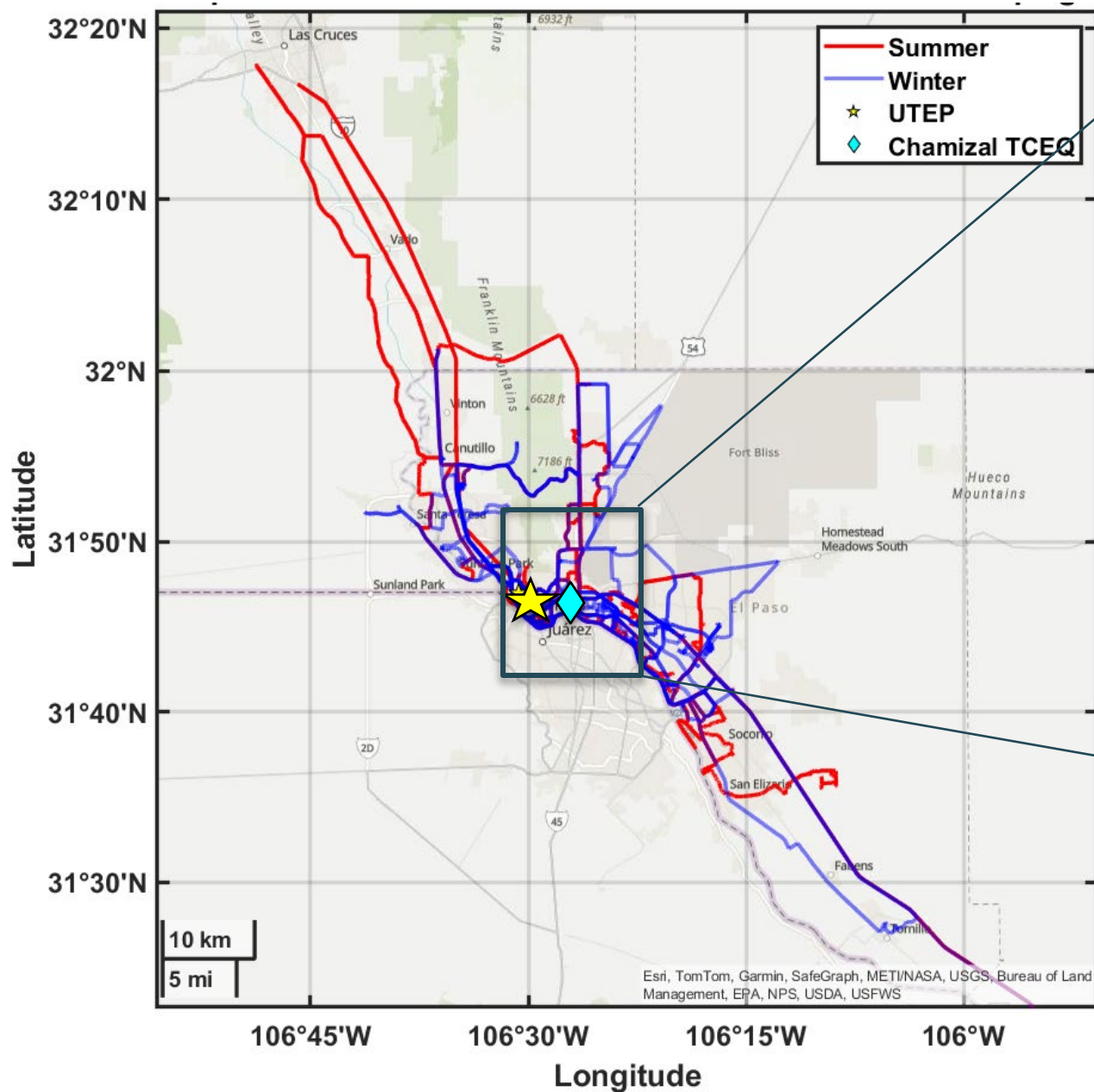
May 13 – 21 & June 5 - 13

1,379 "data km" driven, 1,060,170 1 s datapoints x 1956 VOC ions detected

189 VOC ions above 1 pptv threshold



# Completed Mobile Laboratory Tracks



Survey tracks conducted to scout for hotspots

Focus tracks conducted to enhance statistics *along the border and between monitoring stations and points of interests*

## **Gas-Phase Observations**

# Gas-Phase Observation Objectives

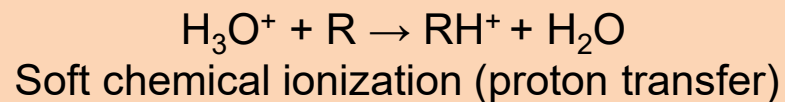


## Objectives:

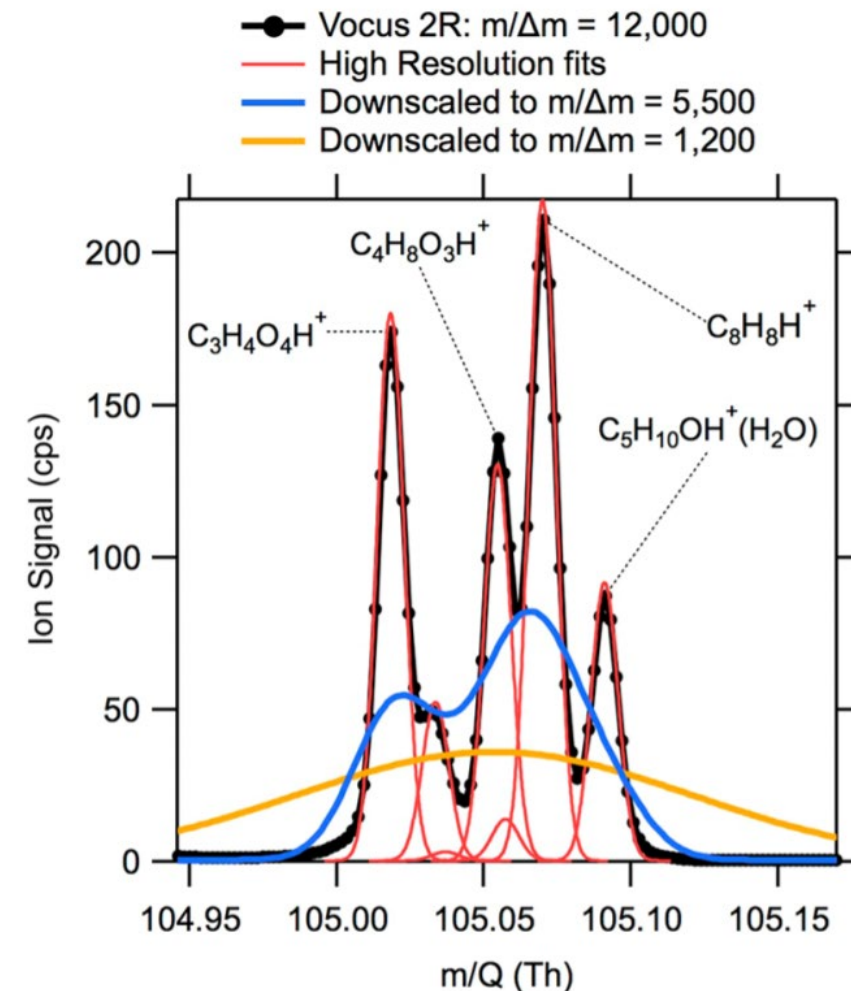
- Map out spatiotemporal variability of VOC source markers and PM precursors
- Understand and fingerprint composition of different source plumes
- Explain high toluene concentrations in El Paso
- Address short-term and high acute events (e.g. burning plumes)
- Conduct preliminary source apportionment
- Assess temporal variability through stationary colocations with TCEQ and other monitoring sites

# Novel Mass Spectrometry for Comprehensive Gas-Phase Measurements

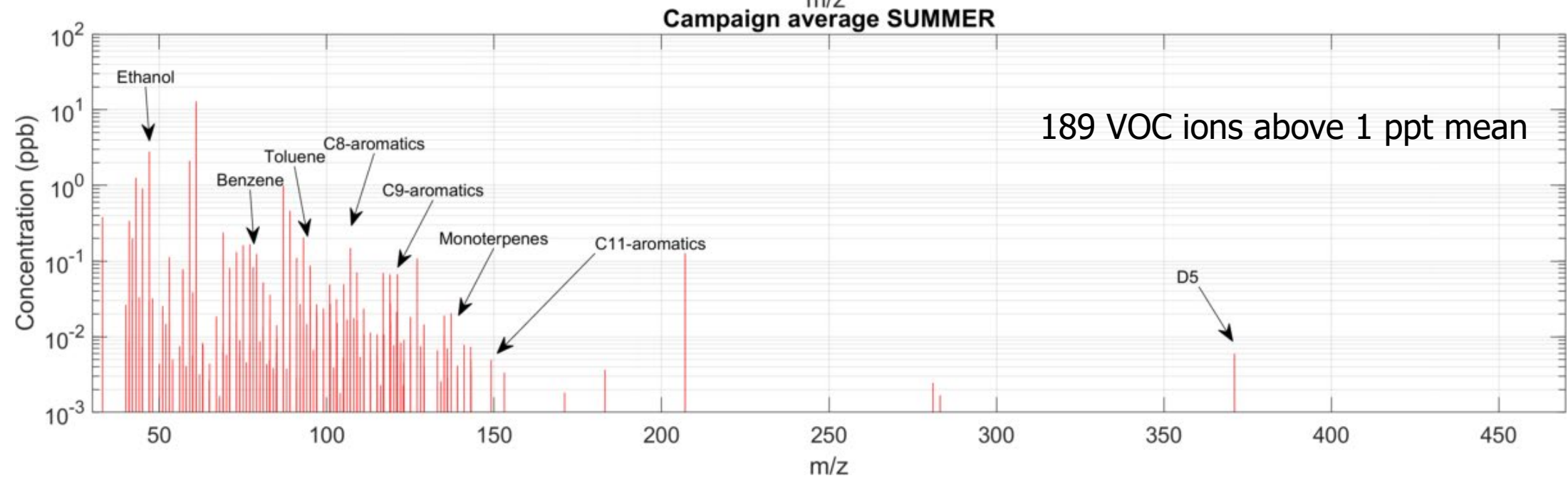
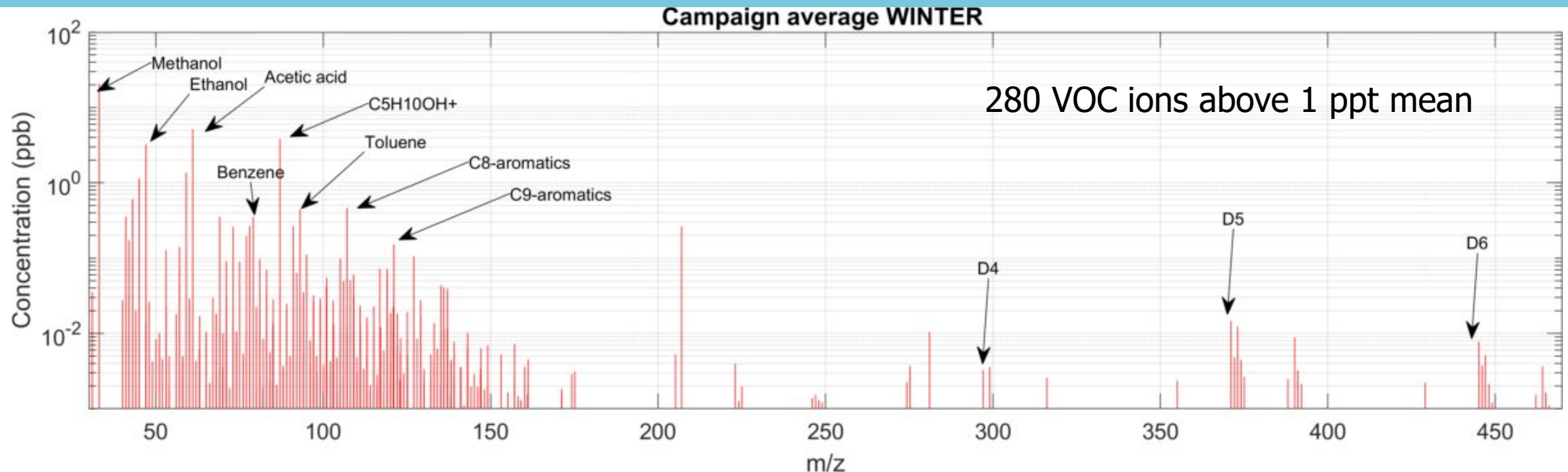
## Vocus 2R PTR-ToF (The “Sniffer”)



- Real Time (<1 s)
- Ultra-high mass resolution
- Sensitive to a broad range of compounds
- Limit of detection <1 ppt
- >1000 VOC ions measured at once
- Revolutionary applications in medical, environmental and industry

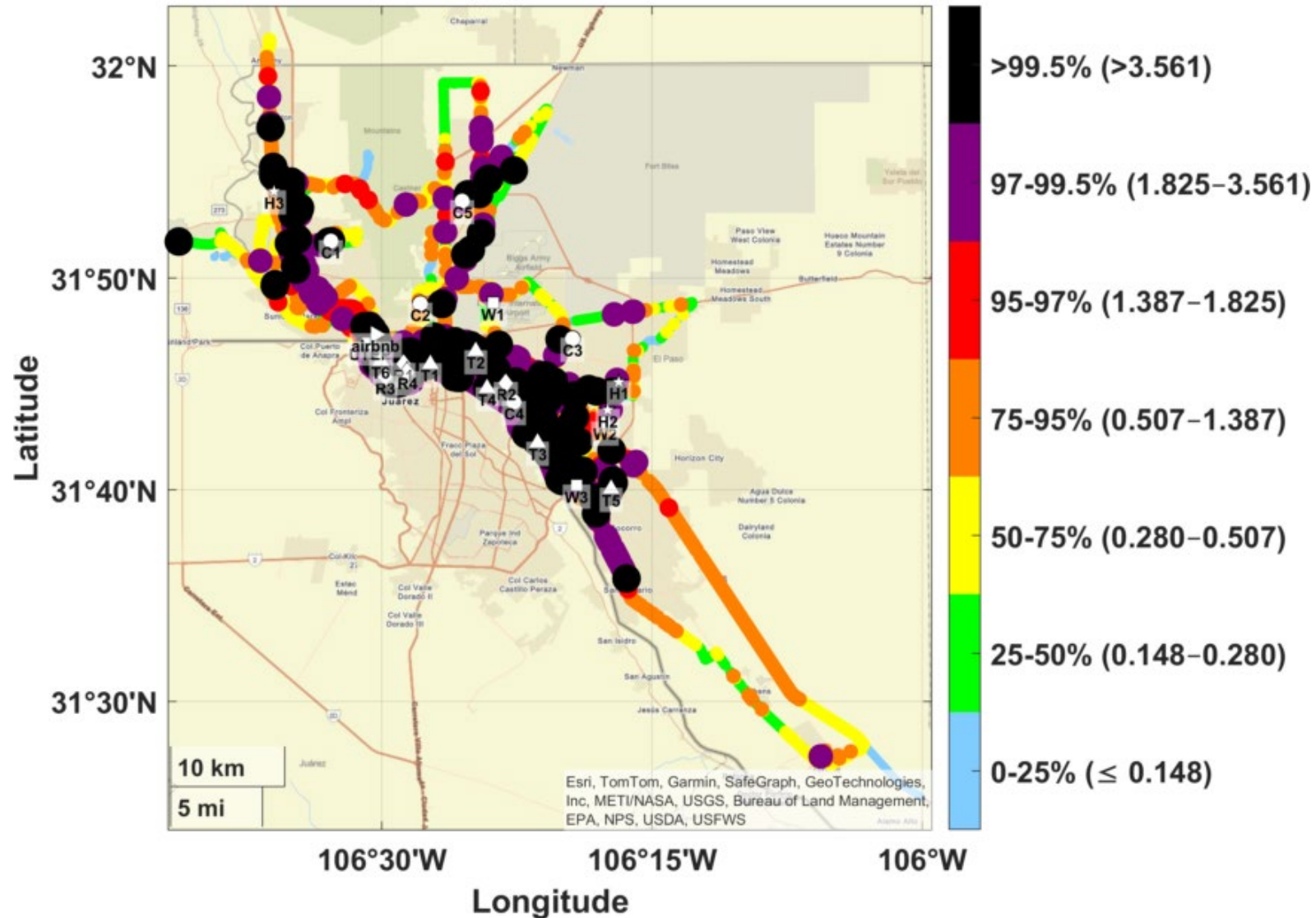


# What is the observed composition of Air in El Paso?



# What is Spatiotemporal Distribution of key VOC Concentrations?

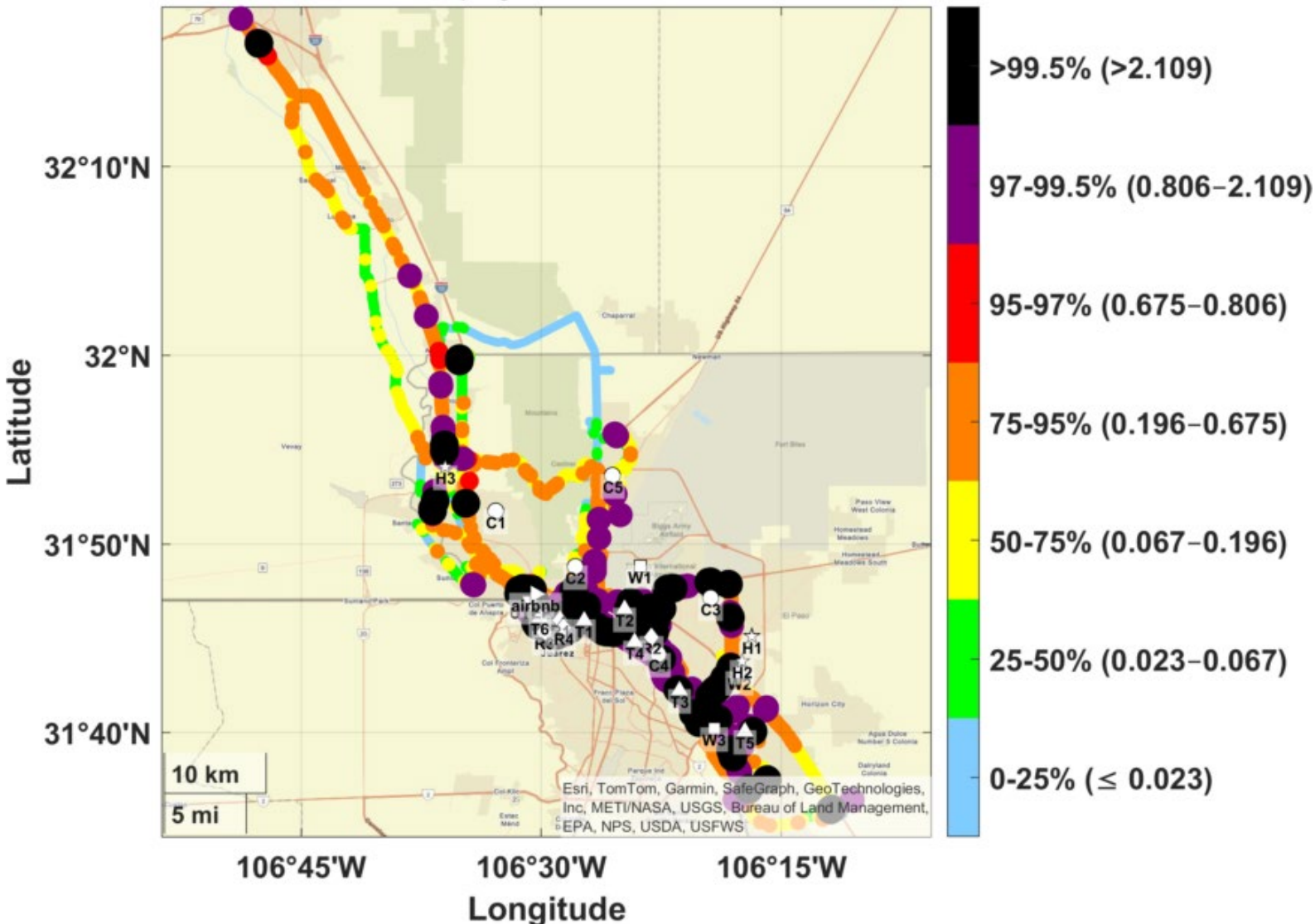
m/z 93.07: C<sub>7</sub>H<sub>8</sub>H<sup>+</sup> (ppb) WINTER



- Winter toluene was enhanced near the border
- Lower concentrations away from the border
- Local enhancements from fossil fuel combustion in New Mexico and north of El Paso

# What is Spatiotemporal Distribution of key VOC mixing ratios?

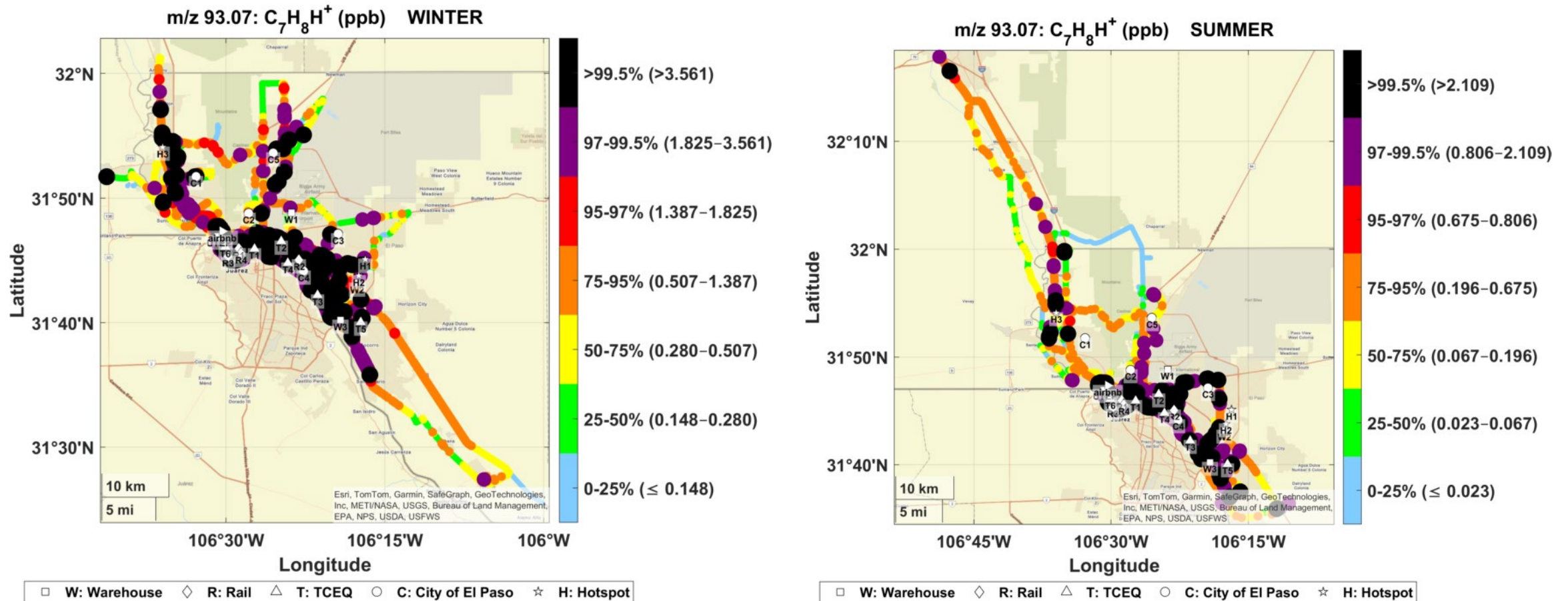
m/z 93.07:  $C_7H_8H^+$  (ppb) SUMMER



- Summer toluene mixing ratios were lower in summer compared to winter
- Consistent enhancements near the border as in winter
- Lower concentrations away from the border and in north El Paso

□ W: Warehouse    ◇ R: Rail    △ T: TCEQ    ○ C: City of El Paso    ☆ H: Hotspot

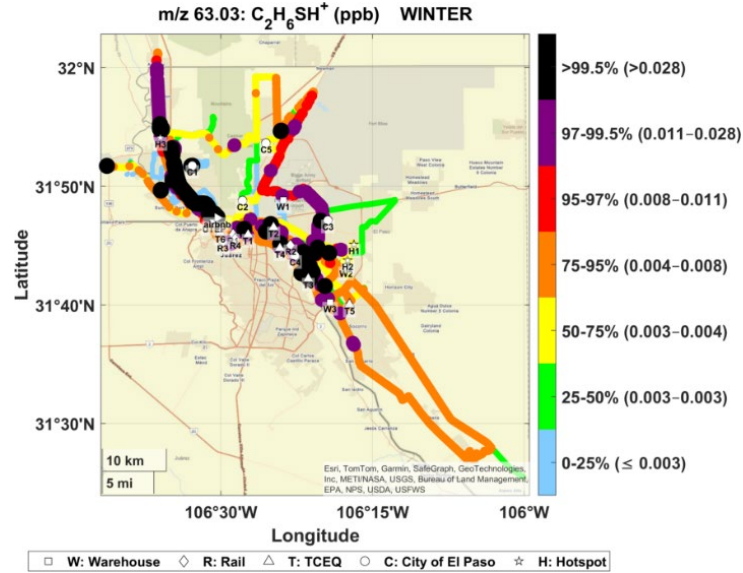
# What is Spatiotemporal Distribution of key VOC Concentrations?



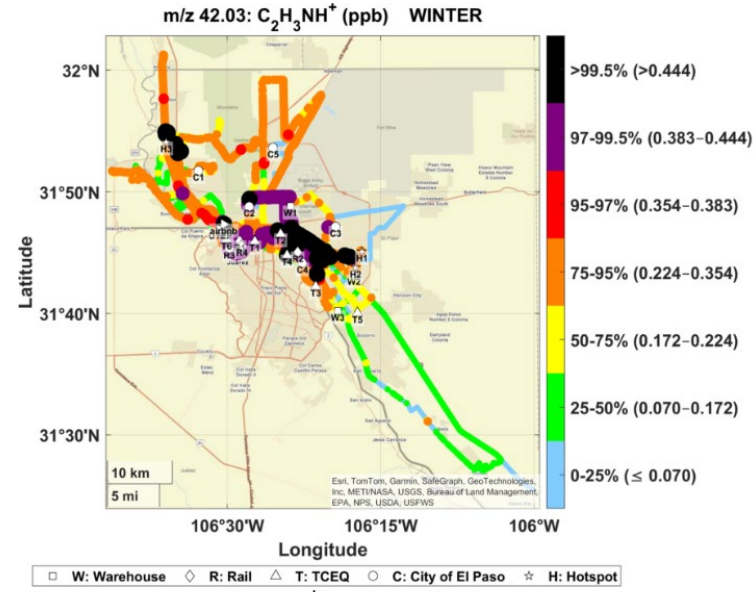
- Similar spatial patterns for toluene in each season
- Higher toluene concentrations in winter

# What is Spatiotemporal Distribution of key VOC Concentrations?

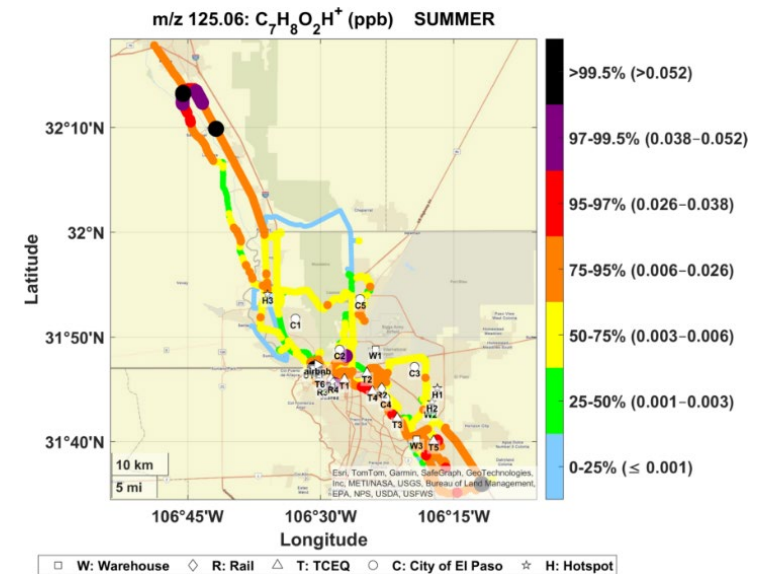
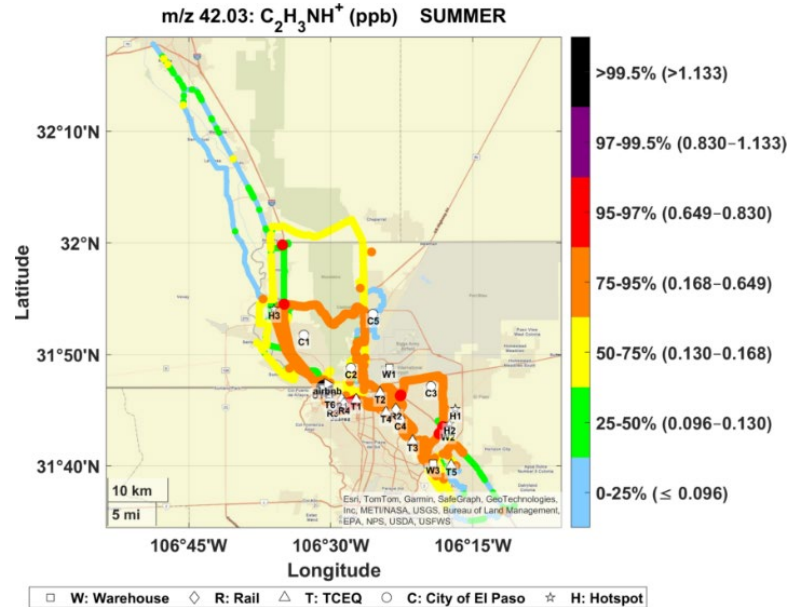
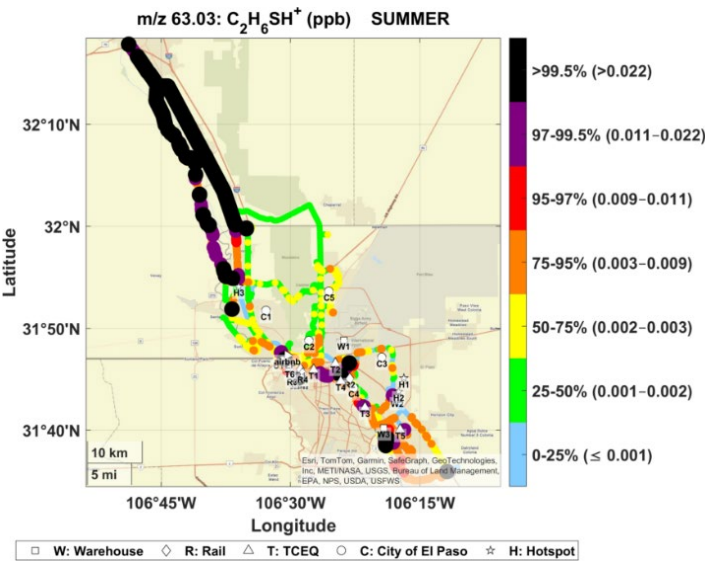
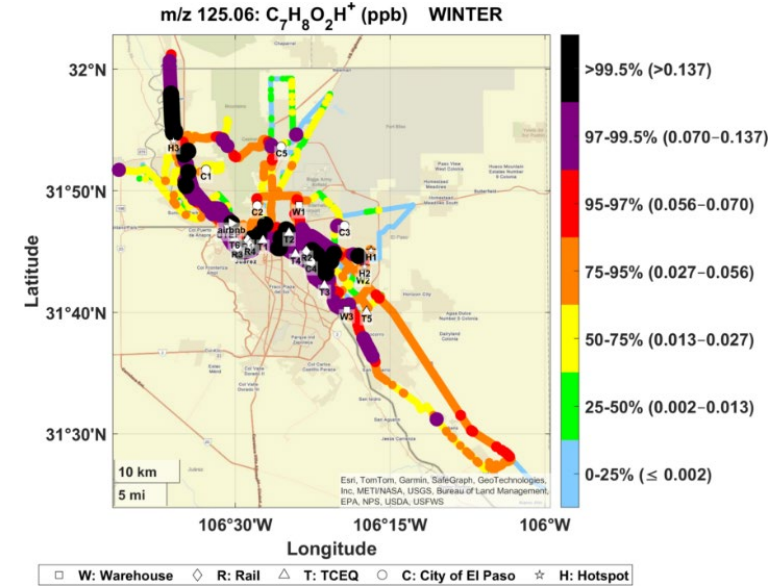
## DMS+ Ethanethiol



## Acetonitrile

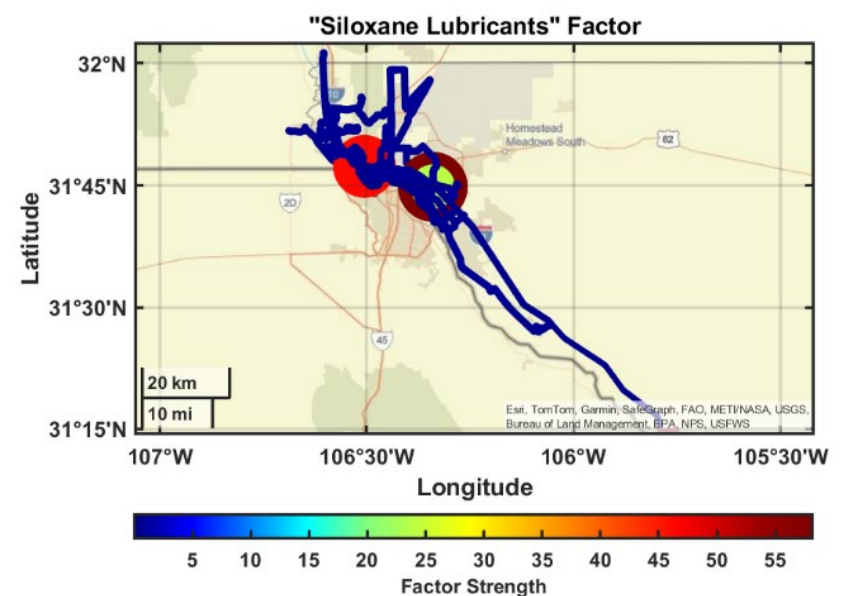
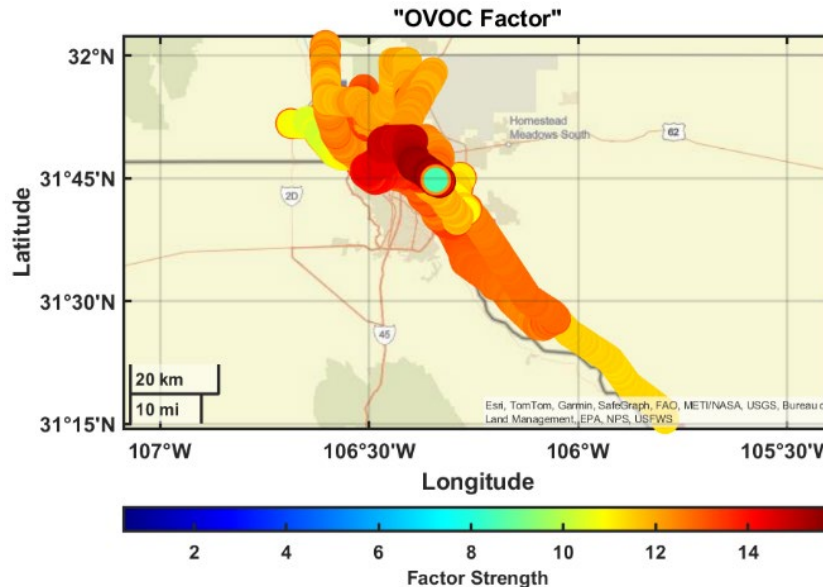
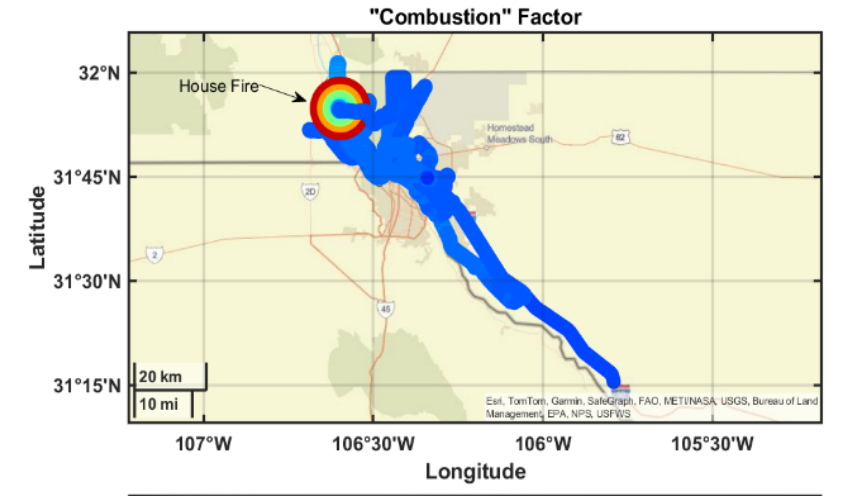
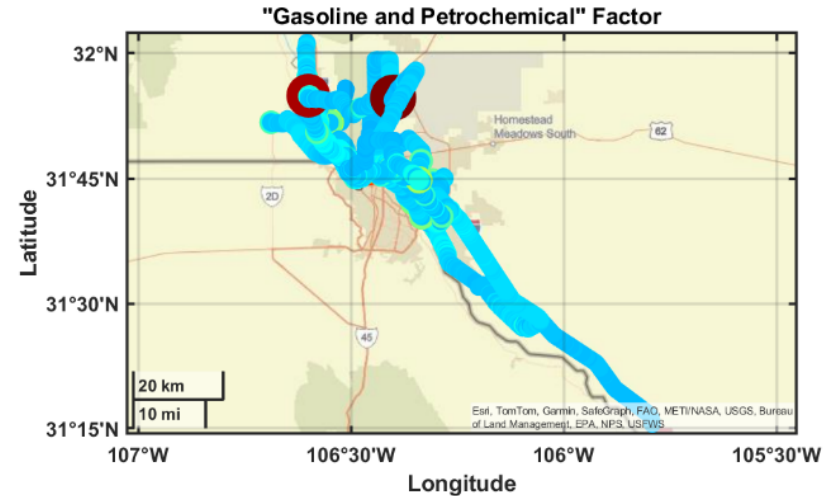
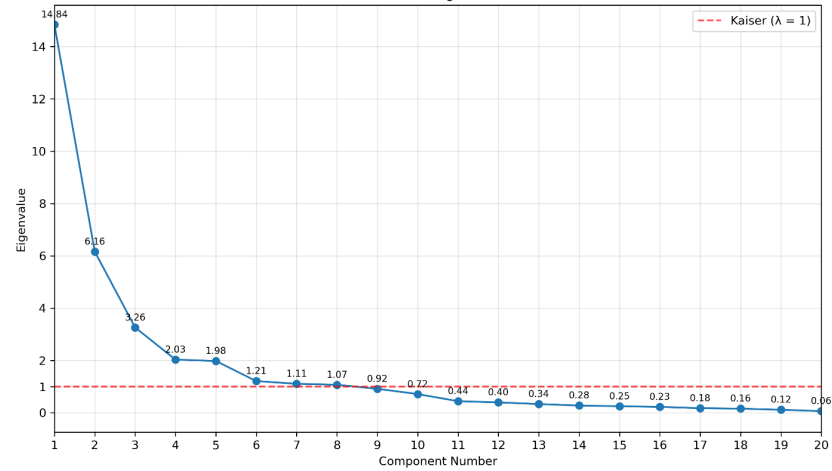


## Guaiacol



# Preliminary Source Apportionment – Factor Analysis

Scree Plot (Eigenvalues)



## Factor Analysis Model on Measurement Data

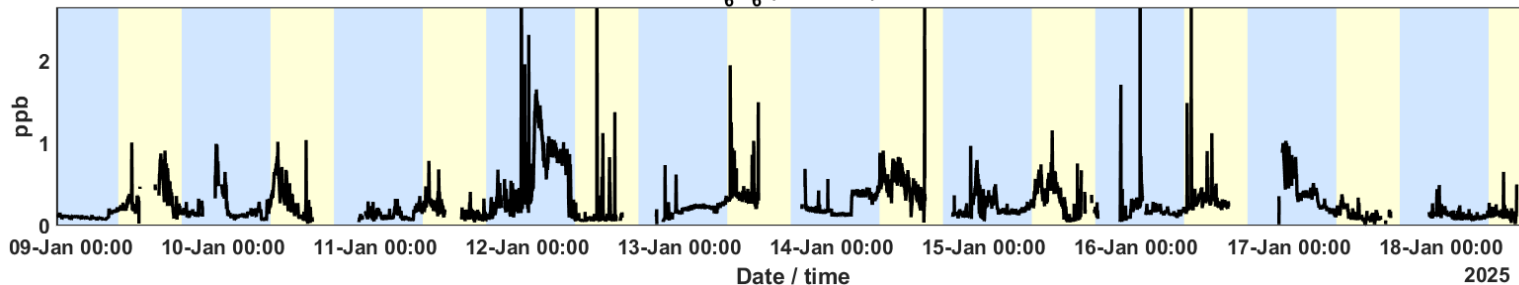
- $X = \Lambda F + \epsilon X$
- $X$  is the vector of observed variables.
- $\Lambda$  is the matrix of factor loadings.
- $F$  is the vector of factors.
- $\epsilon$  is the vector of unique factors (error terms).

Worton, D. R., Goldstein, A. H., Farmer, D. K., Docherty, K. S., Jimenez, J. L., Gilman, J. B., Kuster, W. C., de Gouw, J., Williams, B. J., Kreisberg, N. M., Hering, S. V., Bench, G., McKay, M., Kristensen, K., Glasius, M., Surratt, J. D., and Seinfeld, J. H.: Origins and composition of fine atmospheric carbonaceous aerosol in the Sierra Nevada Mountains, California, *Atmos. Chem. Phys.*, 11, 10219–10241, <https://doi.org/10.5194/acp-11-10219-2011>, 2011.

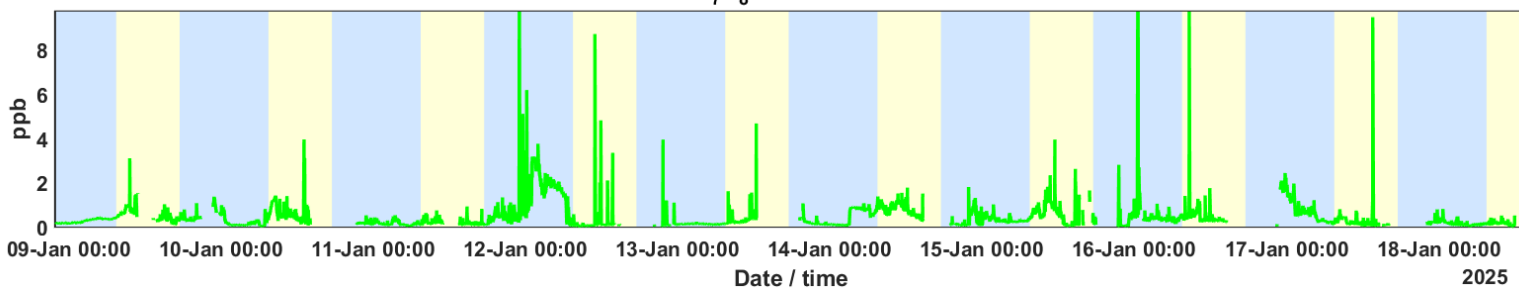
# Stationary Observations at UTEP - WINTER

UTEP - AirbnB site

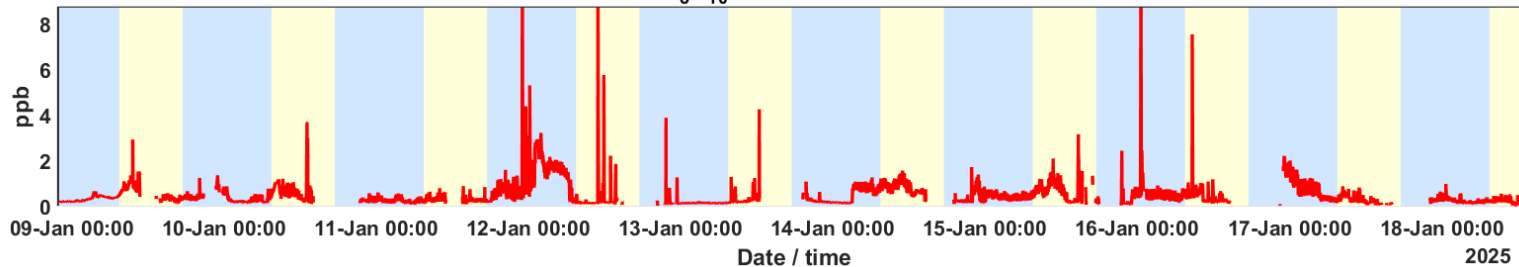
$C_6H_6^+$  (Benzene)



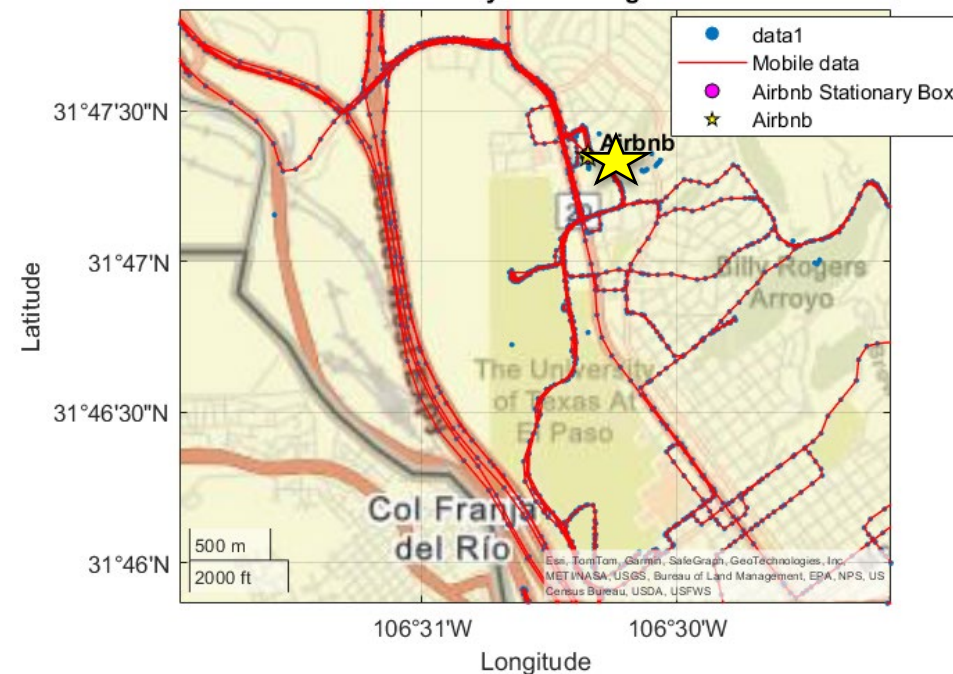
$C_7H_8H^+$  (Toluene)



$C_8H_{10}H^+$  (C8-Aromatics)

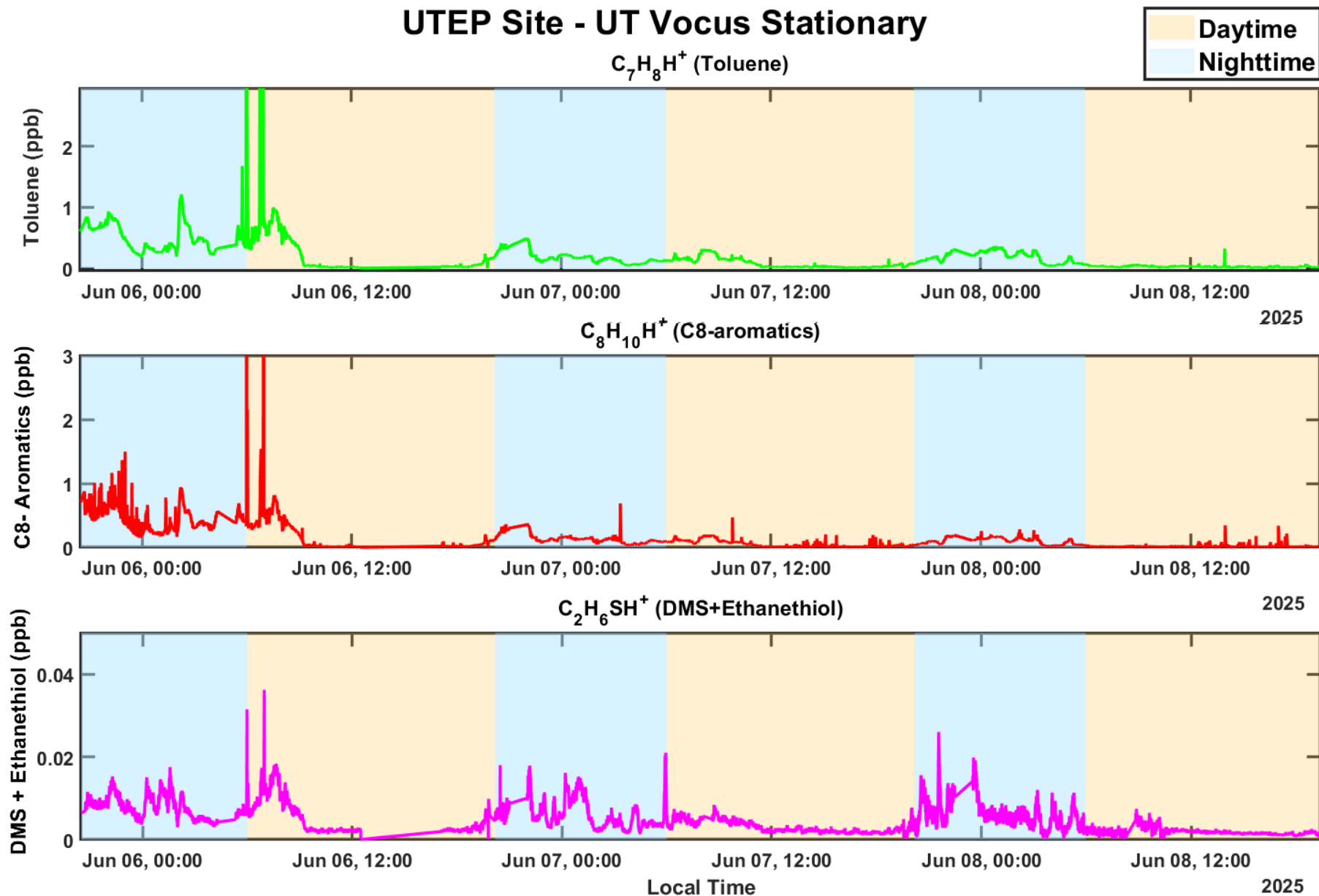


AirBnB Stationary Site during Winter 2025



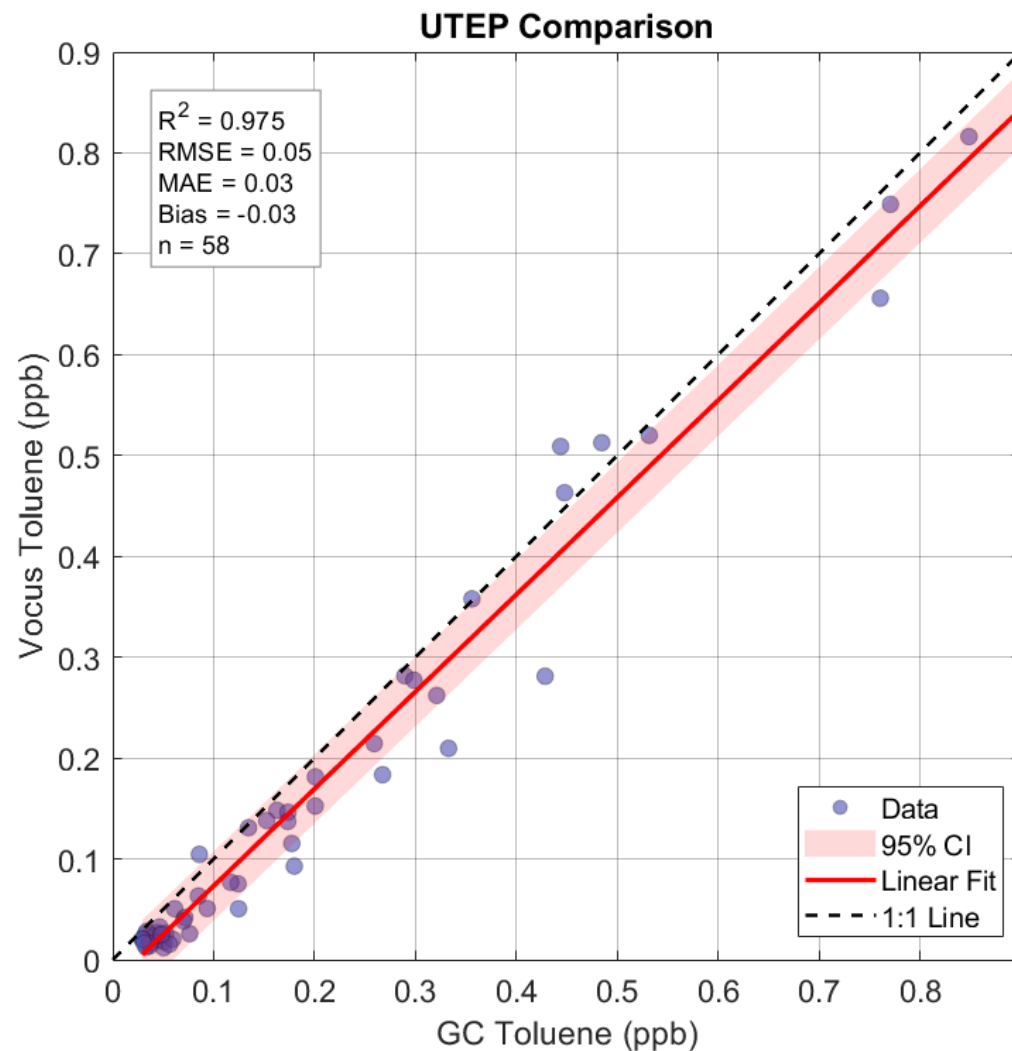
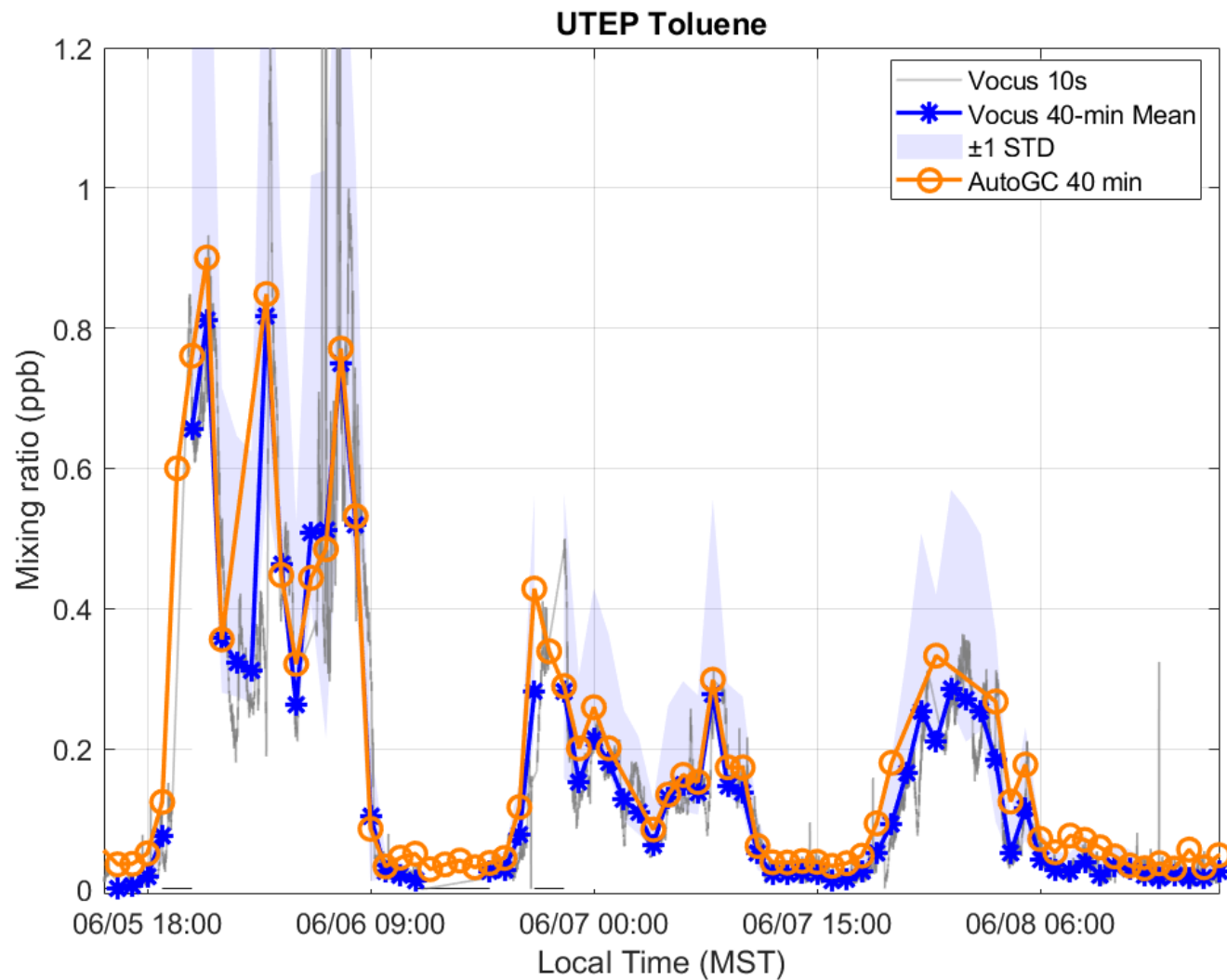
- Nighttime periods higher mixing ratios likely from Juarez air shed. Sometimes, plumes also arriving during the day
- Examples VOCs shown are benzene, toluene, and C8-aromatics

# Stationary Colocation at UTEP Monitoring Site



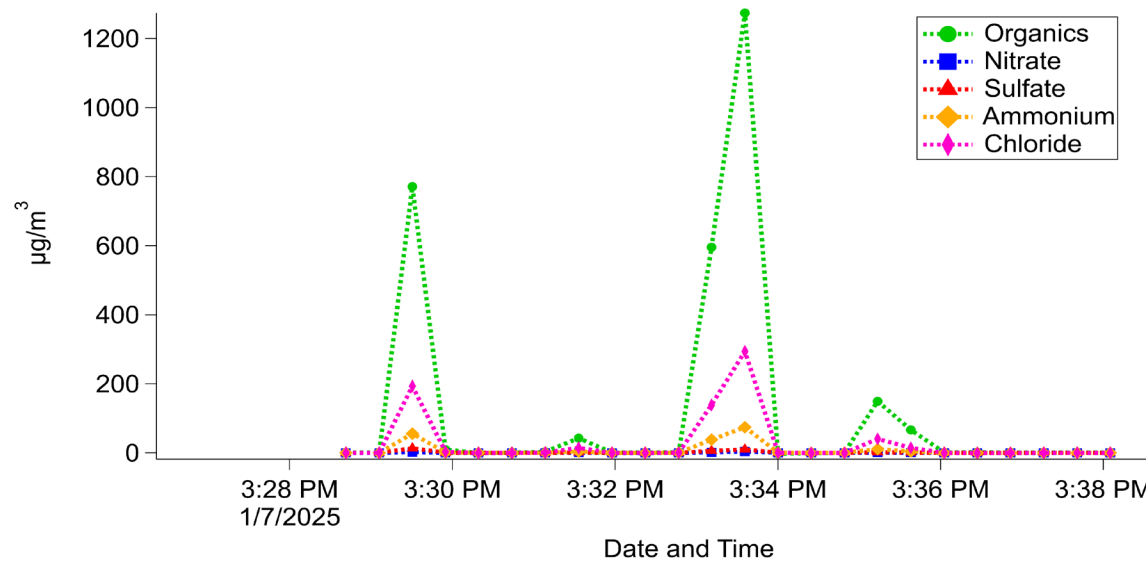
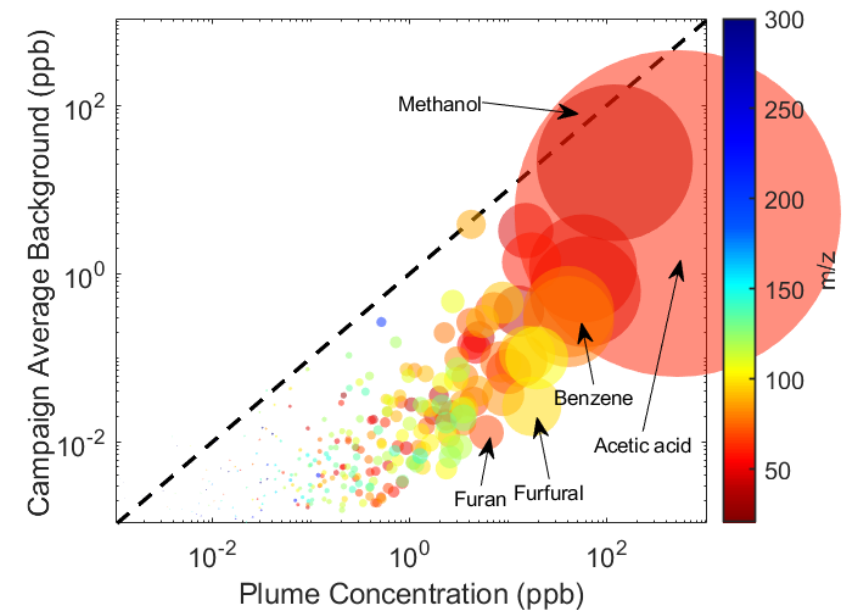
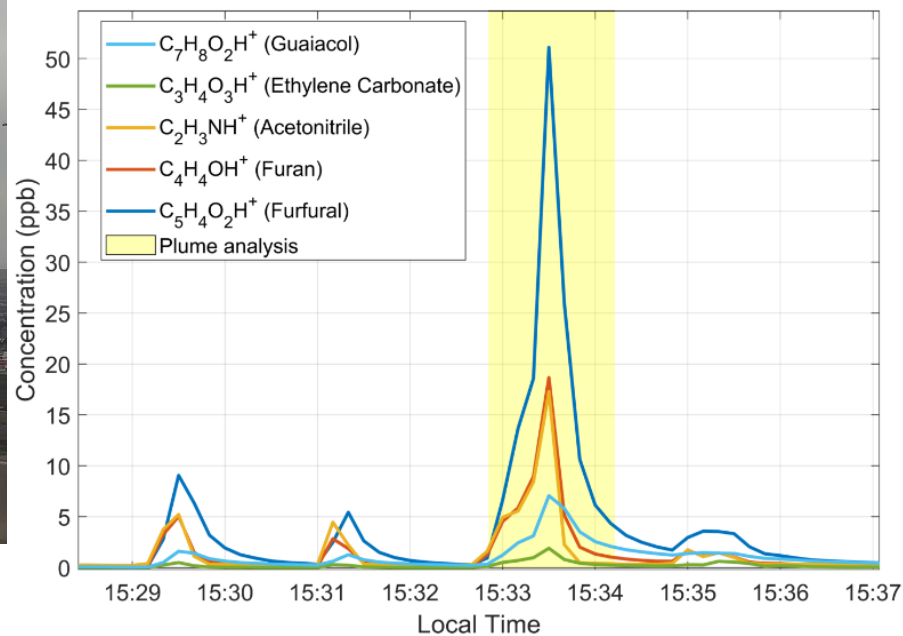
- Nighttime features higher mixing ratios likely from Juarez air shed
- Examples VOCs shown are toluene, C8-aromatics and DMS+Ethanethiol

# Stationary Colocation at UTEP Monitoring Site



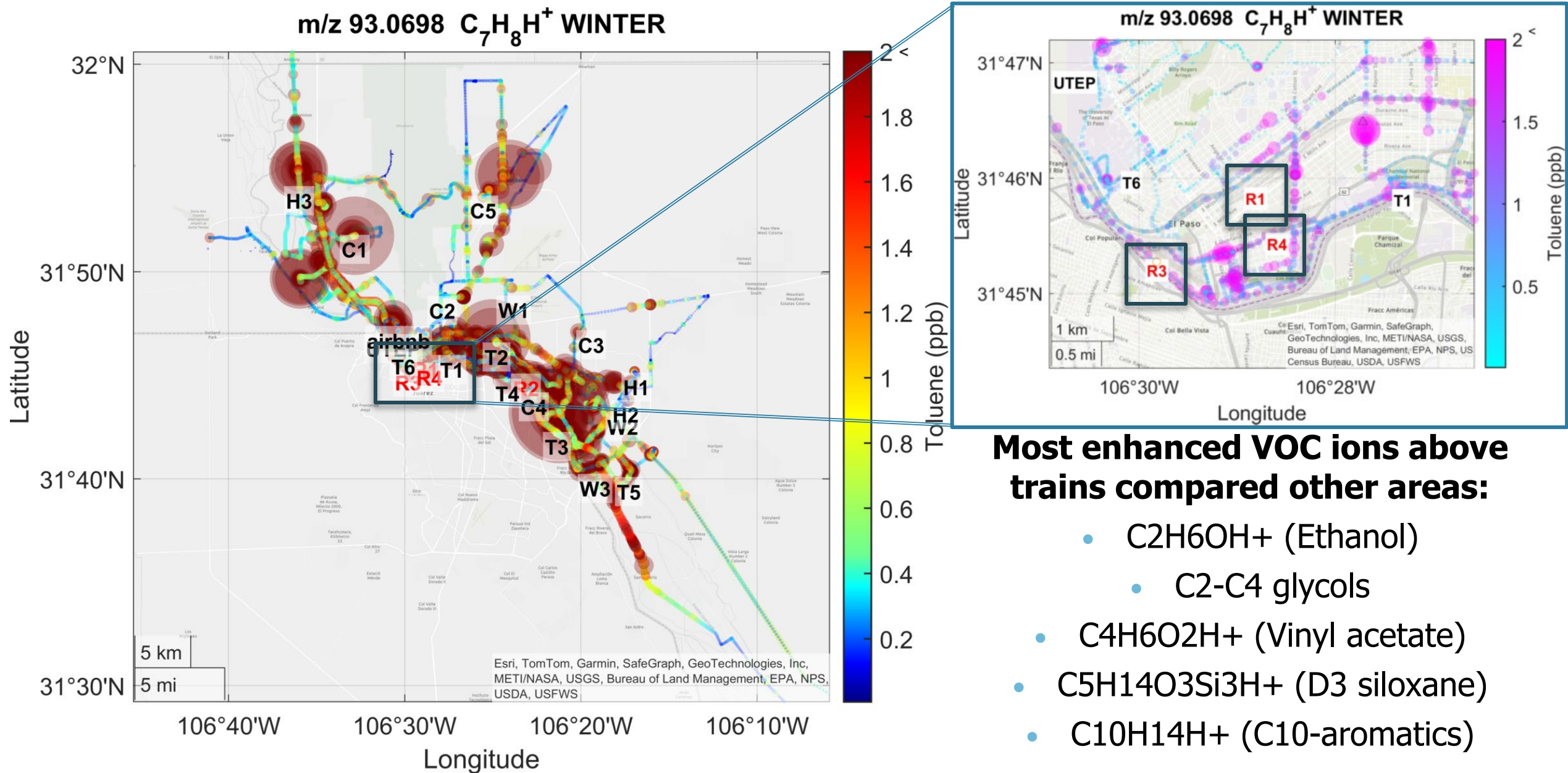
Excellent agreement for toluene between the GC and the Vocus

# Acute Sources: House Fire



Particles and VOCs  
order of magnitude  
increase in the  
dilute smoke

# Special Case - Trains



## Gas Phase - Summary

- Collected comprehensive spatiotemporal gas-phase observations in two seasons in El Paso
- VOC concentrations higher in Winter
- Fingerprinted numerous near-source plumes, acute events, regional backgrounds and collocated with monitoring stations
- Drives near the border featured the highest toluene enhancements along with other combustion and solvent related compounds
- Stationary observations showed high diel variability with VOCs accumulating in the shallow boundary layer at night, often from the Juarez air shed
- The data has potential to complement PM, O<sub>3</sub>, and VOC source apportionment and complement modeling efforts

# Particle Phase Observations

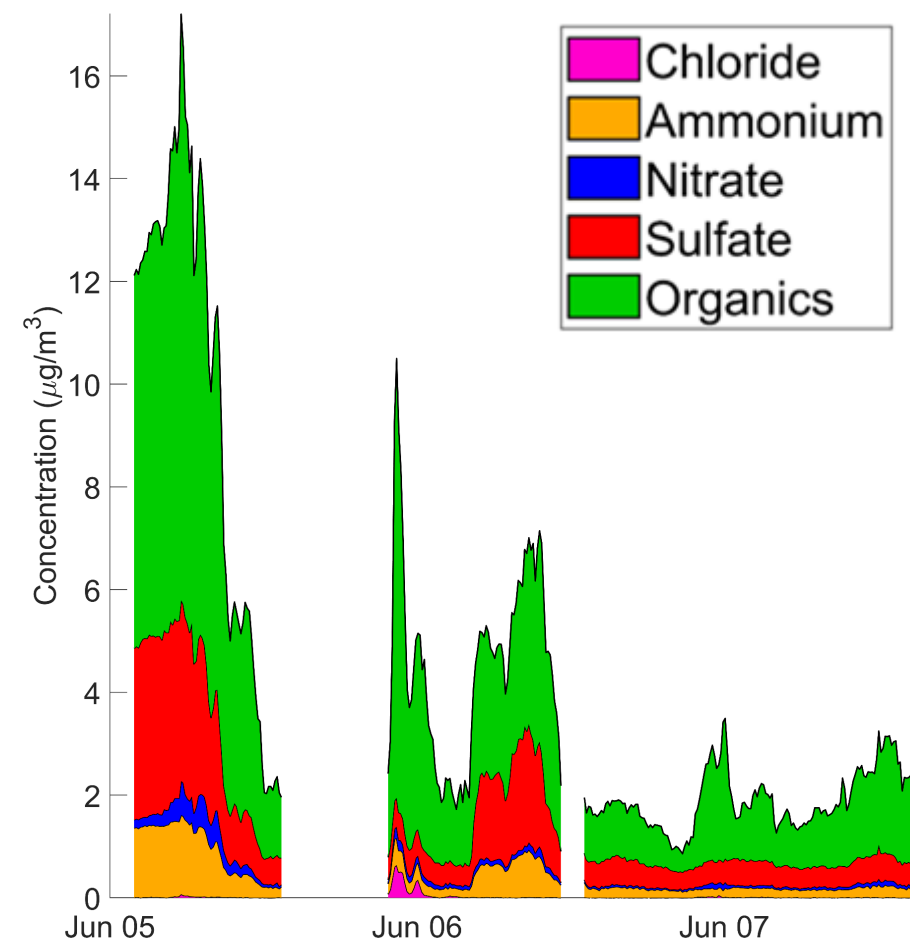
# High Resolution Time of Flight Aerosol Mass Spectrometer (HR-ToF-AMS)



Flash-vaporizes particles at 600°C

Uses electron-impact ionization

Measures size-resolved, non-refractory PM<sub>1</sub> composition.



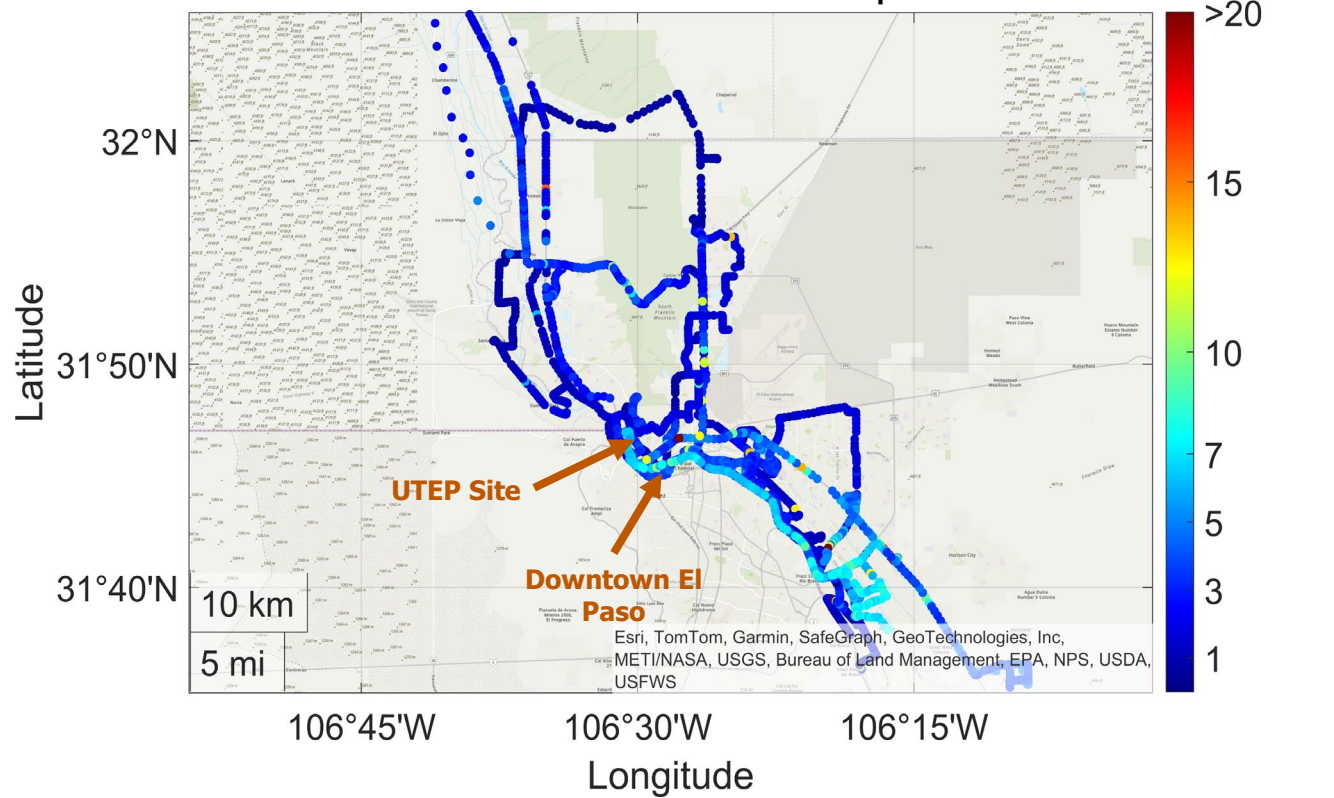
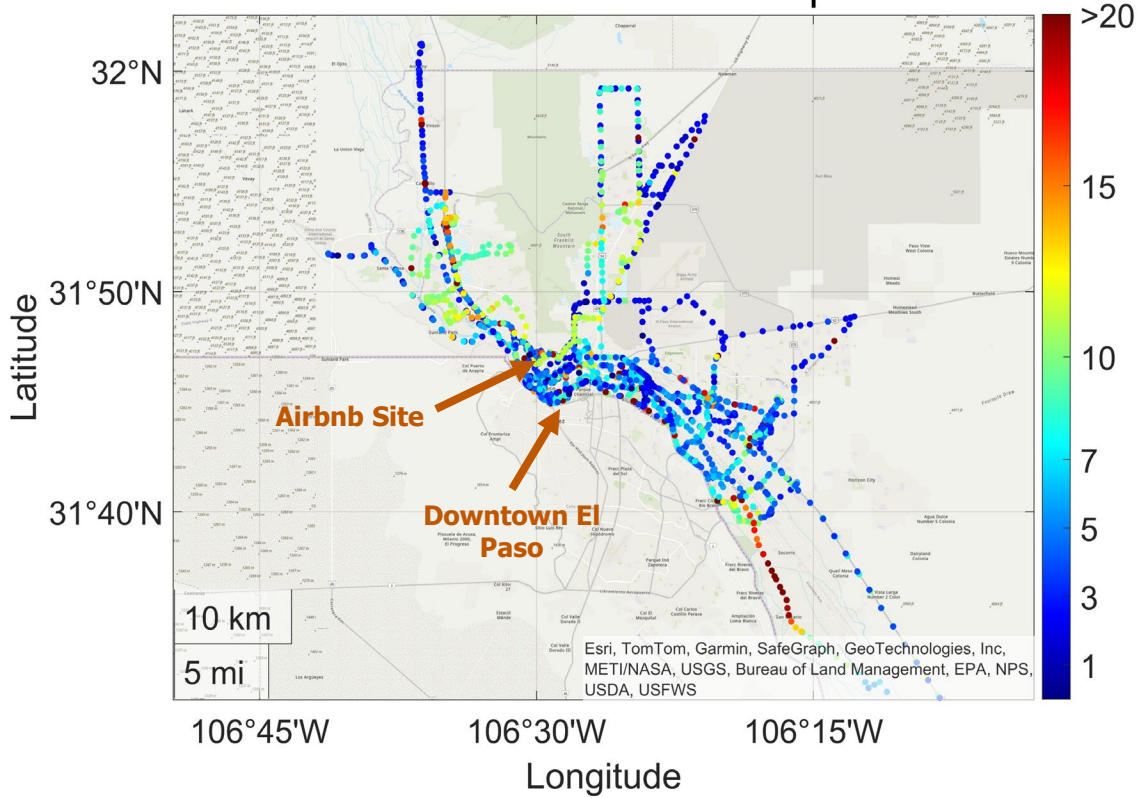
# What is the Spatiotemporal Distribution of Non-refractory PM<sub>1</sub>?

Winter (January 2025)

Summer (May/June 2025)

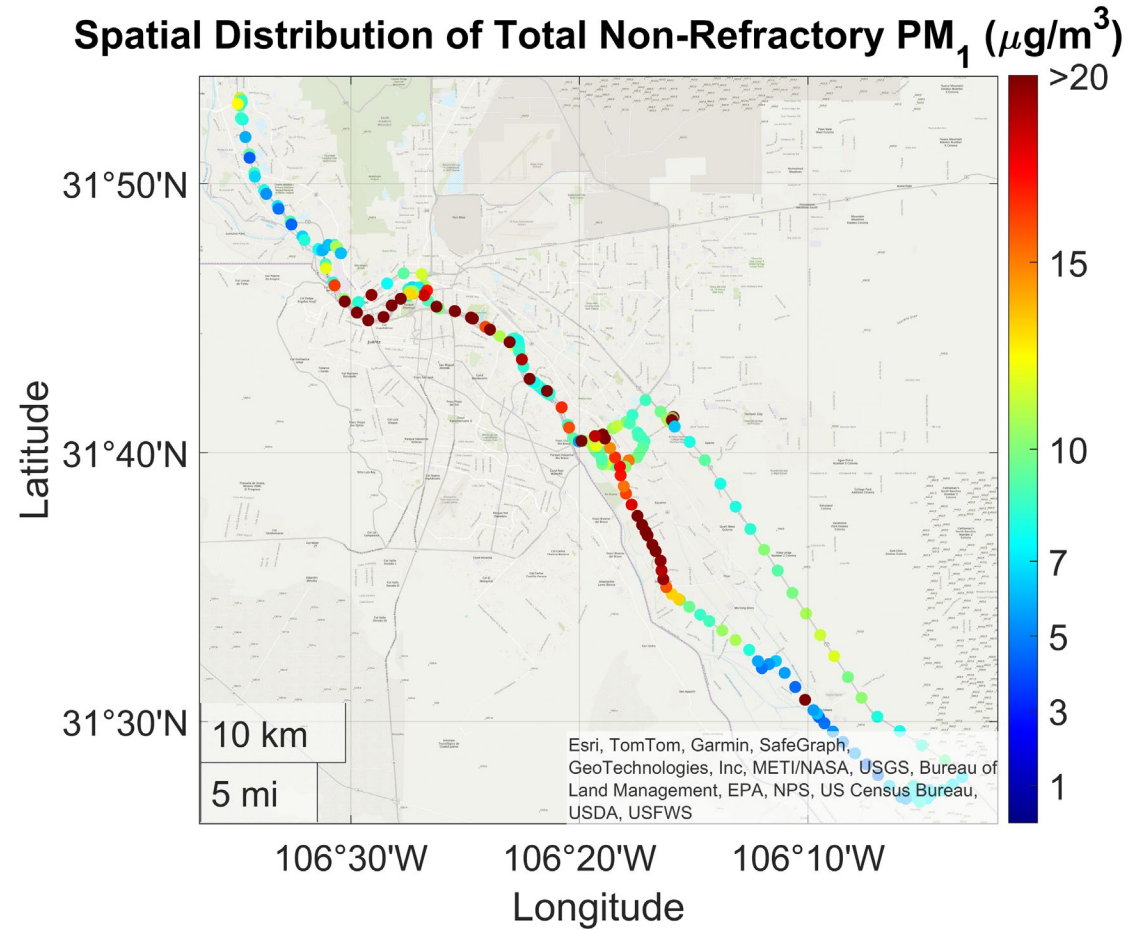
Spatial Distribution of Total Non-Refractory PM<sub>1</sub> (ug/m<sup>3</sup>), January 2025

Spatial Distribution of Total Non-Refractory PM<sub>1</sub> (μg/m<sup>3</sup>), May/June 2025



Overall higher concentrations in the winter than in the summer

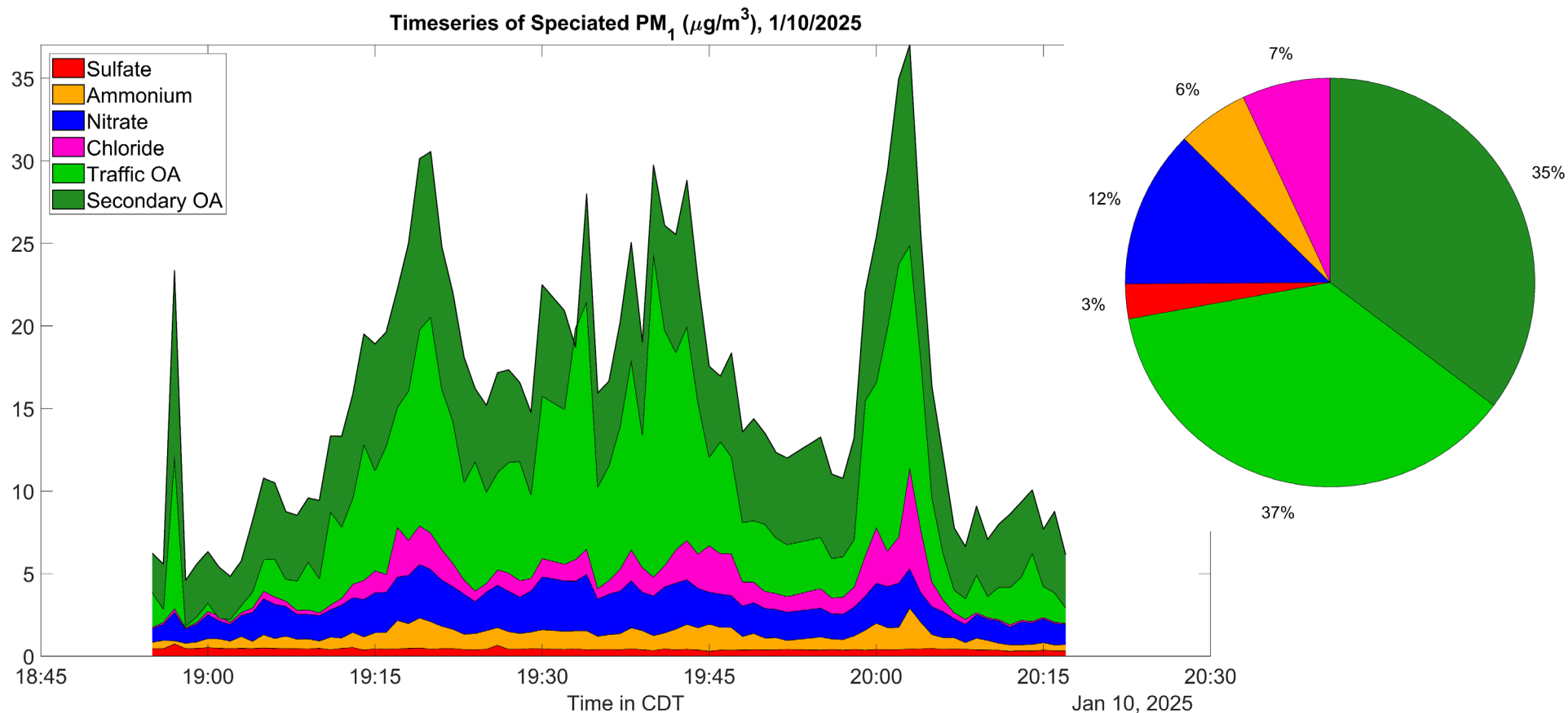
# Periodically Elevated PM1 Near the Mexico/USA Border



Mobile Measurements on January 10, 2025

Wind was coming from the West during this time, consistent with cross border transport

# Mostly Organic Aerosol Along the Border, Strong Influence of Traffic

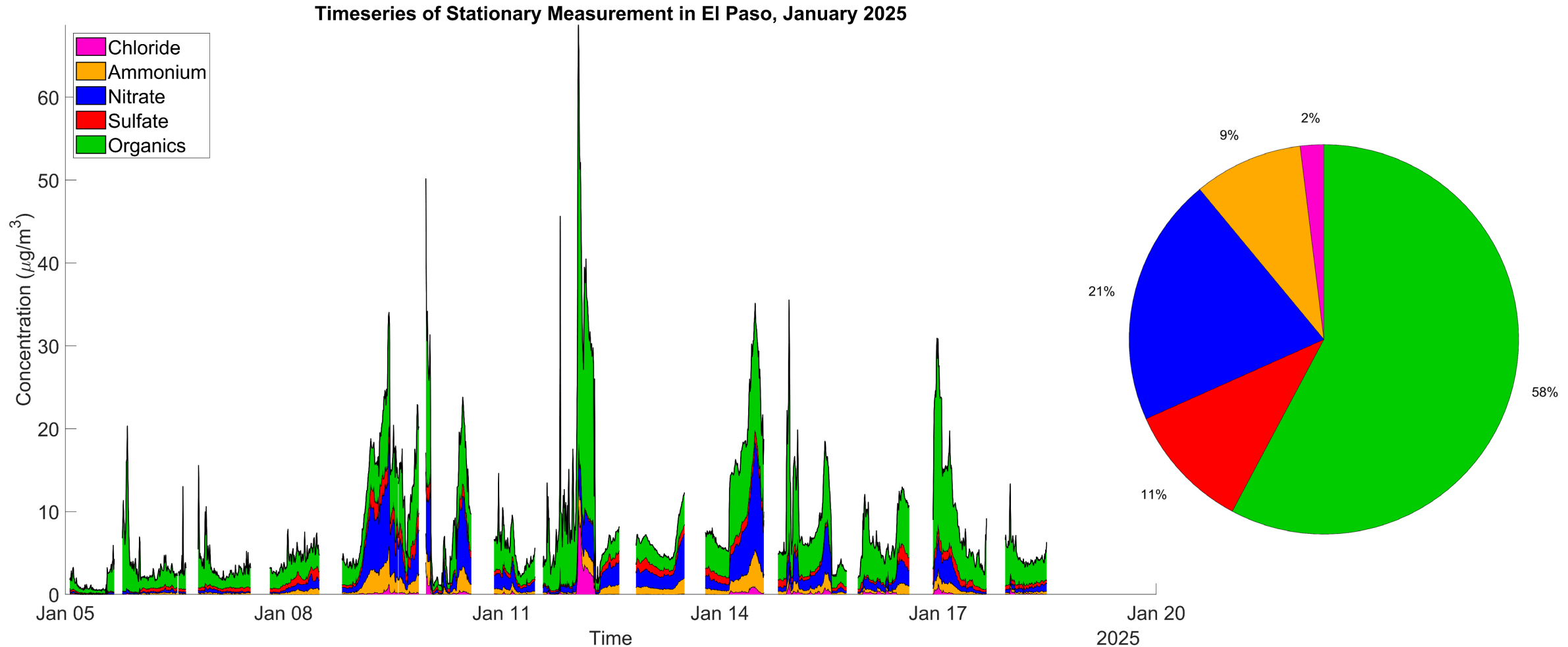


Composition of PM along the border on January 10, 2025

Separation of OA into traffic and secondary is estimated based on correlations.

Full positive matrix factorization, which may resolve additional sources, will be done as part of future/ongoing work

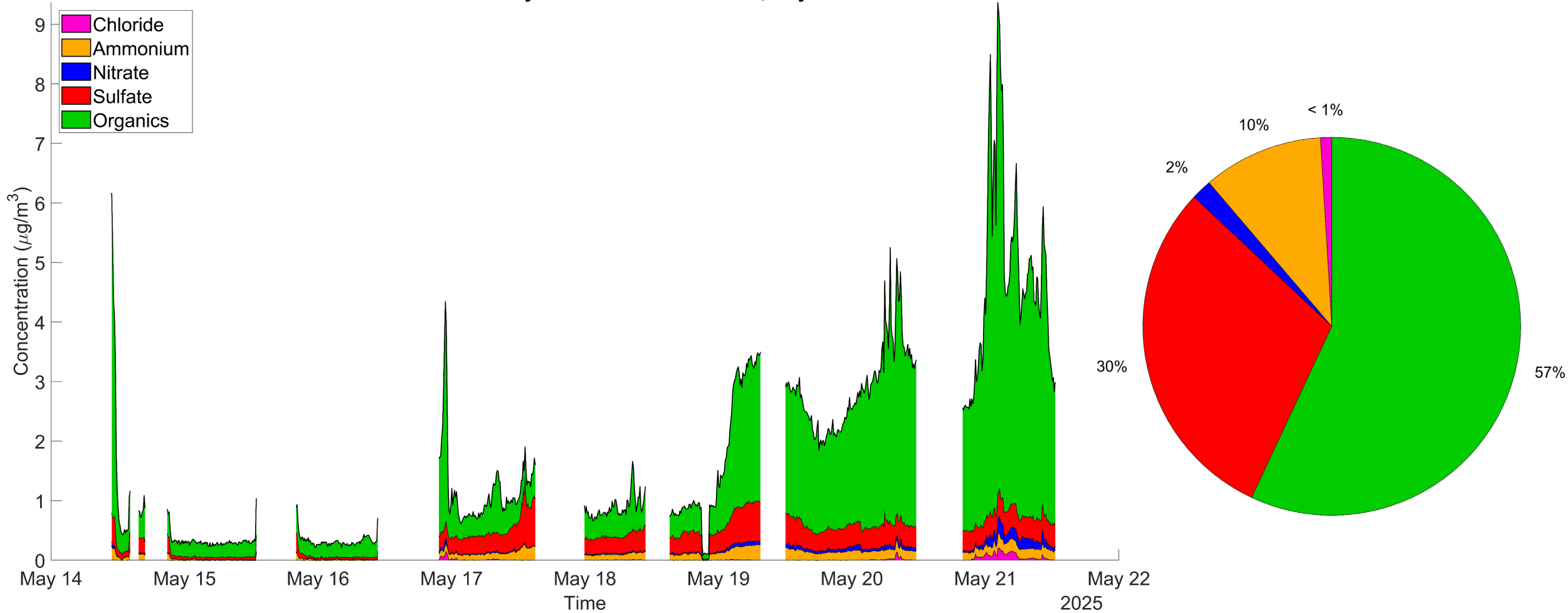
# Stationary Measurements: Winter (Airbnb near UTEP)



High concentrations, and higher levels of ammonium nitrate and ammonium chloride in winter, in part due to semi-volatile nature of PM. Impacts of different sources (vs. thermodynamics) will be clearer after detailed positive matrix factorization analysis.

# Stationary Measurements: Summer 1 (UTEP)

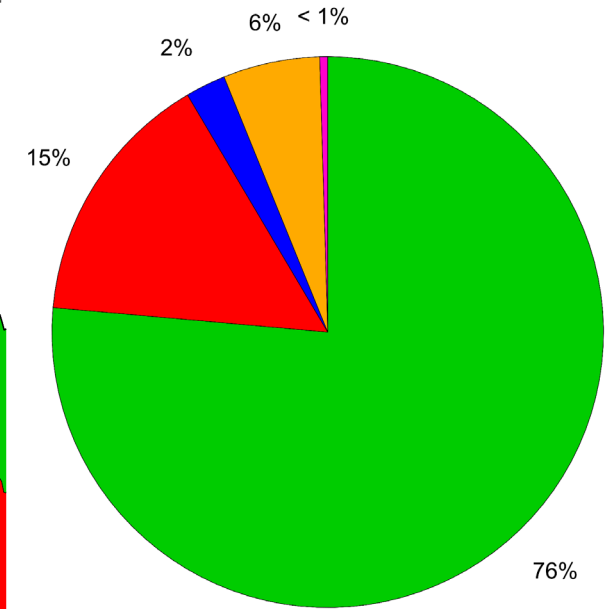
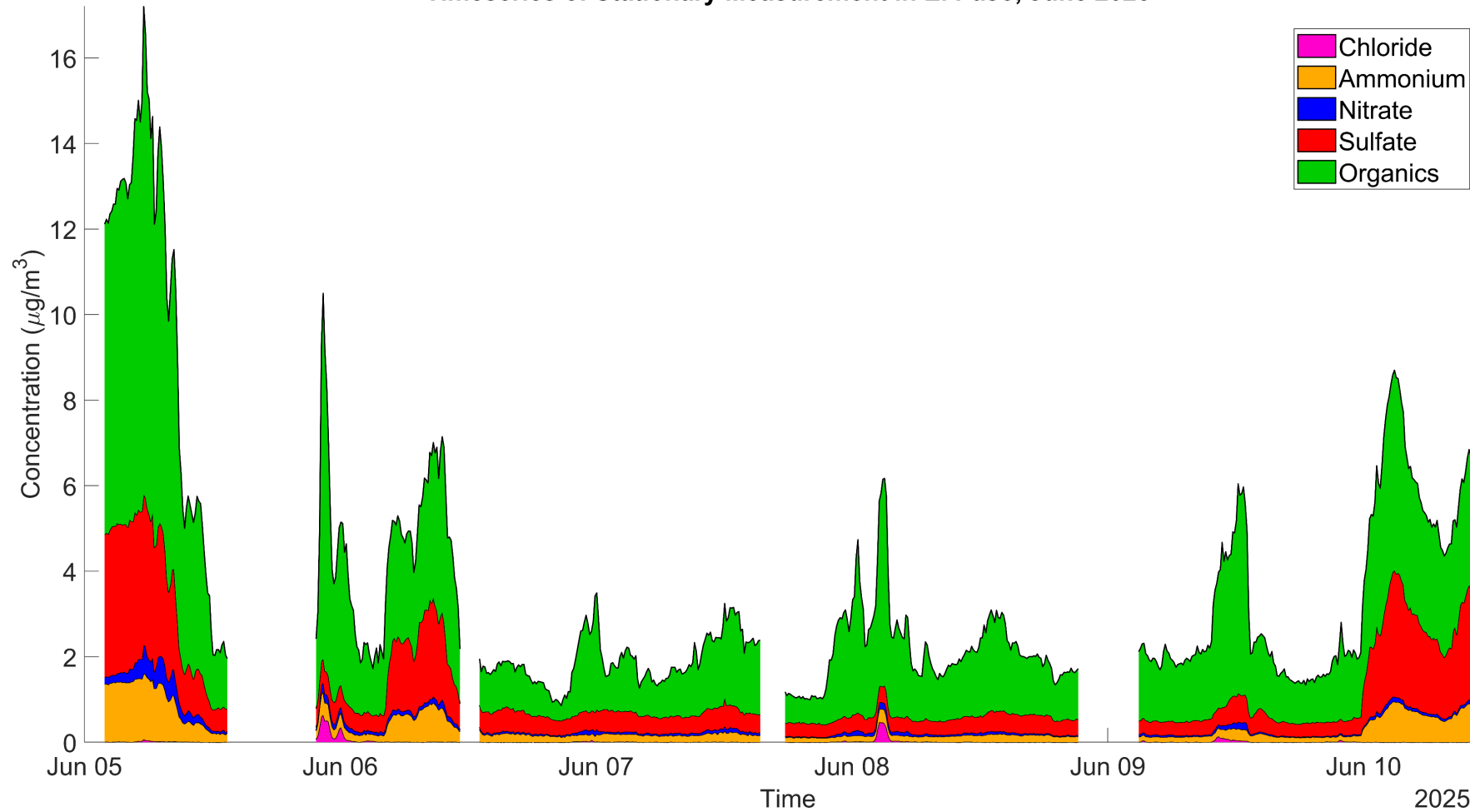
Timeseries of Stationary Measurement in El Paso, May 2025



Overall lower concentrations in summer than winter. Very low concentrations at the beginning of this campaign due to a sand storm (which scavenges small particles)

# Stationary Measurements: Summer 2 (UTEP)

Timeseries of Stationary Measurement in El Paso, June 2025



Heat wave during the measurements in June.

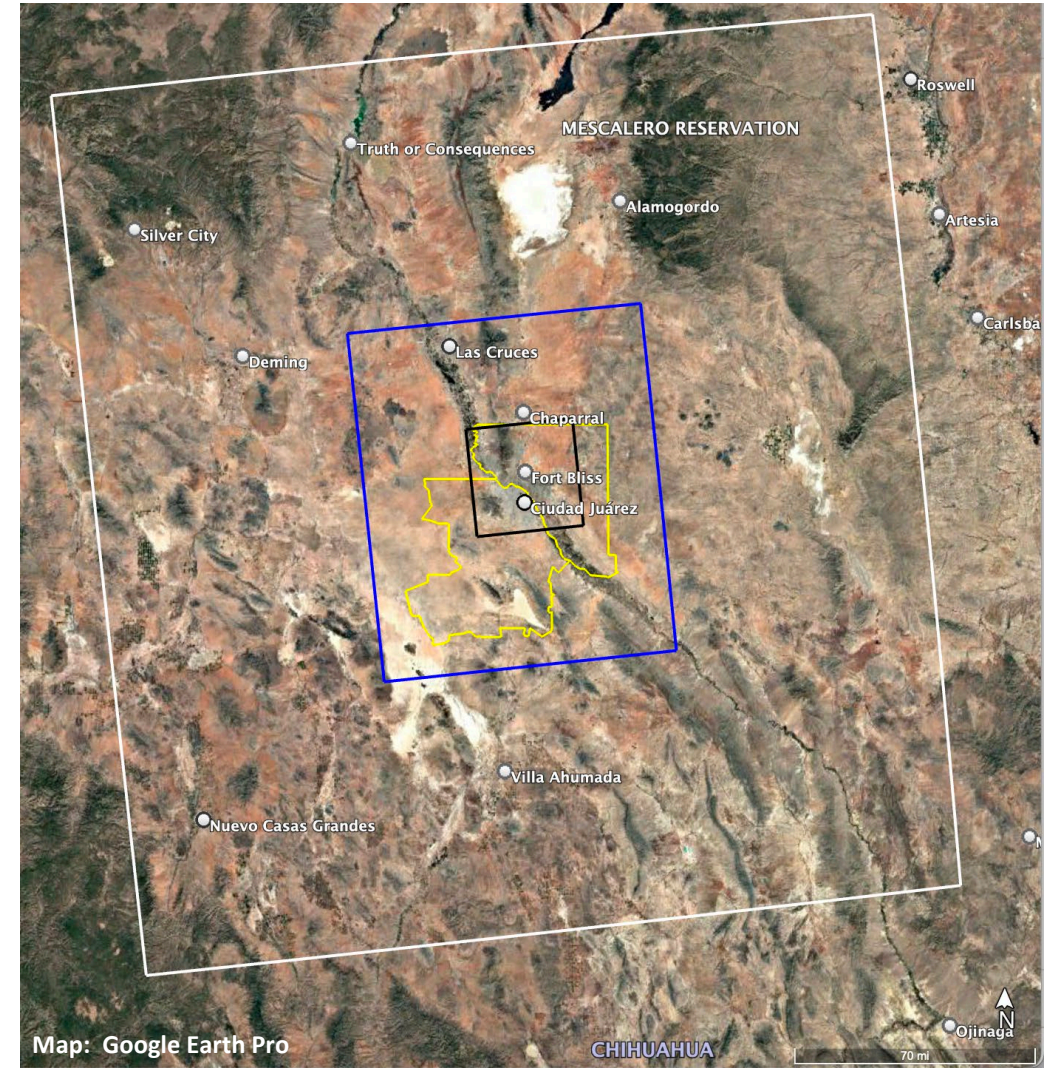
## PM Observations - Summary

- Higher concentrations in winter than summer
- Large spatiotemporal variability in concentrations and composition
- Numerous hotspots measured throughout each campaign
- Cross-border transport appears to influence PM concentration and composition
- Detailed source apportionment methods (e.g. positive matrix factorization) are expected to further identify sources and processes responsible for PM in El Paso

# Modeling

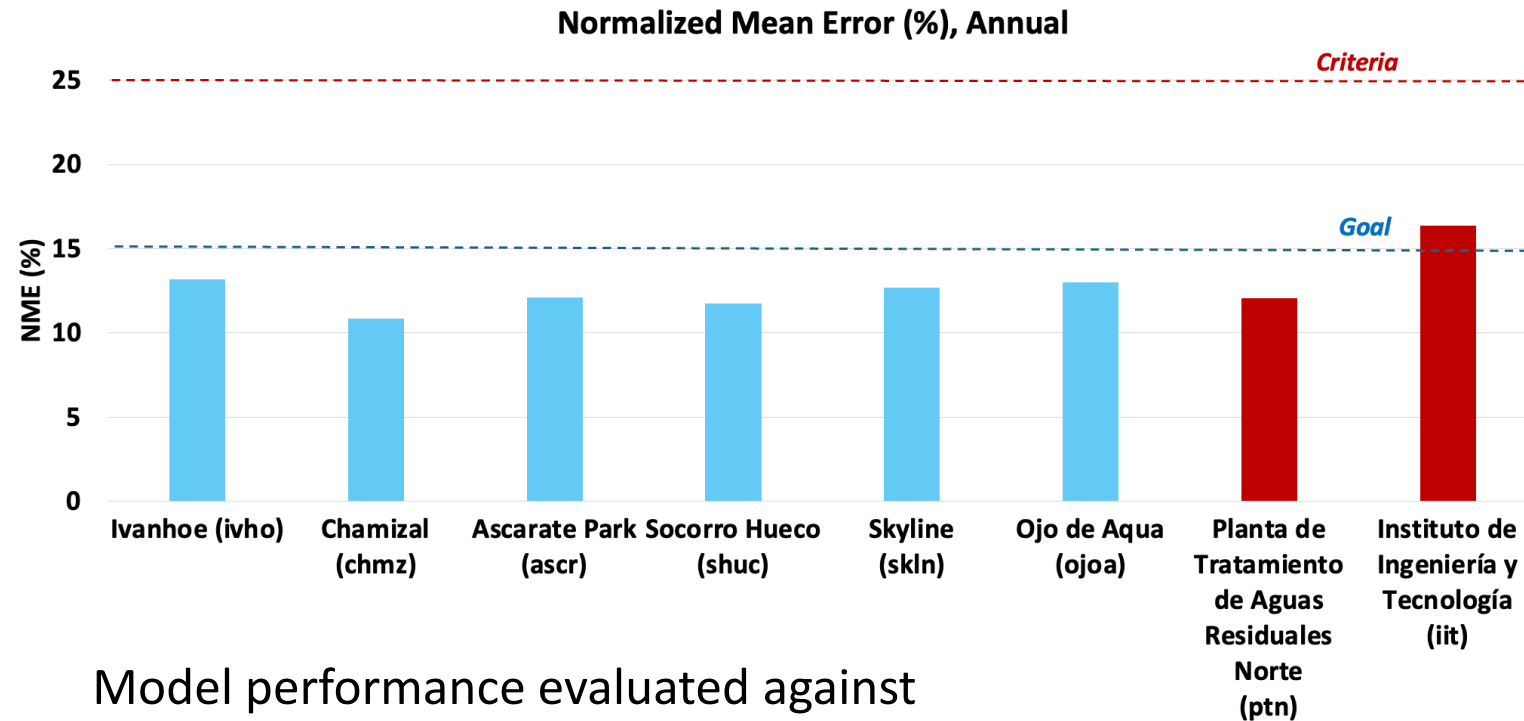
# El Paso-Juárez 2022 Photochemical Modeling Platform

- Developed from EPA Office of Air Quality Planning and Standards (OAQPS) 2022 Modeling Platform that had 12-km horizontal resolution over CONUS and border states in Mexico<sup>1</sup>
- WRF v4.4.2 meteorological fields
- EPA 2022v1 emissions modeling platform<sup>2</sup>
- CAMx version 7.20
  - Reactive Tracer (RTRAC) algorithm for explicit simulation and source tagging for air toxics
  - CB6r5 gas-phase chemical mechanism
  - CF aerosol option
  - Zhang dry deposition



CAMx 12-km (white) and flexi-nested 4-km (blue) and 1-km (black) domains

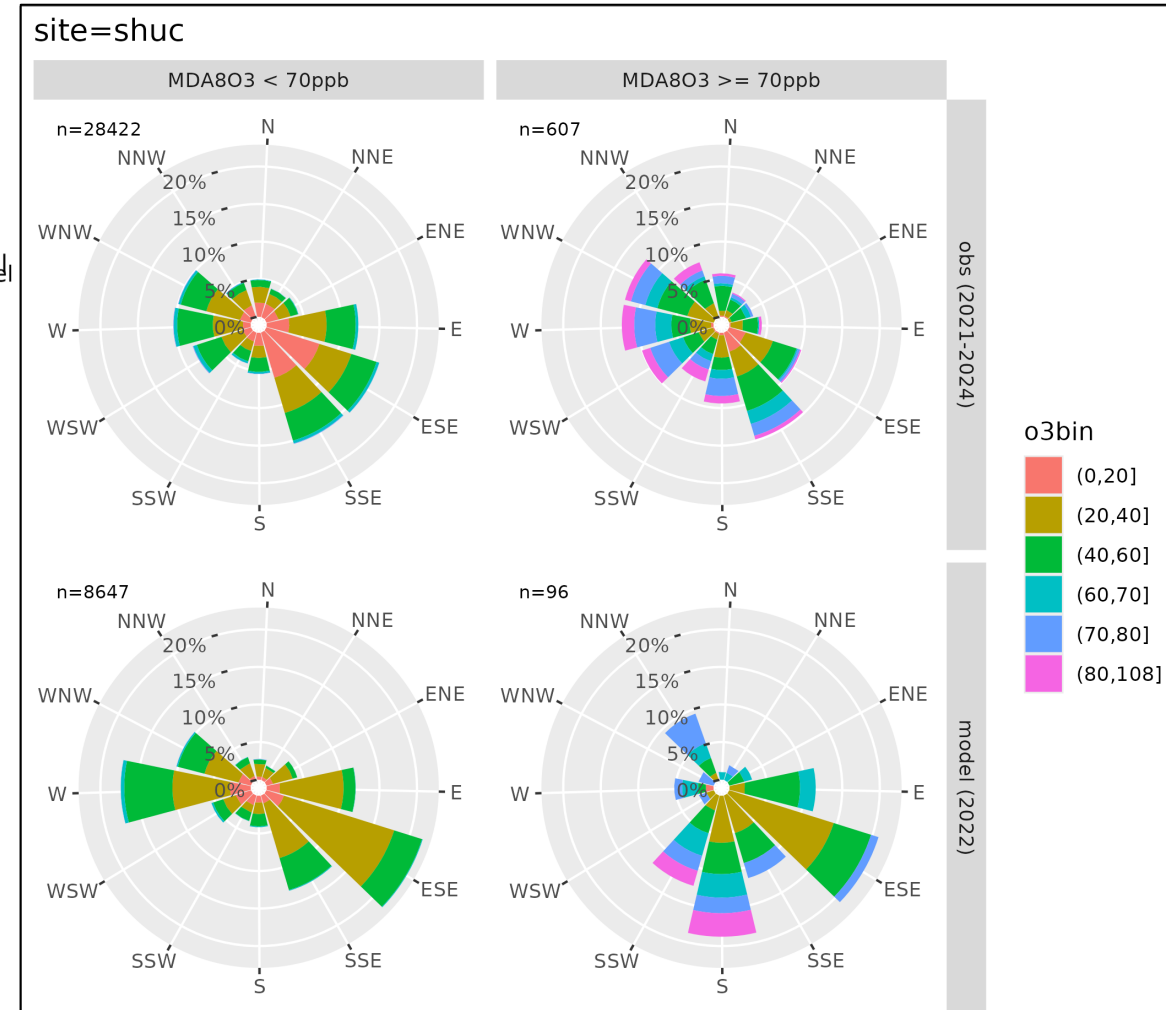
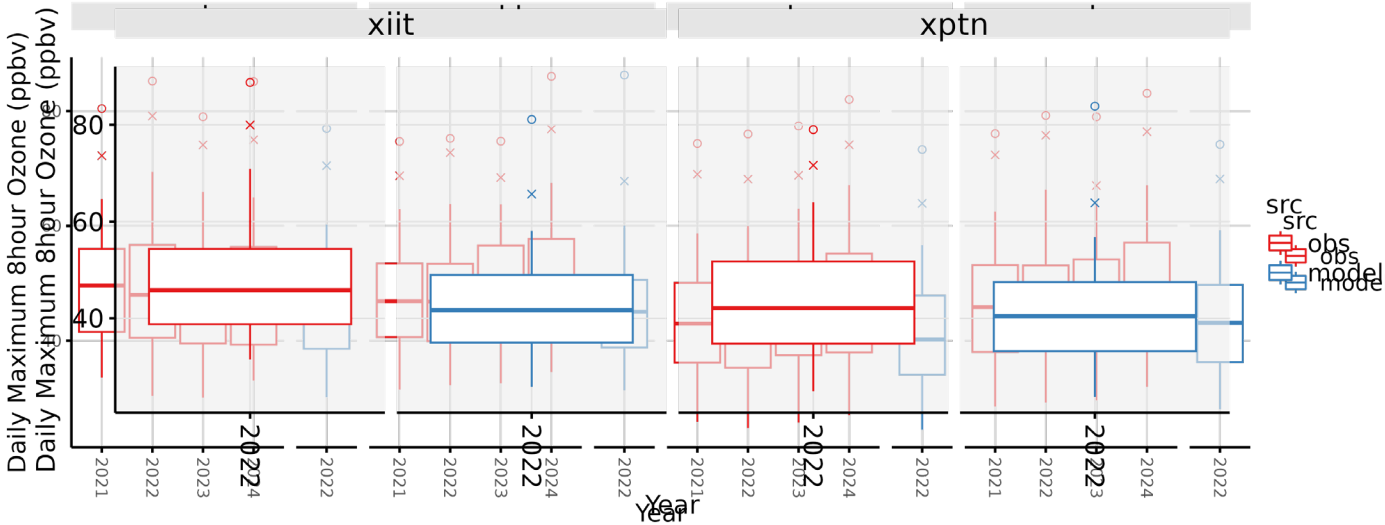
# Model Performance: Maximum Daily 8-Hour Average (MDA8) Ozone



Model performance evaluated against benchmarks established by Emery et al. (2017)

- MDA8 ozone measurements from TCEQ and Mexico's Secretariat of Environment and Natural Resources (SEMARNAT)/National Institute for Ecology and Climate Change (INECC)
- Annual NMB and NME (quarterly NME) statistics at all sites met performance criteria with many achieving goals
- Most quarterly NMB statistics met performance criteria with a few exceptions during Q3 or Q4

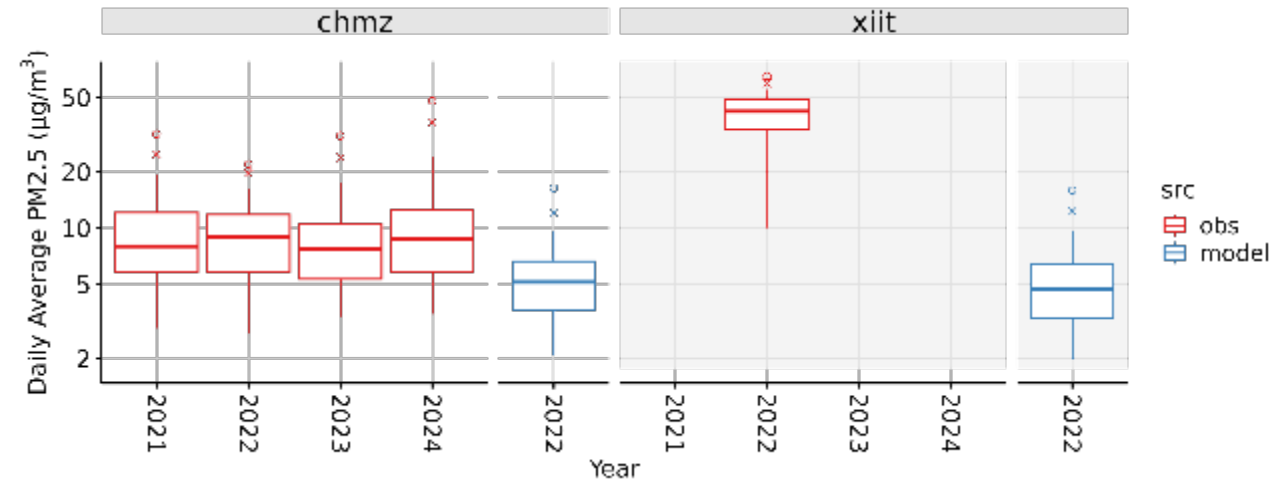
# Ozone Pollution Roses: Non-exceedance vs. Exceedance Days



- EPA 8-hour ozone design values for 2024\* at Ojo de Agua, Skyline Park, and Socorro Hueco > 70 ppb and at Chamizal is 70 ppb
- Variability with complex terrain, channeling of winds along Rio Grande River, emission sources (e.g., urban, border crossing and trade corridor, Chihuahuan desert)
- Exceedance days more often have easterly through west-southwesterly winds in ozone roses

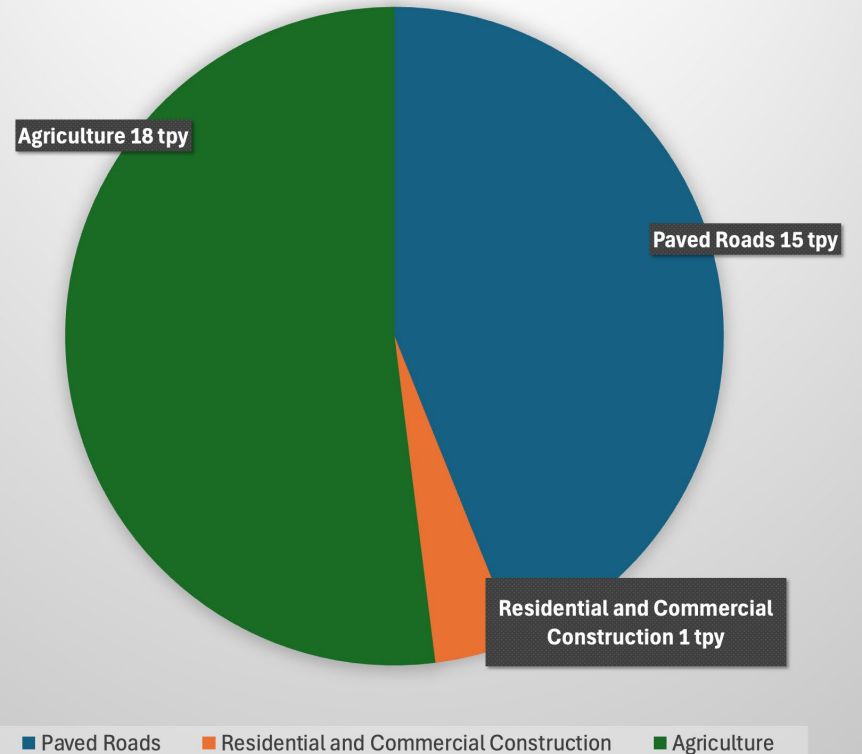
\*Source: <https://storymaps.arcgis.com/stories/86cc46a9348c48289c718f06cae93b1d>

# PM<sub>2.5</sub> Emissions and Model Performance



- Model had pronounced underprediction bias, especially at IIT site in Juárez, and did not meet performance benchmarks
- TCEQ has *Exceptional Events Demonstration for 2023 and 2024 PM<sub>2.5</sub> Exceedances at El Paso County* available for public comment<sup>1</sup>
- Ramboll (2025) has developed WBDUST emissions files for TCEQ's 2022 modeling platform that will be critical for El Paso-Juárez

Unadjusted Area Fugitive Dust Emissions (tpy) in Juárez in the EPA 2022v1 Inventory  
(Total emissions are 37 tpy; No adjustments were applied)

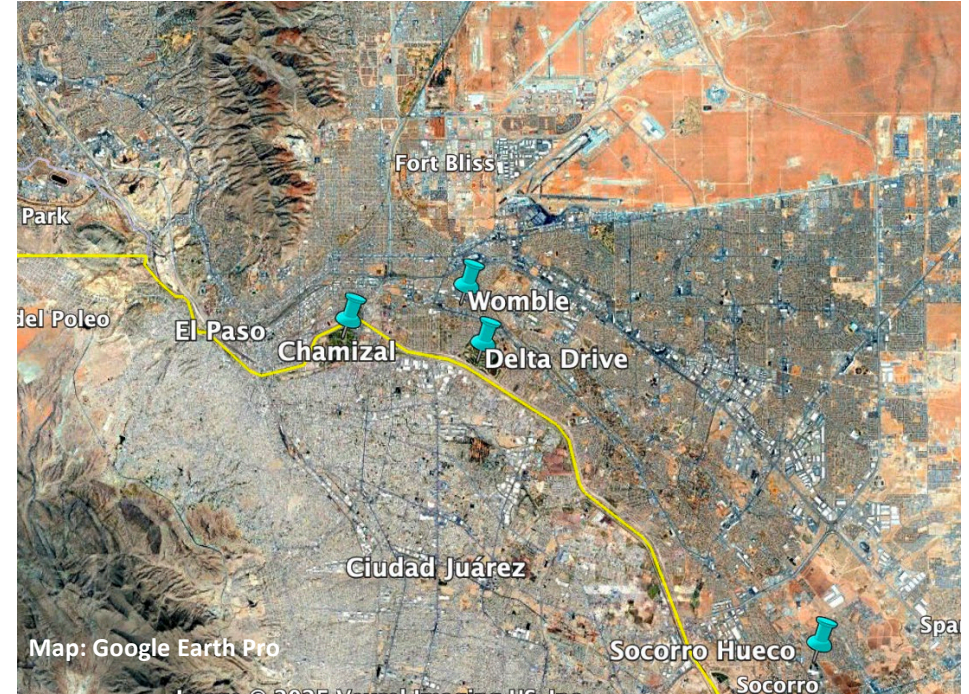
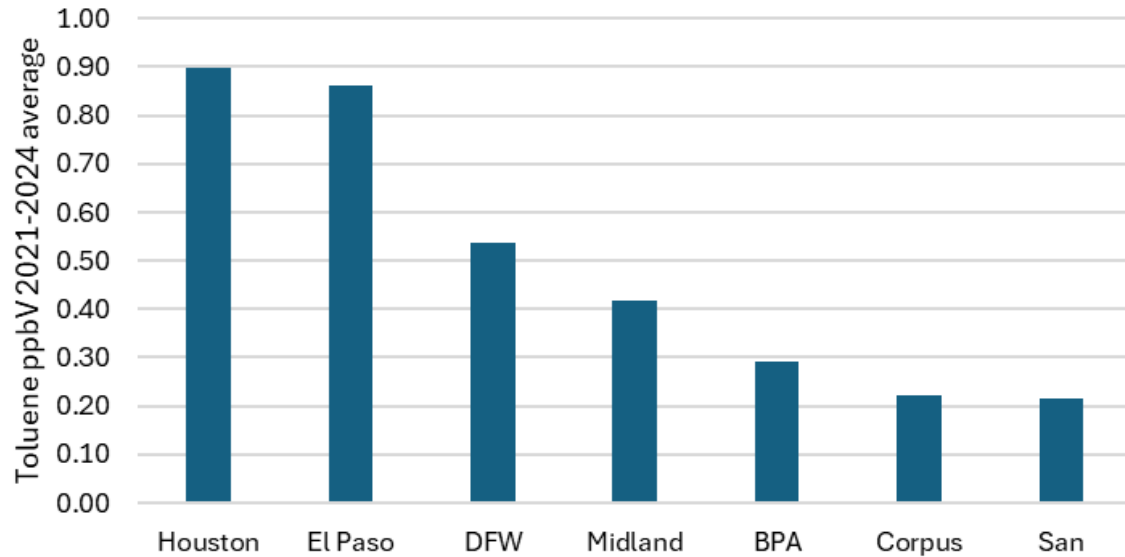


- Afdust sources in Juárez may be missing/under-represented. Total unadjusted afdust sector emissions were 37 tpy versus 1958 tpy in El Paso
- Windblown dust is not in EPA 2022v1 inventory

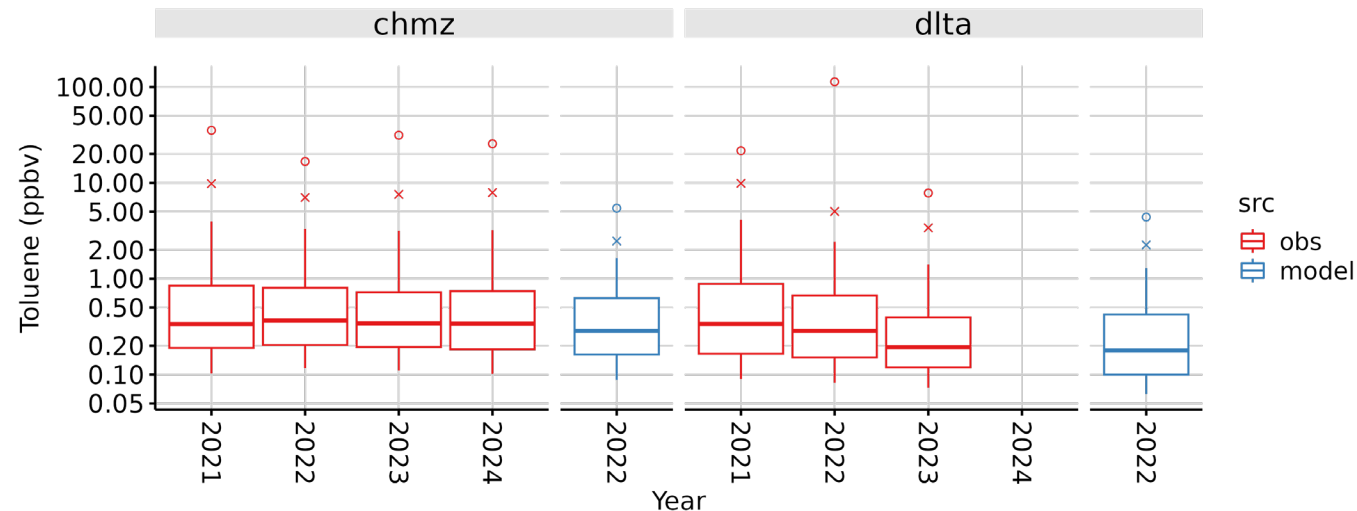
\*Source: <sup>1</sup>[https://www.tceq.texas.gov/downloads/air-quality/air-monitoring/pm/2023-2024\\_elpaso\\_pm2-5\\_ee\\_demonstration\\_final-4aug2025.pdf](https://www.tceq.texas.gov/downloads/air-quality/air-monitoring/pm/2023-2024_elpaso_pm2-5_ee_demonstration_final-4aug2025.pdf)

# Toluene in El Paso-Juárez

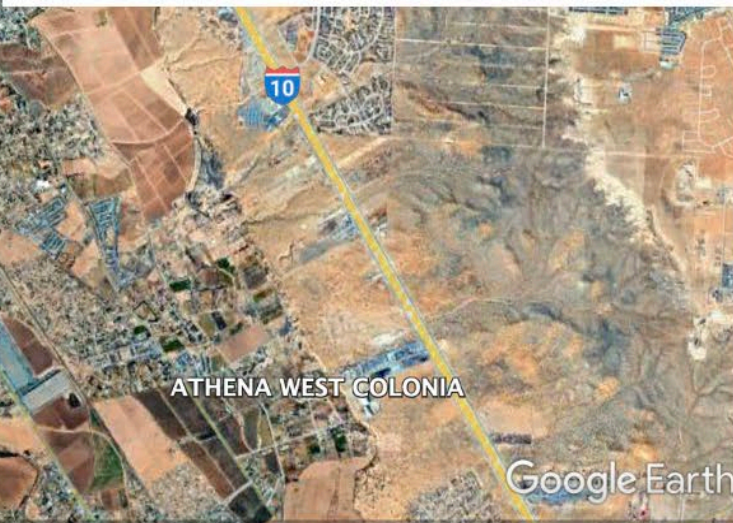
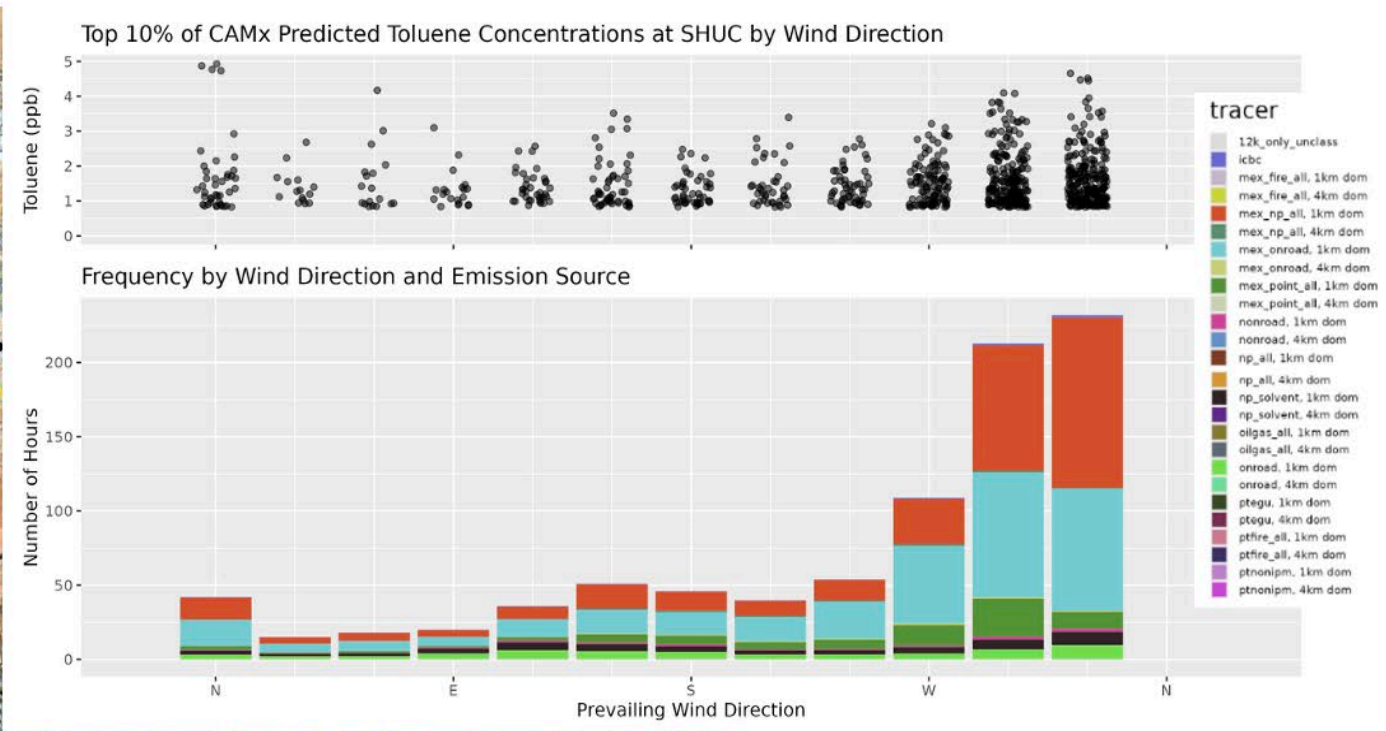
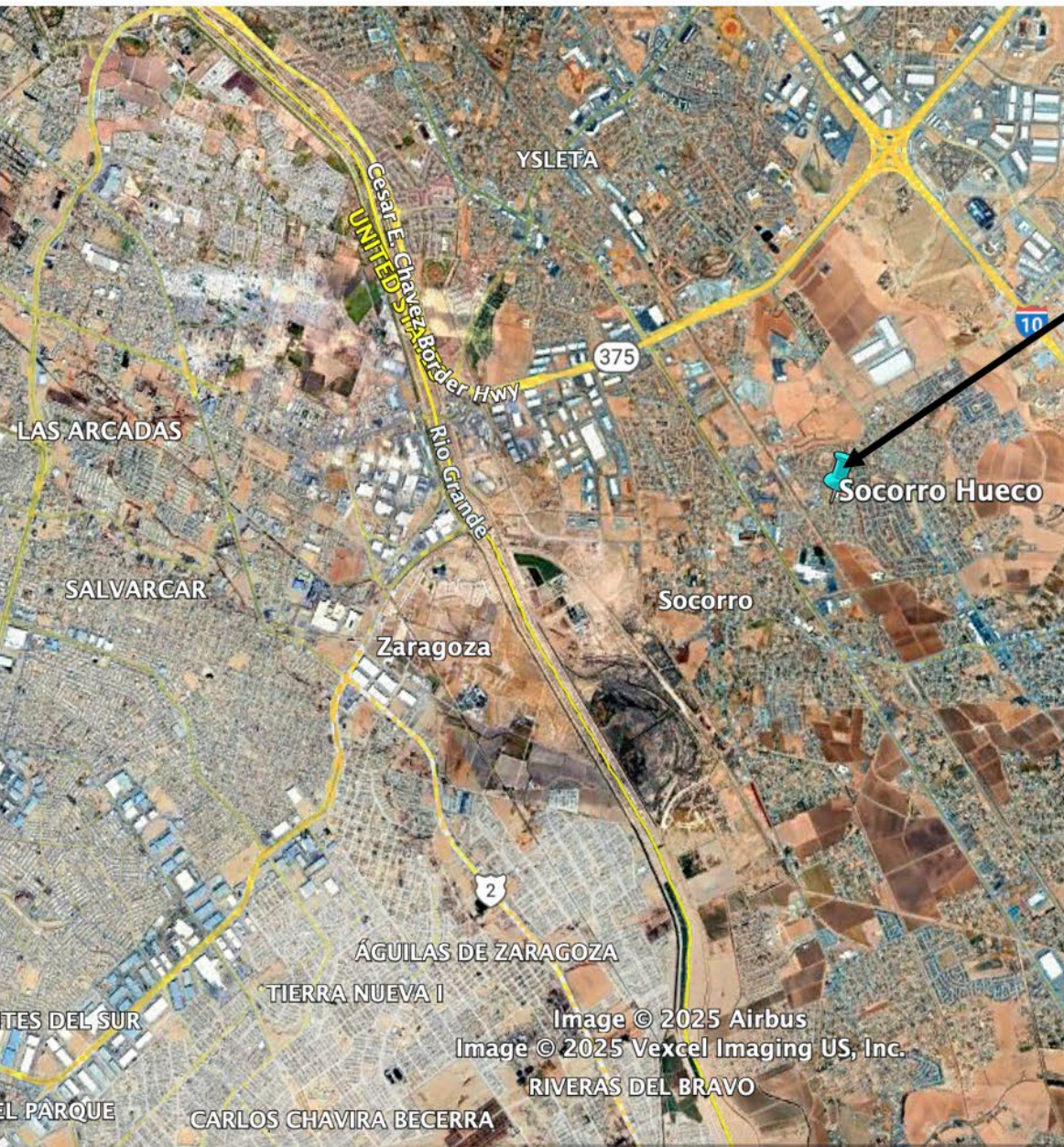
Maximum Observed (auto-GC) Mean Toluene Concentration (ppb) for 2021-2024 by Area



- Chamizal station had second highest mean toluene concentration among 42 Texas auto-GCs for 2021-2024
- Delta Drive is ranked fifth
- Juárez does not have routine VOC observations



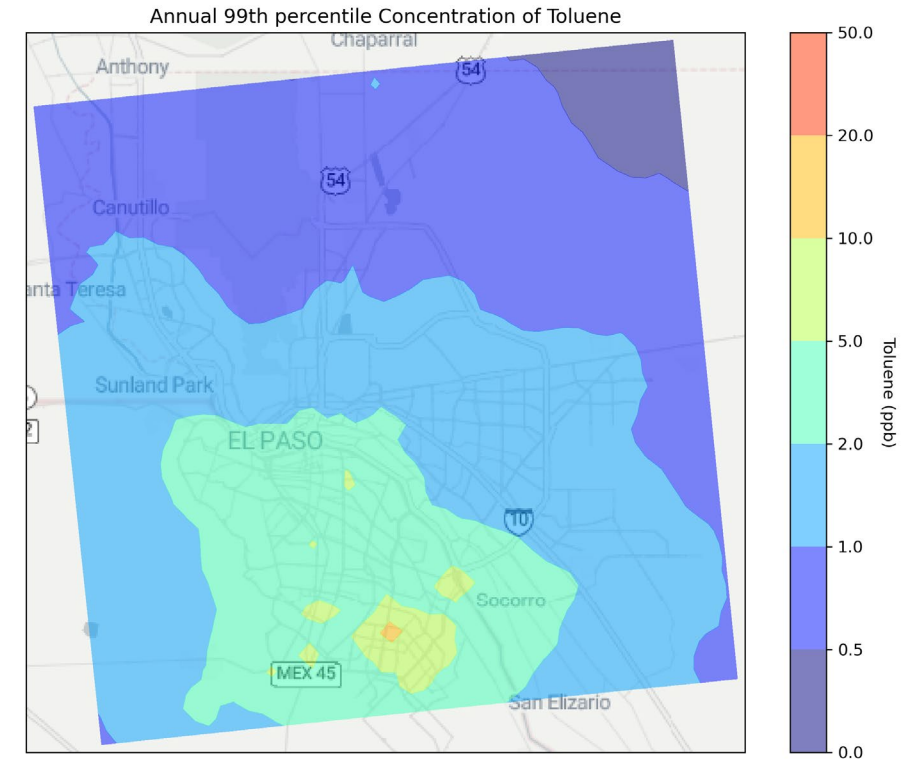
# Emission Sector Contributions to the Top 10% of Modeled Toluene in El Paso



# Toluene Emissions El Paso County & Municipio de Juárez: 2022v1 Inventory

Sources Contributing ~90-95% of Total Toluene Emissions	El Paso (tpy)	Juárez (tpy)
Gasoline Vehicles*	210.33	758.57
Solvent Utilization: Surface Coating	59.24^	346.79^^
Wastewater Treatment		140.49
Plastics Production		55.22
Solvent Utilization: Consumer and Commercial	66.00	
Commercial Equipment	25.38	
Lawn and Garden Equipment	54.78	
Gasoline Service Stations	5.47	16.94
Gasoline Retail Operations		11.53
Industrial Boilers: Coal		11.44
Manufacturing: Misc.	9.58	
Solvent Utilization: Industrial Maintenance	8.86	
Secondary Metal Production		7.38
Industrial Boilers: Natural Gas		7.22
Petroleum Industry: Fugitives	5.28	
Solvent Utilization: Degreasing	3.54	9.01
All Other	41.29	70.42
<b>Total</b>	<b>489.75</b>	<b>1435.12</b>

## CAMx Simulated 2022 Annual 99<sup>th</sup> Percentile Toluene Concentrations

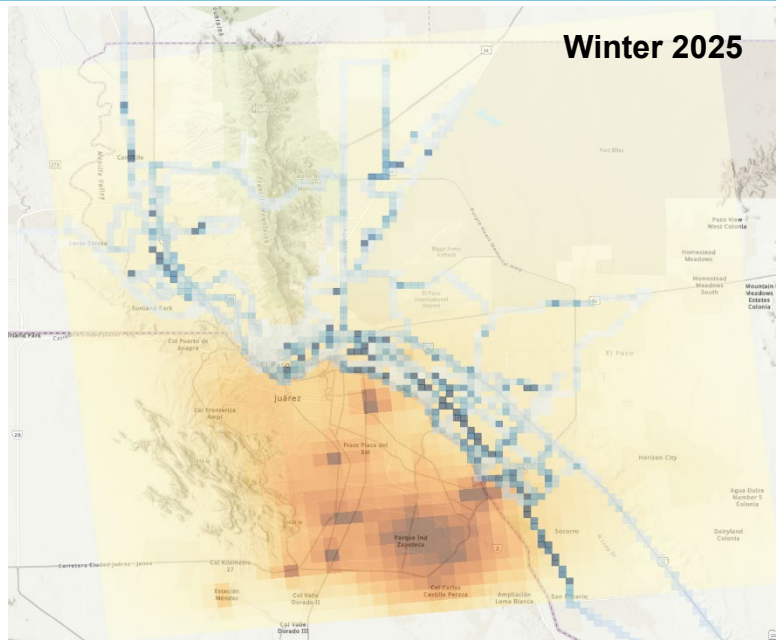


- Binational coordination on VOC monitoring and emissions inventory development could provide mutual benefits for air quality planning and management

\*passenger cars; passenger, light commercial, and short-haul trucks; motorcycles; transit buses

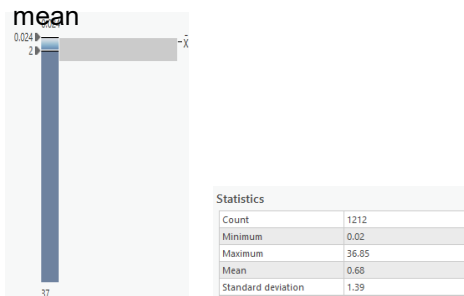
^textiles; traffic markings; industrial maintenance; plastics; ^^misc. manufacturing; motor vehicles; auto refinishing, automotive aftermarket products; wood furniture; electronic and electrical products

# Wrap-up and Future Work – Observations Informing the Model and Vice Versa

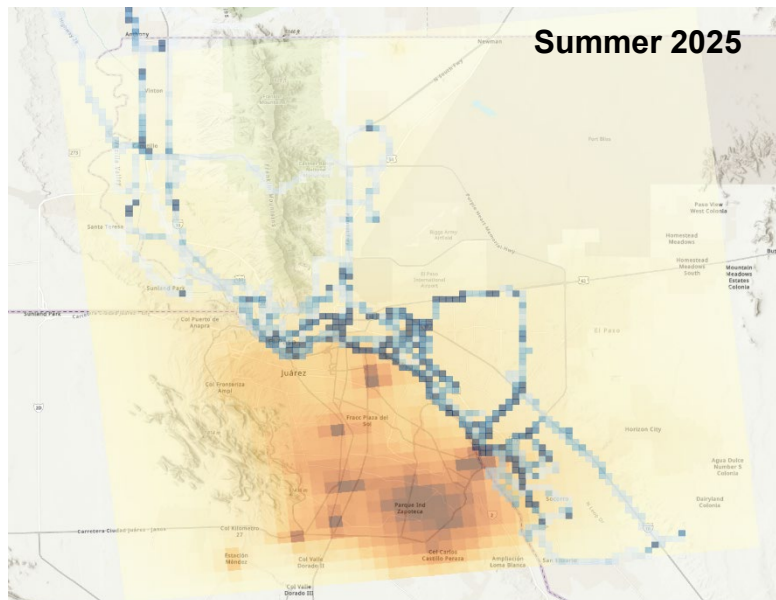
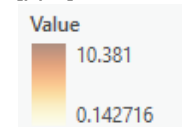


Winter 2025

Toluene – PTR-ToF-MS  
500 m grid 10-second aggregate  
mean

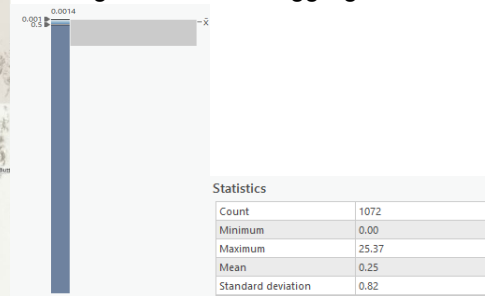


Toluene – CAMx  
1 km annual hourly 95<sup>th</sup> Percentile  
[ppb]

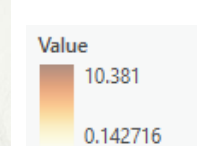


Summer 2025

Toluene – PTR-ToF-MS  
500 m grid 10-second aggregate mean

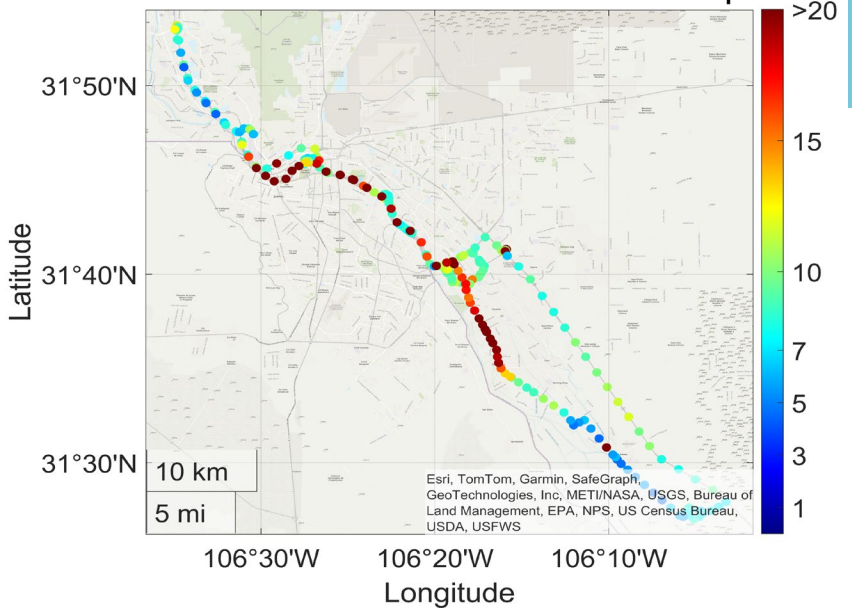


Toluene – CAMx  
1 km annual hourly 95<sup>th</sup> Percentile [ppb]

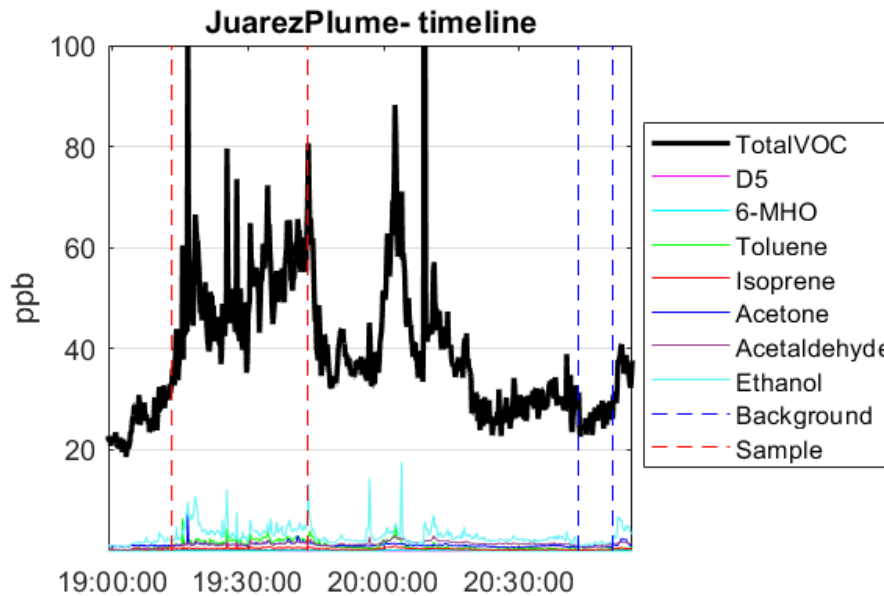


- Model – Observation comparisons are still ongoing on the vast datasets.
- Preliminary work on toluene indicates good spatiotemporal correspondence between the observations and the model.
- Can the sniffer observations identify areas that have enhanced concentrations that could focus inventory improvement effort and identification novel compounds.
- The ongoing goal is to develop a framework for model – observation comparisons.

## Spatial Distribution of Total Non-Refractory PM<sub>1</sub> (μg/m<sup>3</sup>)

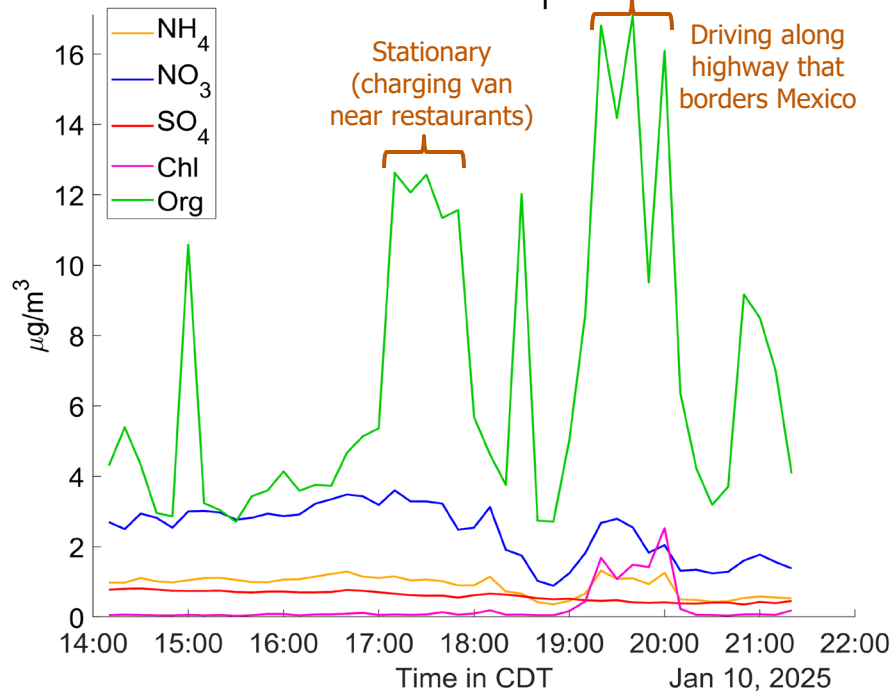


# What is potentially transported from Juarez?

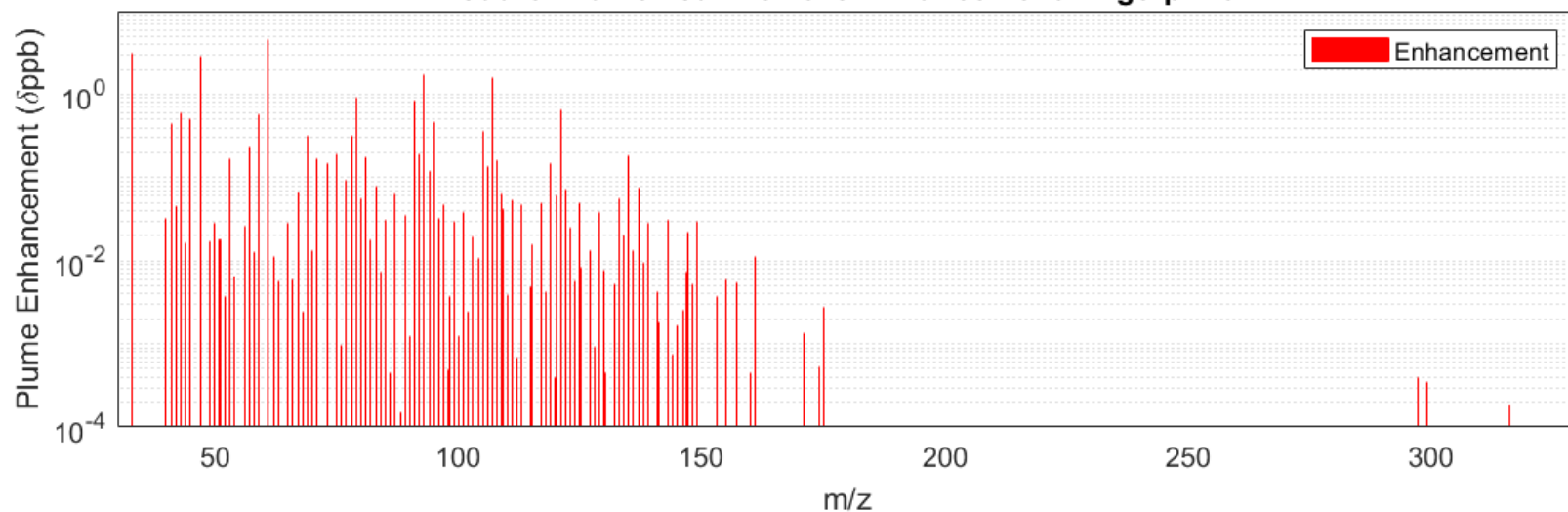


m/z	VOC ion	δppb	%TVOC
61.0284	C2H4O2H+ (Acetic acid)	4.565	18.4
33.0327	CH4OH+ (Methanol)	3.125	12.6
47.0498	C2H6OH+ (Ethanol)	2.830	11.4
93.0698	C7H8H+ (Toluene)	1.746	7.04
107.086	C8H10H+ (C8-Aromatics)	1.589	6.41
79.054	C6H6H+ (Benzene)	0.9088	3.67
91.0541	C7H6H+ (Benzyl fragm.)	0.8447	3.41
121.101	C9H12H+ (C9-Aromatics)	0.6427	2.59
43.0175	C2H2OH+ (Acetic acid fr.)	0.6088	2.46
59.0491	C3H6OH+ (Acetone)	0.5744	2.32
45.0333	C2H4OH+ (Acetaldehyde)	0.4969	2.00
95.0492	C6H6OH+ (Phenol)	0.4566	1.84

## Timeseries of NR-PM<sub>1</sub>, 1/10/2025



## JuarezPlume - Jan 10 2025 Enhancement Fingerprint



# Conclusions and Future Work

- This has been a unique and fascinating study in beautiful El Paso.
- Detailed source apportionment combining collected datasets (VOC+PM) could help understand what sources are contributing to air quality in the region including PM and O<sub>3</sub>
- Preliminary work on toluene observation – modeling integration indicates good spatiotemporal correspondence and is consistent with major sources advected from Juarez
- Database of observed source plume compositions could also be beneficial for source understanding while colocation observations could complement compounds monitored by GC.
- Enhanced PM monitoring and characterization of dust emissions in El Paso and Juarez. Open to suggestions and further collaborations with TCEQ and other collaborators in Texas and beyond

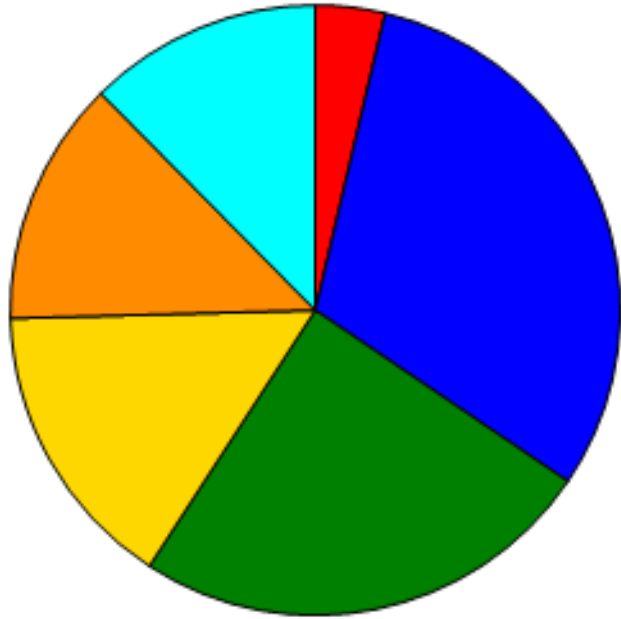
# Acknowledgments

- We thank Weining Zhao and Beata Czader of the TCEQ and Greg Yarwood of Ramboll for their recommendations about the El Paso- Juárez air quality modeling configuration, Jiaoyan Huang of the EPA for assistance with the EPA OAQPS 2022 modeling platform, and Doug Boyer of the TCEQ for insights about El Paso emissions sources
- We appreciate the support and assistance of Vince Torres (AQRP Project Manager), Jocelyn Mellberg (TCEQ Project Manager), Celinda Vallejo-Rodriguez (TCEQ Project Liaison), Joseph Rabago (TCEQ Project Liaison Backup), and RoseAnna Goewey (AQRP Grant & Program Manager) throughout the project



# Offline PM Analysis – Dave Sullivan – complementary PM source apportionment

PM2\_5\_LC - Fpeak = 0.5



Factor Contribution > 0.05 %

- Factor 1 = 0.33163 (3.7 %)
- Factor 2 = 2.77880 (30.8 %)
- Factor 3 = 2.22790 (24.7 %)
- Factor 4 = 1.39060 (15.4 %)
- Factor 5 = 1.17330 (13.0 %)
- Factor 6 = 1.12040 (12.4 %)

PMF 6 factor solution

1. Ammonium Nitrate
2. Crustal material
3. Fires
4. Light duty motor vehicles (LDV)
5. Heavy duty motor vehicles (HDV)
6. Ammonium Sulfate

- Crustal material dominates PM2.5 (31%), followed by motor vehicles (28%), Fires (25%), Ammonium Sulfate (12%) and Ammonium Nitrate (3.7%)