

AQRP Monthly Technical Report

PROJECT TITLE	Advanced Analysis of Ozone Formation Potential, VOC Sensitivity, and Source Apportionment in the El Paso-Juárez Airshed	PROJECT #	26-030
PROJECT PARTICIPANTS	PIs: Pawel K. Misztal, Lea Hildebrandt Ruiz, David W. Sullivan, Elena McDonald-Buller, Yosuke Kimura Graduate Students and Postdocs: Daniel Sung, Shihao Zhai, Hyeonjun Lee, Chun-Ying Chao	DATE SUBMITTED	09/10/2026
REPORTING PERIOD	From: 8/01/2026 To: 8/31/2026	REPORT #	2

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 1: We conducted preliminary VOC prioritization and ozone formation potential analyses for the winter and summer mobile campaigns using four frameworks. Framework 1 (F1) calculates MIR-based ozone formation potential by summing VOC mass concentrations multiplied by their Maximum Incremental Reactivity (MIR) coefficients. F2 additionally applies the molecular-weight factor 48/MW. F3 calculates propylene-equivalent concentrations by weighting VOC mixing ratios by their OH reaction rates relative to propylene, without MIR. F4 uses Carter’s Equal Benefit Incremental Reactivity (EBIR) instead of MIR. These frameworks provide screening metrics rather than measurements of actual ozone production.

We refined F3 to distinguish OH-reaction-rate-based prioritization from the MIR-based ozone formation potential evaluated in F1. The revised formulation omits the MIR term specified in the QAPP and is calculated as follows:

$$T_{3,s,j} = \sum_i C_{i,s,j} \times \frac{k_{OH,i}}{k_{OH,propylene}}$$

Here, C is the VOC mixing ratio in ppbv, i is the formula channel, s is the season, and j is the observation. The propylene reference rate is $2.63 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. F3 is expressed in ppbv propylene-equivalent, not ozone mass or ozone production rate. Further refinement of F3 is planned in the next MTR where MIRi will also be incorporated.

OH rate constants are selected following the QAPP hierarchy: JPL and IUPAC evaluations, peer-reviewed measurements in NIST, and the Kwok and Atkinson (1995) SAR where measured values are unavailable and the method is applicable. Coefficient verification is ongoing, and the results remain preliminary.

Table 1 summarizes the campaign means using isomer geometric-mean coefficients and each framework's eligible channels. We sum channel contributions at each retained 10-second observation and calculate the arithmetic campaign mean and winter-to-summer ratio using Equations (1) and (2).

$$\bar{T}_{k,s} = \frac{1}{N_{k,s}} \sum_{j=1}^{N_{k,s}} T_{k,s,j} \quad (1)$$

$$R_k = \frac{\bar{T}_{k,winter}}{\bar{T}_{k,summer}} \quad (2)$$

T is the framework total for one observation, N is the number of retained observations, and the overbar denotes the arithmetic mean. The subscripts k, s, and j identify the framework, season, and observation. Each retained observation receives equal weight. The winter-to-summer ratio is calculated from the unrounded campaign means; for example, F1 gives $88.418615 / 50.157685 = 1.76$.

Table 1. Preliminary campaign means and winter-to-summer ratios using each framework's eligible channels.

Method	Winter mean	Summer mean	Winter / summer	Channels winter / summer	Units
F1	88.42	50.16	1.76	120 / 129	$\mu\text{g O}_3 \text{ m}^{-3}$
F2	68.86	32.36	2.13	120 / 129	$\mu\text{g O}_3 \text{ m}^{-3}$, MW-rescaled
F3*	4.305	2.484	1.73	74 / 81	ppbv propylene-equivalent
F4	23.68	12.58	1.88	116 / 119	$\mu\text{g O}_3 \text{ m}^{-3}$, EBIR-based

* F3 is preliminary. The next MTR will add the MIR weighting to complete the formulation.

All four frameworks had higher campaign means in winter, with winter-to-summer ratios from 1.73 to 2.13. Their absolute values should not be compared directly because the coefficients differ and F3 has a different unit and chemical interpretation.

The comparison using the same 62 formula channels in both seasons and all four frameworks also showed higher winter means, with ratios from 1.78 to 2.26. Table B1 and Figure B1 in Appendix B present this common-channel comparison.

Figure 1 compares the major VOC contributions within each framework. Methanol is prominent in the winter MIR-based and EBIR-based results, while F3 gives greater weight to the C5H8 channel and other rapidly reacting VOCs. The rankings reflect both abundance and reactivity. Some formula channels represent more than one structural isomer.

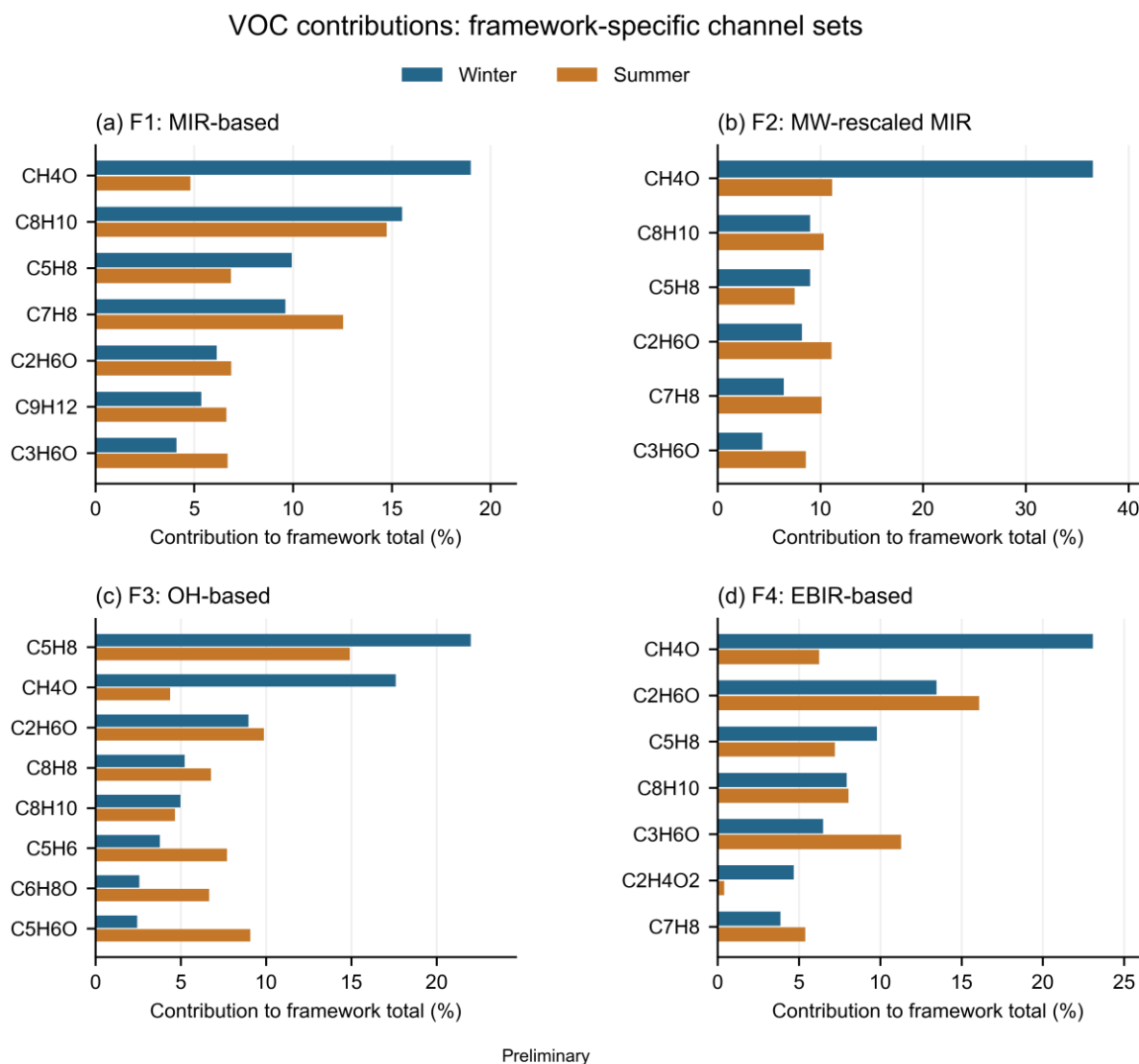


Figure 1. Preliminary winter and summer VOC contribution profiles using each framework's eligible channels. Bars show the percentage contribution to the full framework mean. Each panel includes the six leading channels from either season; displayed contributions therefore need not sum to 100%.

Figure 2 shows the spatial patterns for each framework. Measurements were aggregated into 250 m grids, retaining grids with at least 30 ten-second observations on at least three dates. These criteria were met by 67 winter grids and 35 summer grids. The campaigns sampled overlapping areas, but route coverage differed.

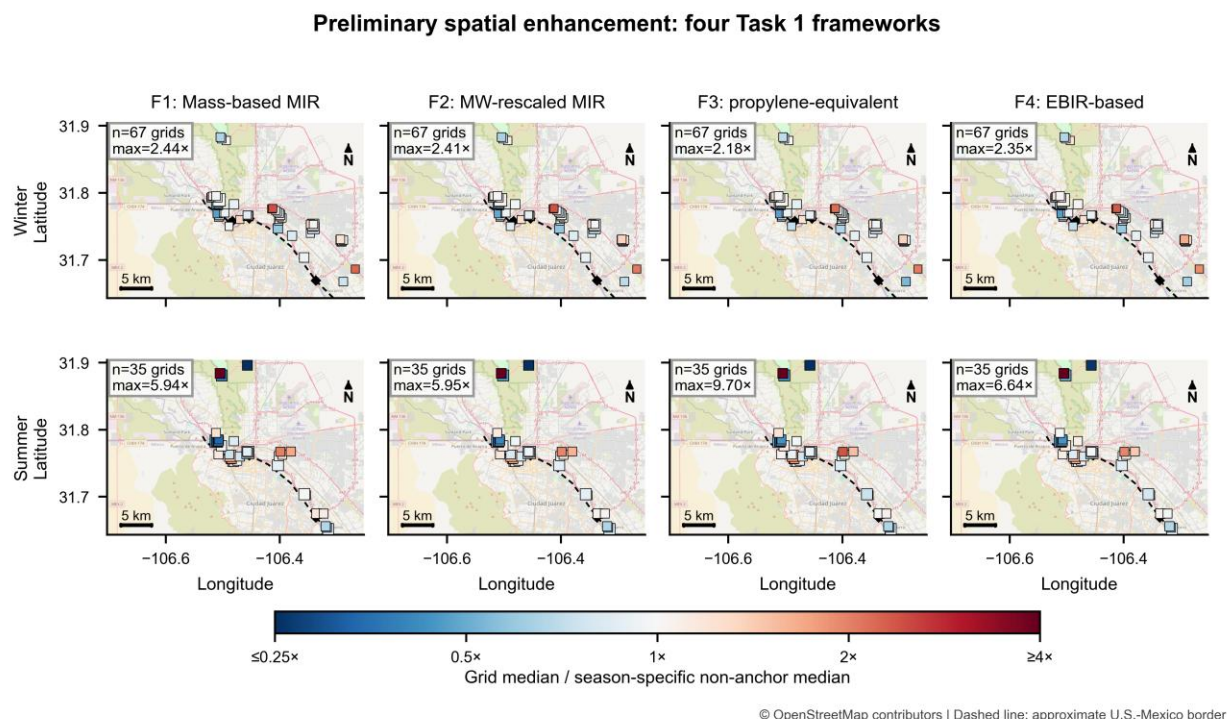


Figure 2. Preliminary repeated-grid spatial enhancement across the four frameworks. Colors represent each grid median divided by the corresponding season- and framework-specific campaign median after excluding repeated stationary coordinates. The common ratio scale compares relative spatial patterns, not absolute values. The dashed U.S.-Mexico border is an approximate visual guide.

Frameworks 1, 2, and 4 produced similar spatial patterns. Framework 3 was also positively related to the other frameworks. We will examine the repeated enhancements using VOC composition and wind-direction data. The maps alone do not identify specific emission sources or quantify transboundary transport.

Task 2: Preliminary observational comparisons. We compared surface NO_2 at Chamizal and Ascarate Park with collocated TEMPO and TROPOMI tropospheric NO_2 columns. We paired observations in time and calculated Spearman correlations without converting satellite columns to surface ppb. TEMPO showed a more consistent relationship at Chamizal than at Ascarate Park. TROPOMI comparisons had fewer matched observations. Figure A1 in Appendix A presents the results.

We also examined the spatial distribution of TEMPO HCHO and NO_2 observations. TEMPO retrievals were assigned to grid cells intersecting the mobile GPS routes, and median column values were calculated for each grid cell over the January and May 2025 campaign periods (Figure 3). HCHO columns were generally higher across the sampled route during the May campaign, whereas NO_2 showed a smaller difference in overall magnitude between the two campaign periods.

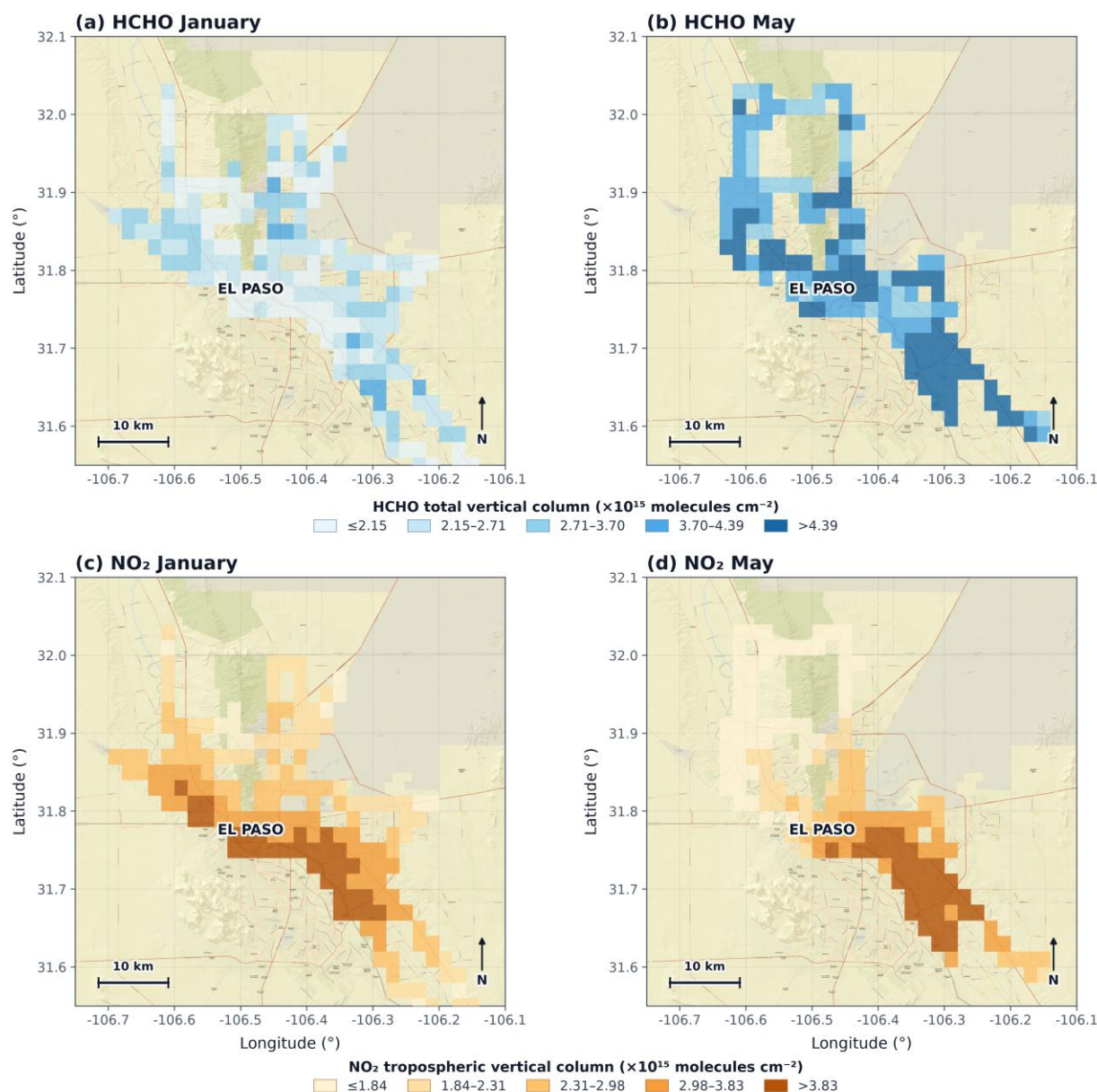


Figure 3. Preliminary campaign-period median TEMPO HCHO total vertical columns (a, b) and NO₂ tropospheric vertical columns (c, d) for January and May 2025 mobile campaign period over sampling route intersecting grid cells.

These preliminary comparisons provide context for ozone-sensitivity analysis but do not by themselves establish a VOC-limited or NO_x-limited regime.

Task 4: Since the completion of AQRP Project 24-024, the U.S. Environmental Protection Agency (EPA) released an update to the 2022v1 (also referred to as 2022hc) emissions modeling platform (EMP). Emissions estimates for most source categories in Chihuahua and five other border states in the 2022v1 platform, were developed by the EPA and Mexico's Secretariat of Environment and Natural Resources (SEMARNAT) for the 2018 base year. The 2022v2 (2022he) emissions modeling platform¹ indicated that only on-road sector emissions differed between the inventories for the state of Chihuahua. The EPA applied an updated version of the MOVES MOtor Vehicle Emission Simulator (MOVES) model for Mexico. The simulation included more extensive on-road sources, adding taxis, buses (school, micro, metro, intercity, transit), and short and long-haul trucks. Three adjustments were also applied: (1) a correction factor of

0.84964 to all on-network emissions from light duty cars and trucks to account for a vehicle miles traveled (VMT) correction; (2) correction factors to VOC-related emissions (total, speciated, and hazardous air pollutants); and (3) correction factors to particulate sulfate emissions in all Mexico municipios except in/around Mexico City, Monterrey, and Guadalajara. A draft 2022v2 (referred to as 2022hd) inventory without the third adjustment for particulate sulfate was also developed. Table 2 summarizes differences in emissions of toluene, carbon monoxide (CO), nitrogen oxides (NO_x), fine (PM_{2.5}) and coarse (PM₁₀) particulate matter, sulfur dioxide (SO₂), and volatile organic compounds (VOCs) between the 2022hc and 2022he inventories for the municipio de Juárez³⁻⁵.

On-road mobile emissions in El Paso County were also revised⁶⁻⁹. The EPA conducted a new simulation with MOVES5.0.0 with updated input data (spatial surrogates, temporal profiles, age distributions, and activity data). Table 3 summarizes differences in emissions of toluene and selected criteria pollutants and precursors between the 2022hc and 2022he inventories for El Paso County. There were no differences between the 2022hd (draft) and 2022he (final) on-road emissions inventories for the United States. Tables 2 and 3 show that on-road emissions from Juárez in the 2022 inventories are substantially greater than El Paso. For example, toluene emissions are more than a factor of four and VOC and NO_x emissions more than a factor of seven in Juárez than in El Paso in the 2022he inventory.

Table 2. On-road emissions of toluene and selected criteria pollutants and precursors and differences between the EPA 2022hc and 2022he inventories for the municipio de Juárez²⁻⁵.

Pollutant	2022hc (tons)	2022he (tons)	2022he-2022hc (tons)	Percent Difference from 2022hc %
CO	76,023.7	125,459.1	49,435.4	65.0
NO _x	22,027.4	31,562.0	9,534.6	43.3
Primary PM _{2.5}	482.1	1,375.9	893.7	185.4
Primary PM ₁₀	803.7	2,269.4	1,465.7	182.4
SO ₂	377.5	252.4	-125.1	-33.1
VOC	8,952.4	19,288.5	10,336.1	115.5
Toluene	800.3	1,155.8	355.5	44.4

Table 3. On-road emissions of toluene and selected criteria pollutants and precursors and differences between the EPA 2022hc and 2022hd inventories for El Paso County².

Pollutant	2022hc (tons)	2022he (tons)	2022he-2022hc (tons)	Percent Difference from 2022hc %
CO	27,375.9	32,530.5	5,154.6	18.8
NO _x	3,770.1	4,123.2	353.2	9.4
Primary PM _{2.5}	117.8	136.1	18.3	15.5
Primary PM ₁₀	377.4	315.5	-61.9	-16.4
SO ₂	16.9	18.3	1.3	7.9
VOC	2,039.4	2,504.5	465.2	22.8
Toluene	220.8	276.8	56.0	25.4

Emissions from other sectors in El Paso had little to no change with the exception of an approximately 15% decrease in criteria and precursor pollutant emissions from residential wood combustion (RWC) in the 2022he inventory. The 2022v2 Technical Support Document (TSD)² indicated for Texas and other states that submitted data for the 2020 National Emissions Inventory (NEI) that 2022v2 platform RWC

emissions were adjusted from 2020 NEI using State Energy Data System (SEDS) data for 2021, and converted to 2023 NEI-consistent source classification codes (SCCs).

Although our workplan for the AQR Project 26-030 project did not include emission inventory updates and a new CAMx simulation, the magnitude of the on-road emissions changes suggests a sensitivity study that applies the 2022he inventories for Juárez and El Paso could be important. To evaluate if this was feasible, we used the EPA Sparse Matrix Operator Kernel Emissions (SMOKE) v.5.0 emission processing system to prepare model-ready emissions for the 4-km and 1-km grids with the 2022he on-road emissions, following a similar approach as for AQR 24-024.

A CAMx simulation with the new on-road inventories was completed at the Texas Advanced Computing Center (TACC). We will provide performance metrics for modeled versus observed toluene concentrations and box and whisker plots at El Paso monitoring sites in the Monthly Technical Report (MTR) for September. Proceeding with the EPA 2022v2 Emissions Modeling Platform would not change the scope, schedule or budget for Task 4. CAMx results with the 2022v2 inventory would be the basis for the Task 4 analyses instead of those from AQR Project 24-024, which used the earlier 2022v1 inventory. We would like to confirm this change meets with the TCEQ and AQR approval.

The modeling team also reviewed Mexico's most recent National Air Quality Report, which is based on 2023 ambient monitoring data¹⁰. Mexico's regulates similar criteria air pollutants and precursors, but standards have different forms than the United States. Compliance with ozone and fine and coarse particulate matter standards remain challenges for Ciudad Juárez.

The abstract submitted for the CMAS Conference (October 19-21, 2026) was accepted for oral presentation by Pawel Misztal and Elena McDonald-Buller.

Preliminary Analysis

As described above, the recent EPA 2022v2 emissions modeling platform was reviewed and compared with the 2022v1 platform used in AQR 24-024.

Data Collected

No new field measurements are reported.

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments

Measurement-based results remain preliminary. Coefficient review and data-quality checks are ongoing.

Goals and Anticipated Issues for the Succeeding Reporting Period

The modeling team will evaluate the results of the updated CAMx simulation, continue with the toluene analysis described in Task 4, and work with the measurement teams to develop approaches for integrated data analyses. Work on the CMAS presentation and extended abstract will also be initiated. We anticipate submission of a draft presentation for review no later than 14 days prior to the start of the conference on October 19th.

For Task 1, we will complete the remaining OH-rate assignments and data-quality checks and compare shared sampling areas and times.

For Task 1, we will also present the complete F3 formulation including MIR, as specified in the Scope of Work, and will report the propylene-equivalent concentrations alongside the four frameworks.

For Task 2, we will evaluate the available observational ozone-sensitivity indicators, considering their timing and spatial coverage.

TCEQ and AQRP suggestions are welcome.

Detailed Analysis of the Progress of the Task Order to Date

Preliminary measurement results are summarized under Tasks 1 and 2 above.

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 (i.e.: 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

Pawel K. Misztal*, Elena C. McDonald-Buller*, Yosuke Kimura, Ling Huang, David W. Sullivan, Lea Hildebrandt Ruiz, Daniel Sung, Shihao Zhai, Evelyn Deveraux, Chun-Ying Chao, Kacper Przykaza, Kyle Druckman, and Chris Emery: Unraveling Transboundary Influences on Air Quality in the El Paso-Juarez Airshed through Complementary Advanced Measurements and Photochemical Modeling, Accepted Abstract for CMAS 2026. *Presenting authors

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.

Measurement-analysis limitations are described in the problems and issues section above.

**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

References

- (1) U.S. Environmental Protection Agency. 2022v2 Emissions Modeling Platform.
<https://www.epa.gov/air-emissions-modeling/2022v2-emissions-modeling-platform>
- (2) U.S. Environmental Protection Agency. Technical Support Document (TSD): Preparation of Emissions Inventories for the 2022v2 North American Emissions Modeling Platform, EPA EPA-454/B-25-002, December 2025. <https://www.epa.gov/air-emissions-modeling/2022v2-emissions-modeling-platform-technical-support-document>
- (3) U.S. Environmental Protection Agency. [2022hc MOVES Mexico on-road emissions inventory]
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- (4) U.S. Environmental Protection Agency. [2022he MOVES Mexico on-road emissions inventory]
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- (5) U.S. Environmental Protection Agency. [Mexico on-road 2022hc, 2022hd, 2022he comparison report]
https://gaftp.epa.gov/Air/emismod/2022/v2/reports/mexico_on-road_2022hc_2022hd_2022he_comparison_report.xlsx
- (6) U.S. Environmental Protection Agency. [2022hc U.S. county-level sector emissions summary]
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- (7) U.S. Environmental Protection Agency. [2022he U.S. county-level sector emissions summary]
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- (8) U.S. Environmental Protection Agency. [2022hc U.S. on-road emissions inventory]
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- (9) U.S. Environmental Protection Agency [2022he U.S. on-road emissions inventory]
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- (10) Instituto Nacional de Ecología y Cambio Climático. Informe Nacional de Calidad del Aire 2023.
<https://sinaica.inecc.gob.mx/archivo/informes/Informe2023.pdf>

Appendix A

Figure A1 compares surface AQS NO_2 with colocated TEMPO and TROPOMI tropospheric NO_2 columns at Chamizal and Ascarate Park. TEMPO showed similar correlations with Chamizal in winter (0.648) and summer (0.629), while the correlations at Ascarate Park decreased from 0.495 in winter to 0.304 in summer. TROPOMI relationships were weaker in summer and were based on fewer matched dates. These results show that satellite column NO_2 provides useful regional context but should not be treated as a substitute for surface NO_2 measurements.

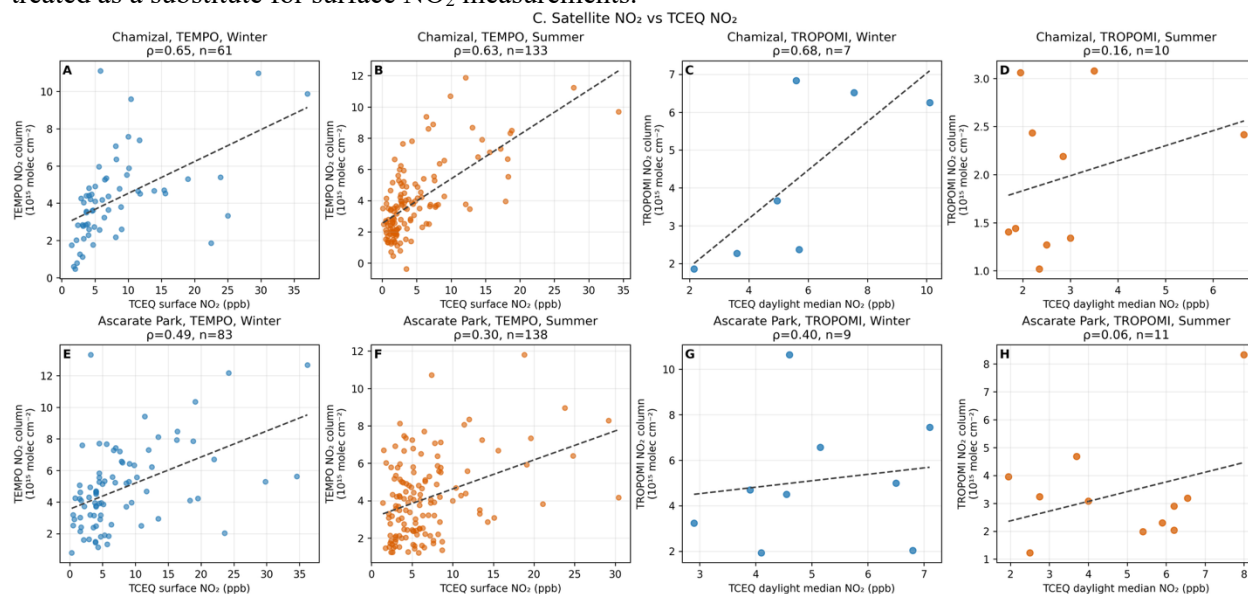


Figure A1. Preliminary surface AQS NO_2 compared with colocated TEMPO and TROPOMI tropospheric NO_2 columns at Chamizal and Ascarate Park. TEMPO observations were paired with the AQS hour corresponding to the satellite subset scan-start time. TROPOMI observations were compared with same-date AQS daylight medians. Spearman correlations describe whether surface and column NO_2 increased and decreased together.

Appendix B. Preliminary common-channel comparison

Table B1 compares campaign means using the same 62 formula channels in both seasons and all four frameworks, including methanol.

Table B1. Preliminary campaign means and ratios for the common 62-channel subset.

Method	Winter mean	Summer mean	Winter / summer	Channels winter / summer	Units
F1	80.45	42.97	1.87	62 / 62	$\mu\text{g O}_3 \text{ m}^{-3}$
F2	65.18	28.84	2.26	62 / 62	$\mu\text{g O}_3 \text{ m}^{-3}$, MW-rescaled
F3	4.017	2.258	1.78	62 / 62	ppbv propylene-equivalent
F4	22.33	11.35	1.97	62 / 62	$\mu\text{g O}_3 \text{ m}^{-3}$, EBIR-based

Figure B1 compares the leading contributions within the common 62-channel subset. Percent contributions use the subset total rather than the full framework total in Figure 1.

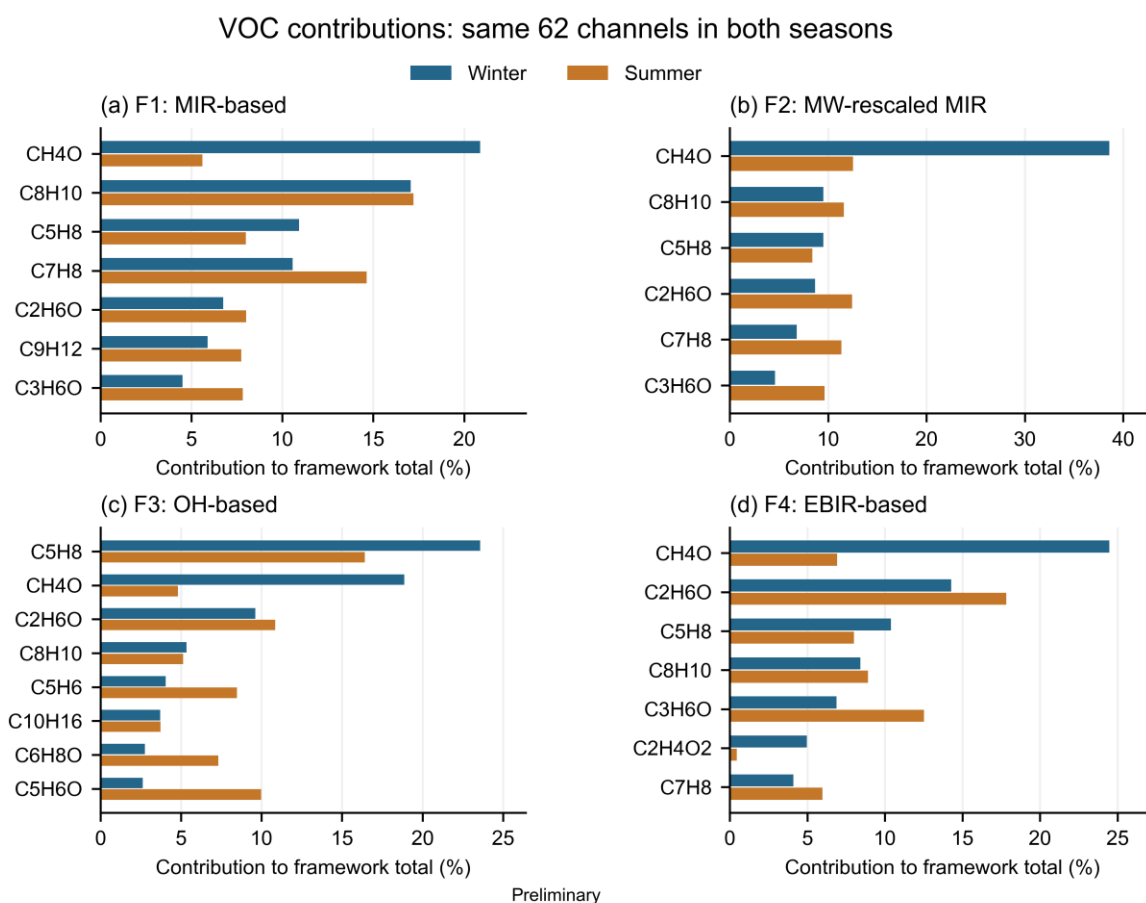


Figure B1. Preliminary VOC contribution profiles for the same 62 channels in both seasons and all four frameworks. Each panel includes the six leading channels from either season. Bars show percentage contributions to the common-subset mean.