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FINAL REPORT

Mexican EGU Impacts on Ozone in El Paso

TCEQ Contract No. 582-19-90498
Work Order No. 582-22-32532-015
Revision 2.0

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List of Acronyms

CAMx – Community Atmosphere Model with Extensions

EGU – Electricity Generating Unit

ELP – El Paso

EPA – Environmental Protection Agency

MDA8 – Maximum Daily 8-hour Average

QAPP – Quality Assurance Project Plan

SCICHEM – Second-Order Closure Integrated Puff Model with Chemistry

TCEQ – Texas Commission on Environmental Quality

WRF – Weather Research and Forecasting Model

Executive Summary

The purpose of this project was to assess the ozone impact of Mexican electrical generating units (EGUs) near Ciudad Juarez on El Paso, Texas. We used v3.3 of the Second-Order Closure Integrated Puff Model with Chemistry (SCICHEM) to assess the impact of four EGUs near Ciudad Juarez on ozone levels in El Paso County, Texas. We examined how large the emissions from hypothetical new point sources in Juarez and surrounding regions would have to be to have a significant impact on ozone in El Paso.

AER modeled the following scenarios for August 2019:

1. Operation of the three incumbent Mexican EGUs (Benito Juarez (Samalayuca I), Samalayuca II, and Transalta Chihuahua III) during the 2019 ozone season.
2. A 2023 scenario where all three incumbent Mexican EGUs have been shut down and replaced by the Central de Combinado 38 CCC Norte III EGU.
3. A 2023 scenario where the oil powered EGU (Benito Juarez (Samalayuca)) has been shut down and the other three natural gas-powered EGUs (Samalayuca II, Transalta Chihuahua III, and Central de Combinado 38 CCC Norte III) operate consistently; and
4. A 2023 scenario where the three natural gas powered Mexican EGUs operate consistently and the oil powered Mexican EGU (Benito Juarez (Samalayuca I)) is used as a peaking unit.

Stack parameters and hourly speciated emissions estimates were developed for each EGU consistent with US EPA data and assumptions. WRF and CAMx output for the El Paso area (180 km x 180 km domain, 4 km resolution) was processed using MMIF and CTM2SCICHEM, respectively, to develop the necessary meteorological and background chemical input data for SCICHEM. A receptor grid at 2 km resolution covering the TCEQ El Paso CAMx domain was used.

Each scenario above was simulated in SCICHEM for August 1-30, 2019. To speed up processing, each day was simulated separately using a 6-hour spin-up period before performing the 24-hour simulation. The maximum daily 8-hour average (MDA8) O₃ impacts at each receptor were calculated, along with the daily 1-hour maximum NO and NO₂ concentrations.

As expected, Scenario IV with all four EGUs running tends to have the largest MDA8 O₃ impacts, with a maximum impact of 12.5 ppbv for August 2019. Replacing the incumbent EGUs (Scenario I) with Norte III (Scenario II) still gives a similar maximum MDA8 O₃ (9.7 ppb to 9.9 ppb, respectively). Adding the two incumbent gas EGUs to Norte III increases the maximum impact from 9.9 ppb to 11.4 ppb. The maximum O₃ impacts of the Mexican EGUs in Texas tend to happen to the northeast and southeast of El Paso, rather than in the city itself.

Our modeling approach could be applied to other months besides August 2019 to better understand the impacts of these EGUs on El Paso air quality. Future work could incorporate future US EPA emission platform data on the EGUs simulated here, updating parameters for Norte III and the other power plants. In addition, future work could further investigate the impact of the MAXPUFF and MAXGRID settings on the final SCICHEM results to find the optimal values for these model parameters.

1. Introduction

1.1 Project Objectives

The purpose of this project was to assess the ozone impact of Mexican electrical generating units (EGUs) near Ciudad Juarez on El Paso, Texas. AER used v3.3 of the Second-Order Closure Integrated Puff Model with Chemistry (SCICHEM) to assess the impact of four EGUs near Ciudad Juarez on ozone levels in El Paso County, Texas. AER examined how large the emissions from hypothetical new point sources in Juarez and surrounding regions would have to be to have a significant impact on ozone in El Paso.

AER modeled the following scenarios for August 2019:

1. **Scenario I:** Operation of the three incumbent Mexican EGUs (Benito Juarez (Samalayuca), Samalayuca II, and Transalta Chihuahua III) during the 2019 ozone season.
2. **Scenario II:** A 2023 scenario where all three incumbent Mexican EGUs have been shut down and replaced by the Central de Combinado 38 CCC Norte III EGU.
3. **Scenario III:** A 2023 scenario where the oil powered EGU (Benito Juarez (Samalayuca I)) has been shut down and the other three natural gas-powered EGUs (Samalayuca II, Transalta Chihuahua III, and Central de Combinado 38 CCC Norte III) operate consistently; and
4. **Scenario IV:** A 2023 scenario where the three natural gas powered Mexican EGUs operate consistently and the oil powered Mexican EGU (Benito Juarez (Samalayuca)) is used as a peaking unit.

The amended schedule of deliverables for this project is given in **Error! Reference source not found.**

1.2 Background

The El Paso area currently has multiple ozone monitors with design values above the 2015 Ozone National Ambient Air Quality Standards (NAAQS). Identifying sources that contribute to ozone concentrations in the El Paso area improve the understanding of ozone formation and help develop strategies to address high concentrations in the State Implementation Plan.

1.3 Report Outline

This Final Report highlights major activities and key findings, provides pertinent analysis, describes encountered problems and associated corrective actions, and details relevant statistics including data, parameter, or model completeness, accuracy and precision. It satisfies Deliverable 7.2 of the Work Plan for Work Order No. 582-22-32532-015:

Deliverable 7.2:	Final Report
Deliverable 7.2 Due Date:	June 30 2022

The modeling protocol used in this project is summarized in Section 2, while our major results are discussed in Section 3. Section 4 discusses the quality assurance findings for this project following the procedures from the project Quality Assurance Project Plan (QAPP). Section 5 summarizes our conclusions and Section 6 makes recommendations for future work based on the results of this project.

Table 1. Projected Schedule for TCEQ Work Order #582-22-32532-015

Milestones	Planned Date
Task 1 - Work Plan	
1.1: TCEQ-approved Work Plan	March 22, 2022
1.2: TCEQ-approved QAPP	March 22, 2022
Task 2 – Progress Reports	
2.1: Monthly Progress Reports	Monthly
Task 3 – SCICHEM Input Data Gathering and Quality Assurance Review	
3.1: Report detailing the input dataset creation and quality assurance/quality control work done	April 30, 2022
Task 4 – SCICHEM Modeling Protocols	
4.1: Modeling protocol for TCEQ project manager review and approval.	April 30, 2022
Task 5 – Developing Tools to Evaluate GEOS-Chem Using Satellite Data	
5.1: SCICHEM output files in formats approved by the TCEQ project manager.	June 15, 2022
Task 6 – Training and on-going technical assistance to train TCEQ staff	
6.1: Technical Support and Review of TCEQ work products.	Upon request throughout the term of this Work Order
6.2: Remote training on SCICHEM and related models.	Prior to June 30, 2022
Task 7 – Draft and Final Reports	
7.1: Draft Report	June 15, 2022
7.2: Final Report	June 30, 2022

2 Modeling Protocol

2.1 Air Quality Model Overview

We used SCICHEM v3.3 to simulate the ozone impact of the four EGUs, along with their various preprocessors. MMIF will be used to convert the TCEQ WRF meteorological data into SCICHEM-ready input files. CTM2SCICHEM will be used to convert the TCEQ CAMx output into model-ready chemical background files. TERSCI will be used to process the complex terrain data and AERMAP will be used to gather elevation data for the receptor grid. BPIPPRM will be used to provide building downwash effects to the modeling scenario.

2.2 Facility Overview

The Samalayuca I (Benito Juarez) Power Plant (EPA NEI Facility ID CFEAD0803711, 31.34138889 °N, 106.4811111 °W, referred to below as “Sam I”) is a 316MW oil fired power project in Samalayuca, Juarez that was commissioned in April 1985. According to the US. EPA 2016v2 Emission Modeling Platform (<https://gaftp.epa.gov/Air/emismod/2016/v2>), in 2016 it emitted 1047 short tons of NO_x and 22 short tons of VOCs.

The Benito Juarez Samalayuca II (Benito Juarez) CCGT Power Station (EPA NEI Facility ID CFEAD0803731, referred to below as “Sam II”) is located at Samalayuca, Juarez (31.3241667 °N, 106.69028 °W). It is a three-unit natural gas power plant with a design capacity of 522 MW that was commissioned in 1998. According to the US. EPA 2016v2 Emission Modeling Platform, in 2016 it emitted 1930 short tons of NO_x and 27 short tons of VOCs.

The Chihuahua III power station is a 275-megawatt (MW) gas-fired power station (EPA NEI Facility ID ECIAD0803711, referred to below as “Chi III”) located in Samalayuca, Juarez, Mexico (31.33333333 °N, 106.4816667 °W). According to the US. EPA 2016v2 Emission Modeling Platform, in 2016 it emitted 785 short tons of NO_x and 13 short tons of VOCs.

The 907MW Norte III natural gas combined-cycle power plant (referred to below as “Norte III”) located in Juárez in Northern Mexico (31.473 °N, 106.7421 °W) commenced operations in June 2020. It is one of the biggest gas-fired combined-cycle facility in Mexico. While this plant was not included in existing EPA modeling platforms, it has the potential to emit 605 short tons of NO_x per year (based on the maximum emission rate of 17.4 g/s used for their NO₂ permitting).

2.3 Receptors

Receptor elevations are from USGS National Elevation Data (NED) at 30-meter resolution and processed by TERSCI and AERMAP. As we are interested in downwind impacts of ozone rather than fence-line concentrations, these receptors will consist of a single 2 km by 2 km resolution grid covering the 4 km El Paso modeling domain used by TCEQ (180 km by 180 km). We use a resolution of 2 km as SCICHEM supplies point estimates of pollutant concentrations at each receptor, and so we will average 4 receptors together for comparisons to the TCEQ 4 km grid.

2.4 Meteorology Data

Meteorology data for August 2019 were provided by TCEQ as WRF output files for the 4 km El Paso modeling domain. These data were processed using MMIF to prepare meteorological input files for SCICHEM.

2.5 Chemical Background Data

Chemical background data is need for this modeling study to provide ambient concentrations of O₃, NO_x, VOCs, and other pollutants. CAMx output data for August 2019 were provided by TCEQ as CAMx netCDF output files for the 4 km El Paso modeling domain. These were converted to the NetCDF classic format and then processed into SCICHEM-ready files using the CTM2SCICHEM preprocessor.

2.6 Stack Parameters

Initial estimates of emissions and stack parameters were taken from the US EPA 2016v2 emission modeling platform (Mexico_2016_point_20191209_27ma). Only Sam I and Sam II had stack parameters listed, and these did not include the temperature of the exhaust gas. Missing stack parameters were filled in using EPA defaults for stack parameters for each SCC code.¹

For Norte III, the environmental impact statement listed most needed stack parameters, with the stack velocity calculated from the given volumetric flow rate (563.55 m³/s) and stack diameter (5.5 m).

The final estimates of the stack parameters are shown in Table 2.

Table 2: Facility Source Parameters. Values estimates by SCC code are in italics.

Plant	unit_id	process_id	scc	longitude	latitude	Height (m)	Diam. (m)	Temp. (°C)	Vel. (m/s)
Sam I	2CH01	2ECM01A	20100201	-106.48111	31.3413889	82.38	3.81	307.39	22.46
Sam I	2CH01	2ECM01B	10100401	-106.48111	31.3413889	82.38	3.81	125.61	22.46
Sam I	2CH02	2ECM02A	20100201	-106.48111	31.3413889	82.38	3.81	307.39	22.92
Sam I	2CH02	2ECM02B	10100401	-106.48111	31.3413889	82.38	3.81	125.61	22.92
Sam II	4CH02	4ECM02	20100201	-106.69028	31.3241667	18.00	1.50	307.39	3.30
Sam II	4CH03	4ECM03	20100201	-106.69028	31.3241667	45.72	5.20	307.39	19.38
Sam II	4CH04	4ECM04	20100201	-106.69028	31.3241667	45.72	5.20	307.39	19.74
Sam II	BLANK	4ECM01	10100601	-106.69028	31.3241667	80.43	3.14	113.33	14.29
Chi III	BLANK	2ECM01	20100201	-106.48167	31.3333333	18.90	3.05	307.39	18.68
Chi III	BLANK	2ECM02	20100201	-106.48167	31.3333333	18.90	3.05	307.39	18.68

¹ See pp. 7-8 of FLAT FILE GENERATION METHODOLOGY Version: Summer 2021 Reference Case using EPA Platform v6. <https://www.epa.gov/system/files/documents/2021-09/flat-file-methodology-epa-platform-v6-summer-2021-reference-case.pdf>

Norte III	N/A	N/A	N/A	-106.4721	31.473	35.00	5.50	89.00	23.72
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2.7 Emissions

NO_x and VOC emission by process were taken from the 2016v2 Emissions Modeling Platform for Sam I, Sam II, and Chi III. Norte III NO_x emissions were estimated based on their maximum possible emissions of 17.4 g/s, while their VOC emissions were calculated by assuming the ratio of NO_x to VOC emissions at Norte III is the same as at Chi III. These annual values are given in Table 3.

Table 3. Annual and August emissions of NO_x and VOCs for each site.

Plant	unit_id	process_id	scc	Annual		August Fraction	August Emissions	
				NO _x (US ton)	VOC (US ton)		NO _x (kg)	VOC (kg)
Sam I	2CH01	2ECM01A	20100201	658.9	15.4	0.0908	54290	1270.6
Sam I	2CH01	2ECM01B	10100401	0.5	0.0	0.0731	33	0.5
Sam I	2CH02	2ECM02A	20100201	59.7	1.4	0.0908	4916	115.0
Sam I	2CH02	2ECM02B	10100401	327.9	5.3	0.0731	21735	351.5
Sam II	4CH02	4ECM02	20100201	846.7	9.3	0.0908	69760	763.0
Sam II	4CH03	4ECM03	20100201	537.1	8.8	0.0908	44248	725.9
Sam II	4CH04	4ECM04	20100201	546.2	9.0	0.0908	45002	738.3
Sam II	BLANK	4ECM01	10100601	0.2	0.0	0.1018	22	0.5
Chi III	BLANK	2ECM01	20100201	395.0	6.5	0.0908	32542	533.9
Chi III	BLANK	2ECM02	20100201	389.9	6.4	0.0908	32125	527.0
Norte III	BLANK	N/A	20100201	605.0	9.9	0.0908	49845	817.8

We estimated the temporal variation of these emissions following EPA standard procedures. For the 2016v2 platform, each SCC code corresponds to a unique monthly, weekly, and hourly temporal profile (see files `amptref_Canada_2010_tref_19jul2017_v2`). The three SCC types at these four facilities all have the same weekly and daily temporal profiles, shown in Figures 1 and 2. However, their monthly profiles differ, as shown in Figure 3. Natural gas emissions are higher than average in August while oil emissions are lower. Emissions are highest during the weekdays and rising from an overnight low at 3 AM local time to an afternoon peak at 3 PM.

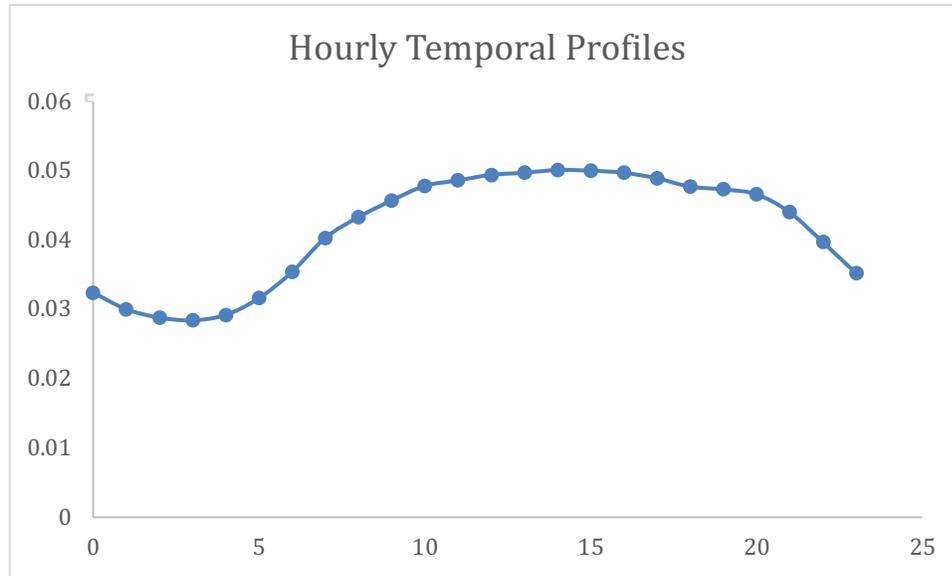


Figure 1. Daily temporal profile (#33 from the EPA 2016v2 Emission Modeling Platform) used for all sites.

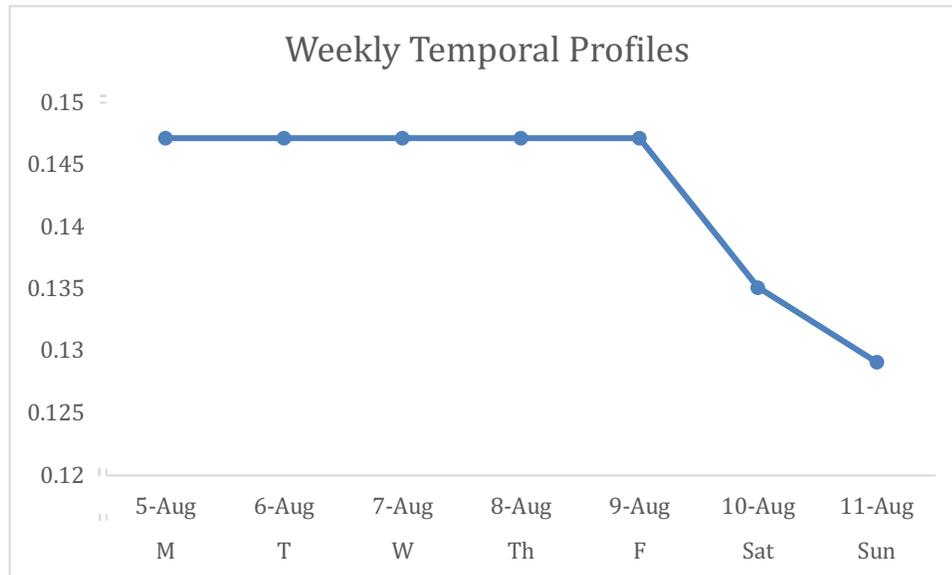


Figure 2. Weekly temporal profile (#8 from the EPA 2016v2 Emission Modeling Platform) used for all sites.

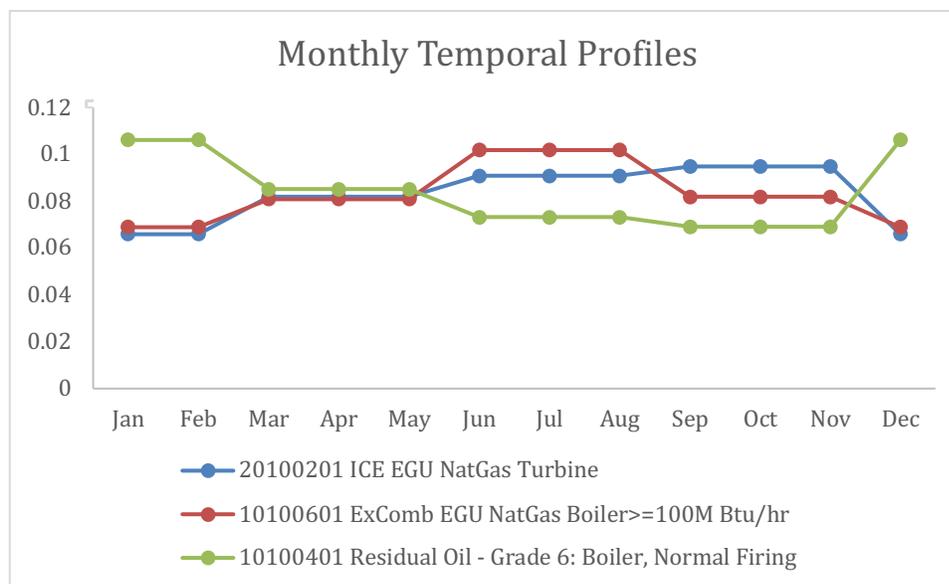


Figure 3. Monthly Temporal profiles used for each site by SCC code.

Thus, we used the SCC codes to determine how much of the annual emission for each process were emitted in August, and the August fractions and total emissions in kg are shown in Table 2. These August total emissions will be used to calculate the hourly emission for each source using the formula:

$$E_{hourly}(D, H) = \frac{7 \text{ days}}{31 \text{ days}} E_{Aug} f_{week}(D) f_{day}(H)$$

where $E_{hourly}(D, H)$ is the total emission of the species in a given day and hour (units kg/hour), $f_{week}(D)$ is the fraction of weekly emissions on day of week D shown in Figure 2 and $f_{day}(H)$ is the fraction of daily emissions for hour H shown in Figure 1. The fraction of 7/31 is used to convert total August emissions (31 days) to weekly emissions (7 days), assuming each week is the same.

The emissions of NO_x and VOCs also need to be speciated to the CB6 chemical mechanism for use in SCICHEM. We will follow the speciation profiles used in the EPA 2016v2 emission modeling platform. For NO_x , we first convert from kg/hour to moles using the molecular weight of NO_2 (0.046 kg/mol), as stated in <https://www.epa.gov/air-emissions-inventories/how-are-oxides-nitrogen-nox-defined-nej>. Then we assume that 15% of the in-stack NO_x by mole is emitted as NO_2 based on an EPA survey of 106 natural gas plants in Texas (available from <https://www.epa.gov/scram/nitrogen-dioxidenitrogen-oxide-stack-ratio-isr-database>). The moles/hour of NO and NO_2 emitted will then be converted to g/s for input into SCICHEM.

For VOCs, the speciation profiles by SCC code are given in Table 4 (see also `gsref_othpt_cmaq_cb6ae7_2016fj_16j_nf.txt` from the 2016v2 platform). Given only Sam I has any appreciable emissions of non-methane VOCs, we do not expect the VOC emissions or their speciation to have much effect on the O_3 impacts of these sources.

Table 4. VOC speciation profiles (mass fractions, normal text) and molecular weights (g/mol, italics) by SCC code.

SCC	VOC/ NONHAPTOG Profile	CH ₄	ACET	PAR	PRPA	TOL	UNR
10100401	0001	0.1897 <i>(16.042)</i>	0.4828 <i>(14.4859)</i>	0.3276 <i>(14.4859)</i>	0	0	0
10100601	0003	0.6364 <i>(16.042)</i>	0	0.2951 <i>(14.446)</i>	0.0455 <i>(44.096)</i>	0.0227 <i>(92.138)</i>	0.0003 <i>(14.3632)</i>
20100201	0007	1.0 <i>(16.042)</i>	0	0	0	0	0

3 Results and Discussion

3.1 Example Output for a Single Day, August 16th

Figure 4 below shows the MDA8 O₃ impact of Scenario I where the three incumbent Mexican EGUs (Benito Juarez (Samalayuca I), Samalayuca II, and Transalta Chihuahua III) for August 16, while Figure 5 shows the impact for Scenario II where all three incumbent Mexican EGUs have been shut down and replaced by the Central de Combinado 38 CCC Norte III EGU. The maximum MDA8 O₃ impact is lower for the second scenario, as expected (7.8 ppb in Figure 1, 5.4 ppb in Figure 2). On this day, the impacts on the Texas side of the border were negligible due to the wind blowing the plumes primarily to the SW.

Figure 6 shows the same plot for Scenario III. In this case the oil plant (Samalayuca I) is shut down, but all three gas plants operate continuously. The maximum O₃ impact is 7.4 ppb. This means that the addition of the Samalayuca II and Transalta Chihuahua III to the Norte III plant increased the MDA8 O₃ impact by 2 ppb, such that it is only slightly smaller (0.4 ppb) than Scenario I where all three older plants are operating.

Figure 7 then shows all four power plants operating, assuming Samalayuca I is used as a peaking unit. As expected, this shows the largest impact on MDA8 O₃ of all of the scenarios (8.8 ppb). The addition of the older oil plant as a peaking unit on this day only adds 1.4 ppb to the impact of the three gas plants from Scenario III.

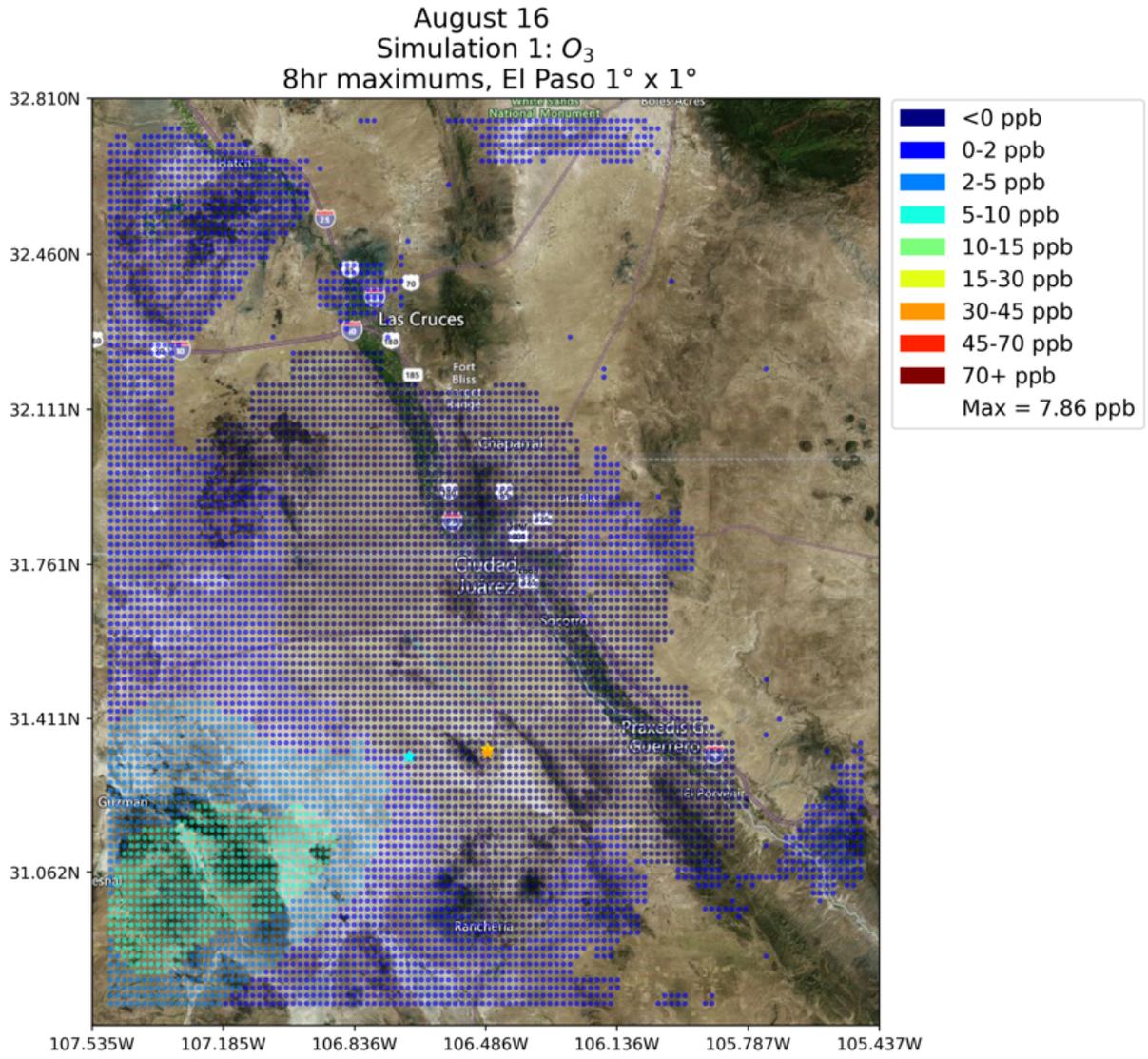


Figure 4. MDA8 O₃ impact of the three incumbent Mexican EGUs (Benito Juarez (Samalayuca), Samalayuca II, and Transalta Chihuahua III) for August 16.

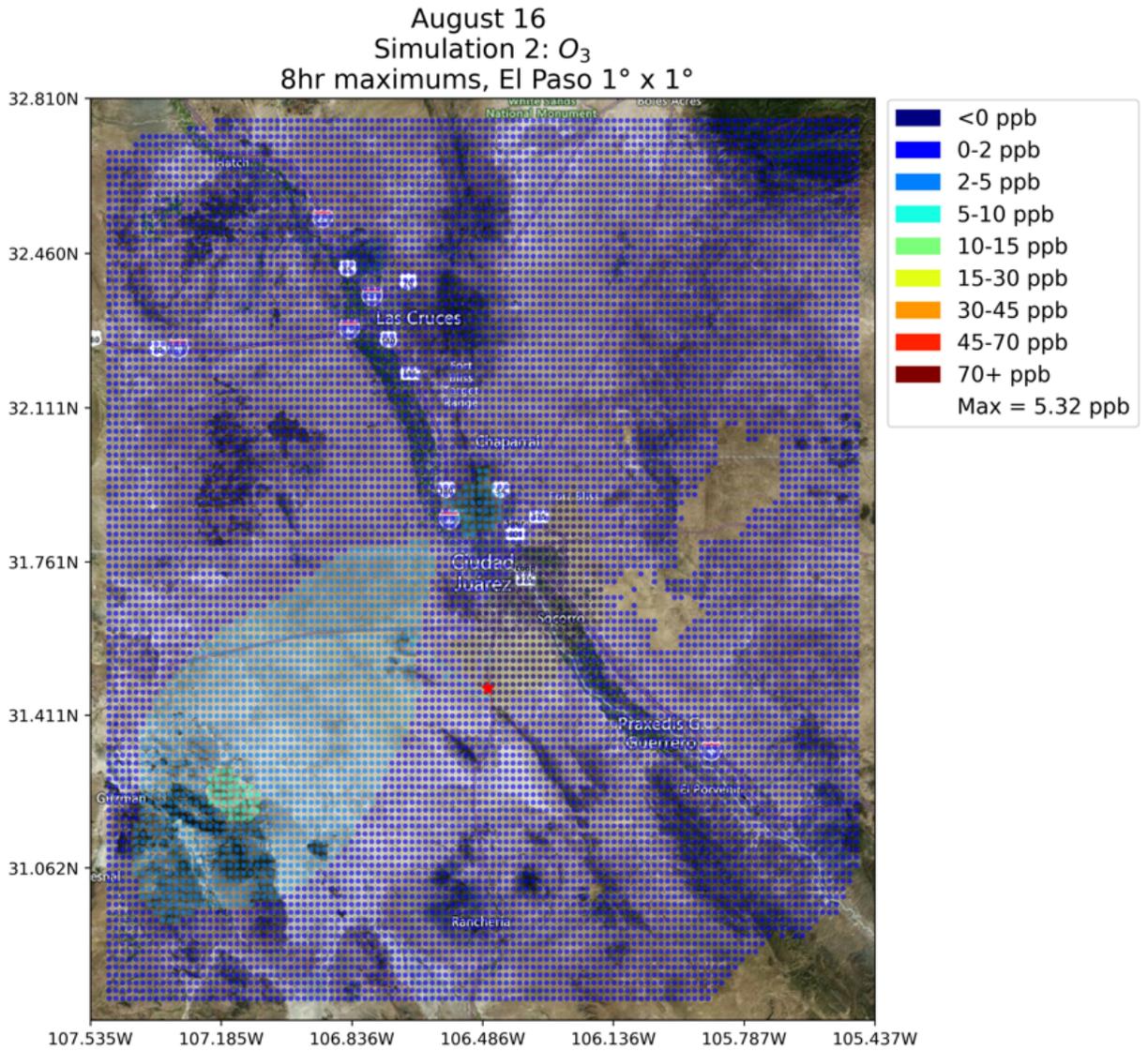


Figure 5. As in Figure 4 but for Scenario II, where all three incumbent Mexican EGUs have been shut down and replaced by Norte III.

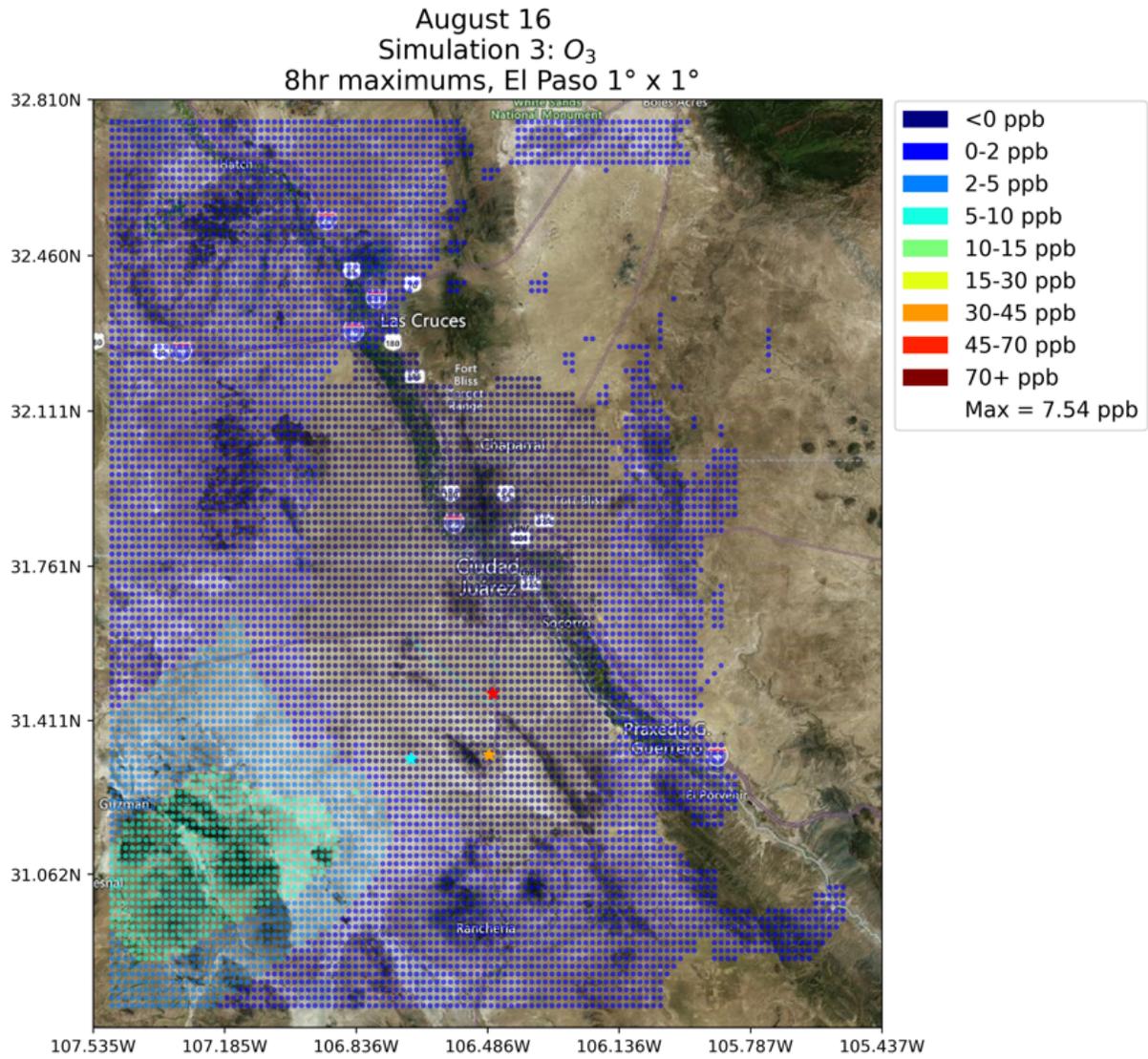


Figure 6. As in Figure 4 but for Scenario III, where all three gas plants are operating.

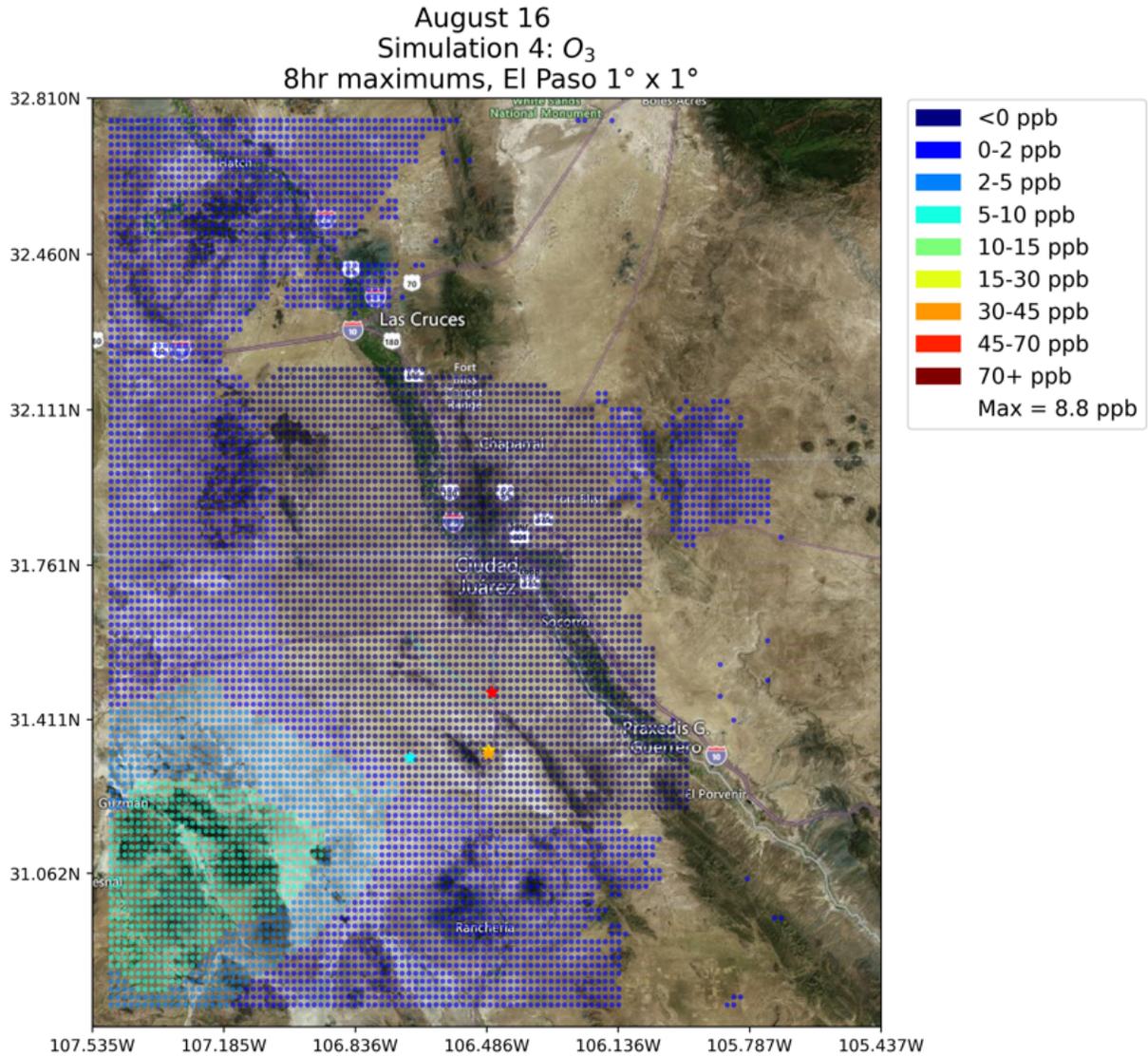


Figure 7. As in Figure 4 but for Scenario IV, where all four plants are operating with the oil plant as a peaking unit.

3.2 Maximum observed MDA8 O₃, August 1-30, 2019

Figure 8 and Figure 9 below shows the MDA8 O₃ average and maximum, respectively, for August 1-30, 2019, for Scenario I, where around it averages -5 ppb for August near the sites. Most of the region averages around 0-1 ppb with a localized area to the northeast. The maximums during this time shows two different areas of 5-10 ppb to the southwest and northeast of El Paso, TX, with a maximum impact of 9.7 ppb.

Figure 10 and Figure 11 shows the average and maximum, respectively, below for Scenario II, where the impact is much less of around -1 ppb for August near Norte III. Most of the region averages around 0-1 ppb with a section in the Northeast of about 1.44 ppb. The maximums during this time shows two different areas of 5-10 ppb to the

southwest and northeast of El Paso, TX. However, the overall maximum over the 30 days is slightly more compared than Scenario I (9.9 ppb vs 9.7 ppb). This suggests that replacing the incumbent EGUs with Norte III reduces the average MDA8 O₃ impact on the surrounding area, but that the worst impacts are still similar.

Figure 12 and Figure 13 shows average and maximum, respectively, for Scenario III where, and the average is similar to Figure 8a. The maximum shows multiple areas of 5-10 ppb with a localized region >10 ppb to the southeast. The absolute maximum is much higher for this Scenario than Scenario II (11.4 ppb vs 9.9 ppb), suggesting that adding the incumbent gas EGUs to Norte III increases the maximum O₃ impact by 1-2 ppb.

Figure 14 and Figure 15 shows average and maximum, respectively, for Scenario IV where, and the average is similar to Figure 8 and Figure 12. The maximum shows multiple areas of 5-10 ppb with a localized region of 10-15 ppb to the northeast. Figure 15, as expected, shows the largest maximum (12.54 ppb) across all scenarios, as all four EGUs are operating, but it should be noted that Scenario I has the highest average (1.44 ppb).

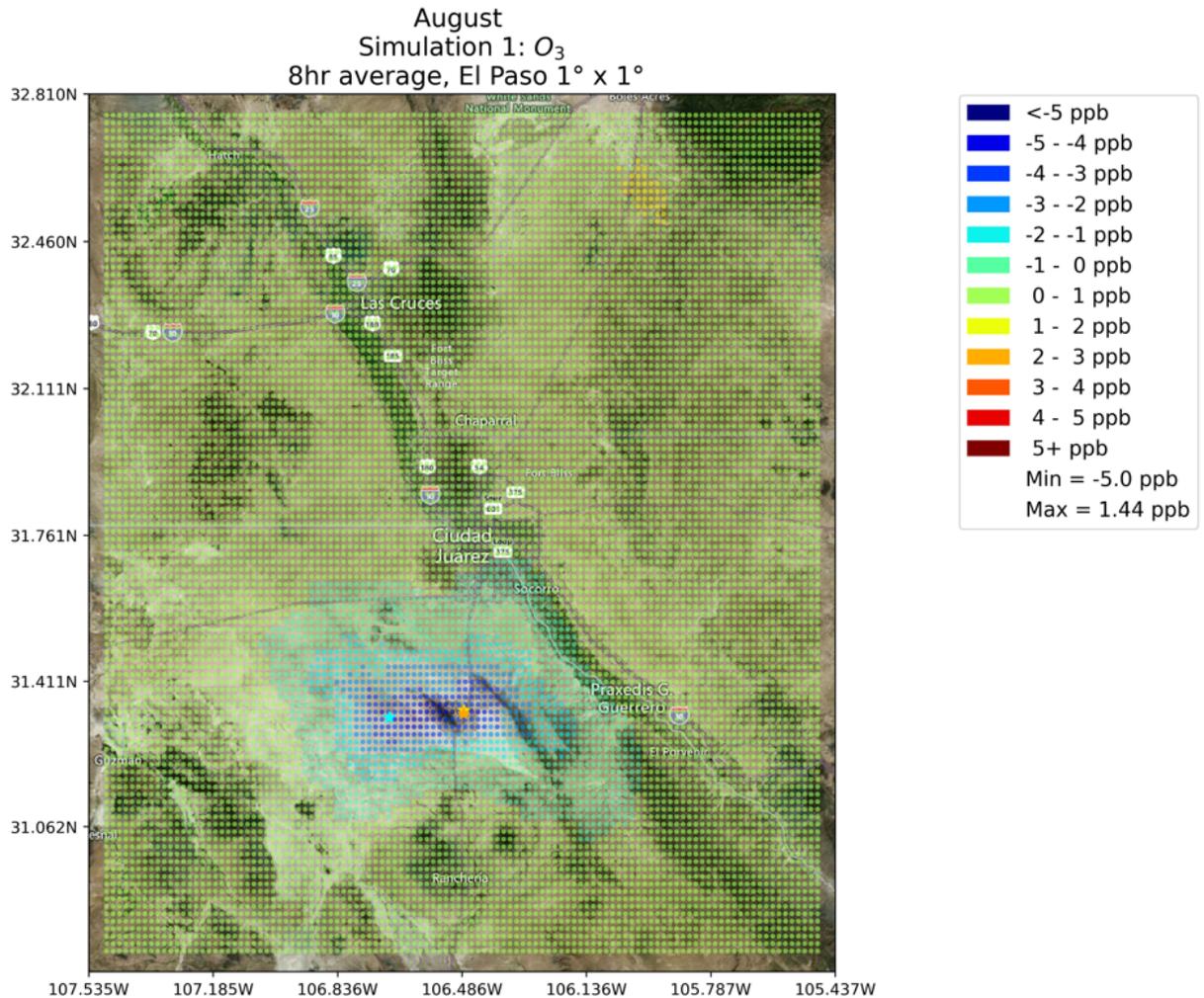


Figure 8. Scenario I average MDA8 O₃ for the period August 1-30.

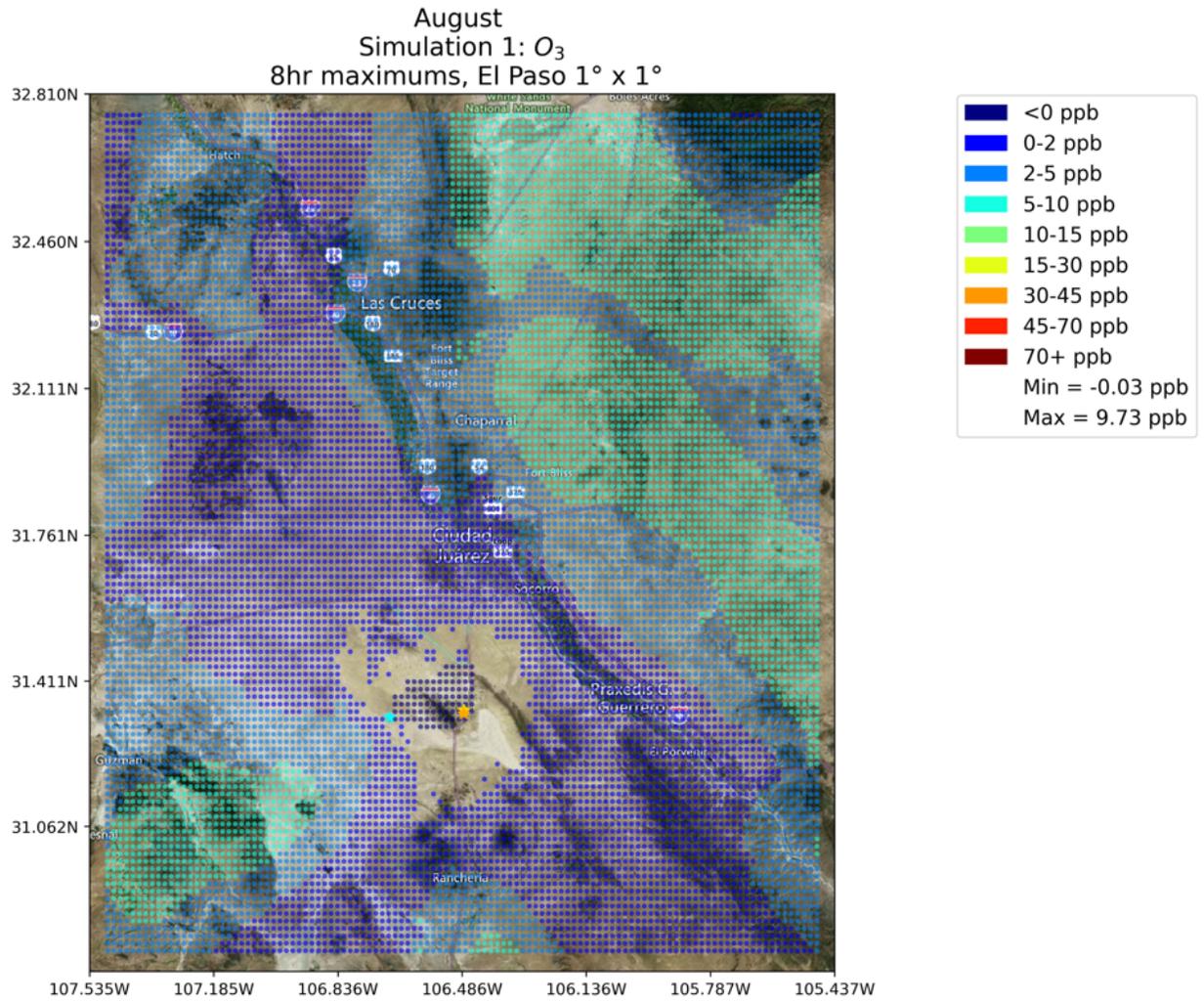


Figure 9. Scenario I maximum MDA8 O₃ or the period August 1-30.

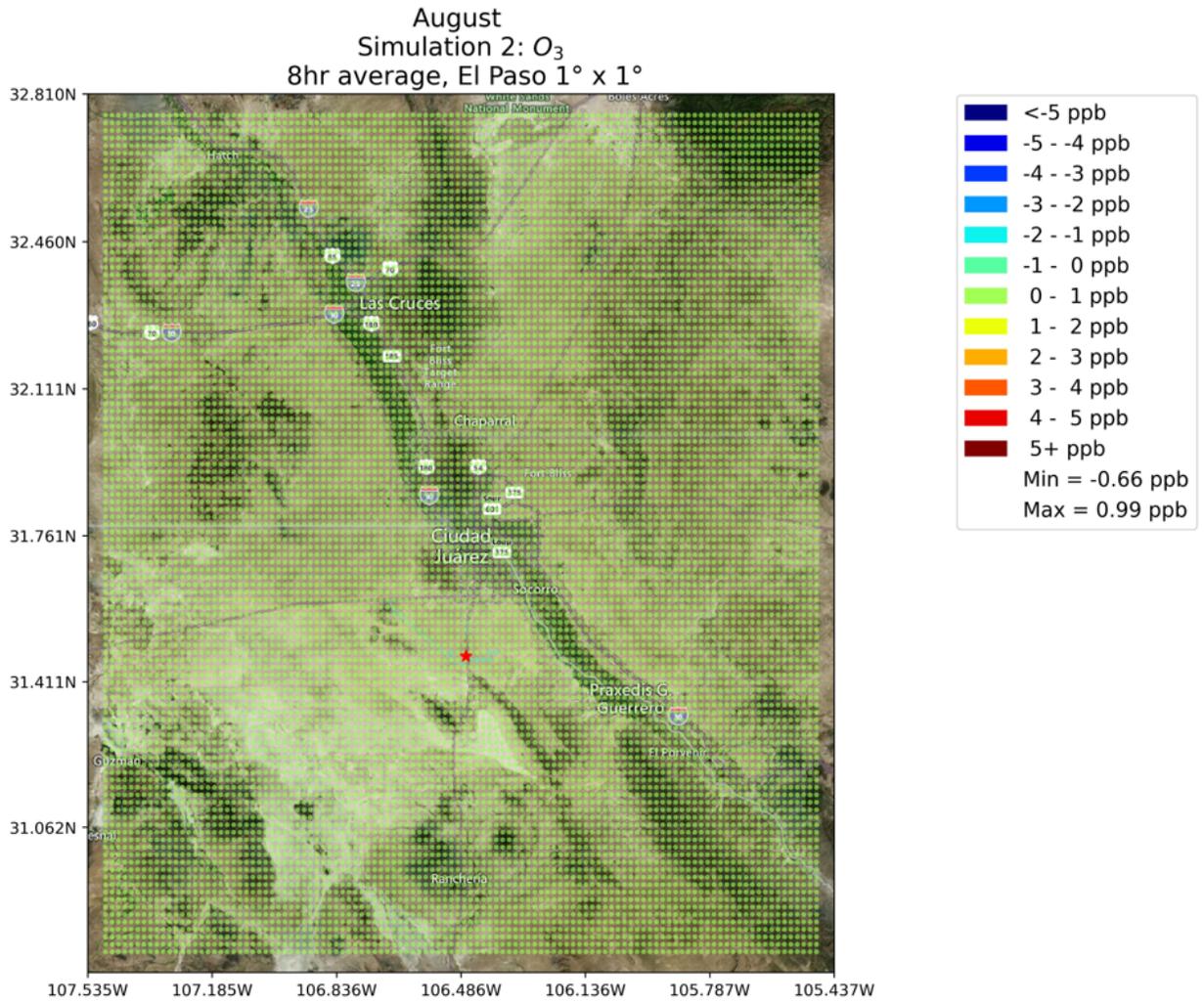


Figure 10. Same as Figure 8, but Scenario II with only Norte III operating.

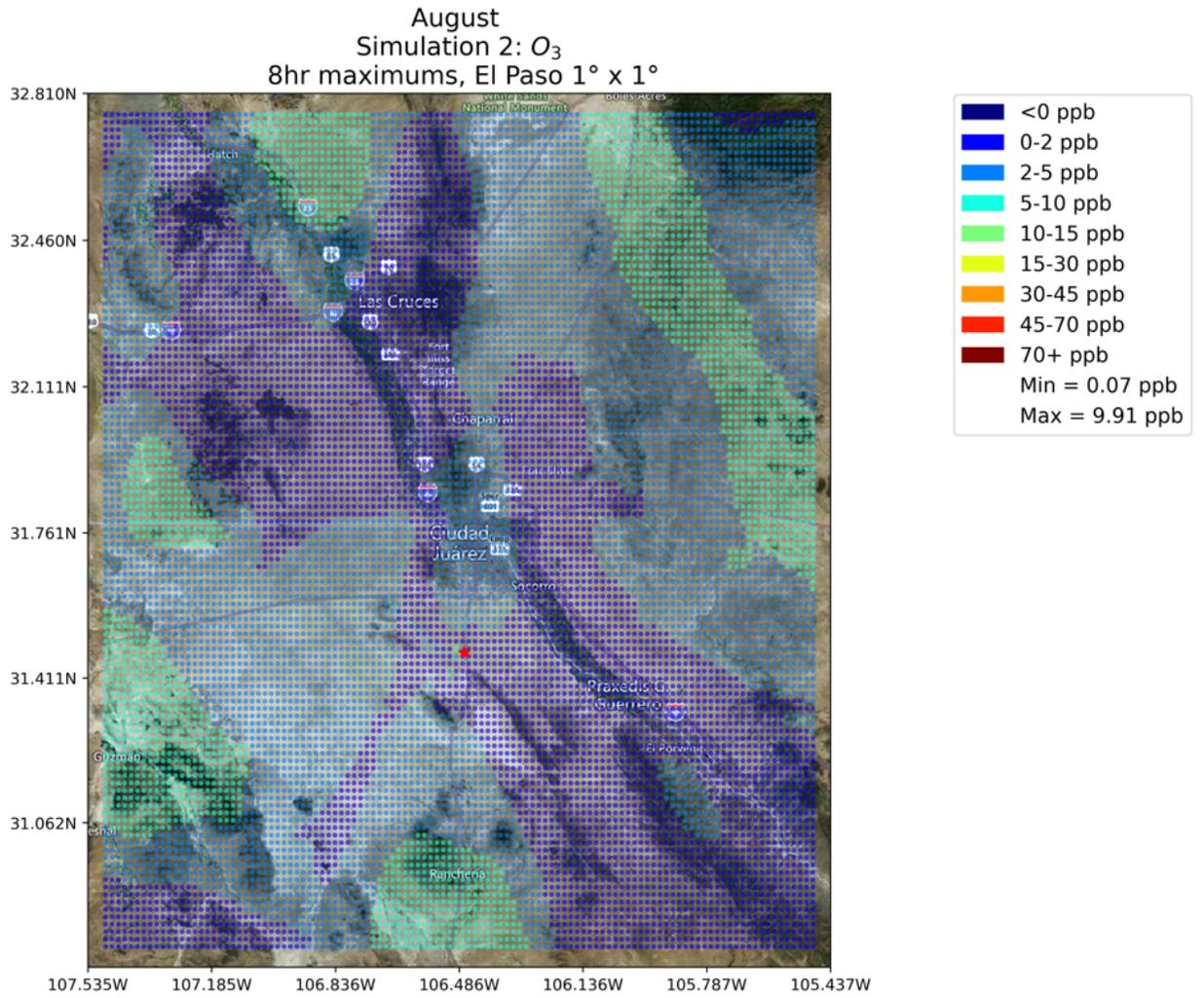


Figure 11. Same as Figure 9, but Scenario II with only Norte III operating.

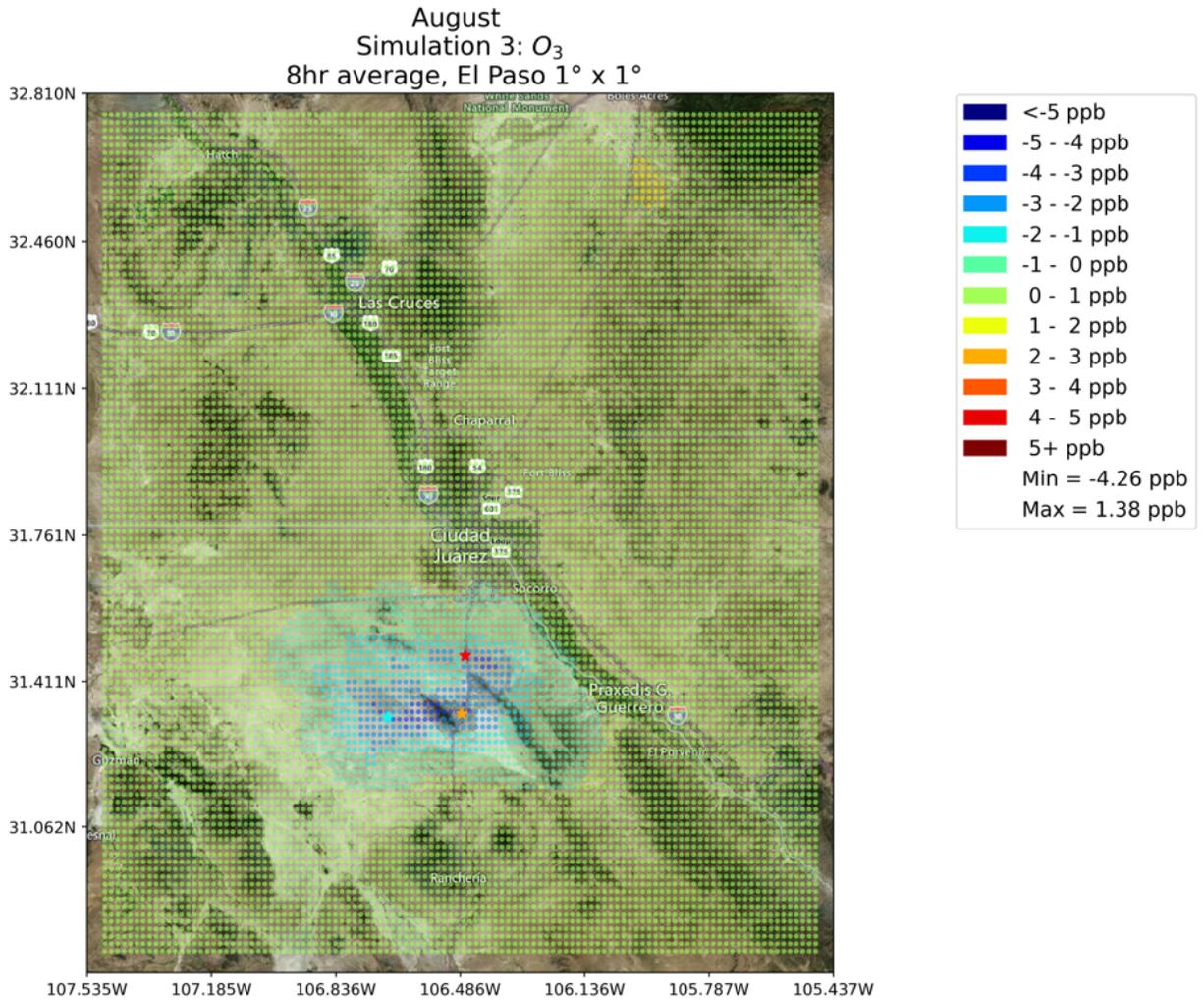


Figure 12. Same as Figure 8, but for Scenario III where all three gas plants are operating.

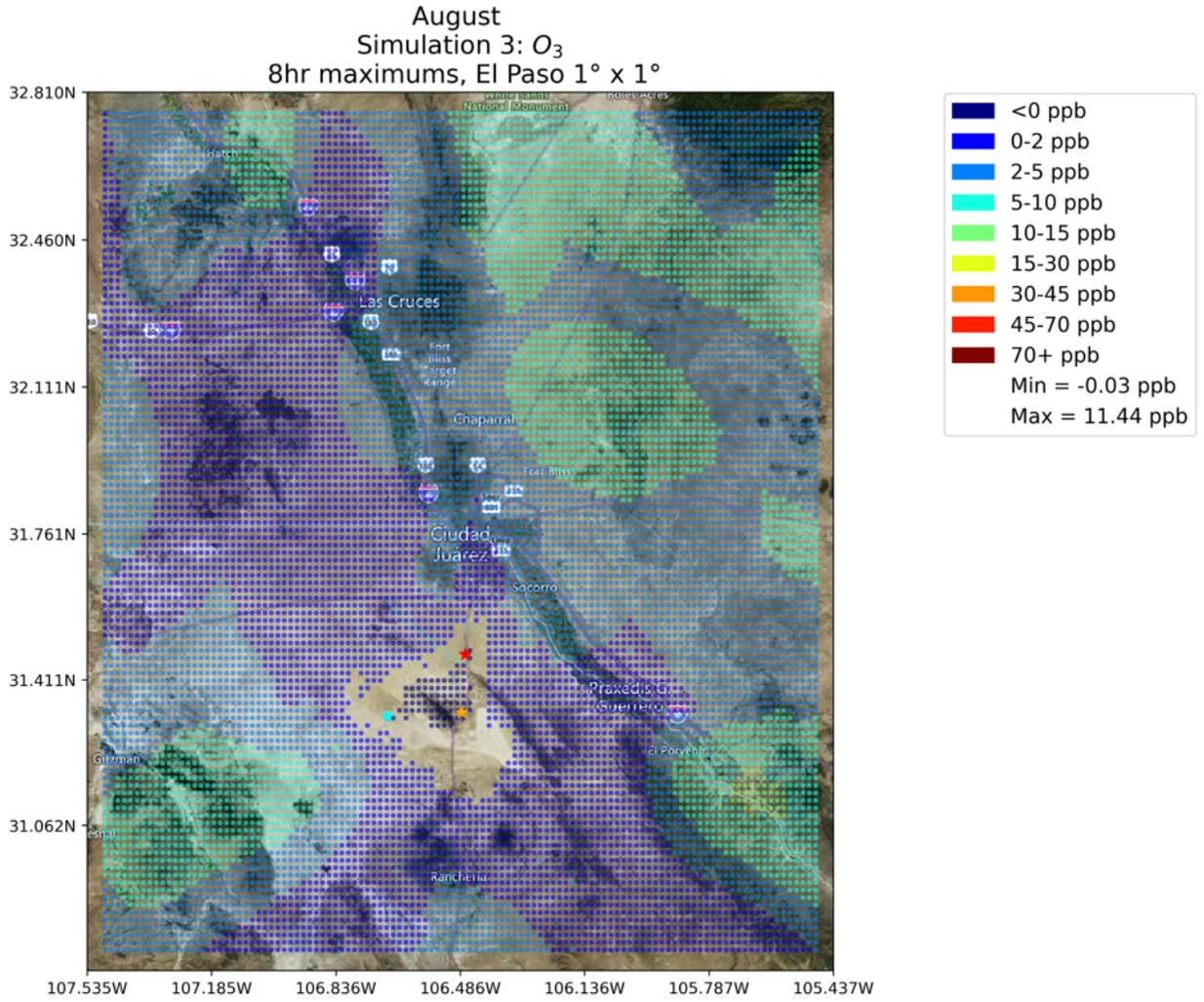


Figure 13. Same as Figure 9, but for Scenario III where all three gas plants are operating.

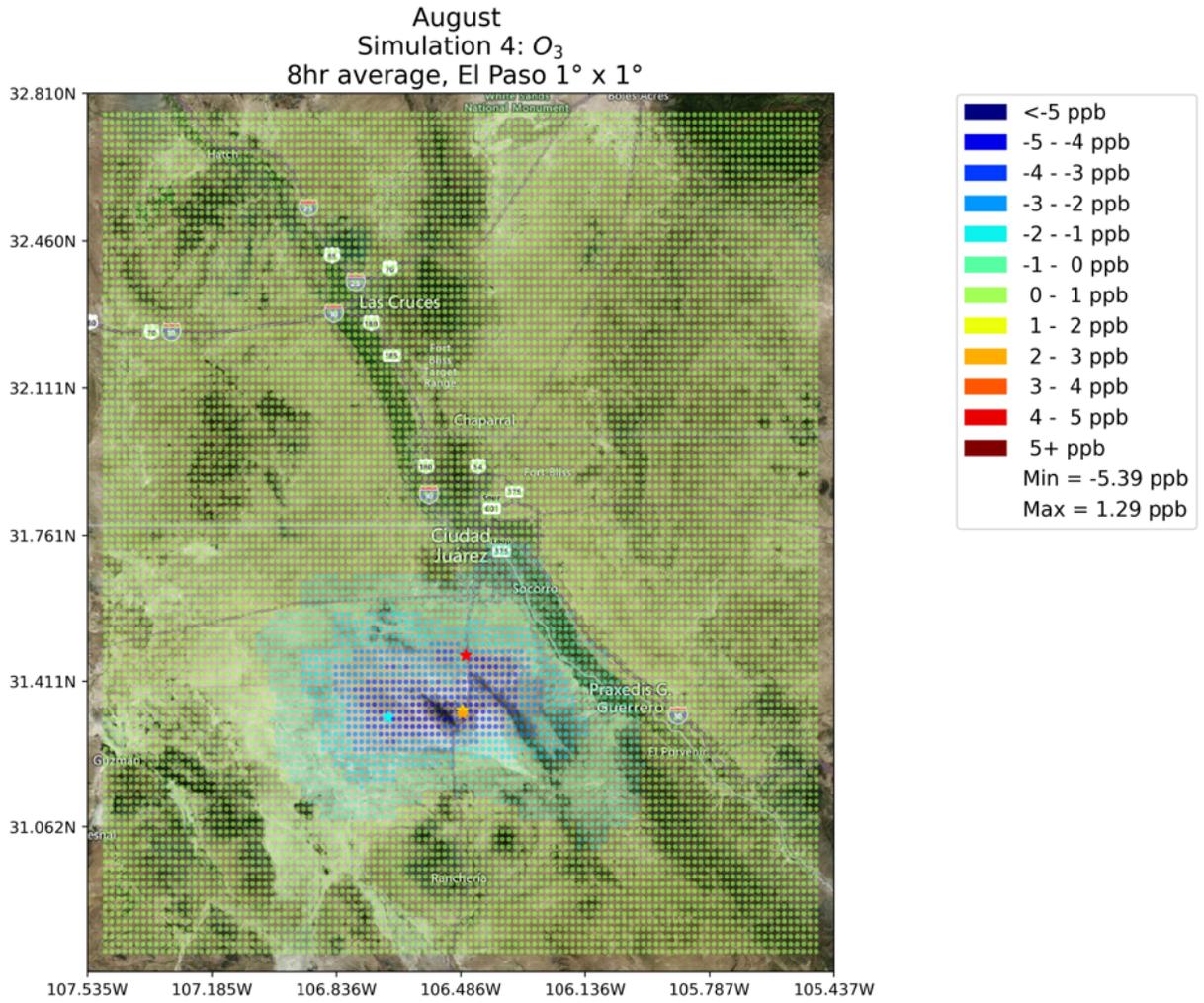


Figure 14. Same as Figure 8a, but Scenario IV where all four plants are operating with the oil plant as a peaking unit.

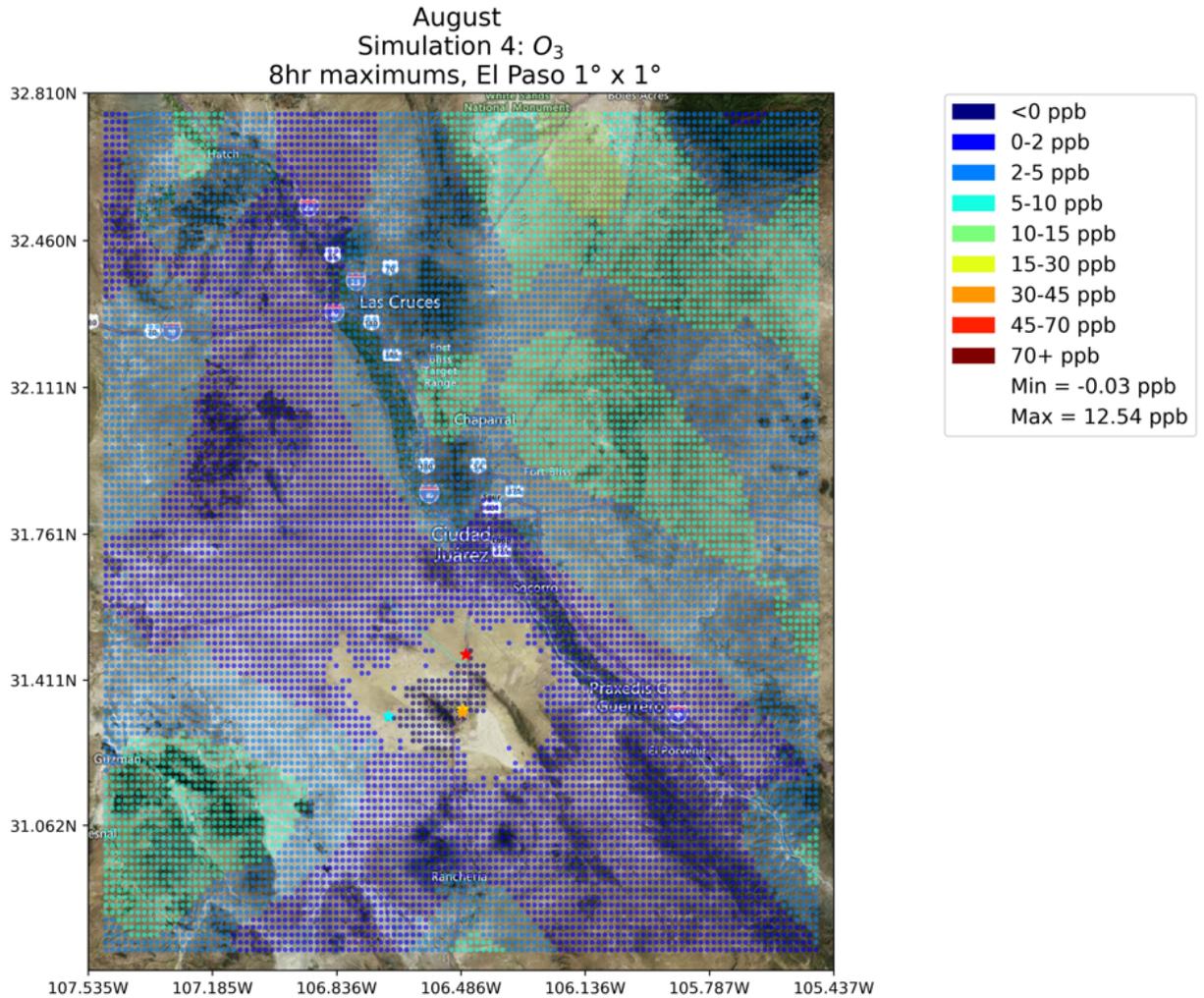


Figure 15. Same as Figure 9, but Scenario IV where all four plants are operating with the oil plant as a peaking unit.

3.3 Comparison with TCEQ Monitors

Table 5 shows the list of regulatory O₃ monitoring location in and around El Paso that will be used to validate the model in this study. Cumulative MDA8 O₃ values and cumulative maximum hourly NO_x concentrations at each location were calculated with SCICHEM for each day in August and compared to the monitor values. To compare with the ambient monitors, the O₃, NO, and NO₂ concentrations from the EGUs in each of the three scenarios need to be added to the ambient estimate. While SCICHEM does add in the ambient background to the calculation, it does so as a constant domain-average value for each hour (see Figure 16) and so these “cumulative” values are not a direct replacement for a full CAMx simulation. Furthermore, the monitoring sites are generally near the border, and so are in the region where the MDA8 impacts from the EGUs are fairly small (< 5 ppb), and so the SCICHEM simulations show little variation at these sites. With those caveats, here we compare the SCICHEM-calculated cumulative MDA8 O₃ and MDA1 NO_x concentrations on each day to the available monitoring data.

Table 5. Nearby O₃ and NO_x monitoring stations for model validation

Site ID	Name	Address	Lat	Lon	O ₃	NO _x
481410057	Socorro Hueco	320 Old Hueco Tanks Road	31.6675457	-106.28798	Y	N
481410029	Ivanhoe	10834 Ivanhoe	31.7857585	-106.32363	Y	N
481410055	Ascarate Park SE	650 R E Thomason Loop	31.7467485	-106.4028	Y	Y
481410037	El Paso UTEP	250 Rim Rd	31.7683021	-106.50126	Y	Y
481410044	El Paso Chamizal	800 S San Marcial Street	31.7656923	-106.45523	Y	Y
481410058	Skyline Park	5050A Yvette Drive	31.8939195	-106.42582	Y	N

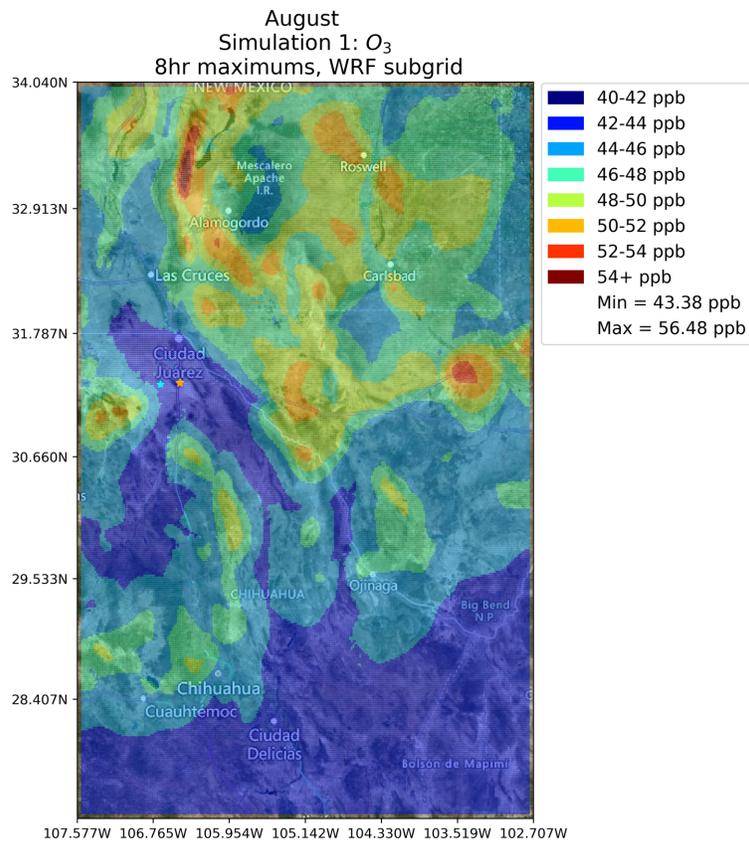


Figure 16. Maximum total MDA8 O₃ over the modeling domain for Simulation 1. Note near-constant background of 43 ppb.

Table 6 shows the mean, standard deviation, and range of MDA8 O₃ at each monitoring site in the observations and for each of the four SCICHEM simulations. In general, the SCICHEM simulations are biased low by 18-25 ppbv. This is due to the spatially constant regional background used in SCICHEM, which thus underestimates the variability of O₃ and impact of local sources on O₃. We have also done spot checks on the MDA8 O₃ values in the original CAMx output. Using this higher-resolution background improves the bias by 5-15 ppb, but this suggests that CAMx is still greatly underestimating MDA8 O₃ in El Paso. For example, at Chamizal on August 10, the observed MDA8 was 104 ppbv, but the CAMx value was only 57 ppbv, with the SCICHEM value of 45 ppb. This suggests that the main issue for the negative bias in SCICHEM is due to the underestimates in CAMx, with a smaller impact (5-15 ppb) coming from the use of a regional average background in SCICHEM.

Table 6. Mean \pm standard deviation of MDA8 O₃ (ppbv) at different monitoring sites in the observations and in each SCICHEM simulation. Min-Max MDA8 at each site is in italics.

Site	Observations	Simulation I	Simulation II	Simulation III	Simulation IV
Ascarte	66.3 \pm 10.8 <i>45-97</i>	44.8 \pm 1.3 <i>44-52</i>	44.8 \pm 0.5 <i>44-47</i>	44.9 \pm 1.3 <i>44-53</i>	44.5 \pm 2.3 <i>42-50</i>
Chamizal	69.5 \pm 14.3 <i>48-108</i>	44.8 \pm 1.3 <i>44-51</i>	44.8 \pm 0.7 <i>44-48</i>	45.0 \pm 1.6 <i>44-52</i>	44.9 \pm 1.5 <i>44-50</i>
El Paso UTEF	67.4 \pm 13.0 <i>48-94</i>	44.9 \pm 1.4 <i>44-51</i>	44.8 \pm 0.7 <i>44-48</i>	44.9 \pm 1.4 <i>44-51</i>	44.9 \pm 1.6 <i>44-52</i>
Ivanhoe	66.3 \pm 10.8 <i>49-89</i>	44.8 \pm 1.3 <i>43-51</i>	44.8 \pm 0.5 <i>44-46</i>	44.9 \pm 1.3 <i>44-51</i>	44.5 \pm 2.3 <i>34-50</i>
Skyline Park	66.1 \pm 12.1 <i>49-103</i>	45.0 \pm 1.6 <i>44-52</i>	44.9 \pm 0.8 <i>44-48</i>	45.0 \pm 1.4 <i>44-51</i>	45.0 \pm 1.9 <i>43-54</i>
Socorro Hueco	63.3 \pm 8.4 <i>48-82</i>	44.7 \pm 1.3 <i>42-51</i>	44.6 \pm 0.2 <i>44-45</i>	44.7 \pm 1.1 <i>43-50</i>	44.4 \pm 2.1 <i>34-49</i>

Table 7 shows the mean, standard deviation, and range of MDA8 O₃ at each monitoring site in the observations and for each of the four SCICHEM simulations. These generally compare well with the observations, except for Simulation II which tends to underestimate the total NO_x. However, as noted above the simulation may be missing the impact of local NO_x sources on the total. Furthermore, Simulations I, III, and IV all show higher max NO_x impacts than seen in the data, suggesting that we may be overestimating the NO_x emissions from the older power plants.

Table 7. Mean \pm standard deviation of MDA1 NO_x (ppbv) at different monitoring sites in the observations and in each SCICHEM simulation. Min-Max MDA1 at each site is in italics.

Site	Observations	Simulation I	Simulation II	Simulation III	Simulation IV
Ascarte	27.0 \pm 15.1	18.0 \pm 17.6	5.0 \pm 6.8	17.8 \pm 21.2	21.5 \pm 23.6
	<i>2.4-65.8</i>	<i>2.2-48.0</i>	<i>2.0-32.0</i>	<i>2.2-66.2</i>	<i>2.2-81.4</i>
Chamizal	26.6 \pm 15.5	19.0 \pm 28.5	4.9 \pm 6.4	18.3 \pm 32.0	21.7 \pm 30.8
	<i>5.7-71.0</i>	<i>2.2-140.8</i>	<i>2.1-32.6</i>	<i>2.1-156.9</i>	<i>2.2-133.5</i>
El Paso UTEP	17.1 \pm 9.8	22.5 \pm 37.4	6.2 \pm 10.4	22.9 \pm 47.3	44.9 \pm 1.6
	<i>3.8-43.3</i>	<i>2.2-169.3</i>	<i>2.2-49.7</i>	<i>2.2-228.3</i>	<i>2.2-185.6</i>

4 Quality Assurance

The WRF and CAMx data supplied by TCEQ has already undergone quality control by TCEQ. We have verified that this data can be successfully preprocessed using MMIF and CTM2SCICHEM, respectively, to produce the necessary meteorological and chemical background files for CAMx. Terrain data has similarly been processed with TERSCI

Hourly emissions files were checked to ensure that the total emissions match with the expected total for August for each facility and process, that the speciation is correct, and that the temporal profiles are correct. This was done by summing every constituent into daily and monthly values, summing up different species to check for consistency with the original NO_x and VOC emission estimates, and plotting the daily and hourly emissions for all species as a timeseries.

All SCICHEM input files were reviewed by an independent AER scientist before modeling begins for consistency with this modeling protocol. The model output was evaluated quantitatively with comparisons to O₃ and NO_x monitoring locations (Section 7) and qualitatively for consistency with expected chemical and transport behavior. This satisfies the requirement to review 10% of all model calculations.

Each of the scene parameters were offset by 10 meters. Stacking each scene on top of each other at the given latitude and longitude resulted in lower values than having each stack offset.

The SCICHEM runs returned a few warnings asking us to increase the values for MAXPUFF and MAXGRID in the model to ensure the accuracy of high-resolution results near the source. We did increase the values of these parameters to the maximum values recommended in the SCICHEM User's Guide (MAXPUFF = 60,000, MAXGRID = 100,000) but continued to get the warnings. We did not increase the values further as we noticed that doing so had a non-negligible effect on the results, and we didn't want to push the model outside of the settings that it had been evaluated with by the developers. Sensitivity tests were performed to see the impact of these settings, as shown in Figures 12-14 below. Note that the O₃ impacts in these plots are artificially high, as these tests were performed with no background O₃. We can see that the increasing MAXGRID from 50,000 (Figure 12) to 250,000 (Figure 13) has a small relative impact on the model results. However, increasing MAXPUFF to 120,000 and MAXGRID to 500,000 resulted in half the initial estimate, likely because the model is not supposed to operate with such extreme settings.

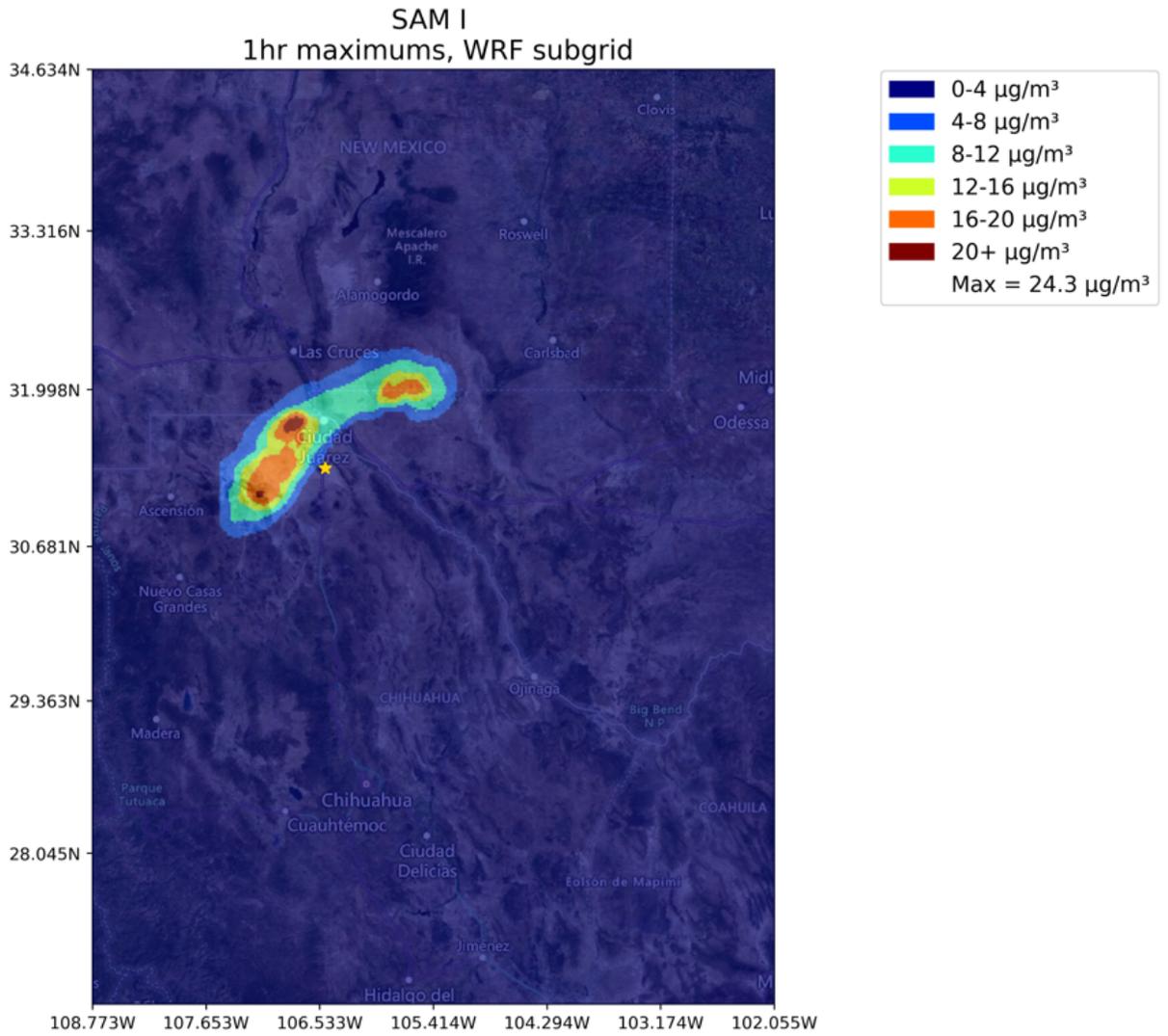


Figure 17. 1 scene used for Samalayuca 1 hour max daily O₃. MaxPuff set to 50000 and MaxGrid 50000.

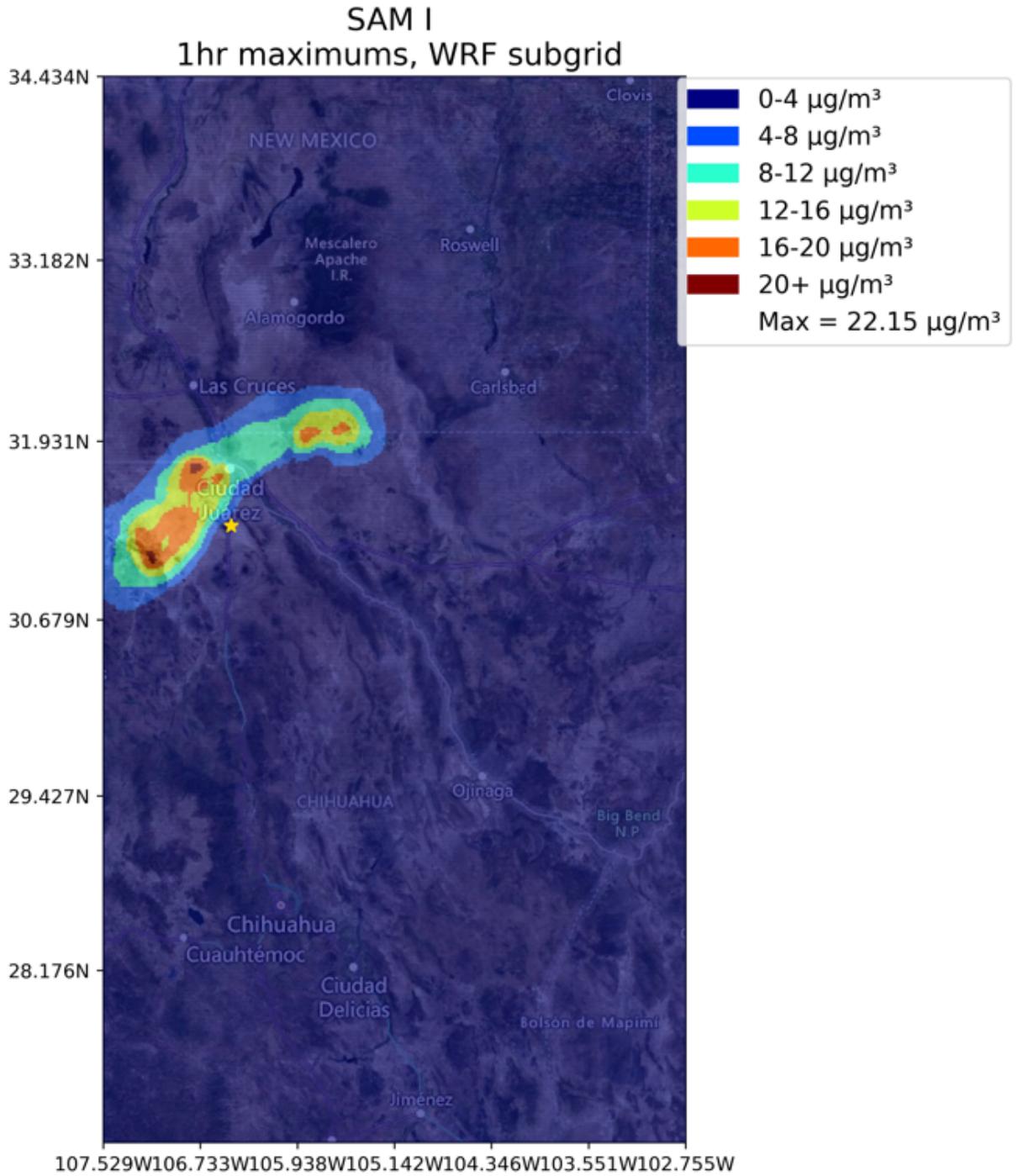


Figure 18. Same as Figure 16 but with MaxPuff 50000 and MaxGrid 250000

Figure 14. Same as Figure 12. MaxPuff 50000 and MaxGrid 250000

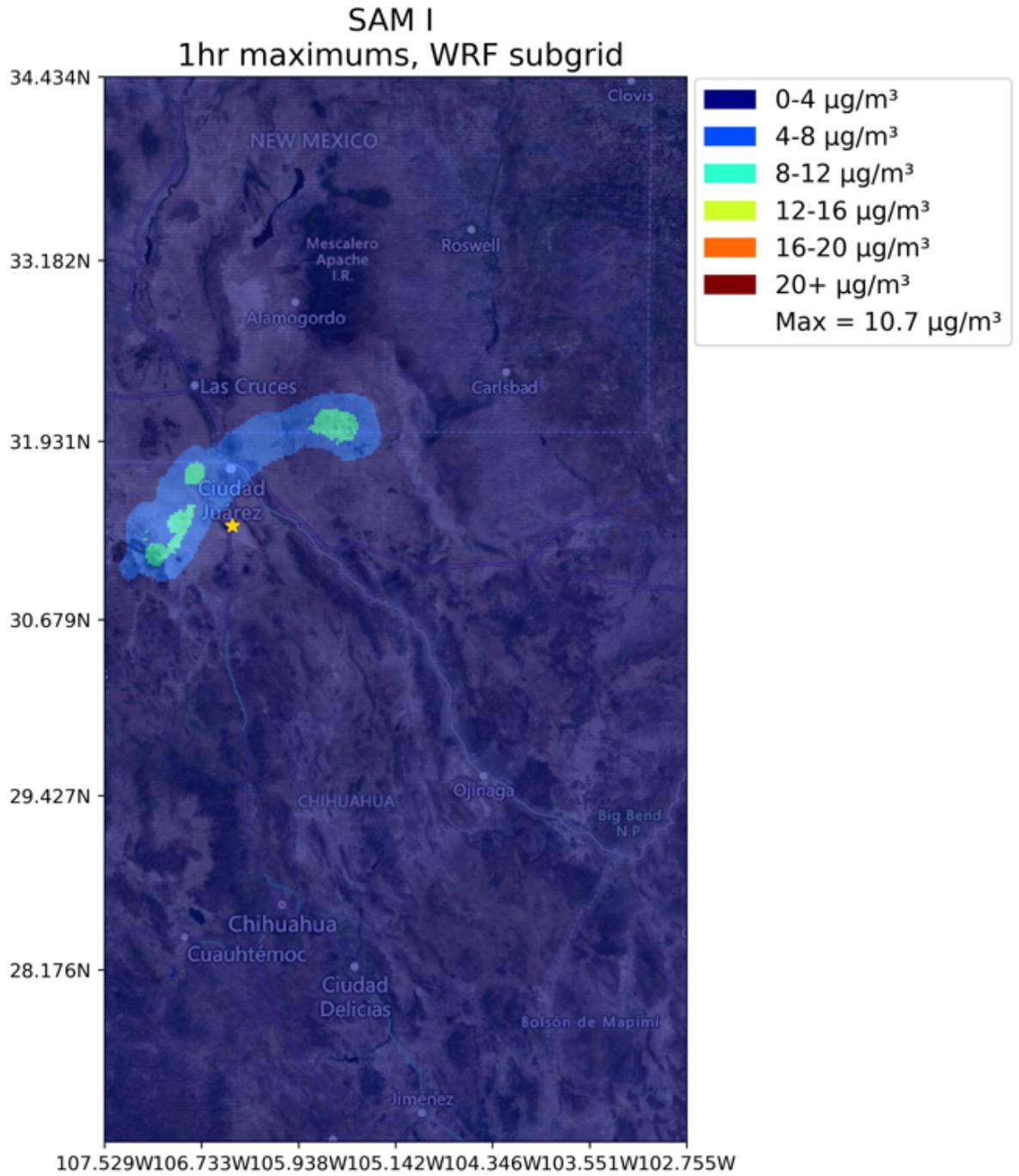


Figure 19. Same as Figure 16 but with MaxPuff 120000 MaxGrid 500000

5 Conclusions

Here we summarize the conclusions of our project, with reference to the corresponding report section.

- We used EPA emission modeling platform data to estimate the emissions and stack parameters for the four Mexican EGUs (Section 2).
- VOCs had a negligible impact on the emissions, but ACET and PAR emissions were included in the SCICHEM modeling for completeness. CH₄ emissions were ignored, and emissions of all other VOCs were negligible (Section 2).
- As expected, Scenario IV with all four EGUs running tends to have the largest MDA8 O₃ impacts, with a maximum impact of 12.5 ppbv for August 2019 (Section 3.2).
- Replacing the incumbent EGUs (Scenario I) with Norte III (Scenario II) still gives a similar maximum MDA8 O₃ (9.7 ppb to 9.9 ppb, respectively, Section 3.2).
- Adding the two incumbent gas EGUs to Norte III increases the maximum impact from 9.9 ppb to 11.4 ppb (Section 3.2).
- The maximum O₃ impacts of the Mexican EGUs in Texas tend to happen to the northeast and southeast of El Paso, rather than in the city itself (Section 3.2).
- Background concentrations in SCICHEM are averaged over the month for each hour (24 total background values for each species) and over the domain rather than giving a true background concentration that CAMx would provide. In addition, CAMx itself underestimates the MDA8 O₃ on several of the high O₃ days in August 2019. These combined effects lead to an underestimate in the total MDA8 O₃ and its variability (Section 3.3).

6 Recommendations for Further Study

Based on the results of this work, we make the following recommendations for further study:

- The Norte III emission and stack parameters used in this study were derived from their maximum possible emissions given the lack of other data. Future US EPA Emission platforms may include more accurate data on annual emissions from Norte III which could be used to refine the estimates made here.
- We only examined August 2019 in this project, but the same method could be applied to the entire ozone season for multiple years to get a better understanding of the impacts.
- The impact of the MAXPUFF and MAXGRID settings on the final SCICHEM results needs to be investigated further to find the optimal values for these model parameters.