PROJECT TITLE	Modeling analysis of TRACER-AQ and over-water measurements to improve prediction of on-land and offshore ozone	**PROJECT #**	22-008
PROJECT PARTICIPANTS	Yuxuan Wang, James Flynn, Paul Walter, Xueying Liu, Evelyn Martinez	**DATE SUBMITTED**	04/10/2023
REPORTING PERIOD	**From:** 3/01/2023 **To:** 3/31/2023	**REPORT #**	7

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

Detailed Accomplishments by Task for reporting period

To continue with Task 4 (Photochemical model evaluation and model inter-comparison), we run WRF-Chem model, starting from the configuration described in the previous MTR (Monthly Technical Reports), Best Performance modified configuration (BPm). We conducted the modeling considering the 2017 National Emission Inventory (NEI) from Environmental Protection Agency (EPA) and this emissions inventory scaled with the TCEQ (Texas Commission on Environmental Quality) emissions inventory (EPAsTCEQ). In the first case, the EPA emissions were taken for all modeling domains (d01, d02). In the second case the EPA emissions inventory scaled with TCEQ was used in the two modeling domains, while for the third case the EPA emissions were taken for the coarser domain d01 (4 km), while for the finer domain d02 (1.33 km), the EPA inventory scaled with TCEQ was taken (See **Table 1).**

Table 1: WRF-Chem model experiments

	Period	**Emission Inventory**
Case 1	First september episode	2017 NEI (EPA) (d01, d02)
Case 2	First september episode	2017 NEI (EPA) scaled with TCEQ (d01, d02)
Case 3	Full september, three episodes	2017 NEI (EPA) (d01), 2017 NEI (EPA) scaled with TCEQ (d02)

Preliminary Analysis
The modeled outputs were compared spatially within the TCEQ continuous ambient monitoring stations (CAMS) across the greater Houston area. The results shown below correspond to the first (6-11) and third (23-26) ozone episodes, the most important episodes during September 2021.

Figure 1 shows the spatial distribution of CAMS-observed and modeled ozone for Cases 1 (EPA), Case 2 (EPAsTCEQ 4.2.2) and Case 3 (EPAsTCEQ 4.0) at 00 UTC (19 h local time). The modeling with the EPA inventory and the scaled inventory with TCEQ emissions data, for both domains (Case 2), show better results than in the case of combining both inventories because in the latter case the modeled data overestimates the observed values too much.

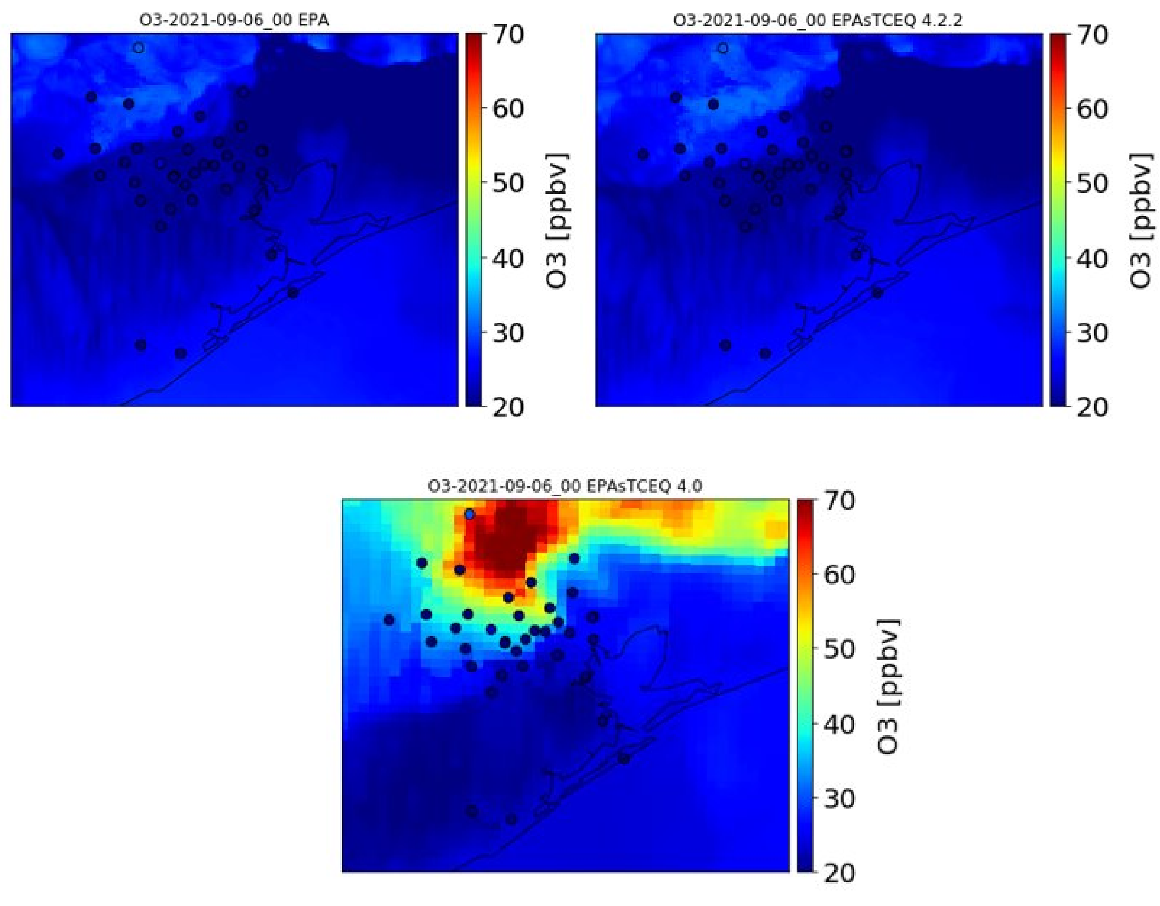


Figure 1: Spatial distribution of CAMS-observed and modeled ozone for Cases 1 (EPA), Case 2 (EPAsTCEQ 4.2.2) and Case 3 (EPAsTCEQ 4.0) at 19 h local time, domain d02.

Figure 2 shows the spatial distribution of CAMS-observed and modeled ozone for Cases 2-3, in the first two days of the first high ozone episode (Sept. 6, 2021 and Sept. 7, 2021) at 21 UTC (16 h local time). In the hours around the ozone maximum, the behavior is different from that observed in Figure 1, because it is Case 3 that shows a better correspondence between the observed and modeled data, mainly in the areas where the maximum values are found.

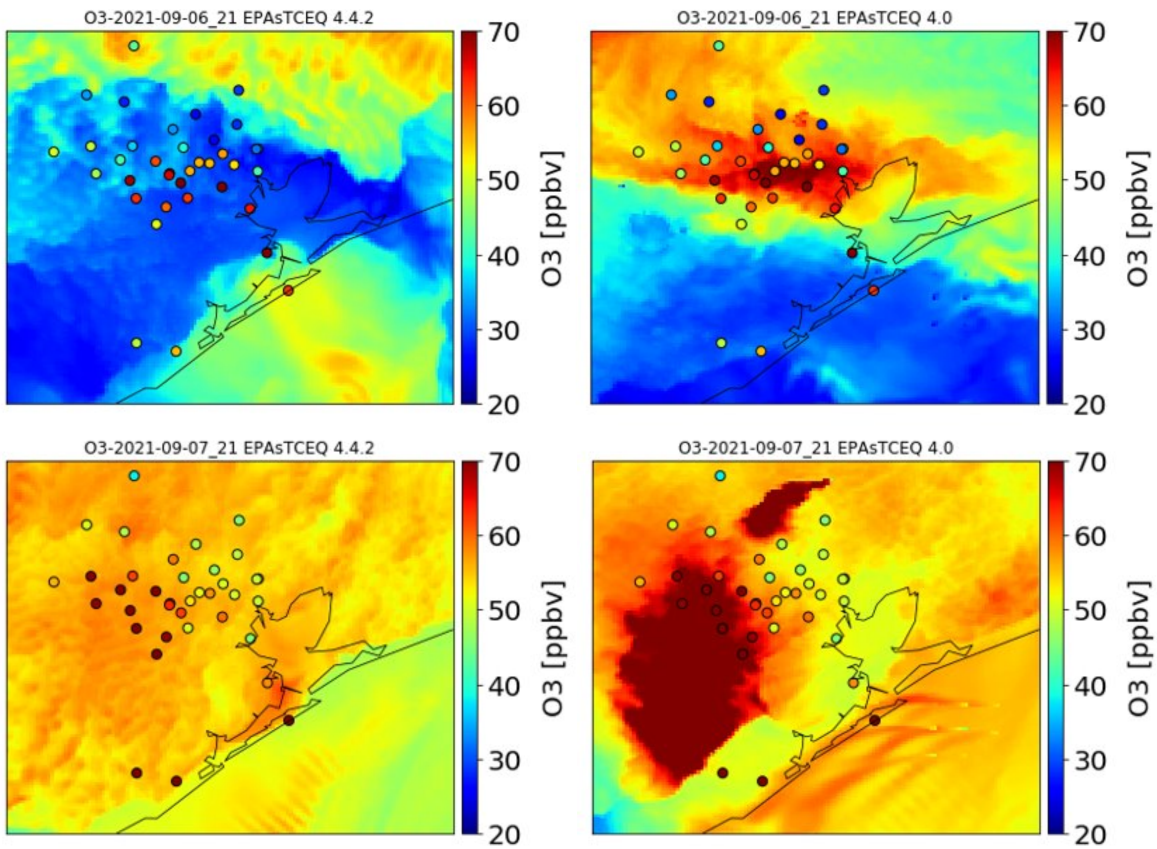


Figure 2. Spatial distribution of CAMS-observed and modeled ozone for Cases 2 (left) and Case 3 (right) at 16 h local time (Sept. 6, 2021, and Sept. 7, 2021), domain d02.

Figure 3 shows spatial distribution of modeled meteorological values (temperature T2, wind velocity and direction) and ERA 5 reanalysis output at 16 h local time, domain d02. The range of values of the model for the temperature and wind direction and speed is in accordance with the obtained by the ERA5 (Fifth generation of the European Centre for Medium-Range Weather Forecasts (ECMWF) atmospheric reanalysis of the global climate).

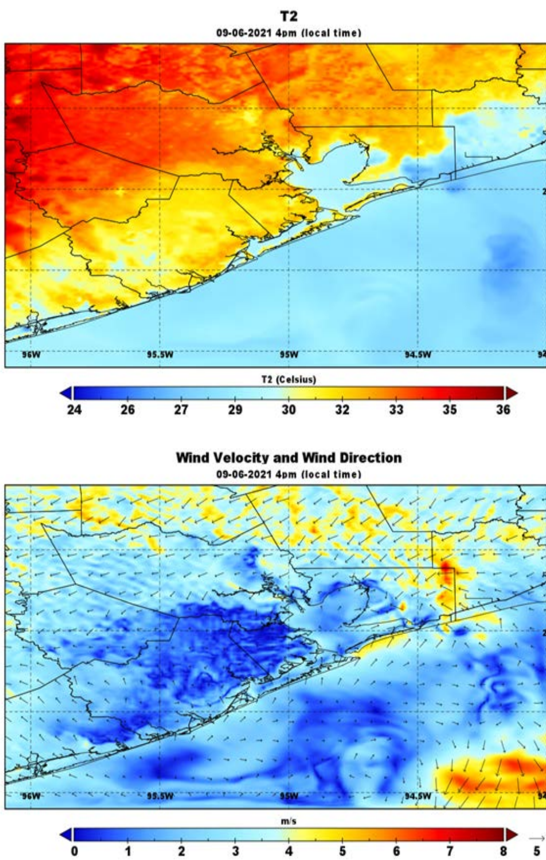
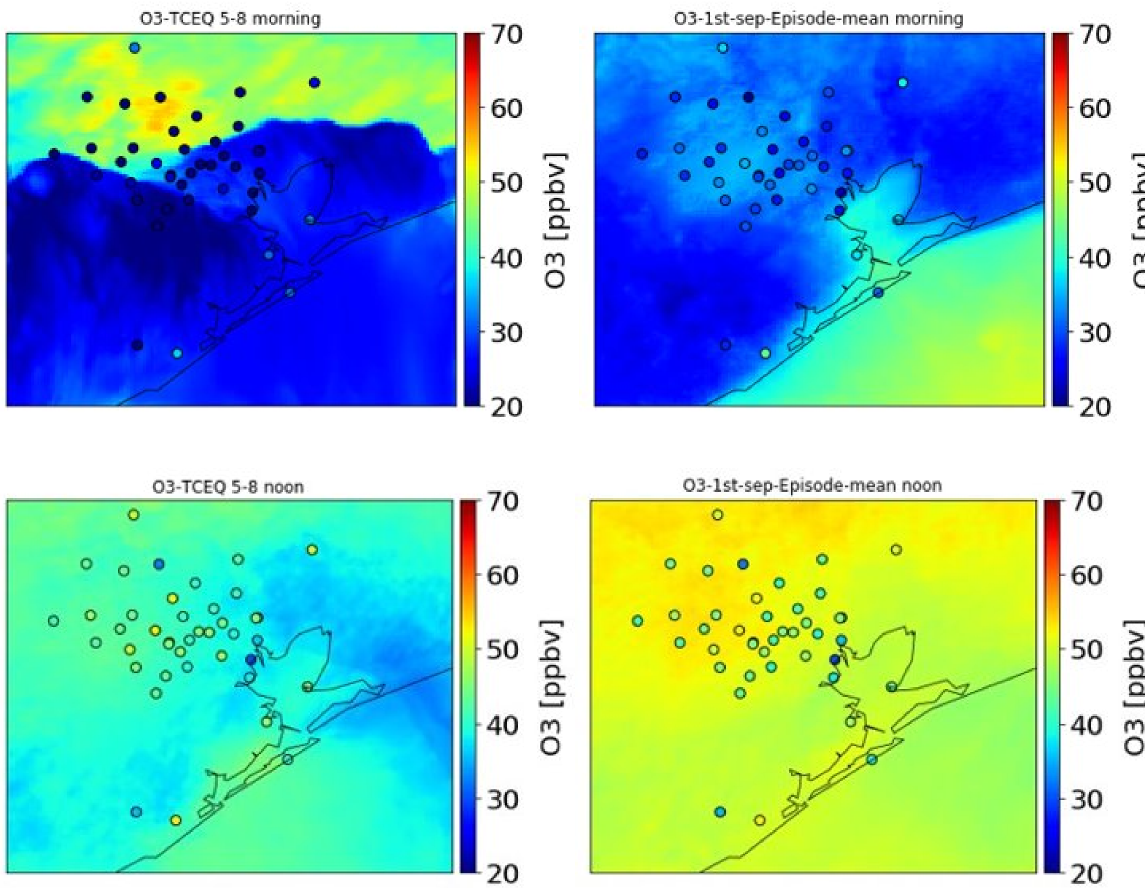


Figure 3. Spatial distribution of modeled meteorological values (temperature T2, wind velocity and direction) and ERA 5 reanalysis output at 16 h local time, domain d02.

Figure 4 shows the spatial distribution of CAMS-observed and modeled mean ozone for Cases 2 and 3 at morning, noon, night, and midnight for the first high ozone episode (Sept. 6-11, 2021). In general, the best correspondence is obtained for Case 3, when using the EPA inventory for domain one and the EPA inventory scaled with TCEQ for domain two. The best correspondence times are morning and noon, while for the case of night and midnight, the modeled values tend to overestimate the observations. For Case 2, the hours of night and midnight have a better correspondence than Case 3, reflecting better ability to describe the mean values of the background.



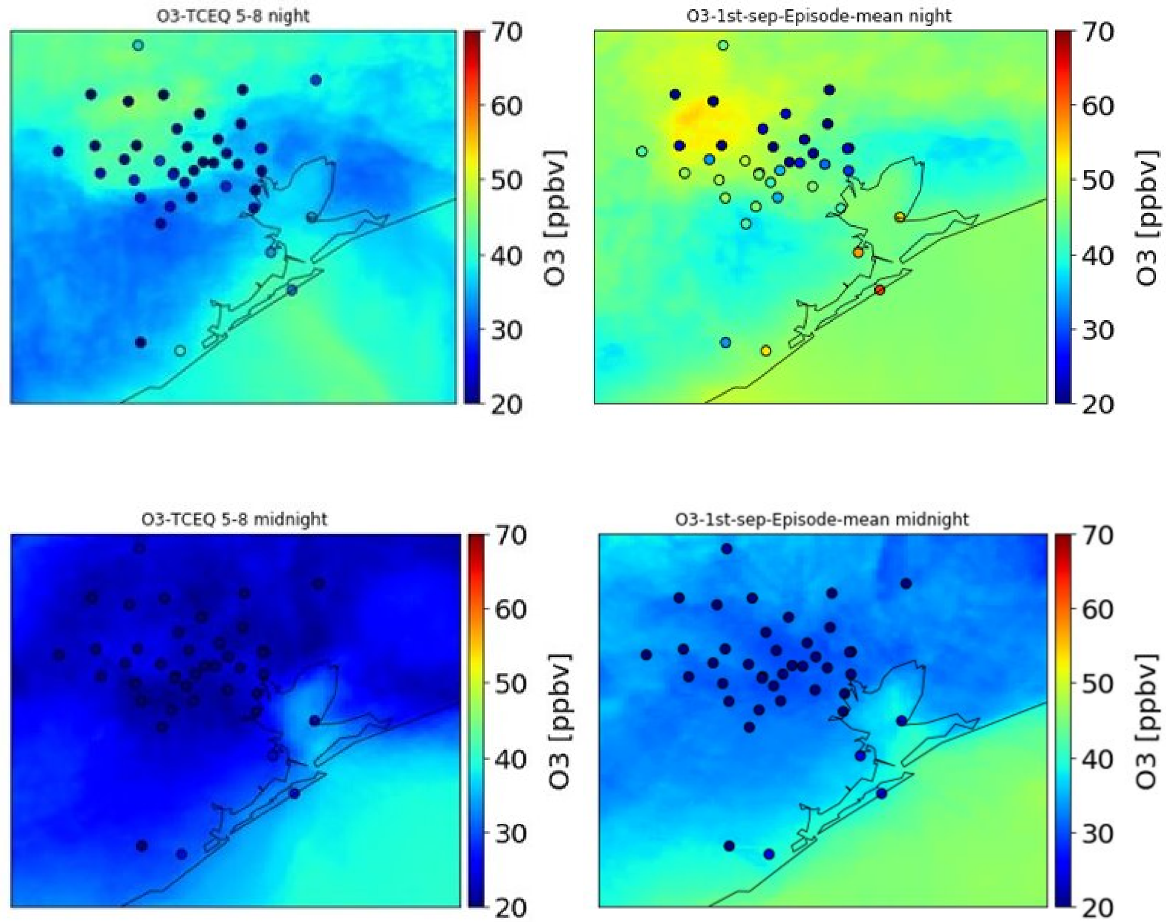


Figure 4. Spatial distribution of CAMS-observed and modeled mean ozone for Cases 2 (left) and Case 3 (right) at morning, noon, night, and midnight for the first high ozone episode (Sept. 6-11, 2021).

Figure 5 shows the spatial distribution of CAMS-observed and modeled mean ozone for Case 3 at morning, noon, night, and midnight for the third high ozone episode (Sept. 23-26, 2021). The best correspondence times are morning and noon again. At night and midnight, the modeled values overestimate the observations.

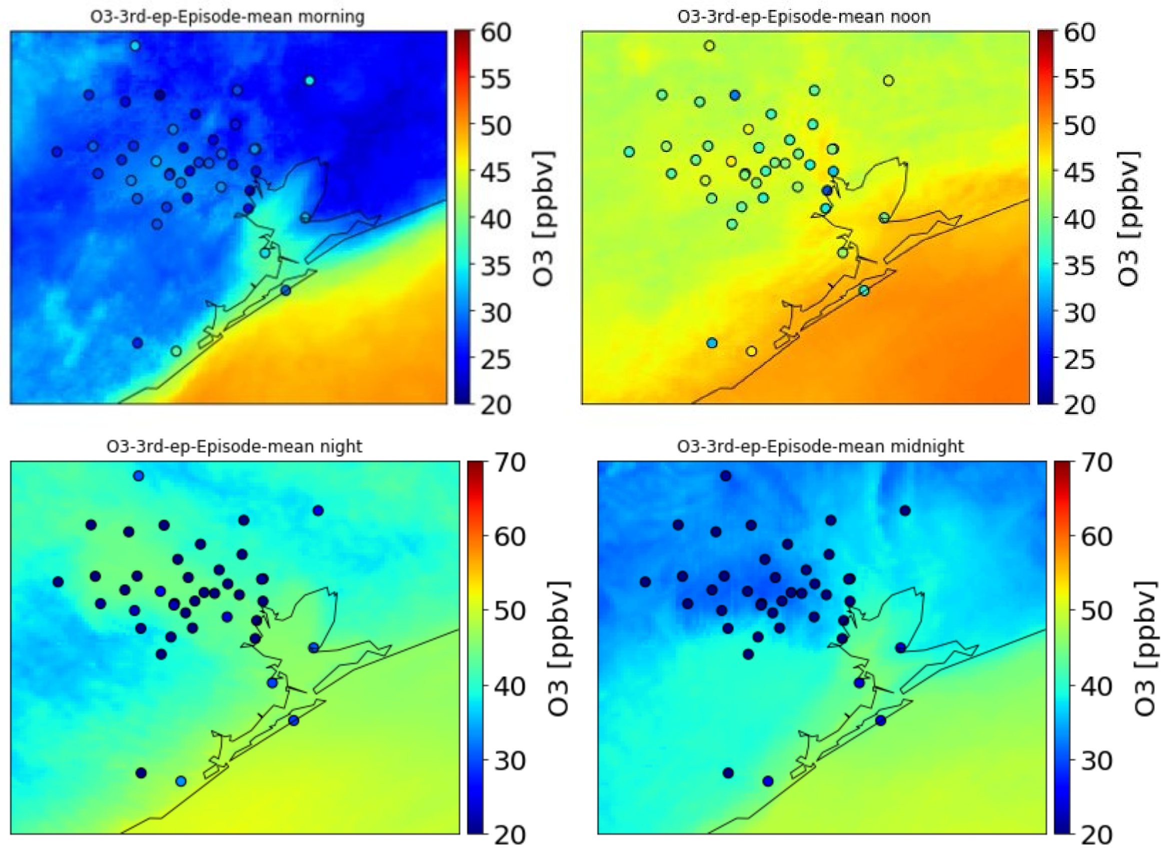
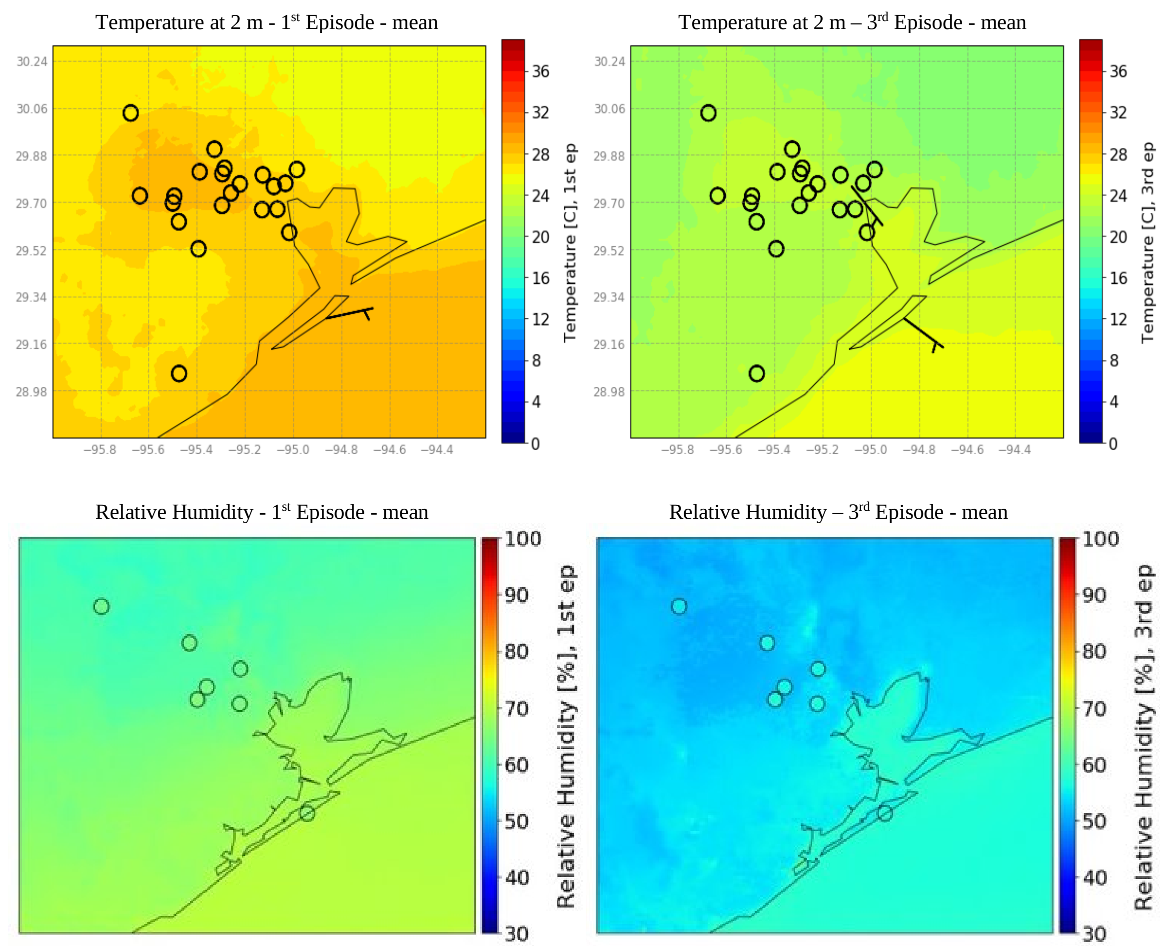


Figure 5. Spatial distribution of CAMS-observed and modeled mean ozone for Case 3 at morning, noon, night, and midnight for the third high ozone episode (Sept. 23-26, 2021).

Figure 6. shows spatial distribution of CAMS-observed and modeled mean meteorological variables (temperature, relative humidity, wind speed and direction) for the first (Sept. 6-11, 2021) and third (Sept. 23-26, 2021) high ozone episodes. For temperature, in both cases, the modeled values correspond to the observed ones adequately, the mean modeled values oscillate around 27.10 °C with 1.73 of standard deviation, and the observed values mean is 27.32 with 0.57 of standard deviation. For relative humidity, Case 1 shows better results, while in Case 2 the model underestimates the value of the variable by up to 10%. Regarding the wind, the correspondence is better in wind speed than in direction. In this variable, the model's outputs for the first episode have a better performance with respect to the observed values.



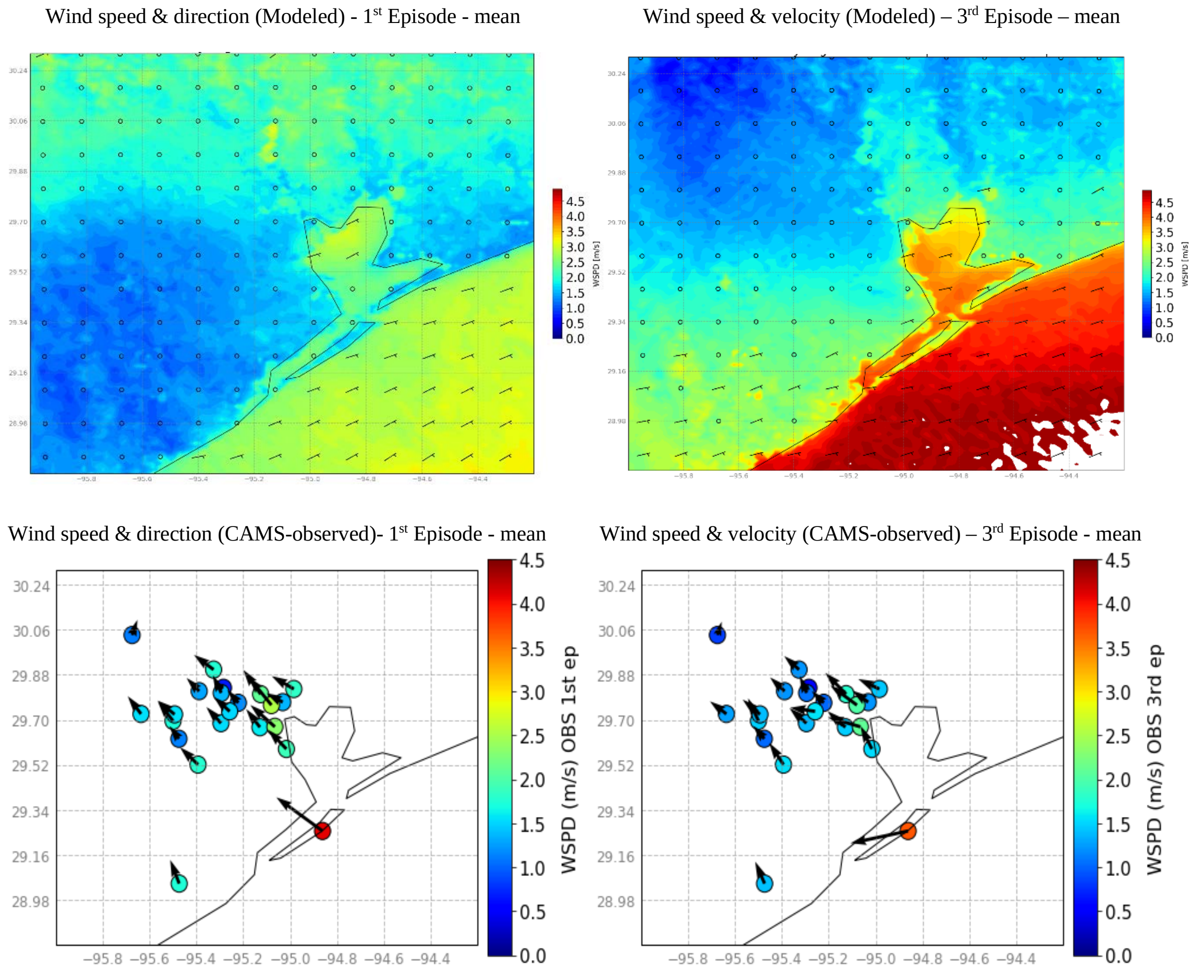


Figure 6. Spatial distribution of CAMS-observed and modeled mean meteorological variables (temperature, relative humidity, wind speed & direction) for the first (Sept. 6-11, 2021) and third (Sept. 23-26, 2021) high ozone episodes.

Figures 7 and 8 show the spatial distribution of CAMS-observed O_3 and modeled mean O_3, CO, SO_2 and NO_2 for first (Sept. 6-11, 2021) and third (Sept. 23-26, 2021) high ozone episodes. The third period shows the best results overall for O_3, since the modeled values are closest to the observations. For the other variables, the model simulates their spatial behavior according to the average normal values in the study area.

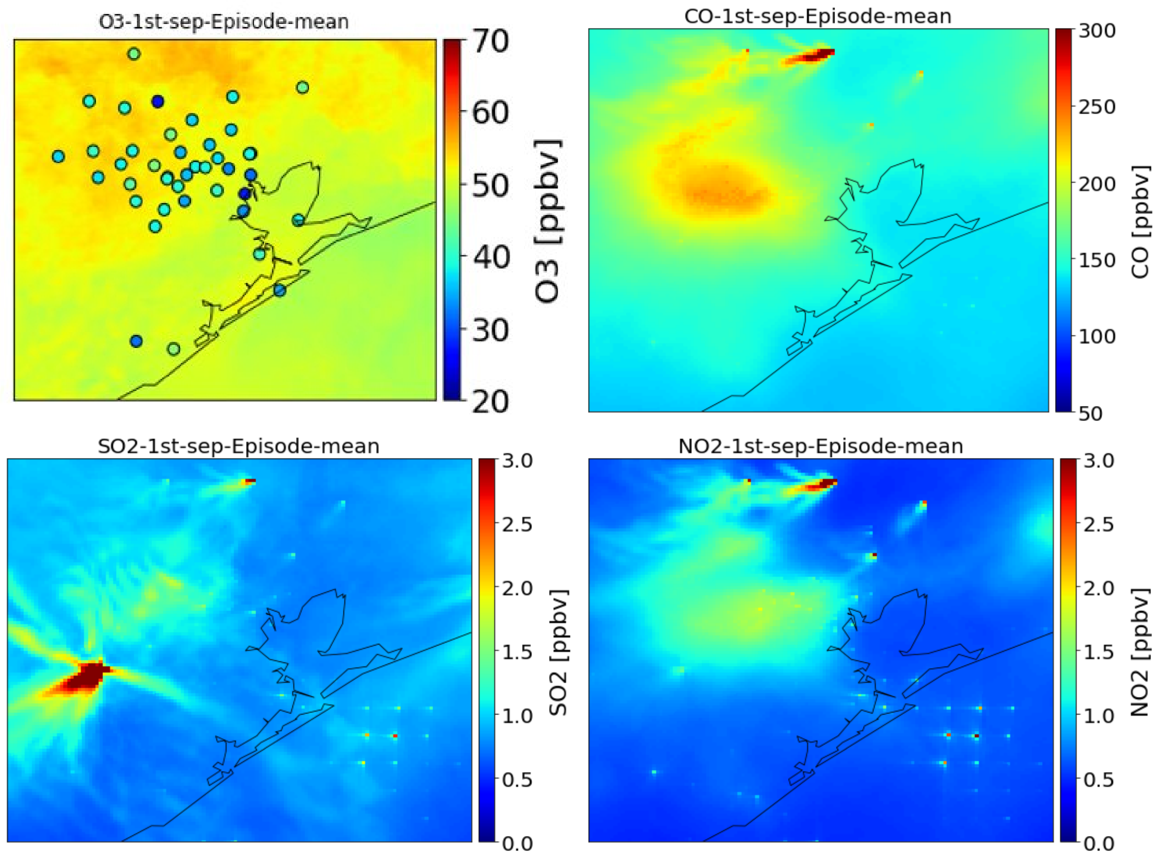


Figure 7. Spatial distribution of CAMS-observed O_3 and modeled mean O_3, CO, SO_2 and NO_2 for first (Sept. 6-11, 2021) high ozone episodes.

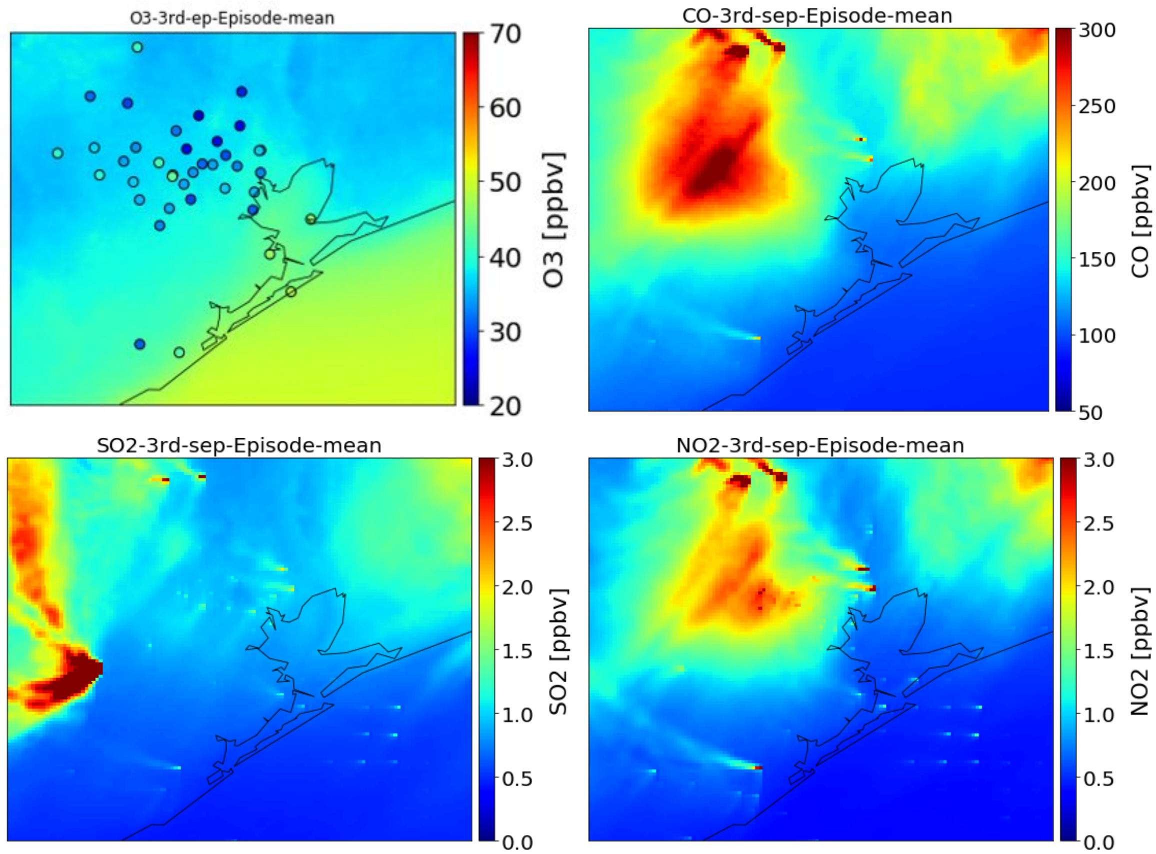


Figure 8. Spatial distribution of CAMS-observed O_3 and modeled mean O_3, CO, SO_2 and NO_2 for third (Sept. 23-26, 2021) high ozone episodes.

Data Collected
None

Identify Any Problems or Issues Encountered and Proposed Solutions or Adjustments
N/A

Goals and Anticipated Issues for the Succeeding Reporting Period

We will evaluate the model statistically and the intercomparison between the three models selected in the project will be conducted for the next period..

Detailed Analysis of the Progress of the Task Order to Date
N/A

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 (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
Yuxuan Wang