

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	03/10/2023
REPORTING PERIOD	From: 2/01/2023 To: 2/28/2023	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

For Task 4 (Photochemical model evaluation and model inter-comparison), we installed and configured the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to conduct photochemical modeling, considering the best-performing meteorology identified in Task 3.

WRF-Chem simulates the emission, transport, mixing, and chemical transformation of trace gases and aerosols simultaneously with the meteorology. It is a powerful integrated modeling system that can support a wide range of applications including air quality forecasting services, case study modeling of chemistry-meteorology feedbacks and climate change assessment studies focusing on chemistry.

We installed the latest version of the WRF-Chem (4.2.2) using Intel compilers and taking into account the characteristics of Carya Cluster. We use the model to perform meteorological and air quality modeling for one of considered high ozone episodes September 6-11. We also considered two nested domains with horizontal resolutions of 4 km x 4 km and 1.33 km x 1.33 km (**Figure 1**), due to the temporal resolution of the High-Resolution Rapid Refresh (HRRR) from [National Oceanic and Atmospheric Administration \(NOAA\) Amazon Web Service](#) is hourly and the horizontal resolution is 3 km (d02 and d03, shown in **Figure 1**).

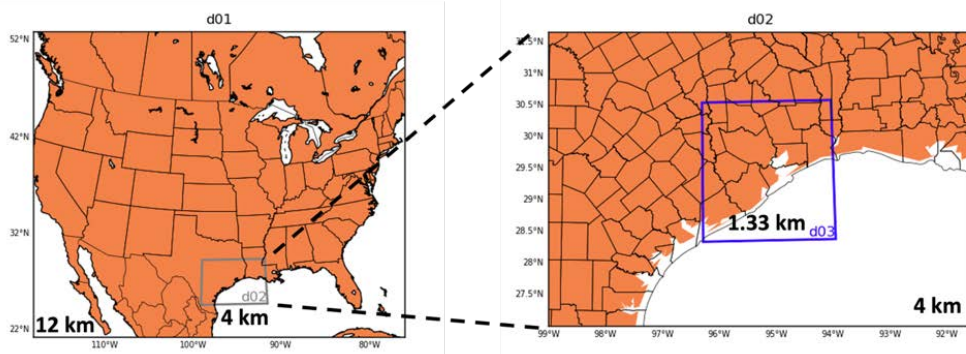


Figure 1. WRF-Chem nested modeling domains and horizontal resolutions.

The outermost domain (d01=d02 Figure 1) contains 129 x 186 grid points and cover Southeast Texas region. The second domain (d02 = d03 **Figure 1**) contains 183 x 171 grid points and focuses over Houston-Galveston region. All domains have identical vertical resolutions with 50 vertical layers. The model spin-up time was of 24 hours for the first forecast.

In order to have optimal representation of the meteorological and chemical fields, we are using physics parameterization showed in **Table 1**.

Table 1. Physics parameterizations used in the simulations with WRF-Chem

Process	Scheme
Cloud microphysics	Morrison 2-moment scheme (mp_physics)
Longwave and shortwave radiation	RRTMG scheme (ra_lw_physics/ ra_sw_physics)
Cumulus parameterization	Grell 3D ensemble scheme (cu_physics)
Planetary boundary layer	MYNN (bl_pbl_physics)

Regarding the bl_pbl_physics option, the same configuration proposed by the best performance configuration form Task 3, was chosen. However for cu_physics, it was necessary to choose a different configuration, because for the compiled version of the model, [an error is documented](#) when it is choose the combination of that physical option with the rest physics desired for this parameterization, for example cu_rad_feedback=.true. . Important option to describe the interaction between aerosol and radiation which has an important role in ozone formation. When running with this combination, the model was not able to generate initial conditions. Therefore, we follow the recommendation of the [user guide](#) where it refers that cu_rad_feedback will only work with cu_phys=3 or 5.

To test the operation of WRF-Chem model, a total of five different configurations shown in **Table 2** were assumed. At first, the best performance configuration with the new cumulus parameterization will be called best performance for WRF-Chem or Best Performance modified (BPm). BPm configuration was used together with the [EDGAR-HTAP](#) anthropogenic emission files (2010) emissions inventory for the MOZART-MOSAIC chemical mechanisms with 10 levels in the vertical (z_dim_stag), case 1, while in case 2, was used [Edgar HTAPv5](#) (2015) () for the MOZART-MOSAIC. [The 2017 National Emission Inventory \(NEI\)](#) was taken in case 3 through anthro_emis utility, cases 4 and 5 have the same characteristics as cases 1 and 3 but with WRF-Chem version 4.0 installation. It was decided to do these tests with a different model version than the one initially installed, because this is a version that is still compatible with version 3.9.1.1 (Task 3 performed version).

The MOZART gas-phase chemistry coupled with MOSAIC aerosol chemistry was used as chemical mechanism. Biogenic emissions are generated using the model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN 2.1) and adapted through WRF-Chem Tool Preprocessor. The Fire INventory from NCAR (FINN), a high-resolution global model, was used to estimate the emissions from open burning of biomass, which includes wildfire, agricultural fires and prescribed burning.

Table 2: WRF-Chem model experiments

	Best Performance (HRRR)	WRF Version	Emission Inventory
Case 1	BPm	v 4.4.2	EDGAR – HTAP v2 (2010)
Case 2	BPm	v 4.4.2	EDGAR – HTAP v5 (2015)
Case 3	BPm	v 4.4.2	2017 NEI (EPA)
Case 4	BPm	v 4.0	EDGAR – HTAP v5 (2015)
Case 5	BPm	v 4.0	2017 NEI (EPA)

Preliminary Analysis

Figure 2 shows the spatial distribution of ozone at 18 h (local time) for the cases shown in **Table 2** (Domain d01). The highest values of the variable and with the highest level of detail for domain 1 are observed in case 2, which uses the latest version of the WRF-Chem model and the most up-to-date EDGAR inventory (2015). Cases 1, 3 and 5 show a similar pattern to each other, although they were built through different versions of the model and the emissions inventory. Case 4 presents the lowest and smoothest O₃ values in the domain, using Edgar_HTAPv5 (2015) but an older version of the model (v 4.0).

Figure 3 shows the spatial distribution of ozone at 18 h (local time) for the cases shown in Table 2 (Domain d02). In addition, the result of another simulation for O₃ using Environmental Protection Agency (EPA) scaled with TCEQ data is shown. Taking this last simulation as a reference, we can see similar patterns for cases 1, 2, O₃ and 5, and the range of modeled values does not present great difference.

Figures 4 and 5 show emissions of Nitrogen Monoxide (E_NO) (Domain d01) and Nitrogen Dioxide (E_NO₂) (Domain d01) respectively, from the emissions inventories EDGAR-HTAPv5, NEI 2017 (EPA) and EPA scaled with TCEQ respectively, at 18 h Local time. The highest values are observed in the emissions generated through EDGAR-HTAPv5, which is in correspondence with what was described in case 2, Figure 1. The emissions generated from EPA and EPA scaled with TCEQ show a similar pattern, the first being slightly higher.

Based on what was observed in the previous Figures, cases O₃ and 5 are the most comparable with the reference case, in terms of emissions source. Therefore, the following modeling and chemical evaluation, for the six cases of high ozone, will be carried out taking the above into account.

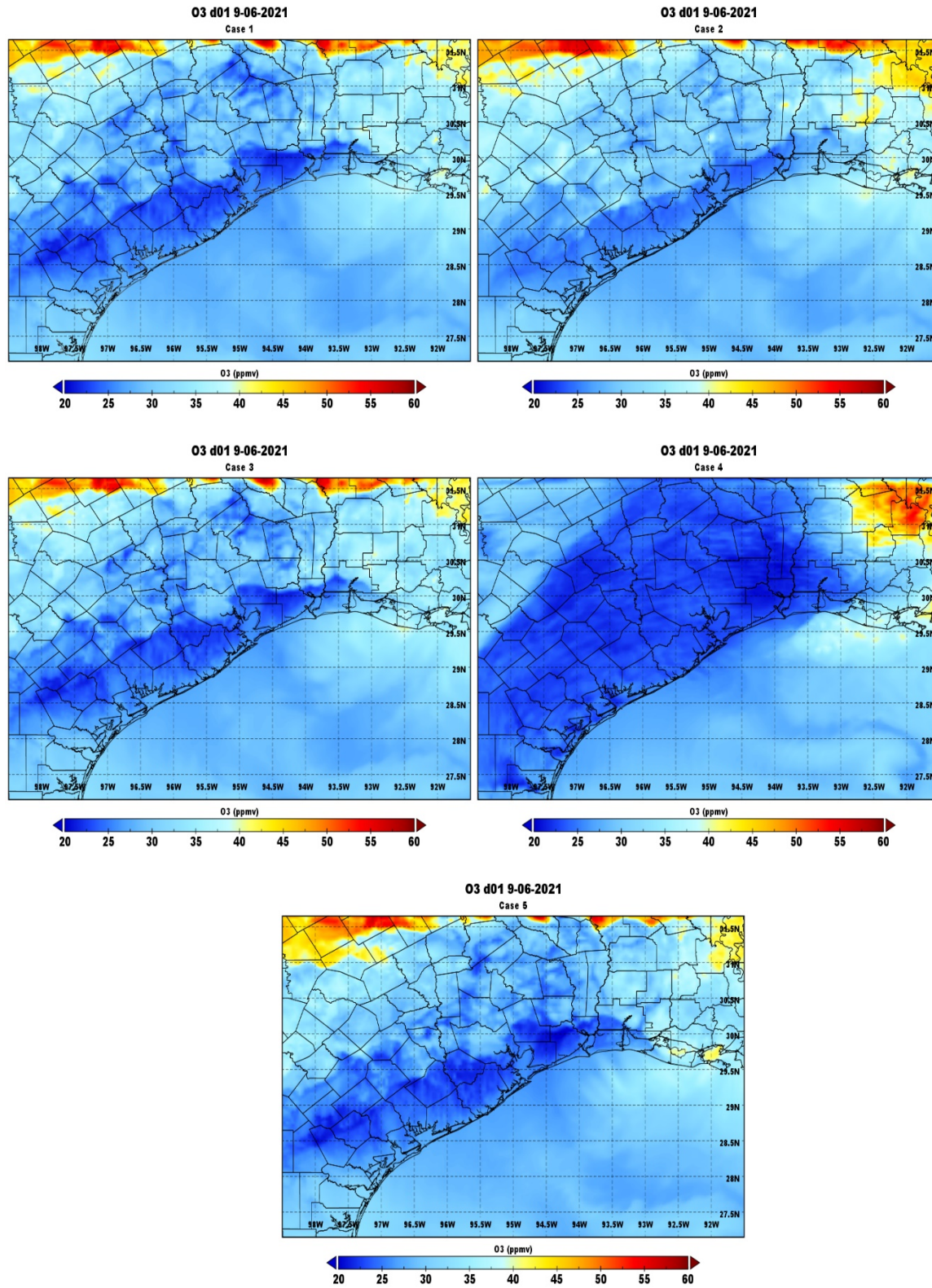


Figure 2: Spatial distribution of Ozone (O_3) (Domain d01), at 18 h (local time) for the cases shown in **Table 2**.

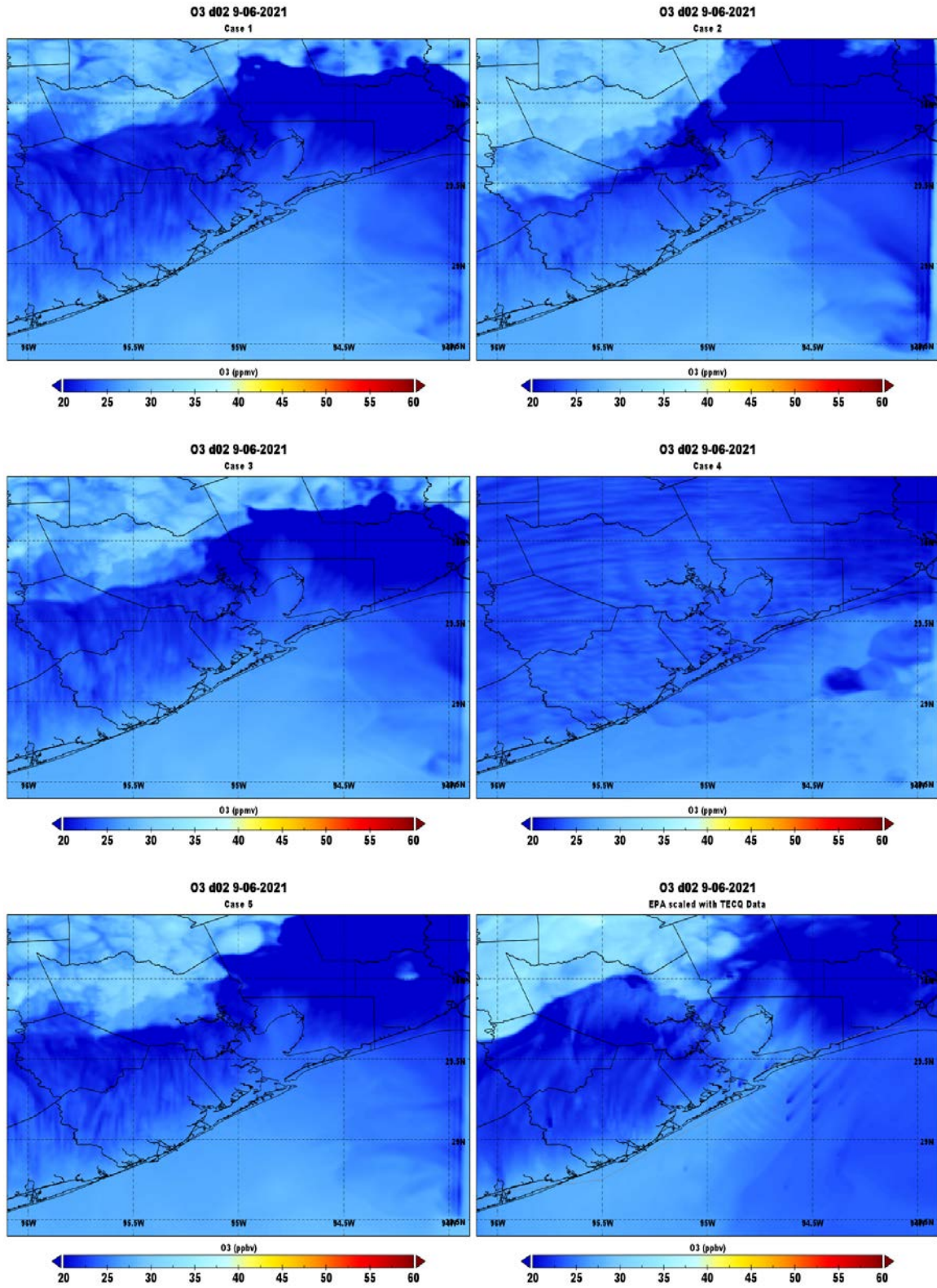


Figure 3. Spatial distribution of Ozone (O₃) (Domain d02), at 18 h (local time for the cases shown in **Table 2**).

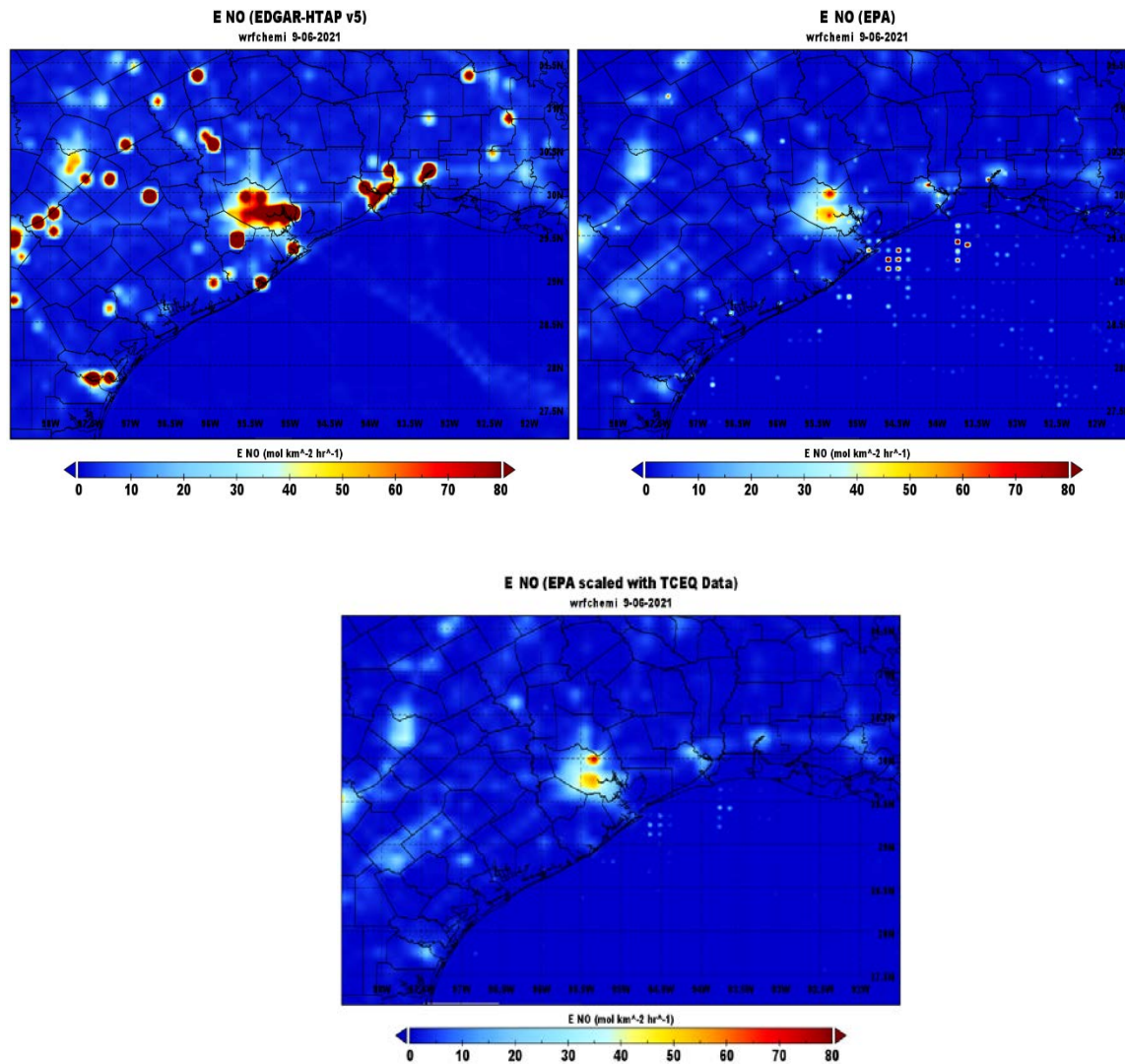


Figure 4. Emissions of Nitrogen Monoxide (E_{NO}) (Domain d01), from the emissions inventories EDGAR-HTAPv5, NEI 2017 (EPA) and EPA scaled with TCEQ respectively, at 18 h (local time).

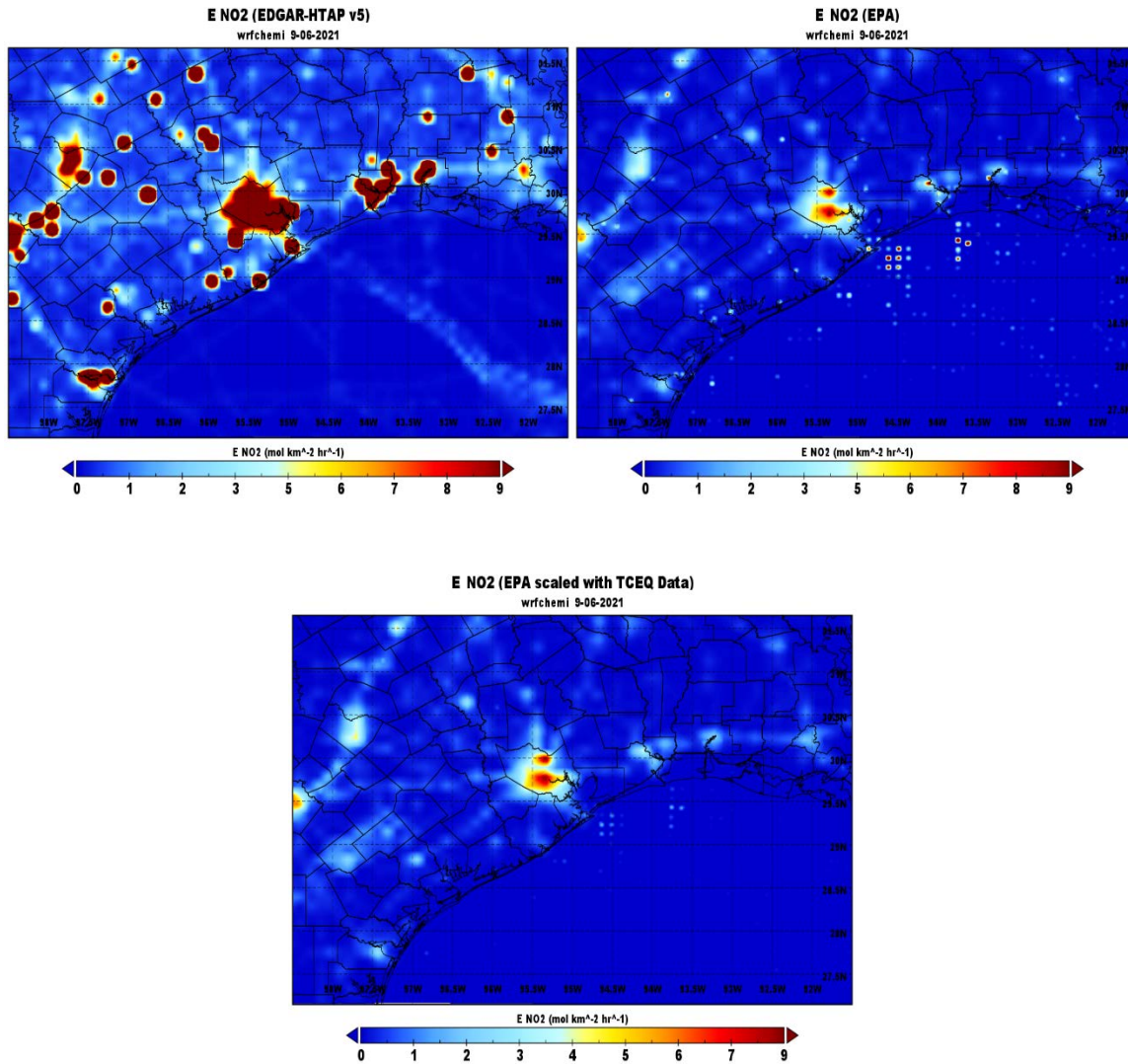


Figure 5. Emissions of Nitrogen Dioxide (E_NO₂) (Domain d01), from the emissions inventories EDGAR-HTAPv5, NEI 2017 (EPA) and EPA scaled with TCEQ respectively, at 18 h (local time).

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
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