Global Modeling Simulations from the Hemispheric Community Multiscale Air Quality (HCMAQ) model: 2017 and 2023

Chemical transport modeling requires information about the atmosphere at the start of the simulation and at the edges of the modeling domain. These are provided by initial and boundary conditions, respectively, which are generally derived from global or hemispheric-scale simulations. “Sensitivity” simulations that test the effect of a change outside of the modeling domain—an emission reduction—will generally use initial and boundary conditions that reflect the change. For example, sensitivity simulations that set anthropogenic emissions outside of the United States to zero can be used to assess the impact of international emissions on US air quality.

This document details global modeling simulations that US EPA conducted using the hemispheric-scale version of the Community Multiscale Air Quality model, i.e.,

1) “BASE” simulation with a standard set of domestic and international emissions,
2) “ZROW” (i.e., zero-out rest-of-world) that removes all anthropogenic emissions outside of the US,
3) “ZOPROW” (i.e., zero-out ozone precursors, rest-of-world) that removes only nitrogen oxide (NO_x = NO + NO_2), carbon monoxide (CO) and volatile organic compound (VOC) anthropogenic emissions outside of the US.

These global modeling results were then used to develop initial and boundary condition data (ICON and BCON, respectively) for regional modeling domains used by Utah Division of Air Quality (UDAQ) for 2017 and by the Maricopa Association of Governments (MAG) for 2023.

Hemispheric Modeling Overview

This section provides details on the H-CMAQ model configuration and the model performance evaluation.

Model Configuration

EPA develops and maintains the Community Multiscale Air Quality (CMAQ; e.g., Appel et al. 2021: https://doi.org/10.5194/gmd-14-2867-2021) chemical transport model. CMAQ simulates key processes relevant to projecting and interpreting air pollution, such as emission trends, transport, chemistry and fate. CMAQ simulations can span a hemispheric domain with a horizontal grid resolution of 108 square km, and the model run on this domain is known as Hemispheric CMAQ (H-CMAQ). As discussed in the introduction, global or hemispheric models such as H-CMAQ are used to generate initial and boundary conditions (IC/BCs) for finer scale simulations. As shown in Table 1, both of the 2017 and 2023 simulations include the update to aerosol nitrate photolysis incorporated in Carbon Bond 6, as described in Sarwar et al., 2024 (https://doi.org/10.1016/j.scitotenv.2024.170406).

Table 1. Summary of the 2017 and 2023 model configurations

Model option	2017	2023[1]
Base model version	CMAQv5.5	CMAQv5.4+
Initialization date	Base: October 1, 2016 Sensitivities: January 1, 2017	Base: October 1, 2022 Sensitivities: January 1, 2023

Chemical mechanism		Carbon Bond 6 with aero 7, including marine halogen updates (cb6r5m_ae7_aq) (following Sarwar et al., 2024)	
Horizontal domain		108 km over the Northern Hemisphere (108NHEMI2)	
Vertical resolution		44 layers from the surface to 50 mb	
Meteorology		WRFv4.1.1[2]	WRFv4.4.1[2]
Emissions	**Anthropogenic**	International anthropogenic emissions are generally from 2010 HTAPv2.0[3] and adjusted for year 2017 using CEDS[4]. Over China, emissions are for 2015 from Tsinghua University. Over USA, emissions are year-specific and based on 2017 NEI (following EQUATES) [5].	Both international and domestic emissions are from HTAP v3.0 for 2018[6], with domestic emissions following EQUATES for 2018 emission year[5].
	Fire	Year-specific (2017) FINNv1.5[7]	Year-specific (2023) FINN v1.5[7]
	Biogenic	Year-specific (2017) CAMSv2.1[8]	Hourly, year-specific (2023) MEGAN v3.2[9] for VOCs, BDSNP (no version) soil NO[10]
	Lightning	Offline GEIA monthly climatology[11]	Year-specific (2023) WWLLN[12]
	Sea Salt	Online[13]	
	Windblown dust	Online[14]	
Deposition		STAGE E20[15,16]	
Bi-directional exchange		Off	

1. An evaluation of the 2023 base simulation is available in the document, "CMAQ Initial and Boundary Input Data: 4/1/2023 to 9/30/2023 MAG 36 km horizontal grid," by K. Baker.
2. Skamarock et al., 2019. doi:10.5065/1dfh-6p97
3. Janssens-Maenhout et al., 2015. doi:10.5194/acp-15-11411-2015
4. McDuffie et al., 2020. doi.org/10.5194/essd-12-3413-2020
5. Foley et al., 2023. doi.org/10.1016/j.dib.2023.109022
6. Crippa et al., 2023. doi.org/10.5194/essd-15-2667-2023
7. Wiedenmyer et al., 2011. doi.org/10.5194/gmd-4-625-2011
8. Sindelarova et al., 2014. doi.org/10.5194/acp-14-9317-2014
9. Kang et al., 2021. pmc.ncbi.nlm.nih.gov/articles/PMC10793874/
10. Huber et al., 2023. doi.org/10.1029/2022JD037611
11. Price, Penner & Prather. doi.org/10.1029/96JD03504
12. Kang et al., 2022. doi.org/10.5194/egusphere-2022-348
13. Gantt, Kelly & Bash, 2015. doi.org/10.5194/gmd-8-3733-2015
14. Foroutan et al., 2017. doi.org/10.1002/2016MS000823
15. Galmarini et al., 2021. doi.org/10.5194/acp-21-15663-2021
16. Emerson et al., 2020. doi.org/10.1073/pnas.2014761117

Model tools leveraging source apportionment functionality may also require IC/BCs from a global or hemispheric simulation with modified inputs that reflect the intended perturbation. For example, tracking the role of international anthropogenic emissions in the "OSAT" source apportionment module the CAMx air quality model requires IC/BCs from a global or hemispheric simulation that that has shut off international anthropogenic emissions. This type of perturbation can be implemented with tools like the Detailed Emissions Scaling, Isolation, and Diagnostic (DESID) module in CMAQ (Murphy et al., 2021; https://doi.org/10.5194/gmd-14-3407-2021). Here we use DESID to adjust emissions outside of the United States for the sensitivity simulations (Figure 1).

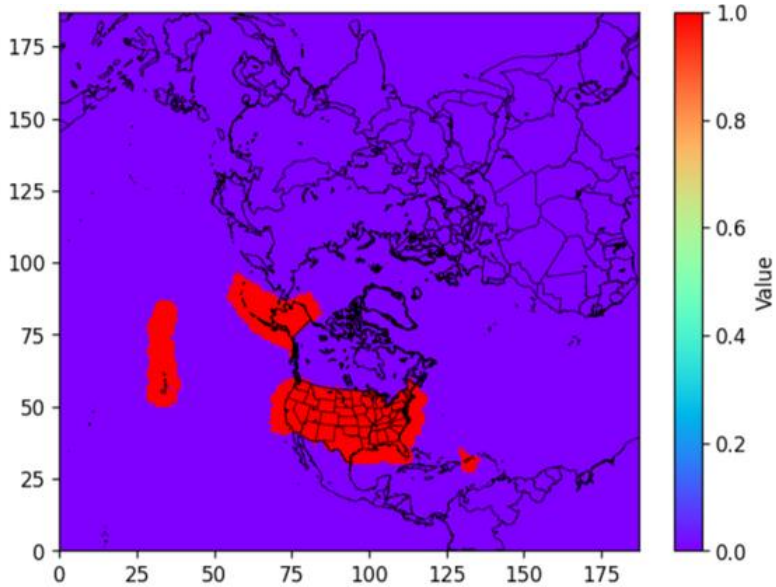

Figure 1. Spatial mask used by the DESID module to shut off emissions outside of the United States. Emissions are retained for the area shown in red (value = 1.0) and set to zero for the area shown in purple (value = 0.0) (Figure created by K. Baker).

BASE simulation results

Figure 2 illustrates monthly average estimates over the Northern Hemisphere at the surface in the BASE simulation for ozone (top) and nitrogen oxide (NO_x = NO + NO_2; bottom) concentrations in July of 2017 (left) and 2023 (right). See Table 1 for more information on the specifics of this configuration. NO_x emissions are a key precursor to ozone formation, so that their spatial distributions show some similarities. Overall, the ozone projection reflects a combination of precursor emissions (NO_x and volatile organic compounds, VOCs), photochemistry, transport and deposition.

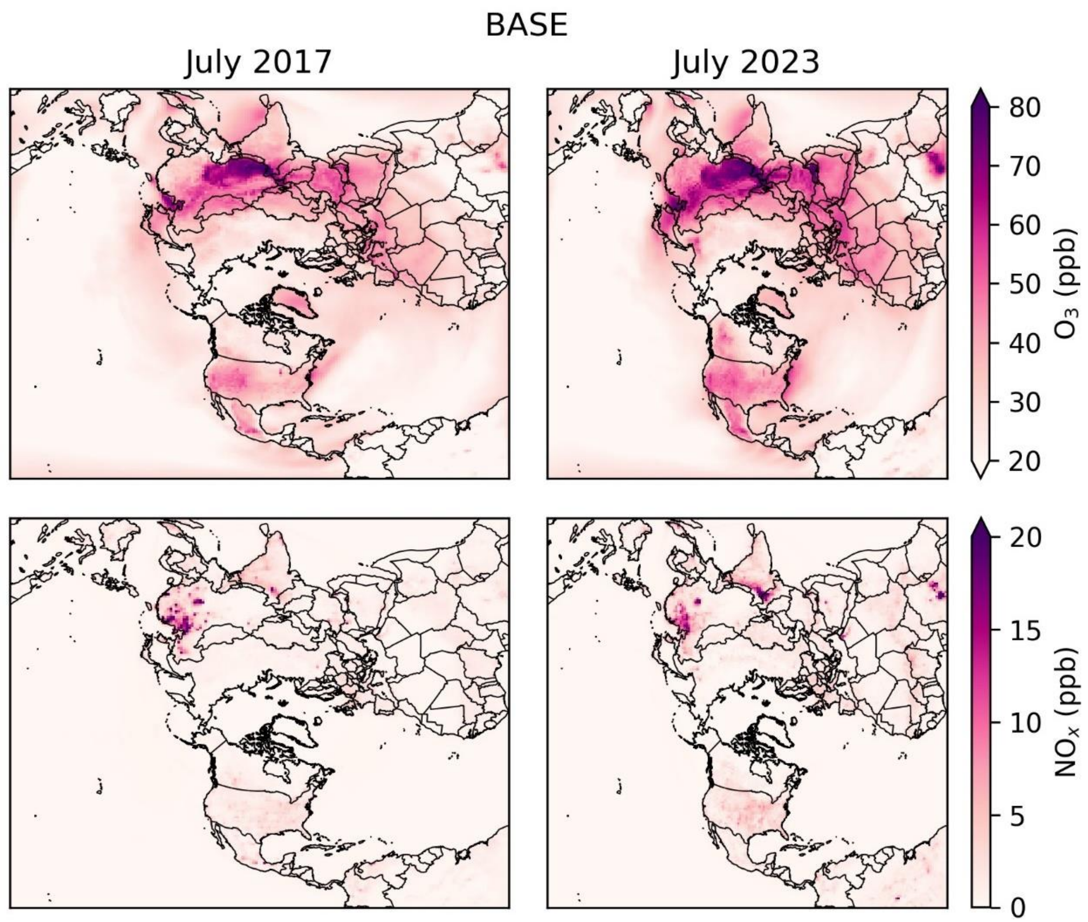

Figure 2. Monthly average ozone (O_3) and NO_x ($NO_x = NO + NO_2$) concentration at the surface in parts per billion (ppb) in the BASE simulation for July 2017 (left) and July 2023 (right).

Model sensitivity to international anthropogenic emissions

We use DESID to conduct a sensitivity simulation that is identical to BASE, except that all international anthropogenic emissions are shut off ("ZROW" for "zero-out rest-of-world"). We compare ozone concentrations in ZROW and BASE to assess the role of international anthropogenic emissions. Both simulations include the nitrate photolysis model update, which provides a mechanism for aerosol emissions and chemistry to affect ozone. To investigate differences related to this novel update, we conduct an additional sensitivity that removes only gas phase ozone precursor emissions (NO_x and VOC) and is referred to as "ZOPROW" for "zero-out precursors rest-of-world."

Comparing chemical species associated with direct emissions (e.g., NO_2) in the base and sensitivity simulations demonstrates that the DESID mask works as intended to shut off anthropogenic emissions outside of the United States (Figure 3). Small changes in NO_2 concentrations over the USA don't reflect the direct change to emissions that DESID imposes, but rather indicate a role for other processes (e.g., nitrate transport prior to photolysis).

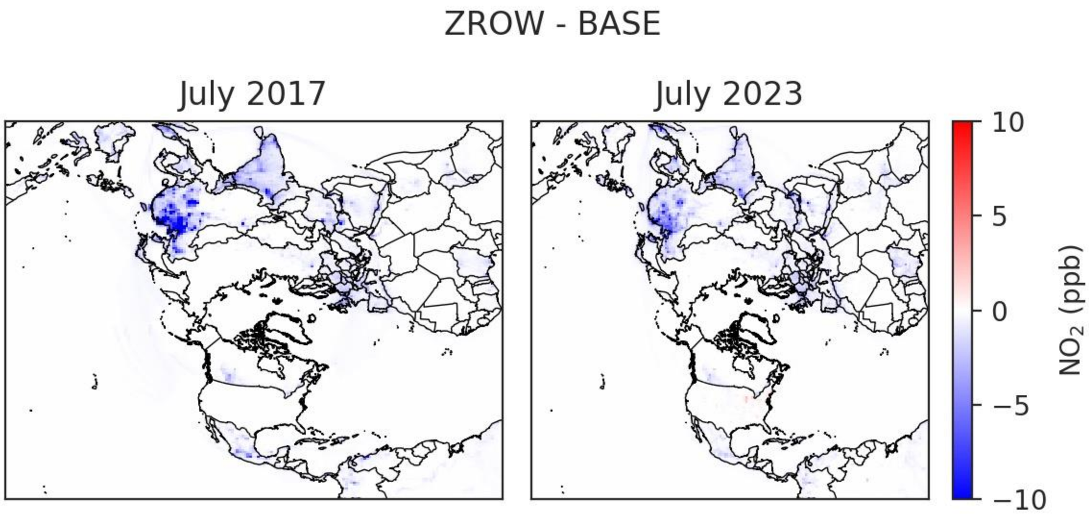

Figure 3. Change in the monthly average nitrogen dioxide (NO_2) concentration at the surface in parts of NO_2 per billion parts of air (ppb) between the ZROW and BASE simulations for July 2017 (left) and July 2023 (right). Negative values (blue) indicate lower concentrations in the ZROW simulation than in the BASE simulation, while positive values (red) indicate higher concentrations in the ZROW simulation than in the BASE simulation.

A counterintuitive result in ZROW is that ozone increases in some regions of the troposphere and especially near the Sahara (Figure 4). This feature is present in both the 2017 and 2023 simulations. Ozone is not emitted directly but is formed through photochemical reactions between NO_x and VOC species, suggesting that NO_x and/or VOC have increased in this region despite the imposed emission reduction. The following discussion identifies likely contributors to these localized ozone increases, but more investigation is needed to conclude which processes lead to these results.

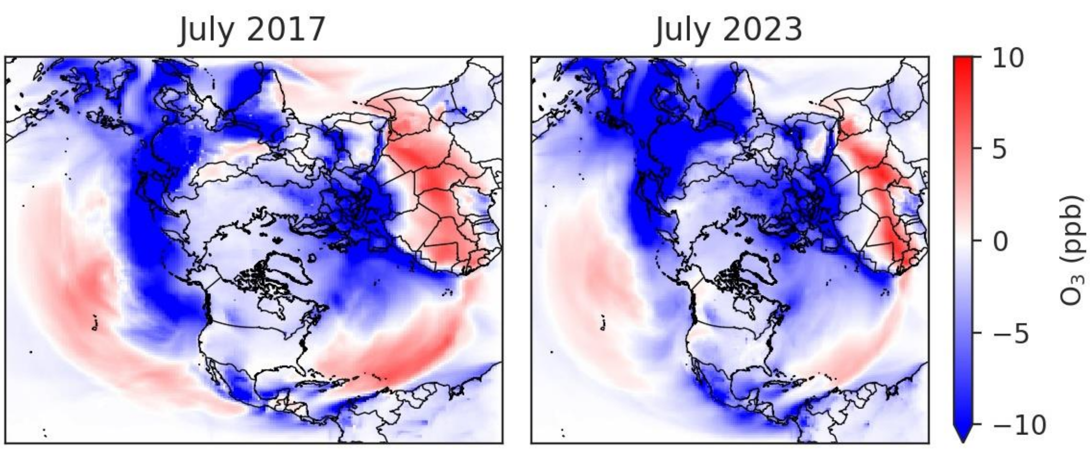

Figure 4. As in Figure 2, but for ozone (O_3).

The most likely possibility is that the nitrate photolysis update, in combination with pre-existing aerosol representation in the model, contributes to this ozone “disbenefit.” Photolysis converts nitrate to NO_x, so that this recently updated process allows transported nitrate, converted to NO_x, to contribute to downwind ozone formation (Sarwar et al., 2024; https://doi.org/10.1016/j.scitotenv.2024.170406).

Nitrate photolysis has been parameterized in CMAQ following field and laboratory studies, but it may not be well constrained for all environmental circumstances, especially under relatively extreme conditions like those of the Sahara or for counterfactual scenarios, such as removing all international anthropogenic emissions.

Total aerosol decreases in the ZROW simulation. However, the response of individual aerosol components varies. The ZROW simulation produces localized increases in nitrate in the accumulation mode (diameter between 0.1 and 2.5 µm) compared to the BASE simulation. Other inorganic aerosol components, ammonium and sulfate, decrease (Figure 5). Thermodynamics support the replacement of sulfate with nitrate following a decrease in oxidized sulfur (SO_x) emissions. This transition, coupled with a shift from gas phase nitric acid to nitrate aerosol, may increase the total modeled nitrate (aerosol nitrate + nitric acid) lifetime and contribute the observed localized nitrate increases in the ZROW model simulation relative to BASE.

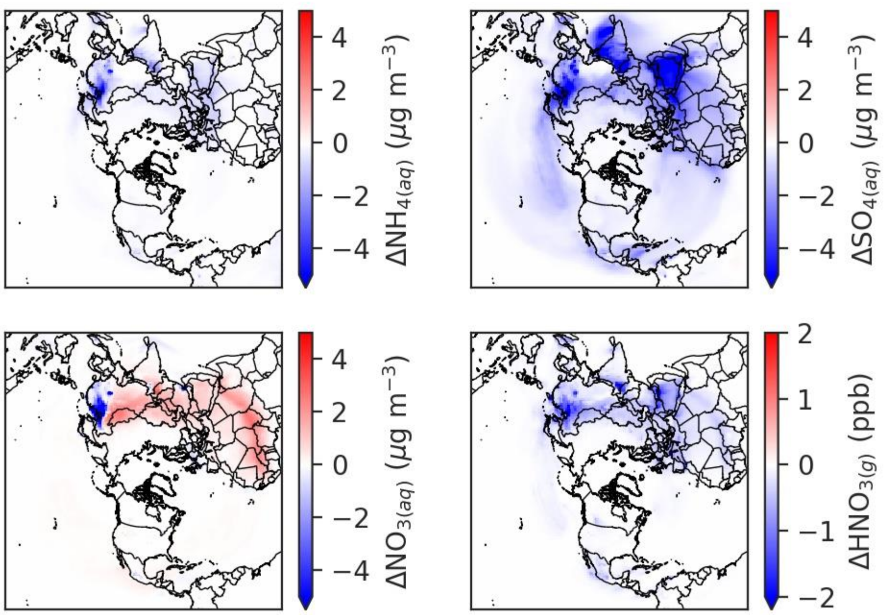

Figure 5. Change in the monthly average sum of the Aitken (I) and accumulation (J) mode concentration for ammonium (NH_4, top left), sulfate (SO_4, top right), nitrate (lower left) and the gas phase concentration of nitric acid (HNO_3, lower right) between the ZROW and BASE simulations for July 2017.

The signal is especially strong over the Sahara, where there is an abundance of nonvolatile cations consistent with a large source of dust. The removal of international anthropogenic SO_x, NO_x, VOC and ammonia emissions pushes the model into a different chemical regime, and the aerosol model ISORROPIA brings nitrate into the particle phase to satisfy the equilibrium of fine mode aerosols (diameter <2.5 µm) when sulfate decreases. These interactions between aerosol component species through the ISORROPIA module are a longstanding representation of aerosol dynamics in the CMAQ model. However, the newer model representation of nitrate photolysis provides an atmospheric feedback pathway by which nitrate increases can lead to subsequent gas-phase ozone increases.

The ZOPROW sensitivity removes international anthropogenic NO_x and VOC emissions and does not perturb emissions of aerosols or the aerosol precursors SO_2 and NH_3. The ZOPROW simulation does not show the same ozone disbenefit as ZROW when ZOPROW is compared to the BASE simulation (Figure 6).

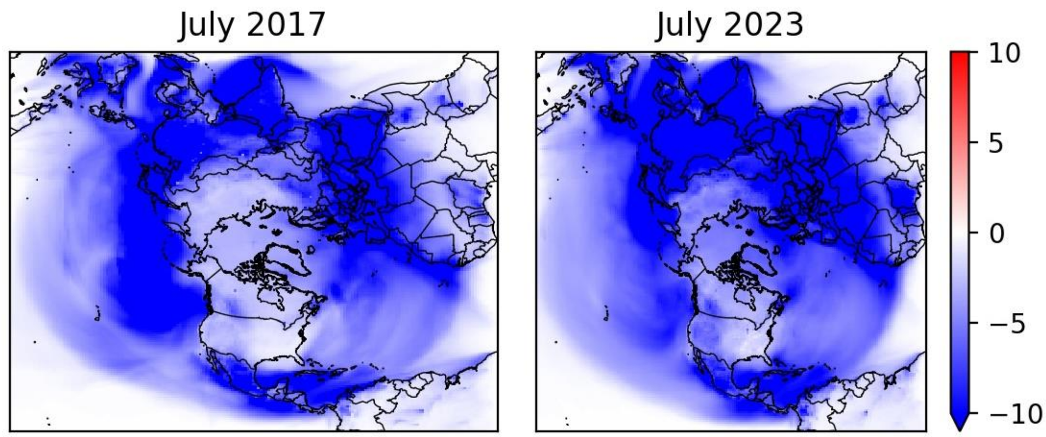

Figure 6. Change in the monthly average O_3 concentration at the surface between ZOPROW (shutting off only NO_x + VOC international anthropogenic emissions) and BASE for July 2017 (left) and July 2023 (right).

Development of IC-BCs for Regional Modeling Domains

Initial and boundary conditions for UDAQ and MAG's custom regional domains were created using CMAQ's ICON and BCON functionality for the BASE, ZROW and ZOPROW HCMAQ simulations. The 108 km CMAQ northern hemisphere domain was horizontally interpolated to a 36 km domain matching the spatial extent shown in Figure 7 for 2023 (relevant for MAG) and 12 km domain matching the spatial extent shown in Figure 8 for 2017 (relevant for UDAQ). The 44 vertical layers resolving the troposphere between the surface and 50 mb were interpolated to fewer layers resolving the troposphere between the surface and 100 mb for 2023 (Figure 7) and 50 mb 2017 (Figure 8) simulations.

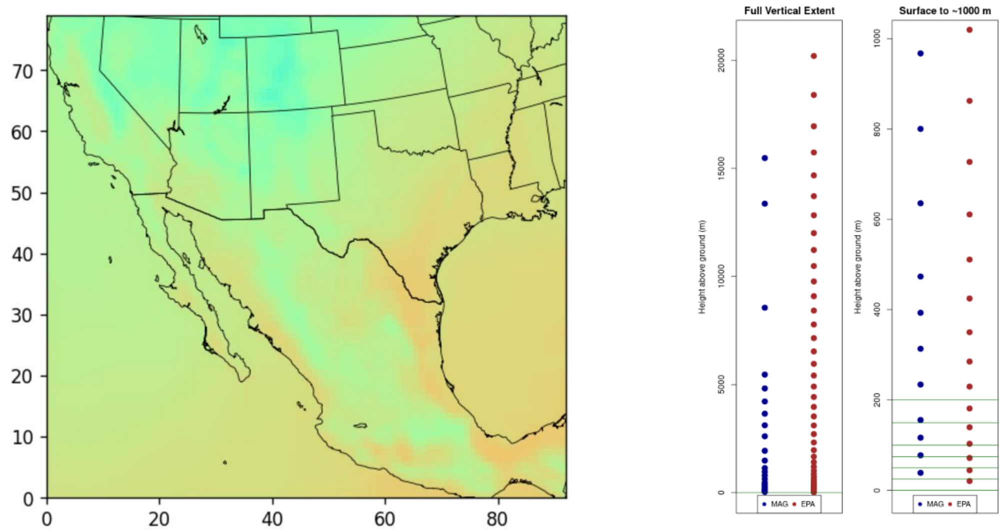

Figure 7. Spatial extent of the MAG 36 km domain (left) and domain average height of each vertical layer for the 36 km domain and 108 km domain (right). Vertical layer mapping is shown for the entire vertical atmosphere represented in CMAQ and for the surface to ~1,000 m to more clearly distinguish the thinner layers nearest the surface.

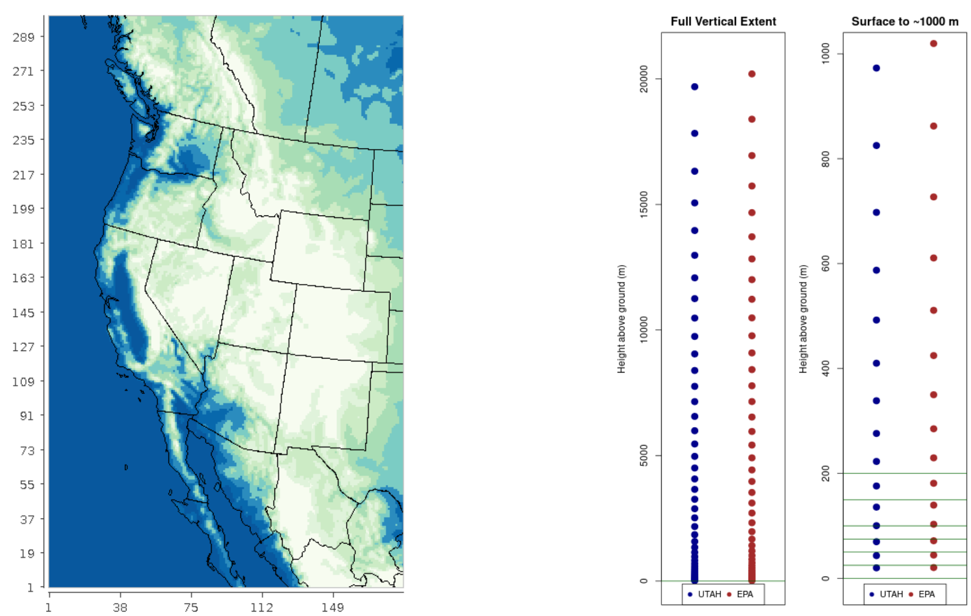

Figure 8. Spatial extent of the UDAQ 12 km domain (left) and domain average height of each vertical layer for the 12 km domain and 108 km domain (right). Vertical layer mapping is shown for the entire vertical atmosphere represented in CMAQ.

Summary

Boundary and initial conditions were created using 2017 and 2023 base and sensitivity simulations from the hemispheric-scale CMAQ model including updates to aerosol nitrate photolysis. Additionally, the two sensitivity simulations (ZROW and ZOPROW cases) bound the range of influence of international anthropogenic emissions on US air quality related to differing representations of the effect of aerosol and aerosol precursor emissions on reactive gas phase species like ozone. ZOPROW (only NO_x + VOC off) case estimates a higher contribution from international emissions at the domain boundaries, while ZROW reflects a lower estimate.

A preliminary analysis has identified that ZROW projects increases in ozone in some regions, which is highly uncertain. The change in ozone in the simulation that only removes NO_x and VOCs is more consistent with previous model versions that did not include such a strong pathway for interactions between gas and aerosol-phase chemistry. The simulation that only perturbs NO_x and VOCs includes the same representation of chemistry as ZROW, so that some of the disbenefit-relevant feedbacks may still be present but are masked by the size of the perturbation.

Data Availability

The ICON and BCON are available as of July 2, 2025 at the following FTP sites.

- 12 km domain used by UDAQ: https://gaftp.epa.gov/aqmg/baker/utah/
- 36 km domain used by MAG: https://gaftp.epa.gov/aqmg/baker/feng/

The simulation used in creating each file is specified in its name (Table 2).

Table 2. File nomenclature specifying the simulation used to create the ICON and BCON files.

Originating simulation	2017 (UDAQ domain)	2023 (MAG domain)
BASE	[unspecified]	qrt2023_r1
ZROW	ZROW	zrow2023
International anthropogenic emissions set to zero for NO_x and, VOC only	ZROW2	zrow2023onlyNOXVOC

Staff in the EPA's Office of Air Quality Planning and Standards (OAQPS) and the Office of Research and Development (ORD) contributed to this work, including Colleen Baublitz, Kirk Baker, Golam Sarwar, Barron Henderson, Havala Pye, Rohit Mathur, Christian Hogrefe, and Heather Simon.

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