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Updates and evaluation of NOAA's online-coupled air quality model version 7 (AQMv7) within the Unified Forecast System

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Abstract. Air quality forecasting system is an essential tool widely used by environmental managers to mitigate adverse health effects of air pollutants. This work presents the latest development of the next generation regional air quality model (AQM) forecast system within the Unified Forecast System (UFS) framework in the National Oceanic and Atmospheric Administration (NOAA). The UFS air quality model incorporates the U.S. Environmental Protection Agency (EPA)'s Community Multiscale Air Quality (CMAQ) model as its main chemistry component. In this system, CMAQ is integrated as a column model to solve gas and aerosol chemistry while the transport of chemical species is processed by UFS. The current AQM version 7 (AQMv7) is coupled with an earlier version of CMAQ (version 5.2.1). Here we describe the development of the updated AQMv7 by coupling to a 'state-of-the-science' CMAQ version 5.4. The updates include improvements in gas and aerosol chemistry, dry deposition processes, and structural changes to the Input/Output (IO) interface, enhancing both computational efficiency and the representation of air-surface exchange processes. A simulation was conducted for the period of August 2023 to assess the effects of these updates on the forecast performance of ozone (O_3) and fine particulate matter ($PM_{2.5}$), two major air pollutants over the continental United States (CONUS). The results show that the updated model demonstrates a significantly enhanced capability in simulating O_3 over the CONUS by reducing the positive bias during both day and night, leading to a reduction of the mean bias by 50% and 72% for hourly and the maximum daily 8-hour average O_3, respectively. Spatially, the updated model lowers the positive bias of hourly O_3 in all of the ten EPA regions, particularly within the Great Plains. Similarly, the updates induce uniformly lower

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fine particulate matter ($PM_{2.5}$) concentrations across the CONUS domain, reducing the positive bias in the northeast and central Great Plain and exacerbating the negative bias in the west and south. The updated model does not improve model performance for $PM_{2.5}$ in the vicinity of fire emission sources as compared to AQMv7, thus indicating a focal point of model uncertainty and needed improvement. Despite these challenges, the study highlights the importance of the ongoing refinements for reliable air quality predictions from the UFS-AQM model, which is the future replacement of NOAA's current operational air quality forecast system.

1 Introduction

Air quality, affected by the amount and type of gaseous and particulate pollutants in the ambient air, has a wide range of impacts on human health, the ecosystem, and the economy. Criteria pollutants, such as ground-level ozone (O_3) and particulate matter with an aerodynamic diameter of less than 2.5 µm ($PM_{2.5}$), can cause cardiovascular and respiratory diseases (Cohen et al., 2005; Lee et al., 2014), worsen symptoms and complications of people with pre-existing health conditions (Balbus and Malina, 2009; Hooper and Kaufman, 2018), and lead to nearly 4.2 million premature deaths worldwide in 2019 with 89% of these deaths occurring in low- and middle-income countries (WHO, 2023). Acidic air pollutants, such as sulfur dioxide (SO_2) and nitrogen oxides (NO_x), can deposit onto soil and watershed and harm plant growth and aquatic life, leading to changes in ecosystems and the loss of biodiversity (Taylor et al., 1994; Lovett et al., 2009). O_3 can also damage forest and crop leaves and interfere with photosynthesis, resulting in yield reduction and food quality deteriorating with an estimated economic loss between 14 to 26 billion dollars globally (Van Dingenen et al., 2009; Tai et al., 2014).

To address the global concern of air pollution and alleviate its health and environmental damage, both international and national agencies play essential roles in air quality regulation and monitoring. Internationally, the World Health Organization (WHO) sets global standards for air quality and provides guidance on its health implications (WHO, 2021). The United Nations Environment Programme (UNEP) coordinates global efforts, with a specific focus on reducing short-lived climate pollutants (UNEP, 2021). In Europe, the European Environment Agency (EEA) provides information and supports the European Union's air quality efforts (EEA, 2022). In the United States, the Environmental Protection Agency (EPA) enforces the Clean Air Act and establishes national ambient air quality standards (NAAQS). Additionally, most countries maintain their own national environmental agencies, which set air quality standards and regulations tailored to local conditions. These agencies follow a comprehensive process, which includes establishing air quality standards, regulating emissions from various sources, monitoring air quality through networks of monitoring stations, and making data accessible to the public. Stringent enforcement measures are in place to ensure compliance, and research initiatives and public awareness campaigns further contribute to informed decision-making and citizen engagement. Importantly, air quality forecasts issued from some of these

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agencies are an effective way to combat air pollution because accurate air pollutant predictions can protect public health by offering advance warnings to at-risk individuals and aid in mitigation strategies by guiding industrial activities and urban planning.

The National Oceanic and Atmospheric Administration (NOAA) has taken on the responsibility of providing operational air quality forecast guidance since 2004 through the National Air Quality Forecasting Capability (NAQFC) system. The initial phase of the NAQFC is offline coupled between NOAA's ETA meteorological model and EPA's Community Multiscale Air Quality (CMAQ) model, providing O_3 forecast guidance over the northeast United States (Otte et al., 2005; Eder et al., 2006). Continued development and evaluation of the NAQFC enabled the system to issue O_3, $PM_{2.5}$, wildfire smoke and dust forecast guidance for the entire contiguous United States (CONUS), Alaska, and Hawaii in order to protect human health, the environment and economy (Mathur et al., 2008; McKeen et al., 2009; Eder et al., 2009; Stajner et al., 2012; Huang et al., 2017; Lee et al., 2017). With the National Weather Service (NWS) transition to use a new Finite-Volume Cubed-Sphere (FV3) dynamical core in the Global Forecast System (GFS) model, in combination with GFS's improvement in data assimilation and physical parameterizations, both short and long weather forecasts are considerably improved (Harris and Lin, 2013; Zhou et al., 2019; Chen et al., 2019), which motivated s NOAA to use FV3GFS as the meteorological driver in the NAQFC (Huang et al., 2017, 2019; Chen et al., 2021). The latest NAQFC, coupled between version 16 of the FV3GFS (FV3GFSv16 hereafter) and CMAQv5.3.1, shows significantly different meteorological and chemical predictions and overall improves the surface O_3 and $PM_{2.5}$ simulations in a 72h forecast relative to its previous version (Campbell et al., 2022) and yields similar results in a historical simulation compared with the commonly-used Weather Research & Forecasting Model (WRF; Tang et al., 2022).

In recent years, NOAA has made extensive efforts to develop the next generation weather forecast model, known as the Unified Forecast System (UFS), which is a community-based, coupled, comprehensive Earth Modeling System with the capability of integrating a number of common components (e.g., land, ocean, atmosphere and sea ice) into different applications. The UFS framework allows for predictions that span local to global domains and range from sub-hourly to seasonal time scales (Krishnamurthy et al., 2021; Bai et al., 2023; Zhu et al., 2023). It is designed to be the unified system for NOAA's operational numerical weather prediction applications while enabling more effective collaboration among government, academia, industry, and beyond (https://ufscommunity.org, last access:30 October 2023).

The Air Quality Model (AQM; https://github.com/NOAA-EMC/AQM) is one of UFS's applications that dynamically couples the CMAQ model with the UFS weather model (https://github.com/ufs-community/ufs-weather-model) to simulate spatiotemporal variations of atmospheric composition and air quality. The chemical component is currently based on the CMAQ model version 5.2.1 (CMAQv5.2.1) in AQM version 7 (AQMv7), which was released in 2018. Hence this version of CMAQ has become scientifically outdated, as EPA is continuously advancing the model with both scientific and structural changes as described in Appel et al. (2021) and Murphy et al. (2021), which can potentially lead to higher biases and errors in

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the air quality forecast. Therefore, there is a need to update the AQMv7 to the latest version 5.4 (at the time of writing) of the CMAQ model (CMAQv5.4; https://github.com/USEPA/CMAQ/tree/5.4, last access: 30 October 2023).

The main objective of this study is to upgrade the chemical component of the current AQMv7 to the latest CMAQ model (see description in Section 2). The simulation design and model inputs are presented in Section 3. In Section 4, we compare the air quality predictive performance between the current and updated AQMv7 (AQMv7_new hereafter) against surface observations in the CONUS. We conclude, in Section 5, that the advancement using a closer state-of-the-science chemical transport model will improve the prediction of atmospheric chemical compositions and therefore result in more accurate air quality forecasts and better protect public health across the US.

2 Methods: Updates to the AQM

The AQM component is a dynamic wrapper that links the UFS weather model with CMAQ through the National Unified Operational Prediction Capability (NUOPC) layer based on the Earth System Modeling Framework (ESMF). AQM has its own input and output (AQMIO) layer that can read in the online-coupled meteorology, initial and boundary conditions (IC/BC), and emissions from different sources, and then pass the updated prognostic and diagnostic chemical tracer fields back to the UFS weather model. CMAQ is treated as a column model for emission mapping, photolysis, gas and aerosol chemistry, and dry deposition at each integration time step, while other transport terms, such as advection and diffusion, are more appropriately handled in the FV3 physics. More details of the AQMv7 structure can be found in Huang et al. (2024).

The updates of AQMv7 are mainly based on the changes from CMAQv5.2.1 to CMAQv5.4, between which there were updates for CMAQ version 5.3 (CMAQv5.3; Appel et al., 2021). The advancements of CMAQv5.3 and CMAQv5.4 are listed in its release notes for each respective version (https://github.com/USEPA/CMAQ, last access: 30 October 2023). Here we only include the features that are used in AQMv7. The newer version usually contains various science, functionality, and computation efficiency upgrades. The following subsections describe the specifics of these changes.

2.1 Chemistry

Of all the three families of gas chemical mechanisms included in CMAQ, the Carbon-Bond version 6 (CB6) scheme is the most widely used for regional air quality simulations, and thus adopted in AQM. The other two chemical mechanisms currently implemented in CMAQ include Statewide Air Pollution Research Center (SAPRC) and the Regional Atmospheric Chemical Mechanism (RACM). The CB6 mechanism has evolved from revision 3 (CB6r3) in CMAQv5.2.1 to revision 5 (CB6r5) in CMAQv5.4 (Yarwood et al., 2010; Emery et al., 2015; Yarwood et al., 2020). The associated aerosol chemistry has also been significantly updated from version 6 (AERO6) to version 7 (AERO7).

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2.1.1 Gas chemistry

The chlorine chemistry in CB6r3 (Sarwar et al., 2012; Luecken et al., 2019) was updated in the 2019 release of CMAQv5.3, which added 5 chemical reactions and one new chlorine species compared with the previous CB6r3 mechanism in CMAQv5.2.1 (github.com/USEPA/CMAQ/blob/5.3/DOCS/Release_Notes/chlorine_chemistry_CB6r3.md, last access 21 February 2024). The same chlorine chemistry was kept in the CB6r5 mechanism. Both detailed and simplified bromine and iodine chemistry schemes (Sarwar et al., 2015) are implemented in CMAQ, the latter of which is used in AQMv7 to reduce the computational demand. The simple halogen chemistry uses a first-order constant to calculate the O_3 loss rate to seawater. With the updates of the detailed halogen chemistry (Sarwar et al., 2019), the O_3 loss rate constant has been recalculated in CMAQv5.3 and further rederived in CMAQv5.4 with an increased and decreased value relative to its previous version, respectively. The final result is a reduction of O_3 in the ocean (https://github.com/USEPA/CMAQ/blob/5.3/DOCS/Release_Notes/simple_halogen_chemistry.md, last access: 22 March 2024). Other chemistry changes in CB6r5 (Burkholder et al., 2019) include updates in reaction rate constants, reaction products and yields, photolysis rates of some species, and the addition of new reactions. The overall impacts of the mechanism migration from CB6r3 to CB6r5 are marginal increases in both summer and winter months (https://github.com/USEPA/CMAQ/wiki/CMAQ-Release-Notes:-Chemistry:-Carbon-Bond-6-Mechanism-(CB6), last access: 31 October 2023).

2.1.2 Aerosol chemistry

AERO7 has extensive changes from AERO6 incorporating a number of key improvements, such as updating the yields of monoterpene secondary organic aerosol (SOA) resulting from the photooxidation by hydroxyl radicals (OH) and O_3 (Saha and Grieshop, 2016), adding the formation and subsequent partitioning of organic nitrate (Pye et al., 2015), introducing the inclusion of water uptake on hydrophilic organic compounds as described in Pye et al. (2017), accounting for the consumption of inorganic sulfate during the formation of isoprene epoxydiol (IEPOX) organosulfates (Pye et al., 2013; Zhang et al., 2018b), and enhancing computational efficiency by replacing the Odum two-product fit (Odum et al., 1996; Henze and Seinfeld, 2006; Carlton et al., 2010) with a new parameterization of anthropogenic SOA yields through a volatility basis set (VBS) approach (Pye et al., 2010, 2019). The updated monoterpene oxidation yield in the VBS fit and the inclusion of water uptake in AERO7 will generally increase organic aerosol and PM2.5 primarily in the vegetated southeast US during summertime (Xu et al., 2018; Zhang et al., 2018a), the latter of which will also affect deposition and aerosol optical depth (AOD) by modulating aerosol size (Pye et al., 2017).

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2.2 Dry deposition

There are two air-surface exchange models starting from CMAQv5.3: the Models-3 dry (M3Dry) deposition model and the Surface Tiled Aerosol and Gaseous Exchange (STAGE) model. Currently, only M3Dry is adopted in AQMv7. Some important updates have been made for O_3 and aerosol deposition depending on land use types since the release of CMAQv5.2.1. The O_3 dry deposition resistance to snow was raised by 10 times from 1000 to 10 000 s m^{-1} following the observed evidence in Helmig et al (2007), leading to a significant increase of ambient O_3 over snow-covered regions. The ground O_3 resistance over soil has also been modified to be dependent on soil moisture (Mészáros et al., 2009; Fares et al., 2012) with a generally decreased value relative to the previous dry deposition scheme and thus result in more O_3 depositing to the soil surface and less remaining in the ambient air.

The aerosol dry deposition scheme has been updated in both CMAQv5.3 and CMAQv5.4. The revised parameterization of aerosol dry deposition in CMAQv5.3 added a leaf area index (LAI) factor in the boundary layer resistance to account for large depositions over forest canopies, which greatly reduces the coarse-mode particle dry deposition velocity (Shu et al., 2022; Appel et al., 2021). The scheme is further improved in CMAQv5.4 by introducing a two-term impaction efficiency to represent macroscale and microscale obstacles, which differ by land use categories including needleleaf forest, broadleaf forest, and grassland (Pleim et al., 2022). The most significant changes of mass dry deposition velocity are found for the accumulation mode over the forested areas with an increase by almost an order of magnitude, causing an overall reduced $PM_{2.5}$ in the continuous US relative to CMAQv5.3.

2.3 Structural changes

A number of changes have been made to the Input/Output (IO) framework of CMAQ (Figure 1). Emission reading, mapping, and scaling are controlled in the Detailed Emissions Scaling, Isolation, and Diagnostic (DESID) module in CMAQv5.3 and beyond. The module can read any number of offline gridded and point emission files by their sources (defined as streams) and apply scaling factors on a per-species and per-region basis for each stream, allowing users to perform emission scaling and perturbation tests with great ease and flexibility (Murphy et al., 2021). The opening, description, extraction, and interpolation of the meteorological and emission variables are encapsulated in the centralized I/O (CIO) module from CMAQv5.3, lowering computational memory requirements and easing code maintenance. The Introduction of the Explicit and Lumped air quality Model Output (ELMO) module is included in CMAQv5.4, which can synthesize the definition, calculation, and maintenance of individual or aggregate gas and particulate matter parameters (e.g., $PM_{2.5}$) online, saving time and storage to run post-processing tools. Implementing these changes requires new control name lists and extensive code updates in AQMv7_new.

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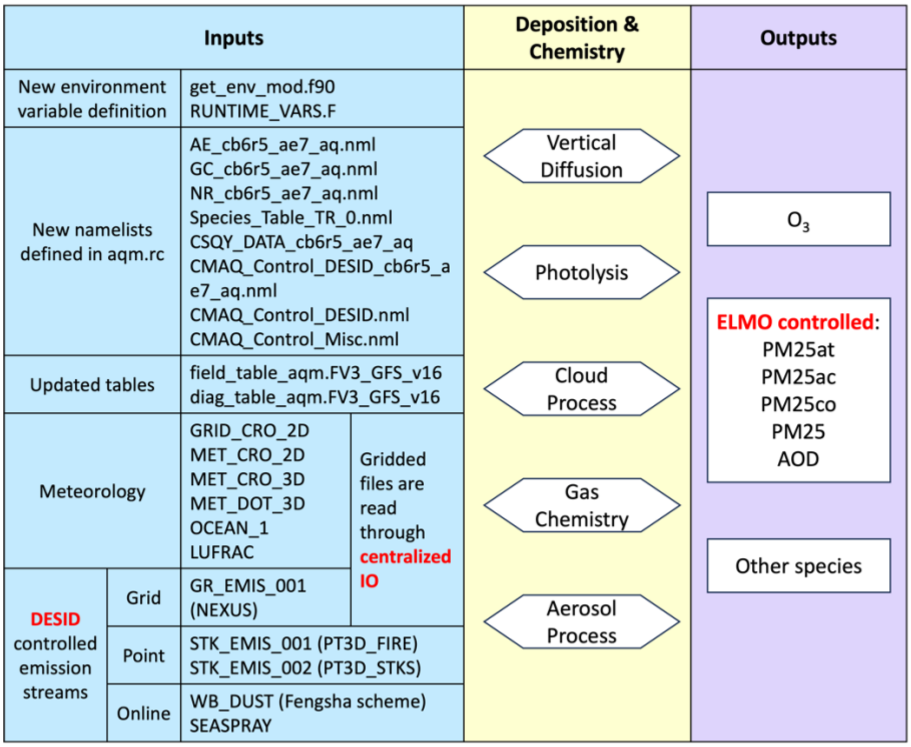

Figure 1: Summary of the IO changes in the AQMv7_new model. Three major structural changes are highlighted in red.

3 Simulation design and evaluation protocol

Despite the chemistry and dry deposition updates described in the last section, other model components and configurations are the same in order to isolate the model performance changes caused by the updates. Table 1 summarizes the model domain, physical settings and emission inputs, as well as some additional information.

Table 1: UFS-AQM model components and configurations. The abbreviation N/A stands for not applicable in this table.

Model attributes	Configuration	Reference
Domain	North America Cantered on 50° N 118° W	N/A
Horizontal resolution	13km	N/A
Vertical resolution	64 levels from near the surface up to the top of the stratosphere	N/A
Meteorological ICs and BCs	FV3GFSv16.3	https://nws.weather.gov/ (last access: 25 November 2023)

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Chemical ICs and BCs	Static monthly AM4 for gases and aerosol species and GEFS-Aerosol for dynamic smoke and dust	Horowitz et al. (2020); Tang et al. (2021)
Microphysics	GFDL six-category cloud microphysics scheme	Lin et al. (1983); Lord et al. (1984); Krueger et al. (1995); Chen and Lin (2011, 2013)
PBL physics scheme	sa-TKE-EDMF	Han and Bretherton (2019)
Shallow and deep cumulus parameterization	SAS scheme	Han and Pan (2011); Han et al. (2017)
Shortwave and longwave radiation	RRTMg	Mlawer et al. (1997); Clough et al. (2005); Iacono et al. (2008)
Land surface model	Noah land surface model	Chen and Dudhia (2001); Ek et al. (2003); Tewari et al. (2004)
Surface layer	Monin-Obukhov	Monin and Obukhov (1954); Grell et al. (1994); Jimenez et al. (2012)
Anthropogenic emissions (CONUS)	Area Sources: NEIC2016v1 Point Sources: NEIC2016v1 with Briggs plume rise	NEI (2019); Briggs (1965)
Anthropogenic emissions (Outside CONUS)	CEDSv2; HTAPv2.2; OMI-HTAP SO_2 2019	O'Rourke et al. (2021); Janssens-Maenhout et al. (2015); Liu et al. (2018)
Biogenic emissions	MEGAN2.1 driven by GFSv16 meteorology	Guenther et al. (2012)
Wildfire emissions	RAVE with Sofiev plume rise	Li et al., (2022); Sofiev et al. (2012)
Other inline/Offline emissions	FENGSHA windblown dust scheme	Fu et al. (2014); Huang et al. (2015); Dong et al. (2016)
	Sea spray emissions	Kelly et al. (2010); Gantt et al. (2015)

The model domain covers North America (NA) with a horizontal resolution of ~13km and 64 vertical layers spanning from the surface up to the top of the stratosphere (~ 0.4 hPa). The Common Community Physics Package (CCPP) FV3GFSv16.3 physics suite (Heinzeller et al., 2023) is used to provide meteorological conditions, where its physical configurations include the Monin-Obukhov Similarity surface layer (Monin and Obukhov, 1954; Grell et al., 1994; Jiménez et al., 2012), the Noah land surface scheme (Chen and Dudhia, 2001; Ek et al., 2003; Tewari et al., 2004), the Rapid Radiative Transfer Model (RRTM) longwave and shortwave radiation schemes (Mlawer et al., 1997; Clough et al., 2005; Iacono et al., 2008), the Simplified Arakawa Schubert (SAS) cumulus parameterization (Han and Pan, 2011; Han et al., 2017), the Geophysical Fluid Dynamics Laboratory (GFDL) six-category cloud microphysics scheme (Lin et al., 1983; Lord et al., 1984; Krueger et al., 1995; Chen and Lin, 2011, 2013), and the sa-TKE-EDMF planetary boundary layer (PBL) scheme (Han and Bretherton, 2019).

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Anthropogenic emissions outside of the CONUS are from CEDSv2-2019 for all gases, except for sulfur dioxide (SO_2) only in the ocean, organic carbon (OC), and black carbon (BC) (Table 1). The blended Ozone Monitoring Instrument-HTAP (OMI-HTAP) 2019 dataset (https://so2.gsfc.nasa.gov/measures.html, last access: 15 March 2024) provides SO_2 emissions over land, and the emissions of coarse particulate matter (PMC) and $PM_{2.5}$ are from HTAPv2-2010. Within the CONUS, all gas and aerosol anthropogenic emissions are from the National Emissions Inventory Collaborative (NEIC) 2016 version 1 (2016v1). The NEIC2016v1 provides both area and point emissions, the latter of which is further calculated inline in AQM using the Briggs plume rise method. The same plume rise method is also applied to the wildfire emissions from the Regional ABI and VIIRS fire Emissions (RAVE) inventory. Both the windblown dust and sea salt emissions are calculated inline. The dust scheme is based on a novel FENGSHA model (Fu et al., 2014; Huang et al., 2015; Dong et al., 2016), which is dependent on the land cover, soil type, soil moisture, and friction velocity. Biogenic emissions are from the Model of Emissions of Gases and Aerosols from Nature version 2.1 (MEGAN2.1) driven by the GFSv16 meteorology. The area source anthropogenic and biogenic emissions are both processed and calculated inline using the NOAA Emissions and eXchange Unified System (NEXUS) component (Campbell et al., 2020), which is based upon the Harmonized Emissions Component (HEMCO) 3.0 (Lin et al., 2021). The chemical initial and boundary conditions (ICs/BCs) are from the monthly mean Atmospheric Model version 4 (AM4) outputs for gas and aerosol species with additional dynamic BCs for dust and smoke aerosols from the aerosol forecast member in the Global Ensemble Forecast System (GEFS-Aerosols), which can better capture the aerosol intrusion events from outside of the domain and thus improve the prediction of air quality (Tang et al., 2021).

The simulations for both AQMv7 and AQMv7_new were performed for the entire month of August 2023, during which there were extensive wildfire activities over the northwest U.S. and Canada. The air quality observations from the EPA AirNow network are used to evaluate the model performance and the evaluation is conducted using the publicly available software MELODIES-MONET (Model EvaLuation using Observations, DIagnostics and Experiments Software (MELODIES) with the Model and ObservatioN Evaluation Toolkit; Baker and Pan, 2017; https://csl.noaa.gov/groups/csl4/modeldata/melodies-monet/, last access: 15 March 2024). The software can produce flexible diagnostic assessments by pairing models and observations, plotting spatial maps, and calculating statistics such as mean bias (MB), normalized mean bias (NMB), median bias (MdnB), normalized median bias (NMdnB), coefficient of determination (R^2), root-mean-square error (RMSE), and the index of agreement (IOA). A meteorological evaluation was also conducted using the U.S. EPA Atmospheric Model Evaluation Tool (AMET; Appel et al., 2011; https://www.cmascenter.org/amet/, last access: 15 March 2024) against the observations collected from the Surface Weather Observations and Reports for Aviation Routine Weather Reports (METAR) and Earth System Research Laboratory's (ESRL's) Radiosonde Database (RAOB).

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4 Results: Assessment and evaluation of updates

In this section, we compared the performance of the current and updated models in their capability of predicting summer season (August) O_3 and $PM_{2.5}$ as they are the most important air pollutants of concern. Although both models are driven by the same CCPP GFSv16 physics suite, we evaluated the simulation of some meteorological factors critical for O_3 and $PM_{2.5}$ formation and transport in Figure S1-4 and Table S1, including surface temperature (TEMP2) and specific humidity (Q2) at 2m, wind speed (WS10) and direction (WD10) at 10m and their vertical distributions, which can provide insights into the overall model performance in air quality predictions. TEMP2, Q2 and WS10 in the CONUS were well simulated with high correlation coefficients (CORR) of 0.95, 0.92 and 0.65 and low mean bias of -0.03 °C, -1.41 g kg^{-1}, and -0.15 m s^{-1}, respectively (Table S1). While cold bias is found in the northeastern and western US (Figure S1) at the surface mainly driven by nighttime underpredictions (Figure S2-3), the vertical distribution shows a nationwide warm bias (Figure S4). Specific humidity has a universally dry bias within the domain both at the surface and vertically with the latter showing higher bias up to 10 g kg^{-1} at some sites. Such biases in TEMP2 and Q2 suggest an overly stable atmosphere in the GFSv16 physics during summer, which may influence overpredictions in trace gases in the lowest model layers. The diurnal evaluations also indicate overpredictions in TEMP2 during the daytime both in the western and eastern US, where the warm and dry biases may further exacerbate O_3 formation and overpredictions, especially in the eastern U.S. (See Section 4.1 below). The WD10 demonstrated relatively worse predictions, especially in its vertical distributions, with low CORR values smaller than 0.6 and a high mean bias greater than 20° at most sites. AMET accounts for the wind direction vector issue in its calculation of the evaluation statistics.

4.1 O_3 evaluation

Figure 2 displays the spatial maps of hourly O_3 distribution in the CONUS averaged in August 2023 from two model simulations and AirNow observations, as well as the model mean bias at each site. The western US generally has a higher level of O_3 relative to the eastern US, reflecting the overall O_3 spatial distribution during summertime. The AQMv7 captures this spatial pattern, yet with a positive bias at most of the AirNow sites. A higher positive bias of more than 20 ppb can be found near the west and east coast compared to the smaller or even negative bias in the central US, indicating the land-sea interactions may not be well represented in the model. The relatively large O_3 overestimates are also impacted by the near-surface meteorological biases described previously (i.e., too warm and dry during the day and too cool and dry at night), as well as an overly stable boundary layer. The AQMv7_new model shows a nation-wise decrease in O_3 mixing ratios, which greatly reduces the high positive bias over the coastal sites. In contrast, the negative bias at some sites in the southcentral regions (e.g., northern Texas and Oklahoma) becomes bigger.

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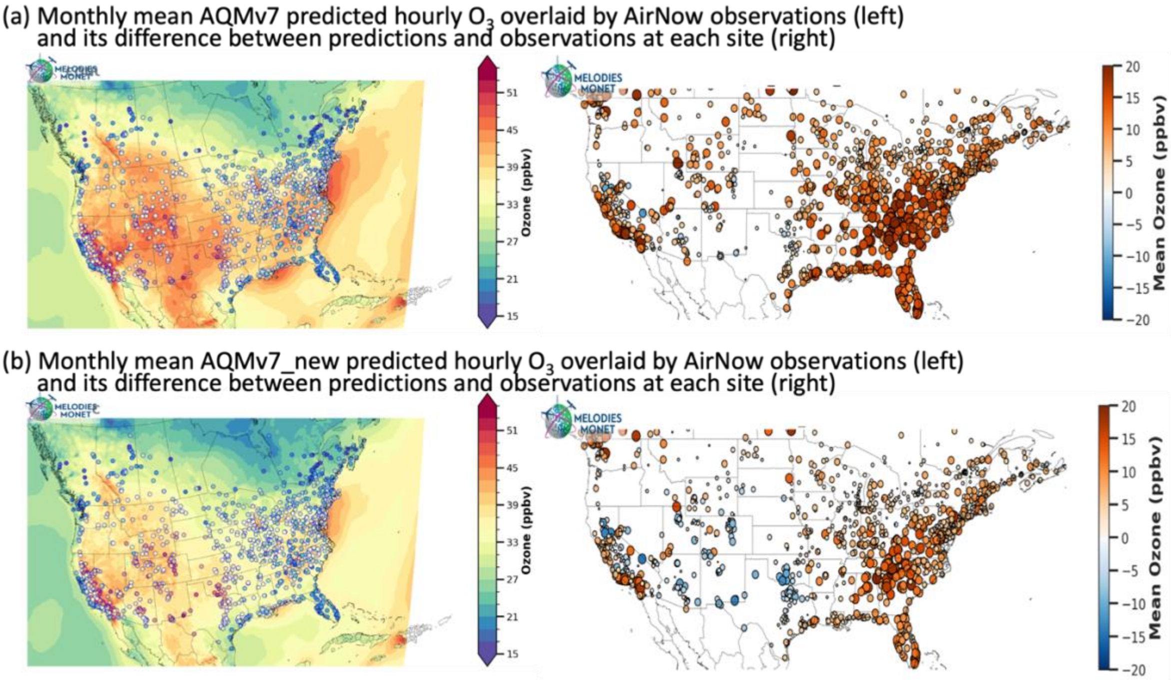

Figure 2: Maps of monthly mean hourly O_3 in the CONUS predicted by AQMv7 (a) and AQMv7_new (b) overlaid by AirNow observation sites (left column) and its bias between simulations and observations (model - AirNow) at each site (right column).

Averaging across the CONUS, the hourly O_3 time series from the AQMv7 simulation (red line in Figure 3a) show that the model captures the temporal variation with an R^2 value of 0.50 (Table 2). However, the model overestimates both the peak values at noon and the low values at night with a mean bias of 7.06 ppb (22.64%), which explains the widespread positive bias shown in Figure 2. Such overestimation of O_3 during daytime and nighttime is alleviated by the updated model, reducing the mean bias by 50% to 3.55 (11.38%). We also evaluated the model performance of the maximum daily 8-hour average (MDA8) O_3 simulation in Figure 3b with the statistics listed in Table S1. Similarly, the AQMv7 overpredicts MDA8 O_3 by 4.99 ppb (11.44%), which is greatly lowered by 72% in the updated model with a mean bias value of 1.37 ppb (3.15%). Furthermore, the RMSE and IOA values of both hourly and MDA8 O_3 are also improved by the model updates, indicating an overall enhanced model performance in simulating O_3 in the CONUS.

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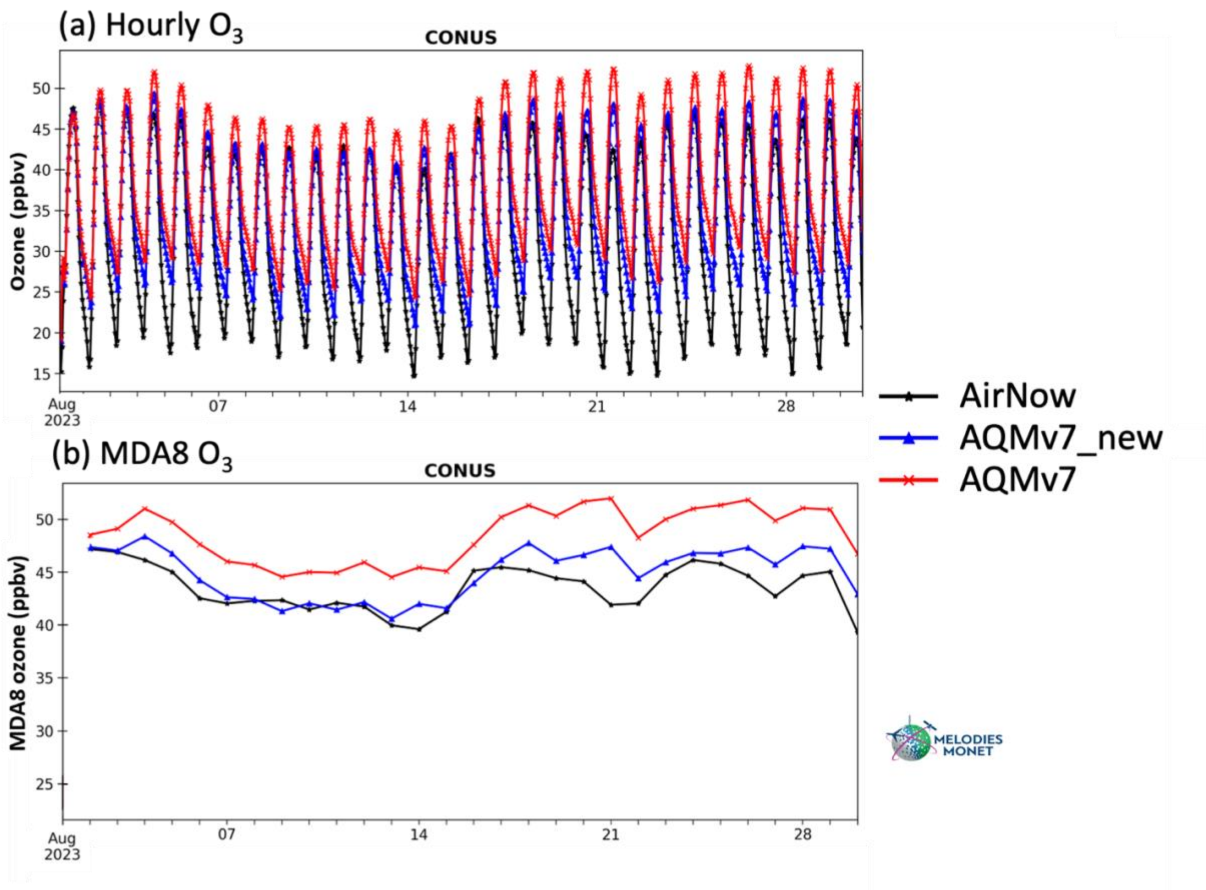

Figure 3: Time series of hourly (a) and MDA8 (b) O_3 in the CONUS from AirNow observations (black line), AQMv7 (red line) and AQMv7_new (blue line) predictions.

Table 2: Hourly O_3 evaluation statistics of the AQMv7 and AQMv7_new simulations against the AirNow network in the CONUS and different regions in August 2023. The bold numbers in AQMv7_new indicate an improvement relative to those in AQMv7.

Region	Model	MB (ppb)	NMB (%)	MdnB (ppb)	NMdnB (%)	R^2	RMSE (ppb)	IOA
CONUS	AQMv7	7.06	22.64	6.35	21.16	0.50	13.36	0.79
	AQMv7_new	**3.55**	**11.38**	**2.79**	**9.28**	**0.51**	**11.71**	**0.82**
Region 1 (northeast)	AQMv7	7.17	25.60	6.33	21.82	0.44	12.01	0.74
	AQMv7_new	**4.82**	**17.19**	**3.77**	**12.99**	**0.45**	**10.54**	**0.77**
Region 2 (NY-NJ)	AQMv7	6.82	23.02	5.94	19.82	0.45	12.65	0.77
	AQMv7_new	**4.47**	**15.11**	**3.36**	**11.20**	**0.47**	**11.17**	**0.80**

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Region 3 (mid-Atlantic)	AQMv7	9.11	29.04	7.87	24.59	0.42	14.39	0.72
	AQMv7_new	**5.37**	**17.13**	**3.92**	**12.27**	**0.44**	**12.04**	**0.76**
Region 4 (southeast)	AQMv7	13.00	47.09	12.21	45.23	0.51	16.85	0.69
	AQMv7_new	**8.67**	**31.40**	**7.89**	**29.23**	0.50	**13.82**	**0.74**
Region 5 (upper Midwest)	AQMv7	6.66	21.37	5.82	18.79	0.48	12.42	0.78
	AQMv7_new	**3.03**	**9.71**	**2.06**	**6.64**	**0.51**	**10.38**	**0.82**
Region 6 (south)	AQMv7	4.77	13.79	4.91	14.44	0.66	11.79	0.85
	AQMv7_new	**-0.34**	**-0.99**	**0**	**-0.01**	0.66	**10.97**	**0.86**
Region 7 (central Great Plain)	AQMv7	7.97	24.53	7.15	21.65	0.49	12.73	0.76
	AQMv7_new	**3.05**	**9.40**	**2.23**	**6.76**	**0.50**	**10.21**	**0.81**
Region 8 (northern Great Plain)	AQMv7	4.18	10.96	3.17	8.13	0.36	12.09	0.73
	AQMv7_new	**-0.30**	**-0.78**	**-1.32**	**-3.38**	**0.43**	**10.61**	**0.78**
Region 9 (southwest)	AQMv7	5.73	15.96	5.13	15.09	0.56	13.06	0.82
	AQMv7_new	**2.45**	**6.82**	**1.83**	**5.39**	**0.58**	**11.79**	**0.86**
Region 10 (northwest)	AQMv7	5.39	18.63	4.12	14.72	0.54	12.07	0.83
	AQMv7_new	**3.39**	**11.72**	**1.93**	**6.91**	0.53	**11.55**	**0.84**

In addition to the statistics listed in Table 2, hit rate, false alarm rate, and critical success index (CSI) are metrics commonly used to evaluate the performance of predictions, providing valuable insights into different aspects of forecast accuracy and reliability. Figure 4 compares these three metrics between AQMv7 and AQMv7_new at different hourly O_3 thresholds across the CONUS. Although both models have difficulties in predicting higher levels of O_3 indicated by the decrease of hit rate and CSI and the increase of false alarm rate as the threshold changes from 0 ppbv to 100 ppbv, the new model yields a higher hit rate and a lower false alarm rate when O_3 is greater than 20 ppb. The CSI value was also improved when the threshold is higher than 60 ppbv. All these changes denote that our updates make the model simulate O_3 more accurately, especially for high O_3 events.

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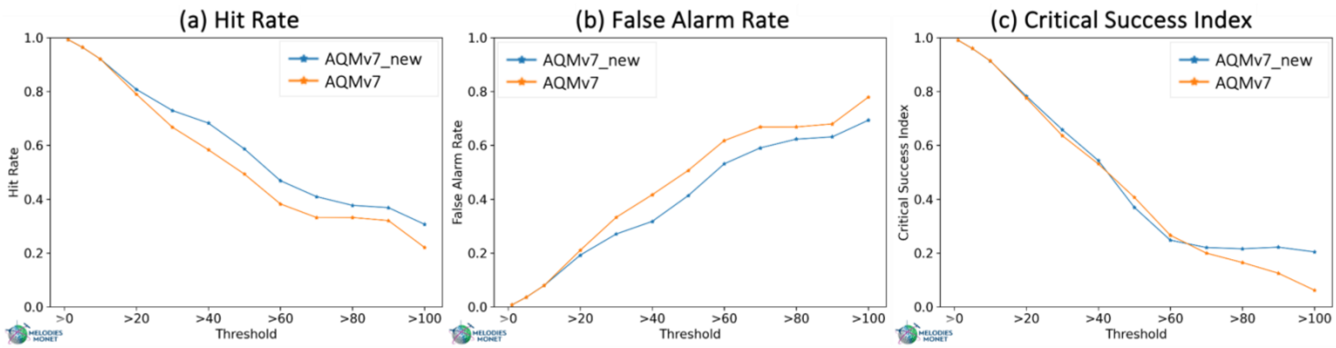

Figure 4: Hit rate (a), false alarm rate (b), and critical success index (c) of hourly O_3 at different thresholds across the CONUS.

We also assessed the model simulations in each of the 10 EPA regions (R1-R10 hereafter) in Figure 5a and Table 2 to further examine how the updates will affect the model performance regionally. The AQMv7 model overestimates hourly O_3 at all regions with the mean bias values ranging from 4.18 ppb (10.96%) in the northern Great Plain (R8) to 13.00 ppb (47.09%) in the southeast (R4). Compared to the AQMv7 model, the statistical distributions of hourly O_3 from the AQMv7_new model move to the lower end, which reduces the respective positive bias by 2.35 ppb, 2.35 ppb, 3.74 ppb, 4.33 ppb, 3.63 ppb, 5.11 ppb, 4.92 ppb, 4.48 ppb, 3.28 ppb, 2.00 ppb from R1 to R10 and makes the mean bias close to zero in R6 and R8. The Great Plain regions (R6-R8) have a higher sensitivity to the model updates relative to other regions, which is likely due to the combined effects of O_3 chemistry and dry deposition. As described in Section 2, the halogen chemistry updates reduce O_3 over sea water, which can be transported into the central U.S. dominated by southerly winds in summer, such as the Great Plain low-level jet (Zhu and Liang, 2013; Li et al., 2020). In addition, the added dependence of O_3 dry deposition velocity to soil moisture leads to more O_3 uptake by dry soil than wet soil (Appel et al., 2021) and the central and western U.S. generally have lower soil moisture than the eastern regions. The RMSE values in the southeast (R4) and central Great Plain (R7) are also improved the most by 3.03 ppb and 2.52 ppb, respectively.

The regional analysis was also conducted by comparing IOA values between these two models on a daily basis and the results are shown in the scorecard plot (Figure 5b). The IOA is a standardized measure of the degree of model prediction error and is defined as the ratio of the mean square error to the potential error. A value of 1 indicates a perfect match between the model and observations, while a value of 0 indicates no agreement at all (Willmott, 1981). The new model has higher IOA values on most of the days in all regions at a 95% confidence level, except for R10 with improved IOA values only on individual days. It is noted that there are some days on which the AQMv7_new model performs worse at both urban and rural sites in a specific region (e.g., August 17 – 20 in R6). The time series focusing on R6 (Figure S5) reveal that the AQMv7 model generally underestimates O_3 on those days and a further reduction in the new model will make the performance worse.

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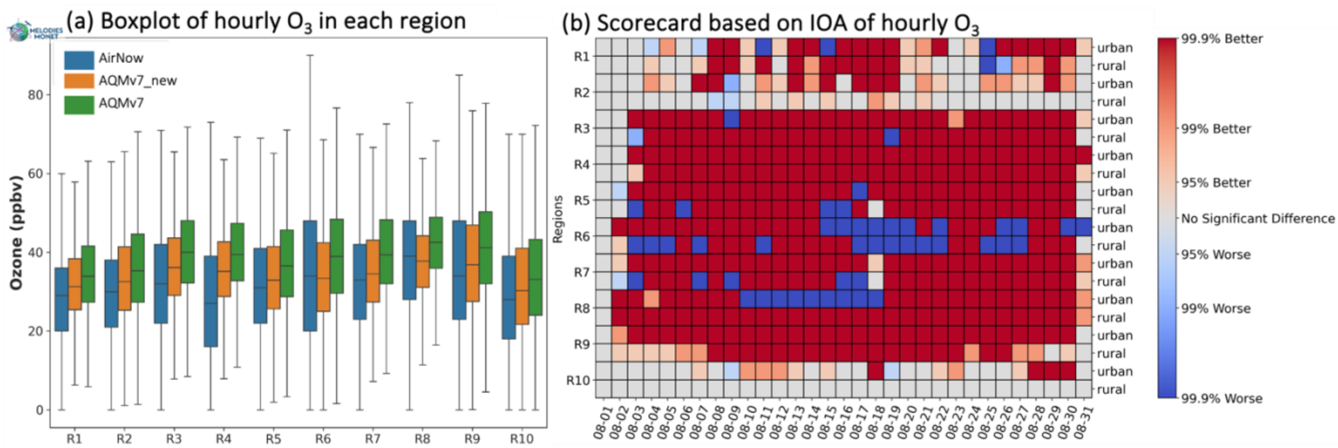

Figure 5: (a) Boxplot of observed and model-simulated hourly O_3 separated by ten EPA regions. (b) Scorecard plot based on IOA values grouped by urban and rural sites (left axis) within each region (right axis) on each day. Red colors indicate the AQMv7_new model performs better, while blue colors indicate that the AQMv7 model performs better. The saturation of the colors varies by significance levels.

In summary, we compared the model performance of two models in their capability of predicting the spatiotemporal patterns of O_3 in the CONUS and found that the updated AQMv7_new model reduces the positive bias and the RMSE values of both hourly and MDA8 O_3, indicating an improved model accuracy. The extent of the model performance improvements also differs by region with the Great Plain area experiencing the highest enhancement likely due to contributions from both halogen chemistry and dry deposition.

4.2 $PM_{2.5}$ evaluation

Following the evaluation process of O_3, we further examined the model performance changes in $PM_{2.5}$ predictions. As shown in Figure 6a, the monthly average of the hourly $PM_{2.5}$ spatial map from AQMv7 displays extremely high values over western Canada and the northwestern US due to wildfire emissions. The fire plumes can be transported to the northeastern US and partly lead to higher $PM_{2.5}$ levels than those in the central and southwestern regions. The mean bias of $PM_{2.5}$ at the AirNow sites near the wildfire locations is also very high with a value of up to ±15 μg/m^3, where generally in the west-northwest U.S., there are $PM_{2.5}$ overpredictions near fire sources and underpredictions downstream. This result implies that there are substantial uncertainties in wildfire emissions, smoke transport, and plume chemistry for AQMv7. The sites over the northeast have a relatively smaller positive mean bias of less than 10 μg/m^3, followed by the close-to-zero mean bias at the sites over the south. The AQMv7_new model also predicts extreme $PM_{2.5}$ values near the wildfire locations and thus shows comparable positive or negative bias as the AQMv7. However, the positive mean bias in the northeastern area is reduced in AQMv7_new, which

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implies that the overall effect of the model updates is to reduce $PM_{2.5}$ in places with less wildfire impact. Such reductions inevitably deteriorate the model performance when AQMv7 is unbiased or already underestimates $PM_{2.5}$ at the sites in the southern US.

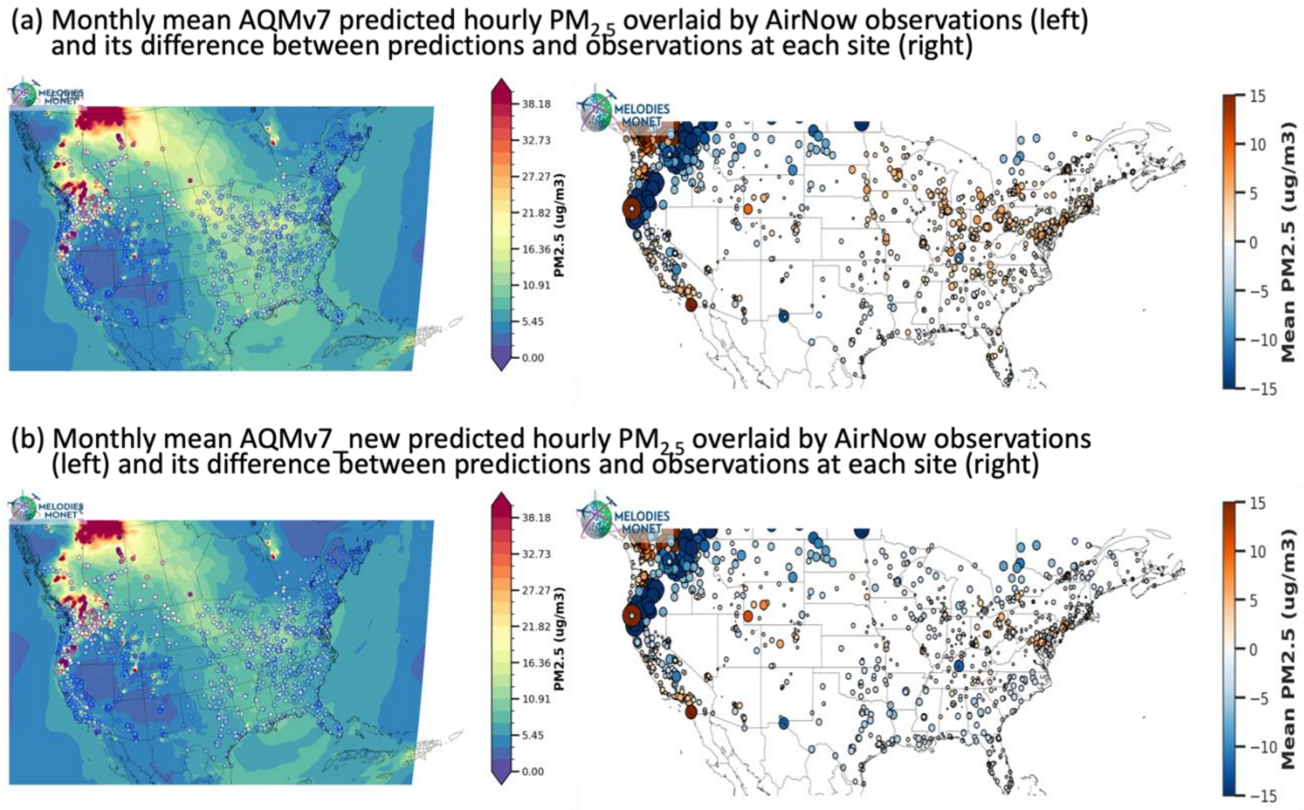

Figure 6: Same as Figure 2 but for $PM_{2.5}$.

The hourly and daily time series of the CONUS-mean $PM_{2.5}$ are shown in Figure 7 and their corresponding statistics are summarized in Table 3 and Table S2. The two models have similar temporal variations and they both well capture the sharp increases in $PM_{2.5}$ values during August 19-21, which are dominated by enhanced fire sources across the U.S. The AQMv7 overall shows an unbiased simulation of hourly $PM_{2.5}$ with a mean bias value of -0.05 μg/m^3 (-0.44%) for the CONUS. The AQMv7_new predicts lower $PM_{2.5}$ values at most hours, which increases the mean bias to -1.40 μg/m^3 (-12.47%). However, the absolute median bias was reduced by more than 50% in the AQMv7_new model from 0.77 μg/m^3 (9.94%) to 0.34 μg/m^3

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(4.35%), indicating that some extreme values may lead to the worsening model performance across the CONUS. RMSE was
335 also slightly reduced by the AQMv7_new. Daily $PM_{2.5}$ from the AQMv7_new is also lower on all days, increasing the negative bias from 0.09 µg/m^3 (0.84%) to 1.47 µg/m^3 (12.94%), but the median bias and RMSE values are similarly improved (Table S2).

The hit rate, false alarm rate, and CSI for $PM_{2.5}$ resemble the changes of O_3 as the threshold varies from low to high, with decreasing hit rate and CSI and increasing false alarm rate (Figure 8). Although CSI values only slightly increase in
340 AQMv7_new when $PM_{2.5}$ is greater than 40 µg/m^3, the values of hit rate and false alarm rate become higher and lower compared to AQMv7, respectively, and the changes are bigger at higher thresholds. This indicates that AQMv7_new can better predict $PM_{2.5}$ at most pollution levels with more improvements found in highly polluted cases.

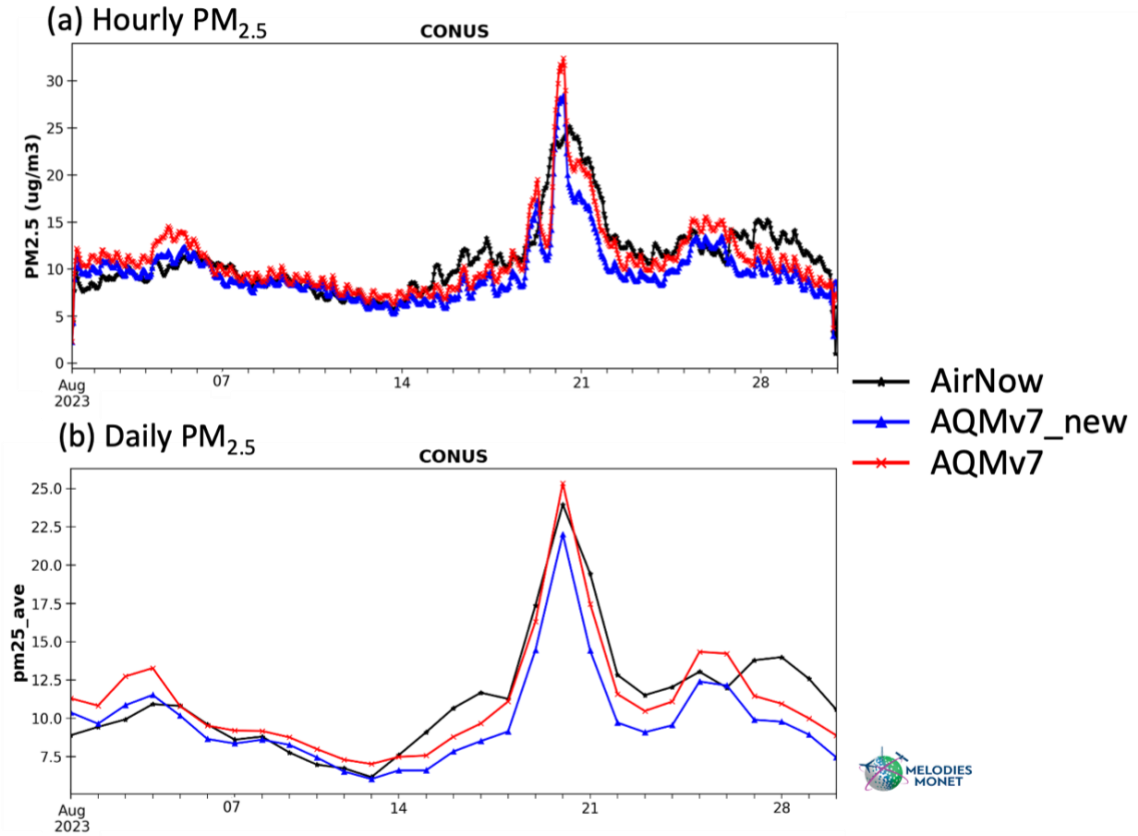

Figure 7: Same as Figure 3 but for $PM_{2.5}$.

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Table 3: Same as Table 2, but for hourly $PM_{2.5}$ evaluation.

Region	Model	MB (μg/m³)	NMB (%)	MdnB (μg/m³)	NMdnB (%)	R^2	RMSE (μg/m³)	IOA
CONUS	AQMv7	-0.05	-0.44	0.77	9.94	0.07	32.43	0.38
	AQMv7_new	-1.40	-12.47	**-0.34**	**-4.35**	0.06	**31.92**	0.38
Region 1 (northeast)	AQMv7	1.63	24.32	1.83	35.23	0.33	4.17	0.71
	AQMv7_new	**0.02**	**0.36**	**0.32**	**6.23**	0.26	**4.11**	0.70
Region 2 (NY-NJ)	AQMv7	2.82	33.94	2.83	38.83	0.28	5.61	0.68
	AQMv7_new	**1.77**	**21.31**	**1.54**	**21.08**	0.24	5.81	0.68
Region 3 (mid-Atlantic)	AQMv7	2.48	26.49	2.09	26.17	0.33	6.24	0.70
	AQMv7_new	**0.98**	**10.48**	**0.47**	**5.84**	0.32	**6.00**	**0.72**
Region 4 (southeast)	AQMv7	0.60	6.16	0.80	9.20	0.28	4.65	0.71
	AQMv7_new	-1.10	-11.24	-0.85	-9.81	0.24	4.89	0.67
Region 5 (upper Midwest)	AQMv7	2.65	22.59	1.90	18.28	0.24	9.84	0.64
	AQMv7_new	**-0.43**	**-3.68**	**-0.41**	**-3.92**	0.24	**7.93**	**0.68**
Region 6 (south)	AQMv7	-1.18	-11.67	-0.68	-7.30	0.22	5.93	0.64
	AQMv7_new	-2.47	-24.36	-2.17	-23.31	0.18	6.64	0.62
Region 7 (central Great Plain)	AQMv7	1.97	19.60	1.80	19.77	0.11	7.80	0.55
	AQMv7_new	**-0.27**	**-2.70**	**-0.17**	**-1.84**	0.09	**7.04**	0.55
Region 8 (northern Great Plain)	AQMv7	-1.19	-13.94	-0.50	-8.27	0.06	12.75	0.45
	AQMv7_new	-1.38	-16.12	-0.71	-11.85	0.05	13.49	0.41
Region 9 (southwest)	AQMv7	-0.15	-1.95	0.57	9.51	0.10	10.57	0.45
	AQMv7_new	-0.54	-6.92	**0.21**	**3.51**	0.10	10.64	0.44
Region 10 (northwest)	AQMv7	-3.33	-19.99	0.44	0.44	0.10	54.25	0.46
	AQMv7_new	-4.11	-24.70	**0.15**	**0.15**	0.10	**51.45**	**0.48**

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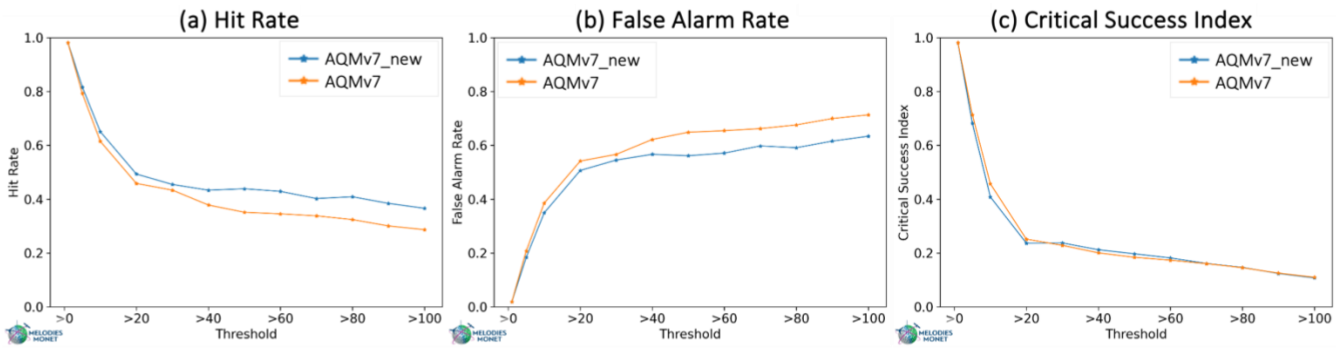

Figure 8: Same as Figure 4 but for $PM_{2.5}$.

The evaluation by each EPA region is illustrated in Figure 9 and the corresponding metrics are listed in Table 3. The AQMv7 shows a general overestimation in the eastern US (R1-R5) and central Great Plain (R7) with the positive bias values ranging from 0.60 μg/m^3 (6.16%) in the southeast (R4) to 2.82 μg/m^3 (33.94%) in the New York-New Jersey area (NY-NJ; R2). Regions in the western US (R6, R8-R10) exhibit an overall underestimation of $PM_{2.5}$ with the lowest negative bias of -0.15 μg/m^3 (1.95%) found in the southwest (R9). The highest mean bias of -3.33 μg/m^3 (-19.99%) among all the 10 regions lies in the northwest (R10), which can be attributed to the larger uncertainties in wildfire emissions, plume rise, chemistry, and transport. The RMSE value of 54.25 μg/m^3 in the southwest is also much higher than those in other regions, which range from 4.17 μg/m^3 to 12.75 μg/m^3. From the boxplot in Figure 9a, the AQMv7_new predicts a uniformly reduced $PM_{2.5}$ level in all regions, which is consistent with the time series in Figure 7. Such effects improve the model performance in regions with a relatively large positive bias, including R1-R3, R5, and R7. However, if the overestimation is small (e.g., R4) or if AQMv7 underestimates $PM_{2.5}$ (R6, R8-R10), a further reduction in AQMv7_new deteriorates the model performance by increasing the mean bias. The upper Midwest (R5) and central Great Plain (R7) experience the highest magnitude of reduction by 3.08 μg/m^3 to 2.24 μg/m^3, respectively. This is likely due to the decrease in the regional-scale transport eastward of wildfire-induced PM2.5 smoke in AQMv7_new (Figure 6). Other regions in the eastern US, including R1-R4 and R6, show a moderate decline ranging from 1.05 μg/m^3 in NY-NJ (R2) to 1.70 μg/m^3 in the southeast (R4). By contrast, the western US areas (R8-R10) witness a lower reduction by 0.19 μg/m^3, 0.39 μg/m^3, and 0.78 μg/m^3, respectively. Since the use of AERO7 generally enhances $PM_{2.5}$ mass concentrations (Section 2), such spatial patterns can be explained by the dominating updates to the dry deposition scheme, which increases the deposition velocity of the accumulation mode aerosol by a factor of 10 in forested areas (Pleim et al., 2022), with less enhancement for low-lying vegetation.

A similar east-west discrepancy can be seen from the scorecard plot in Figure 9b, which compares the daily values of IOA between the two models in each region. Unlike the considerable differences, positive or negative, in the eastern US (R1-R7), most days in the western US (R8-R10) do not have statistically significant changes. The AQMv7_new shows higher IOA values than those from AQMv7 in R1-R5 and R7 before the wildfire outbreak near August 18, after which the AQMv7_new performs worse with lower IOA. This implies an underestimation of $PM_{2.5}$ from wildfire, which can be partly attributed to the fact that VOC emissions from the RAVE inventory are disabled due to uncertainties in its VOC emission factors and the resulting impacts on trace gases and aerosol predictions. R6 has consistently lower IOA values from the AQMv7_new on most days, especially at the urban sites. Similar to O_3 in the same region, $PM_{2.5}$ is underestimated by the AQMv7 regardless of the influence of wildfire (Figure S5), and the reduction in the updated model exacerbates the negative bias.

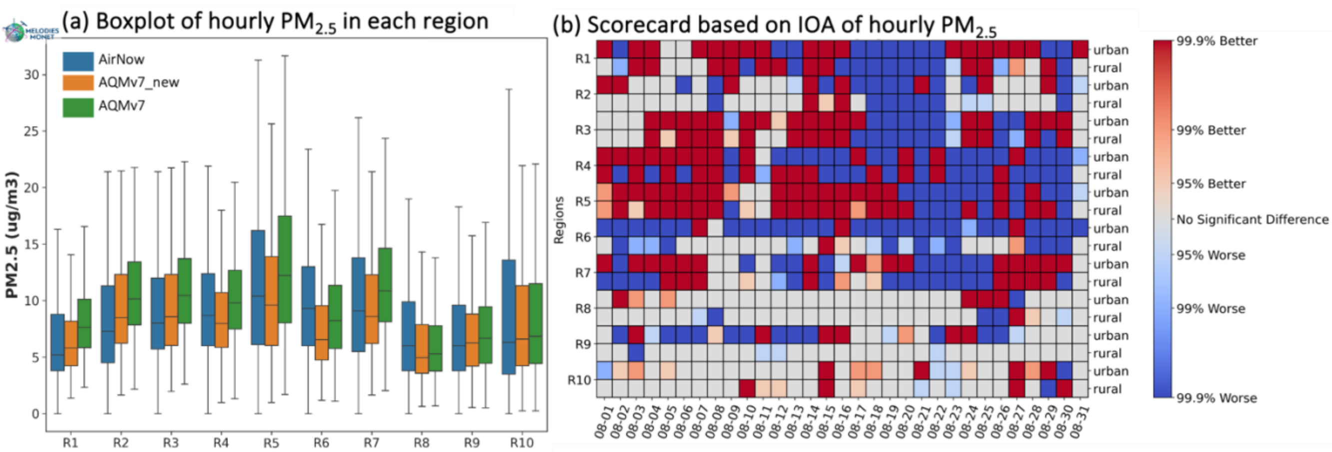

Figure 9: Same as Figure 5 but for $PM_{2.5}$.

In summary, the AQMv7 demonstrates large bias/error for $PM_{2.5}$ near and downstream of wildfire sources in the western U.S., indicating uncertainties in fire emissions, transport, and plume chemistry, while there is an overall overestimation of $PM_{2.5}$ in the eastern US and central Great Plain. The AQMv7_new demonstrates a reduced $PM_{2.5}$ level in all regions, which closes the gap between model and observation in the places where positive biases are found, thus improving the $PM_{2.5}$ predictive accuracy therein. However, the reduction also worsens the model performance in the western regions with a negative bias. The magnitude of the reduction in the AQMv7_new displays an east-to-west discrepancy, which is due to the dependence of the dry deposition velocity on vegetation types introduced by the new scheme.

5 Conclusion and discussion

An updated AQMv7 model (AQMv7_new) within the UFS system was developed to incorporate the recent scientific improvements from CMAQv5.4. The evolution of gas and aerosol chemistry in AQMv7_new is primarily influenced by the

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changes in the CB6 scheme, the introduction of a new aerosol module, and updated air-surface exchange processes. The adoption of CB6r5 in CMAQv5.4 represents an improvement over CB6r3, with updates in halogen chemistry, reaction rates, products, photolysis rates, and the addition of new reactions. The aerosol chemistry scheme, AERO7, introduces key improvements, such as updated monoterpene oxidation yields, organic nitrate formation, water uptake on hydrophilic organic compounds, and a new parameterization for anthropogenic SOA yields. Significant updates in dry deposition processes enhance the representation of air-surface exchange in AQMv7_new. Changes in O_3 dry deposition resistance over snow-covered regions and soil dependence on moisture contribute to a more accurate simulation of ambient O_3 concentrations. The aerosol dry deposition scheme undergoes continuous refinement, incorporating factors like leaf area index (LAI) and impaction efficiency based on land use categories. Structural changes in the IO framework of CMAQ, such as the DESID and CIO modules contribute to an improved computational efficiency and the ease of maintenance. The ELMO module in CMAQv5.4 further streamlines the synthesis of model output parameters, reducing the need for post-processing tools.

To test the performance of the AQMv7_new, a monthly simulation in August 2023 was conducted over the North America domain and the air quality evaluation was performed for the CONUS in comparison to the surface O_3 and $PM_{2.5}$ observations at AirNow sites. AQMv7_new demonstrates improved simulation of O_3 concentrations, reflecting near CONUS-wide better spatiotemporal agreement with observations. Generally, there is a nationwide decrease in O_3 mixing ratios, significantly reducing the persistent high positive bias observed at coastal sites for AQMv7. Temporally, the AQMv_new addresses the persistent positive bias in peak values at noon and low values at night, leading to a substantial reduction (72%) in the overprediction of MDA8 O_3. While AQMv7 with CMAQ 5.2.1 chemistry tends to overestimate hourly O_3 concentrations in all the 10 EPA regions, AQMv7_new with CMAQ 5.4 exhibits a universal shift in the statistical distribution to the lower end, thus reducing the positive bias across all regions. The Great Plain regions particularly benefit from the model updates, possibly due to the enhanced O_3 dry deposition velocity over dry soil and the increased halogen-mediated O_3 loss over the sea.

The spatial distribution of monthly average $PM_{2.5}$ concentrations reflects extreme values over western Canada and the northwestern US, attributed to wildfire emissions, which introduces substantial uncertainties in the model as indicated by the high mean bias values at the AirNow sites close to wildfire sources. AQMv7_new generally predicts lower $PM_{2.5}$ values averaged across the CONUS domain, which reduces the positive bias in the northeast. Despite the worsened mean bias, median bias and RMSE values are improved for both hourly and daily $PM_{2.5}$ prediction. Improvements are also found in the hit rate and false alarm rate at high thresholds, suggesting a better predictive accuracy of $PM_{2.5}$, particularly in highly polluted scenarios. The region-specific evaluation highlights a general overestimation in the eastern US and an underestimation in the western US by AQMv7, with the AQMv7_new uniformly reducing $PM_{2.5}$ levels across all regions. This reduction improves the predictive accuracy in regions with positive bias but exacerbates the negative bias in regions where AQMv7 already underestimated $PM_{2.5}$. Furthermore, the magnitude of the reduction displays an east-to-west discrepancy: higher reduction in

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the east and lower in the west. This spatial pattern can be attributed to the changes in the dry deposition scheme, which greatly increases the dry deposition rate over forests for the accumulation mode aerosol.

AQMv7_new narrows the NMB of MDA8 O_3 and daily $PM_{2.5}$ in all regions to be within -9.35% - 12.40% and -25.30% - 20.25%, respectively. These ranges fall in the benchmark criteria of ±15% for MDA8 O_3 and ±30% for daily PM_{25} as suggested by Emery et al. (2017) by summarizing the model performance statistics reported from 2005 to 2015 in the CONUS. Despite these big improvements, challenges and limitations remain. Uncertainties persist in accurately capturing the complex dynamics of wildfire emissions and their influence on air quality. The AQMv7_new model cannot improve upon the exacerbated $PM_{2.5}$ predictions near and just downstream of wildfire sources (e.g., west-northwest U.S.), partly due to its current omission of fire-related VOC in the simulations. However, the AQMv7_new does demonstrate improved regional transport of fire-related PM2.5 concentration enhancements compared to near-surface observations farther eastward in the U.S. (Figure 6). Continuous efforts should be made to reduce the uncertainties of wildfire emissions and test cases can be conducted to tune the RAVE emission factors of different VOC species. The current UFS-AQM system has limited capabilities in diagnostics and can only write out species concentrations and AOD. This limits our current study to only a qualitative inference that the performance changes are driven by lumped updates to the chemistry, and/or dry deposition schemes based on the CMAQ release notes. However, the verification results in this study showed that the changes from AQM_v7 to AQMv7_new behave similarly to that on the WRF-CMAQ: version 5.2.1 versus 5.4. More process-related diagnostics and tools are currently being added to UFS-AQM to better interpret the performance changes by quantitively attributing them to various processes, such as chemical productions and destructions, dry deposition, and transport. In addition, longer simulations covering both winter and summer and a more comprehensive evaluation with different observational platforms (e.g., surface sites, ozonesondes, aircraft, lidar, and satellite) are also ongoing for a more thorough investigation of the AQM and impacts of the model updates described here. Further refinements to the coupled CCPP physics (e.g., GFS) and the critical driving meteorological parameters are needed, which inherently interact with natural emissions in addition to wildfire, such as biogenic VOCs, soil NO, windblown dust, oceanic dimethyl sulfide (DMS), and lightning NOx emissions, are also highly needed. This study shows that the UFS-AQM framework can well accommodate the community air quality model, like CMAQ, as well as its latest upgrade. The results of this upgrade are consistent with those shown in the WRF-CMAQ systems. This method is proven to be viable for coupling different dynamics, physics and chemistry etc and linked with the authorized repository. Although we did not include some functions of the original CMAQ, such as the decoupled direct method in three dimensions (DDM-3D) (Zhang et al., 2012), Integrated Source Apportionment Method (ISAM) (Kwok et al., 2015) in the UFS-AQM model due to its framework limitation, the online CMAQ prediction model within this framework yields overall reasonable results. As the UFS-AQM model is an upcoming replacement for the existing operational air quality forecast system of NOAA, this study underscores the importance of ongoing scientific investigations, refinement, and quality assurance processes in atmospheric modelling to ensure reliable predictions and advance our understanding of the intricate interactions driving air quality variability.

Code and data availability

The UFS-AQMv7 source codes are available on the following GitHub repository GitHub - ufs-community/ufs-srweather-app at production/AQM.v7 (last access: 15 March 2024). The AQMv7_new codes are reposited at https://zenodo.org/records/10833128 (last access: 19 March 2024) and can also be downloaded via a GitHub tag GitHub - noaa-oar-arl/AQM at CMAQ54_Paper (last access: 15 March 2024).

Author contributions

WL conducted the model updates and drafted the initial manuscript. BT contributed to model updates and performed air quality evaluation. PCC conducted the model runs and meteorology evaluation. PCC, YT, BB, ZM, JH, and RM contributed to model updates, project methodology, analyses, and evaluation. BB, DT, IS, PCC, and YT contributed to project administration, funding acquisition, and supervision. RG helped with meteorology evaluation. All authors contributed to the interpretation of the results and revisions of the paper.

Competing interest

The contact author has declared that neither they nor their co-authors have any competing interests.

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