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Evaluation of the offline-coupled GFSv15-FV3-CMAQv5.0.2 in support of the next-generation National Air Quality Forecast Capability over the contiguous United States

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Abstract

The next-generation National Air Quality Forecast Capability (NAQFC) will use the meteorology from Global Forecast System with the new Finite Volume Cube-Sphere dynamic core (GFS-FV3) to drive the chemical evolution of gases and particles described by the Community Multiscale Air Quality modelling system version 5.3 (CMAQ v5.3). CMAQ v5.0.2, a historical version of CMAQ, has been coupled with the North American Mesoscale Forecast System (NAM) model in the current operational NAQFC. An experimental version of the NAQFC based on the offline-coupled GFS-FV3 version 15 with CMAQv5.0.2 modeling system (GFSv15-CMAQv5.0.2), has been developed by the National Oceanic and Atmospheric Administration (NOAA) to provide real-time air quality forecasts over the contiguous United States (CONUS) since 2018. In this work, comprehensive region-specific, time-specific, and categorical evaluations are conducted for meteorological and chemical forecasts from the offline-coupled GFSv15-CMAQv5.0.2 for the year 2019. The forecast system shows good overall performance in forecasting meteorological variables with the annual mean biases of -0.2 °C for temperature at 2-m, 0.4% for relative humidity at 2-m, and 0.4 m s^{-1} for wind speed at 10-m against the METeorological Aerodrome Reports (METAR) dataset. Larger biases occur in seasonal and monthly mean forecasts, particularly in spring. Although the monthly accumulated precipitation forecasts show generally consistent spatial distributions with those from the remote sensing and ensemble datasets,

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

moderate-to-large biases exist in hourly precipitation forecasts against the Clean Air Status and Trends Network (CASTNET) and METAR. While the forecast system performs well in forecasting ozone (O_3) throughout the year and fine particles with a diameter of 2.5 µm or less ($PM_{2.5}$) for warm months (May-September), it significantly overpredicts annual-mean concentrations of $PM_{2.5}$. This is due mainly to the high predicted concentrations of fine fugitive, coarse-mode, and nitrate particle components. Underpredictions in the southeastern U.S. and California during summer are attributed to missing sources and mechanisms of secondary organic aerosol formation from biogenic volatile organic compounds (VOCs) and semi- or intermediate-VOCs. This work identifies possible underlying causes for systematic region- and time-specific model biases, which will provide a scientific basis for further development of the next-generation NAQFC, in particular, derivation of the science-based bias correction methods to improve forecasting skill for O_3 and $PM_{2.5}$.

1. Introduction

Three-dimensional air quality models (3-D AQMs) have been widely applied in real time air quality forecasting (RT-AQF) since the 1990s in the U.S. (Stein et al., 2000; McHenry et al., 2004; Zhang et al., 2012a). The developments and applications of the national air quality forecasting systems based on 3-D AQMs were conducted in the 2000s (Kang et al., 2005; Otte et al., 2005; McKeen et al., 2005, 2007, 2009). Since then, improvements and significant progress have been achieved in RT-AQF through the further development of AQMs and the use of advanced techniques. For example, more air pollutants in the products, more detailed gas-phase chemical mechanisms and aerosol chemistry, and the implementation of chemical data assimilation were available (Zhang et al., 2012b; Lee et al., 2017). Various AQMs, coupled with meteorological models in either an online or offline manner, were developed and applied in RT-AQF (e.g., Chuang et al., 2011; Lee et al., 2011; Žabkar et al., 2015; Ryan, 2016). The early version of the National Air Quality Forecast Capability (NAQFC) was jointly developed by the U.S. National Oceanic and Atmospheric Administration (NOAA) and the U.S. Environmental Protection Agency (EPA) to provide forecasts of ozone (O_3) over the northeastern U.S. (Eder et al., 2006). Since the first operational version over the contiguous United States (CONUS) (Eder et al., 2009), the NAQFC has been continuously updated and developed to provide more forecasting products (including O_3, smoke, dust, and particulate matter with a diameter of 2.5 μm or less ($PM_{2.5}$)) with increasing accuracy (Mathur et al., 2008; Stajner et al., 2011; Lee et al., 2017).

The forecast skill of a historical NAQFC, which was based on the North American Mesoscale Forecast System (NAM) model (Black, 1994) and the Community Multiscale Air Quality Modeling System version 4.6 (CMAQ v4.6), over CONUS during year 2008 was evaluated by Kang et al. (2010a) for operational O_3 and experimental $PM_{2.5}$ products. Overall, maximum 8-h O_3 was slightly overpredicted over the CONUS

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

during the summer, with the mean bias (MB), normalized mean bias (NMB), and correlation coefficient (Corr) of 3.2 ppb, 6.8 %, and 0.65, respectively. The performance of predicted daily mean $PM_{2.5}$ varied: with an underprediction during the warm season and an overprediction in the cool season. The MBs and NMBs during warm/cool seasons were -2.3/4.5 μg m^{-3} and -19.6%/45.1%, respectively. The current version of the U.S. NOAA's operational NAQFC has provided the air quality forecast to the public for O_3 and $PM_{2.5}$ at a horizontal grid resolution of 12 km over CONUS since 2015. It is currently based on the CMAQ v5.0.2 (released May 2014) (U.S. EPA, 2014) coupled offline with the NAM model. Daily mean $PM_{2.5}$ was underpredicted during warm months (May and July 2014) and overpredicted during a cool month (January 2015) over CONUS still persist (Lee et al., 2017).

Efforts have been made to reduce the seasonal and region-specific biases in the historical and current NAQFC. Development and implementation of an analog ensemble bias correction approach was applied to the operational NAQFC to improve forecast performance in $PM_{2.5}$ predictions (Huang et al., 2017). Kang et al. (2008, 2010) investigated the Kalman Filter (KF) bias-adjustment technique for operational use in the NAQFC system. The KF bias-adjusted forecasts showed significant improvement in both O_3 and $PM_{2.5}$ for discrete and categorical evaluations. However, limitations in the underlying models and the bias correction/adjustment approaches need further improvement. Characterizing the current NAQFC forecasting skill and identifying the

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

underlying causes for region- and time-specific biases can result in further development of the NAQFC system and improved pollutant predictions.

In the next generation NAQFC, the NAM will be replaced by the Finite Volume Cube-Sphere Dynamical Core (FV3), the dynamical core in Global Forecast System (GFS). To support this new development, a prototype of the offline-coupled GFS version 15 (v15) with CMAQv5.0.2 (GFSv15-CMAQv5.0.2) has been developed and applied by the NOAA for RT-AQF over CONUS since 2018 (Huang et al., 2018, 2019, 2020). In this work, the meteorological and air quality forecasts from the offline-coupled GFSv15-CMAQv5.0.2 are comprehensively evaluated for the year of 2019. The main objectives of this work are to: (1) evaluate the forecast skills of the experimental prototype of the GFSv15-CMAQv5.0.2 system; (2) identify the major model biases, in particular, systematic biases and persistent region- and time-specific biases in major species; (3) investigate underlying causes for the biases to provide a scientific basis for improving the model representations of chemical processes and developing science-based bias correction methods for O_3 and $PM_{2.5}$ forecasts. This work will support NAQFC's further development and improvement through enhancing its forecasting abilities and generating a benchmark for the operational version of next-generation NAQFC that is being developed by NOAA based on the offline-coupled GFS-FV3 v16 with CMAQ v5.3 (Campbell et al., 2020). Eventually, the latest version of CMAQ (version 5.3), which has updates in gas-phase chemistry (Yarwood et al., 2010; Emery et al., 2015; Luecken et al.,

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

2019), lightning nitric oxide (LNO) production schemes (Kang et al., 2019a, 2019b), and secondary aerosol formation (in particular, secondary organic aerosol) (e.g., Pye et al., 2013, 2017; Murphy et al., 2017) among others, will be coupled with GFS-FV3 v16 and be implemented into NAQFC.

2. Model system and evaluation protocols

2.1 Description and configuration of offline-coupled GFSv15-CMAQv5.0.2

FV3 is a dynamical core for atmospheric numerical models developed by the Geophysical Fluid Dynamics Laboratory (GFDL) (Putman and Lin, 2007). It is a modern and extended version of the original FV core with a cubed-sphere grid design and more computationally efficient solvers. It was selected for implementation into the GFS as the next generation dynamical core in 2016 (Zhang et al., 2019a). The GFS-FV3 v15 (GFS v15) has been operational since June 2019. The GFS v15 uses the Rapid Radiative Transfer Method for GCMs (RRTMG) scheme for shortwave/longwave radiation (Mlawer et al., 1997; Iacono et al., 2000; Clough et al., 2005), the Hybrid eddy-diffusivity mass-flux (EDMF) scheme for Planetary Boundary Layer (PBL) (National Centers for Environmental Prediction, 2019a), the Noah Land Surface Model (LSM) scheme for land surface option (Chen et al., 1997), the Simplified Arakawa-Schubert (SAS) deep convection for cumulus parameterization (Arakawa et al.,

Geoscientific Model Development
Discussions
Open Access
EGU

1974; Grell, 1993), and a more advanced GFDL microphysics scheme for microphysics (National Centers for Environmental Prediction, 2019b). An interface preprocessor has been developed by NOAA to interpolate data, transfer coordinates, and convert the GFS v15 outputs into the data format required by CMAQv5.0.2 (Huang et al., 2018, 2019). The original outputs from GFS v15, which have a horizontal grid with 13-km resolution and a Lagrangian vertical coordinate with 64 layers in NEMSIO format, are processed to Lambert-Conformal Conic projection by PREMAQ, a preprocessor, to recast the meteorological fields for CMAQ into an Arakawa C-staggering grid (Arakawa and Lamb, 1977) with a 12-km horizontal resolution and 35 vertical layers (Table 1). The first 72 hours in 12:00 UTC forecast cycles from GFS v15 are used to drive the air quality forecast by the offline-coupled GFSv15-CMAQv5.0.2 system.

CMAQ has been continuously developed by the U.S. EPA since the 1990s (Byun and Schere, 2006) and has been significantly updated in many atmospheric processes since then. Chemical boundary conditions for the GFSv15-CMAQv5.0.2 system are mainly from the global 3-D model of atmospheric chemistry driven by meteorological input from the Goddard Earth Observing System (GEOS-Chem). The lateral boundary condition for dust is from the outputs of NEMS GFS Aerosol Component (NGAC) (Lu et al., 2016). The area sources from National Emissions Inventory of year 2014 version 2 (NEI 2014v2), point sources from NEI 2005 with projected sulfur dioxide (SO_2) and nitrogen oxide (NO_X) to year 2019, and U.S. EPA's MOVES 2014 mobile sources along with the biomass burning emission inventory from the Blended Global Biomass Burning Emissions Product system (GBBEPx) (Zhang et al., 2019b) are processed by Sparse Matrix Operator Kerner Emissions (SMOKE) model and the PREMAQ for CMAQ. Biogenic emissions are calculated inline by Biogenic Emission Inventory System (BEIS) version 3.14 (Schwede et al., 2005). Sea-salt emission is parameterized within CMAQ v5.0.2. While the deposition velocities are calculated inline, the fertilizer ammonia bi-directional flux for in-line emissions and deposition velocities is turned off. Detailed configurations of photolysis, gas-phase chemistry, aqueous chemistry, and aerosol chemistry for CMAQ v5.0.2 are listed in Table 1.

2.2 Datasets and evaluation protocols

Comprehensive evaluation of the GFSv15-CMAQv5.0.2 forecasting system is conducted for both meteorological and chemical variables for year 2019, including discrete, categorical, and region-specific evaluations. The products in the first 24-hour of each 72-hour forecast cycle are extracted and combined as a continuous, annual forecast. The evaluation of meteorological variables is carried out for those results from PREMAQ in GFSv15-CMAQv5.0.2 system. Detailed information for datasets used in this study is listed in Table S1. Observed hourly temperature at 2-meters (T2), relative humidity at 2-meters (RH2), precipitation (Precip), wind direction at 10-meters (WD10), and wind speed at 10-meters (WS10) are obtained from the Clean Air Status and Trends Network (CASTNET) and the METeorological Aerodrome Reports (METAR) datasets. The

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions
Open Access
EGU

majority of CASTNET sites are suburban and rural sites. Approximately 1900 METAR sites over CONUS are used in this study (Fig. S1). For evaluation of precipitation, a threshold of ≥0.1 mm is used for valid records because the CASTNET and METAR have different definitions of 0.0 mm values. In CASTNET, the records without any precipitation are filled as 0.0 mm, the same as those records with negligible precipitation. However, in METAR, the records without any precipitation are left as blank, the same as an invalid record. The negligible precipitation is recorded as 0.0 mm.

The air quality forecasting products are evaluated include hourly O_3, hourly $PM_{2.5}$, maximum daily 8-hour average O_3 (MDA8 O_3), and daily average $PM_{2.5}$ (24-h avg $PM_{2.5}$) for chemical forecast. The AIRNow dataset is used for observed hourly O_3 and $PM_{2.5}$. It is a near real time (NRT) dataset which has preliminary quality control (QC). Many abnormal records are not quality controlled completely. To filter the abnormal records, the thresholds of 120 ppb and 100 μg m^{-3} for O_3 and $PM_{2.5}$ are used, respectively. Remote sensing data from the Global Precipitation Climatology Project (GPCP) and the Climatology-Calibrated Precipitation Analysis (CCPA) (Hou et al., 2014; Zhu and Luo, 2015) datasets are also used for evaluation of precipitation. GPCP is a global precipitation dataset with a spatial resolution of 0.25 degree and a monthly temporal resolution. The CCPA uses linear regression and downscaling techniques to generate analysis product of precipitation from two datasets: the National Centers for Environmental Prediction (NCEP) CPC Unified Global Daily Gauge Analysis and the

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

NCEP EMC Stage IV multi-sensor quantitative precipitation estimations (QPEs). The CCPA product with a spatial resolution in 0.125 degree and temporal resolution of an hour is used in this study. Satellite-based Aerosol Optical Depth (AOD) at 550 nm from Moderate Resolution Imaging Spectroradiometer (MODIS) Terra platform (Levy et al., 2015) is used for the evaluation of monthly AOD. The statistic measures such as mean bias, the root mean square error (RMSE), the normalized mean bias, the normalized mean error (NME), and the correlation coefficient are used, more details about evaluation protocols are referring to Zhang et al. (2009, 2016). The Taylor diagram (Taylor, 2001), which includes the correlations, NMBs, and the normalized standard deviations (NSD), is used to present the overall performance (Wang et al., 2015). The NMBs $\leq$ 15% and NMEs $\leq$ 30% by Zhang et al. (2006) and NMBs ($\leq$ 15% and $\leq$ 30%), NMEs ($\leq$ 25% and $\leq$ 50%), and Corr (>0.5 and >0.4) for MDA8 O_3 and 24-h $PM_{2.5}$, respectively, by Emery et al. (2017) are considered as performance criteria. Monthly, seasonal, and annual statistics and analysis are included. Seasonal analysis for O_3 is separated into ozone season (May-September) and non-ozone season (January-April and October-December). Analysis for ten CONUS regions, defined by U.S. EPA (www.epa.gov/aboutepa), are included and listed in Fig. S1c..

3. Evaluation of model forecast skills

3.1 Evaluation of meteorological forecasts

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Discrete performance evaluation is conducted for post-processed meteorological fields from the GFSv15-CMAQv5.0.2 system (Table 2). The GFS v15 can predict well the boundary layer meteorological variables. It has overall cold biases and wet biases for annual T2 and RH2 in 2019, respectively. It also overpredicts WS10, and underpredicts hourly precipitation. Despite CASTNET siting being slightly different from that of METAR, the annual and most of the seasonal performance for the model show similar pattern in terms of bias for both the CASTNET and METAR networks. Mean biases of T2 are mostly within ±0.5 degree Celsius except those in February and March against CASTNET (Table S2). Underprediction is generally larger against CASTNET than METAR. For spatial distribution of MB for seasonal T2 against METAR (Fig. 1), cold biases are mainly found in the Midwest and West U.S. where most of the CASTNET sites are located. GFS v15 usually underpredicts T2 in West Coast, the Mountain States, and the Midwest. Overpredictions of T2 in the states of Kansas, Oklahoma, the areas near the East Coast, and the Gulf Coast offset some underpredictions, resulting in smaller mean biases but similar RMSE for the model against METAR compared to that against CASTNET. The difference between observed T2 from the two datasets is larger in cooler months than warmer months. The largest underpredictions occur in the spring (MAM) season. In general, GFS v15 underpredicts T2 for both CASTNET and METAR, consistent with cold biases found in other studies using GFS v15 (e.g., Yang, 2019). Such underpredictions will affect chemical forecasts, especially the forecast of O_3. Consistent

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

with the overall underpredictions of T2, GFS v15 overpredicts RH2 in general. The largest overprediction is found in spring (MBs of 3.4% and 2.7% with CASTNET and METAR, respectively), corresponding to the largest underprediction of T2 in spring (MBs of -0.5 °C and -0.4 °C with CASTNET and METAR, respectively). GFS v15 shows moderately good performance predicting wind. The annual MB and NMB of WS10 against METAR are 0.4 m s^{-1} and 10.7 %, respectively. A larger overprediction of WS10 is found with CASTNET than other datasets (Zhang et al., 2016). GFSv15-CMAQv5.0.2 also gives higher overpredictions for CASTNET compared to METAR. The largest biases in wind speed are found in summer. GFSv15-CMAQv5.0.2 gives the largest cold biases, wet biases in spring, indicating the necessity of improving model performance in such seasons in future GFS-FV3 development.

By adopting the threshold of ≥0.1 mm, performance against the CASTNET and METAR show similar results: a large underprediction in hourly precipitation. Predicted monthly accumulated precipitation (Fig. S2) shows consistency in spatial distribution with observations from CCPA (Fig. S3) and GPCP (Fig. S4). The high precipitation in the Southeast are captured well in spring while the high precipitation in the Midwest and South are captured well in other seasons. It indicates that GFSv15-CMAQv5.0.2 has good performance in capturing the spatial distributions of accumulated precipitation but has poor performance in predicting hourly precipitation. In the current version of the experimental GFSv15-CMAQv5.0.2 system, the precipitation from original GFS v15

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

output is artificially spread out over time during the preprocessing by the interface preprocessor due to the interpolation using a temporal allocation algorithm. Short rains are interpolated into adjacent time steps (Fig. S5). Such an algorithm leads the model and measurements being more consistent for monthly accumulated precipitation than for discrete hourly precipitation from GFS v15 (which will be resolved by NOAA in the next version of NAQFC based on the GFSv16-CMAQ forecasting system).

An overall comparison of performance with CASTNET and METAR datasets is performed using a Taylor diagram (Fig. 2). The normalized standardized deviations (NSDs), Corrs, and NMBs are considered. The NSDs are ratios of variance of predicted values to variance of observed values, following the equations by Wang et al. (2015). The NSDs represent the amplitude of variability. With the NSDs closer to 1, the predicted values have closer variance as the observed values. Consistent with other analysis in this section, larger biases and lower correlation in model wind speed and wind direction are found for CASTNET compared to METAR. The amplitude of variability of WS10 against CASTNET is overpredicted (with the NSD larger than 1), while it is underpredicted against METAR. Because of the post-processing smearing of hourly precipitation, the variance of predicted precipitation is smaller than the observed one, leading to very small NSDs for precipitation. The location of the T2 and RH2 points near the REF marker in the Taylor diagram indicates that the GFSv15-CMAQv5.0.2 is capturing the magnitude and variability of these variables well.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

3.2 Evaluation of chemical forecast over the CONUS

Performance of chemical forecasts (i.e. O_3 and $PM_{2.5}$) are evaluated on monthly, seasonal, and annual timescales for the studied period of 2019. Performance of the MDA8 O3 and the 24-h average $PM_{2.5}$ (24-h avg $PM_{2.5}$) are considered as the primary objectives. Categorical performance evaluations for MDA8 O_3 and 24-h avg $PM_{2.5}$ are also conducted. Table 3 shows the discrete statistics of predicted MDA8 O_3 and 24-h avg $PM_{2.5}$ against AIRNow.

The GFSv15-CMAQv5.0.2 has good performance for MDA8 O_3 on a seasonal and annual basis with MBs $\leq \pm 1$ ppb, NMB ≤ 2.5 %, and NME ≤ 20%. The monthly NMBs/NMEs are within ±15 %/25 %, respectively. Moderate overpredictions and underpredictions are found in both seasons with MB of 0.9 and -0.9 ppb, respectively. The largest underprediction is found in spring months, especially in March. Underprediction of MDA8 O_3 in spring months is consistent with the largest underprediction of T2 in spring. The ozone temperature relationship was found and studied by previous researches (S. Sillman and Samson, 1995; Sillman, 1999). O_3 is expected to increase with increasing temperature within specific range of temperature (Bloomer et al., 2009; Shen et al., 2016). It indicates biases in predicted T2 could be one of the reasons for the corresponding biases in O_3 prediction. Predicted MDA8 O_3 is lower than observed values in major parts of the Midwest and West regions during the O_3

season (Fig. 3 and S7), which is consistent with underprediction of T2 in summer. But GFSv15-CMAQv5.0.2 gives very high O_3 in the southeastern U.S., especially in areas near the Gulf Coast. Such overpredictions compensate for moderate underpredictions in Midwest and West, causing an overall overprediction in overall CONUS. Prediction and simulation of O_3 in coastal or marine areas are impacted by halogens chemistry and emissions (Adams and Cox, 2002; Sarwar et al., 2012; Liu et al., 2018), including bromine and iodine chemistry (Foster et al., 2001; Sarwar et al., 2015; Yang et al., 2020) and oceanic halogen emissions (Watanabe, 2005; Tegtmeier et al., 2015; He et al., 2016). CMAQ v5.0.2 has only simple chlorine chemistry for CB05 mechanisms, and the reduction of O_3 by reaction with bromine and iodine is not included in CMAQ v5.0.2. Iodide-mediated O_3 deposition over seawater and detailed marine halogen chemistry has been found to reduce O_3 by 1-4 ppb near the coast (Gantt et al., 2017), suggesting the missing halogen chemistry and O_3 deposition processes contribute to overpredicted O_3 in coastal and marine areas seen here. Coastal and marine areas are also impacted by air-sea interaction processes, which are simply represented in the current meteorological models without coupling oceanic models (He et al., 2018; Zhang et al., 2019c,d). For example, coastal O_3 mixing ratios are impacted by predicted sea surface temperatures and land-sea breezes through their influence on chemical reaction conditions and diffusion processes. As discussed in Section 3.1, T2 is significantly overestimated near the Gulf Coast during summer, which could contribute to biases in O_3 predictions directly or indicate missing land-sea breezes and thus missing transport effects in the GFSv15-CMAQv5.0.2 air quality forecasting system. In the non-O_3 season, GFSv15-CMAQv5.0.2 can forecast well the spatial variations of MDA8 O_3 with overall underpredictions in the Northeast.

Unlike the good performance for O_3, GFSv15-CMAQv5.0.2 gives significant overpredictions for 24-h avg $PM_{2.5}$ with annual MB, NMB, and NME of 2.2 μg m^{-3}, 29.0%, and 65.3%, respectively (Table 3). The MBs and NMBs range from -0.2 μg m^{-3} to 5.0 μg m^{-3}, and -2.6 % to 59.7 % across the four seasons. With the exception of California and the Southeast, predicted 24-h avg $PM_{2.5}$ shows overprediction during most of the year in spring, autumn, and winter (Fig. 4). Using the historical emission inventories from NEI 2011 and NEI 2014 instead of the latest version of NEI 2017 is one of the reasons for the overpredictions of $PM_{2.5}$ concentrations in 2019. Moderate underpredictions of $PM_{2.5}$ are found in California in spring, autumn, and summer. Murphy et al. (2017) found that secondary organic aerosols (SOA) generated from anthropogenic combustion emissions were important missing PM sources in California prior to CMAQ v5.2. Higher predicted $PM_{2.5}$, typically SOA, in California is expected in the future using GFS-FV3-CMAQv5.3. The largest underpredictions of $PM_{2.5}$ occur in the Southeast in summer. Biogenic volatile organic compounds (BVOCs) and biogenic SOA (BSOA) are most active in Southeast region in summer. Many missing sources and mechanisms for SOA formation from BVOCs have been identified in recent years (Pye et al., 2013, 2015, 2017; Xu et al., 2018) and have resulted in significant improvements in

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

predicting SOA in the Southeast using CMAQ v5.1 through v5.3. Anthropogenic emissions and aerosol inorganic compounds were found to have impacts on BSOA (Carlton et al., 2018; Pye et al., 2018, 2019). Such interactions and mechanisms are not represented sufficiently in CMAQ v5.0.2, further enhancing the biases in predicted $PM_{2.5}$ in the Southeast. In general, updating NAQFC with CMAQ v5.3 is expected to reduce the biases in California and the Southeast.

Categorical evaluation is conducted to quantify the accuracy of the GFSv15-CMAQv5.0.2 system in predicting events in which the air pollutants exceed moderate or unhealthy categories for the U.S. air quality index (AQI) (www.airnow.gov). The metrics of False Alarm Ratio (FAR) and the Hit Rate (H) are used (Kang et al., 2005; Barnes et al., 2009). The scatter plots for predicted and observed MDA8 O_3 and 24-h avg $PM_{2.5}$ are shown in Fig. 5a and Fig. 5b, respectively. The plots are divided into four areas based on whether the predicted and/or observed data fall above or below the AQI thresholds: (a) observed values ≤ thresholds and predicted values > thresholds; (b) observed and predicted values > thresholds; (c) observed and predicted values ≤ thresholds; (d) observed values > thresholds and predicted values ≤ thresholds. The FAR and H are defined in Eq. (1) and Eq. (2):

$$FAR = \frac{a}{a+b} \times 100\% \qquad (1)$$

$$H = \frac{b}{b+d} \times 100\% \qquad (2).$$

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions
Open Access
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Numbers of the scatters in the four areas (a) to (d) are indicated in the equations. The higher the FAR is, the more GFSv15-CMAQv5.0.2 overpredicts the AQI leading to false air quality warnings. The higher the H is, exceedances are more successfully captured by the GFSv15-CMAQv5.0.2 system. In this study, the thresholds for two categories of "Moderate" and "Unhealthy for Sensitive Groups" are considered. Since 2018, they are defined as 55 ppb and 70 ppb for MDA8 O_3 and 12 µg m^{-3} and 35.5 µg m^{-3} for 24-h avg $PM_{2.5}$. For comparison with previous studies, the historical thresholds are also included into the evaluation: 60 ppb and 75 ppb for MDA8 O_3 and 15 µg m^{-3} and 35 µg m^{-3} for 24-h avg $PM_{2.5}$. The metrics in four categories, corresponding to four thresholds, are shown in Fig. 5c. Categorical performance under stricter AQI standards is better than under historical standards. For example, the FAR decreases from 47.8 % to 41.1 %, and the H increases from 40.3 % to 43.9 % with the "Moderate" thresholds change from 60 ppb to 55 ppb. It could be due to the better performance of the forecast system for values closer to the annual average level (~40 ppb). The scatters are more discrete for extreme values (Fig. 5a). When the thresholds of MDA8 O_3 are closer to the average level, the categorical performance increases. The categorical performance of GFSv15-CMAQv5.0.2 in predicting MDA8 O_3 is close to the performance of the previous NAQFC (Kang et al., 2010). Similar improvement in the FAR and H for predicting categorical 24-h avg $PM_{2.5}$ can be found when the threshold changes from 15 µg m^{-3} to 12 µg m^{-3}: the FAR decreases from 79.7 % to 70.1 %, and the H increases from

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

51.9 % to 57.0 %. However, the FAR is high (over 90%) and the H is much lower under the threshold of 35.5 µg m^{-3}. It is because most of the false alarms occur when observed 24-h avg $PM_{2.5}$ are lower than 20 µg m^{-3} and the predicted values are higher than 20 µg m^{-3} (Fig. 5b). It shows the poorer performance in correctly capturing the category of "Unhealthy for Sensitive Groups" due to the significant overprediction of $PM_{2.5}$ in cooler months.

Evaluation of predicted AOD against observations from MODIS is shown in Fig. 6. High predicted AOD in the Midwest during cooler months show consistency with MODIS and correspond to high surface $PM_{2.5}$ predictions. High predicted AOD are missing in California, corresponding to underprediction of surface $PM_{2.5}$ in California. In summer months, AOD is largely underpredicted in California and the Southeast region, which may be caused by the previously mentioned missing sources of SOA.

To further analyze the major source for spatial and temporal biases in predicted $PM_{2.5}$, key chemical components of $PM_{2.5}$ in January, July, and August are depicted in Fig. 7. Extremely high particulate sulfate and organic carbon, generated by large wildfires, are carried in from the north boundary in July. The forecast spatial pattern agrees well with the observed AOD in July. High concentrations of $PM_{2.5}$ associated with soil components, unspecified coarse mode components, and high particulate NO_3^- concentrations are major contributors to the high $PM_{2.5}$ in the Midwest. The soil components are estimated using the Interagency Monitoring of Protected Visual

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Environments (IMPROVE) equation and specific constituents (Appel et al., 2013). These high concentrations are caused by large emissions of anthropogenic primary $PM_{2.5}$, primary coarse PM, ammonia (NH_3), and NO_x in the Midwest (Fig. S6). The large emissions of anthropogenic primary course PM, as well as the wind-blown dust are the major sources for soil components and unspecified coarse mode components. Appel et al. (2013) also indicated CMAQ overpredicts soil components, sources of which include fugitive and wind-blown dust, in the eastern United States.

3.3 Region-specific evaluation

As discussed in section 3.2, biases in predicted O_3 and $PM_{2.5}$ vary from region to region. To further analyze the region-specific performance of the GFSv15-CMAQv5.0.2 system, evaluation for 10 regions within CONUS is conducted. By identifying the detailed characteristics of region-specific biases and indicating the underlying causes for such biases, this section aims to help the NAQFC to improve its forecast ability for specific regions. A science-based bias correction method will be developed for the operational GFS-FV3-CMAQ system in the future. This section can also contribute to hypotheses that may serve as a scientific basis for future bias correction methods.

Figure 8 shows the annual model performance for MDA8 O_3 and 24-h avg $PM_{2.5}$ in the 10 CONUS regions. In section 3.2, a slight underprediction of MDA8 O_3 on annual

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions
Open Access
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basis was found over the CONUS. MDA8 O_3 is overpredicted in most of the regions except regions 2, 4, and 6 (Fig. 8a). The overpredictions in regions 4 and 6 are mostly from the large biases near the coast area during O_3 season. Correlations between predictions and observations in most of the regions are higher than 0.6, except for 0.55 in region 4 and 0.50 in region 7. Poor performance in regions 4 and 7 is illustrated by the Taylor Diagram (Fig. 8b). Small Corr and NSD, result in the markers of regions 4 and 7 laying farthest from the reference point. The amplitude of variability of the predicted MDA8 O_3 are smaller than observed values in all the regions, especially in regions 4 and 7. The performance in region 2 is the best, with smallest MB/NMB, highest Corr, and similar variability in predictions and observations. The time series of the MDA8 O_3 for the 10 regions during 2019 is shown in Fig. S7. Regions 1, 2, 4, and 6 show different results for the O_3 season and non-O_3 season: GFSv15-CMAQv5.0.2 tends to overpredict MDA8 O_3 during the O_3 season and underpredicts during the non-O_3 season. The underprediction during spring months, which is indicated in section 3.2, can be also found in most of the regions with obvious gaps between observed and predicted curves in March and April. The lowest O_3 predictions occur at 5 am local standard time (LST) in most of the regions (Fig. S8). For regions 4 and 6, significant overprediction occurs not only during the O_3 season for MDA8 O_3 (which mainly occurs during the daytime) but also during the nighttime. During the non-O_3 season, the biases in predicting MDA8 O_3 for regions 4 and 6 are small and consistent with good daytime predictions. However, O_3

is still overpredicted during the nighttime in these regions, associated with the collapse of the boundary layer and difficulty in simulating its time and magnitude (Hu et al., 2013; Cuchiara et al., 2014; Pleim et al., 2016).

Consistent with the analysis in section 3.2, $PM_{2.5}$ is significantly overpredicted in most of the regions except in regions 4, 6, and 9 (Fig. 8c). The underprediction during warmer months, likely due to missing sources and mechanisms for BSOA, compensate for the annual biases in regions 4 and 6, leading to smaller MBs/NMBs but low correlations in these regions. The variability in predictions is much larger than in observations, with the NSDs >1 for all regions (Fig. 8d). The forecast system has best performance in region 9 with an NSD of 1.2, an NMB of -12.0 %, and a Corr of 0.40. As discussed in section 3.2, the performance of predicted $PM_{2.5}$ in region 9 is expected to be further improved with the updates in CMAQ v5.3, specifically the representation of anthropogenic SOA.

Figure S9 shows the time series of 24-h avg $PM_{2.5}$ in the 10 CONUS regions. The gaps between observed and predicted curves are large in cooler months, but the GFSv15-CMAQv5.0.2 system has relatively good performance in warmer months for most of the regions. Less overprediction is found in regions 6, 8, and 9 during cooler months, and those regions generally show the best performance (see Taylor Diagram). The different biases across the regions further indicate that multiple factors likely contribute to them. To further analyze the underlying causes for varied patterns and

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

performance on season- and region-specific basis, diurnal evaluations for $PM_{2.5}$ and chemical components of $PM_{2.5}$ during O_3 season and non-O_3 season are shown in Fig. 9. The GFSv15-CMAQv5.0.2 has a large seasonal variation in diurnal $PM_{2.5}$, inconsistent with the observation. While $PM_{2.5}$ is underpredicted during daytime in regions 4, 6, 8, and 9 during O_3 season, $PM_{2.5}$ is always overpredicted across the day during non-O_3 season except for region 9. Increased OC, particulate nitrates, soil and unspecified coarse mode components contribute to most of the increase in predicted total $PM_{2.5}$. The general cold biases over CONUS, especially in region 5, could make the GFSv15-CMAQv5.0.2 system predict higher nitrate particulates, leading to larger increase in $PM_{2.5}$ from O_3 season to non-O_3 season. Emissions vary from month to month in the year (Fig. S10). Larger emissions for NH_3, NO_x, VOC, primary coarse PM, and primary $PM_{2.5}$ are in O_3 season compared to non-O_3 season. Primary organic carbons (POC) emissions are higher in O_3 season. Changes in emissions are not fully consistent with the changes in $PM_{2.5}$ components, indicating other biases or uncertainty could also contribute to the significant overprediction during non-O_3 season. For example, the implementation of bidirectional flux of NH_3 and the boundary layer mixing processes under more stable condition (during non-O_3 season) in GFSv15-CMAQv5.0.2 system need to be further studied. Pleim et al., (2013, 2019) found that the NH_3 fluxes and concentrations could be better simulated and the monthly variations of NH_3 concentrations were larger comparing to the raw model by implementing the bidirectional flux of NH_3. The absolute biases for diurnal $PM_{2.5}$ are generally larger during nighttime in most of the regions, except for region 9. It is consistent with the analysis by Appel et al. (2013), which suggested that the efforts of improving nighttime mixing in CMAQ v5.0 be further needed, further indicating the need for improvements of CMAQ in predicting dispersion and mixing of air pollutants under stable boundary layer conditions.

4. Conclusion

In this work, the air quality forecast for the year 2019 predicted by the offline-coupled GFSv15-CMAQv5.0.2 system is comprehensively evaluated. The GFSv15-CMAQv5.0.2 system is found to perform well in predicting surface meteorological variables (temperature, relative humidity, and wind) and O_3 but has mixed performance for $PM_{2.5}$. Moderate cold biases and wet biases are found in spring season, especially in March. While the GFSv15-CMAQv5.0.2 system can generally capture the monthly accumulated precipitation compared to remote sensing and ensemble datasets, temporal distributions of hourly precipitation show less consistency with in-situ monitoring data, which is attributed to the interpolation and post-processing in the offline-coupling interface preprocessor.

MDA8 O_3 is slightly overpredicted and underpredicted in ozone and non-ozone seasons, respectively. The cold biases of T2 contribute to the underprediction of MDA8

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

O_3 in spring. The significant overprediction near the Gulf Coast, which is caused by missing halogen chemistry and the missing of model representation of the air-sea interaction processes, compensates for underprediction in the West and Midwest in O_3 season for nation-wide metrics. GFSv15-CMAQv5.0.2 has poorer performance in predicting $PM_{2.5}$, comparing to the performance for O_3. Significant overpredictions are found in spring, autumn, and winter, with the largest overprediction in the Midwest, WA, and Oregon, due mainly to high concentrations of predicted soil, unspecified coarse mode and nitrate components. The overall cold biases in the Region 5/Midwest could contribute to higher predicted nitrate particulate matter but overprediction of $PM_{2.5}$ in the region is likely driven by sources containing trace metals such as anthropogenic fugitive dust and wind-blown dust. The forecasting system may be improved through updating the emissions inventory used (i.e., NEI 2014) to NEI 2016v2 or NEI 2017 which are more presentative to the year of 2019 in the next development of next-generation NAQFC.

Categorical evaluation indicates that the GFSv15-CMAQv5.0.2 can capture well the air quality classification of "Moderate" described by the AQI. However, the categorical performance is poorer for $PM_{2.5}$ at the "unhealthy for sensitive groups" threshold due mainly to the significant overprediction during the cooler months. Region-specific evaluation further discusses the biases and underlying causes in the 10 USEPA defined regions in CONUS. An update from CMAQ v5.0.2 to v5.3.1 is expected to alleviate potential errors in missing sources and mechanisms for SOA formation. The

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

variations of performance in between O_3 and non-O_3 seasons, as well as during the daytime and nighttime, indicate further studies need to be conducted to improve boundary layer mixing processes within GFSv15-CMAQv5.0.2. The varied region-specific performance indicates that improvements, such as bias corrections, should be considered individually from region to region in the following development of the next generation NAQFC.

We have used bias analyses in this work to identify several areas of weakness for further improvement and development of next-generation NAQFC. Further studies are still needed for improving the emissions, the aerosol chemistry, and the boundary layer mixing for the future GFS-FV3-CMAQ system. Our work and the further studies can provide information and scientific basis for the development and implement of a science-based bias correction method in next-generation NAQFC.

Supplement

The supplement related to this article is available in gmd-2020-272_supplement.pdf

Code and data availability

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

The documentation and source code of CMAQ v5.0.2 are available at doi:10.5281/zenodo.1079898. The GFS forecasts in grib2 format are available at https://www.ncdc.noaa.gov/data-access/model-data/model-datasets/global-forcast-system-gfs. The GFS forecast inputs in binary (nemsio) format and the coupler used in this study for the GFSv15-CMAQv5.0.2 system are available upon request. The AIRNow data is available for download through the AirNow-Tech website (http://www.airnowtech.org). The CASTNET data is available for download from https://java.epa.gov/castnet/clearsession.do. The METAR data is available for download from https://madis.ncep.noaa.gov. The GPCP data is available through NOAA website (https://www.ncei.noaa.gov/data/global-precipitation-climatology-project-gpcp-monthly). The CCPA precipitation is available from https://www.nco.ncep.noaa.gov/pmb/products/gens. The MODIS_MOD04 dataset is available at dx.doi.org/10.5067/MODIS/MOD04_L2.006. The data processing and analysis scripts are available upon request.

Author contribution

YZ and DT defined the scope and focus of the manuscript and designed the model simulations. XC and YZ developed the paper outline and structure. PL, JH, YT, and JM performed the forecast simulations. YT generated the emissions and PC generated the lateral boundary conditions for the model simulations. XC performed the model

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

evaluation and drafted the manuscript. XC and KW developed postprocessing and statistical scripts. HP, BM, and DK assisted in analysis of region-specific biases. YZ, HP, DK, BM, JH, PC, PL, DT, and KW reviewed the manuscript.

Competing interests

The authors declare that they have no conflict of interest.

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https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

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References

Adams, J. W. and Cox, R. A.: Halogen chemistry of the marine boundary layer, J. Phys. IV, 12(10), 105–124, doi:10.1051/jp4:20020455, 2002.

Appel, K. W., Pouliot, G. A., Simon, H., Sarwar, G., Pye, H. O. T., Napelenok, S. L., Akhtar, F. and Roselle, S. J.: Evaluation of dust and trace metal estimates from the Community Multiscale Air Quality (CMAQ) model version 5.0, Geosci. Model Dev., 6(4), 883–899, doi:10.5194/gmd-6-883-2013, 2013.

Arakawa, A. and Lamb, V. R.: Computational design of the basic dynamical processes of the UCLA general circulation model, 1977.

Arakawa, A. and Schubert, W. H.: Interaction of a Cumulus Cloud Ensemble with the Large-Scale Environment, Part I, J. Atmos. Sci., 31(3), 674–701, doi:10.1175/1520-0469(1974)031<0674:IOACCE>2.0.CO;2, 1974.

Barnes, L. R., Schultz, D. M., Gruntfest, E. C., Hayden, M. H. and Benight, C. C.: Corrigendum: False alarm rate or false alarm ratio?, Weather Forecast., 24(5), 1452–1454, doi:10.1175/2009WAF2222300.1, 2009.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Binkowski, F. S., Arunachalam, S., Adelman, Z. and Pinto, J. P.: Examining photolysis rates with a prototype online photolysis module in CMAQ, J. Appl. Meteorol. Climatol., 46(8), 1252–1256, doi:10.1175/JAM2531.1, 2007.

Black, T. L.: The New NMC Mesoscale Eta Model: Description and Forecast Examples, Weather Forecast., 9(2), 265–278, doi:10.1175/1520-0434(1994)009<0265:TNNMEM>2.0.CO;2, 1994.

Bloomer, B. J., Stehr, J. W., Piety, C. A., Salawitch, R. J. and Dickerson, R. R.: Observed relationships of ozone air pollution with temperature and emissions, Geophys. Res. Lett., 36(9), doi:10.1029/2009GL037308, 2009.

Byun, D. and Schere, K. L.: Review of the governing equations, computational algorithms, and other components of the models-3 community multiscale air quality (CMAQ) modeling system, Appl. Mech. Rev., 59(1–6), 51–77, doi:10.1115/1.2128636, 2006.

Carlton, A. G., Bhave, P. V., Napelenok, S. L., Edney, E. O., Sarwar, G., Pinder, R. W., Pouliot, G. A. and Houyoux, M.: Model representation of secondary organic aerosol in CMAQv4.7, Environ. Sci. Technol., 44(22), 8553–8560, doi:10.1021/es100636q, 2010.

Carlton, A. G., Pye, H. O. T., Baker, K. R. and Hennigan, C. J.: Additional Benefits of Federal Air-Quality Rules: Model Estimates of Controllable Biogenic Secondary

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Organic Aerosol, Environ. Sci. Technol., 52(16), 9254–9265, doi:10.1021/acs.est.8b01869, 2018.

Chen, F., Janjić, Z. and Mitchell, K.: Impact of atmospheric surface-layer parameterizations in the new land-surface scheme of the NCEP mesoscale Eta model, Boundary-Layer Meteorol., 85(3), 391–421, doi:10.1023/A:1000531001463, 1997.

Chuang, M. T., Zhang, Y. and Kang, D.: Application of WRF/Chem-MADRID for real-time air quality forecasting over the Southeastern United States, Atmos. Environ., 45(34), 6241–6250, doi:10.1016/j.atmosenv.2011.06.071, 2011.

Clough, S. A., Shephard, M. W., Mlawer, E. J., Delamere, J. S., Iacono, M. J., Cady-Pereira, K., Boukabara, S. and Brown, P. D.: Atmospheric radiative transfer modeling: A summary of the AER codes, J. Quant. Spectrosc. Radiat. Transf., 91(2), 233–244, doi:10.1016/j.jqsrt.2004.05.058, 2005.

Cuchiara, G. C., Li, X., Carvalho, J. and Rappenglück, B.: Intercomparison of planetary boundary layer parameterization and its impacts on surface ozone concentration in the WRF/Chem model for a case study in houston/texas, Atmos. Environ., 96, 175–185, doi:10.1016/j.atmosenv.2014.07.013, 2014.

Eder, B., Kang, D., Mathur, R., Yu, S. and Schere, K.: An operational evaluation of the Eta-CMAQ air quality forecast model, Atmos. Environ., 40(26), 4894–4905, doi:10.1016/j.atmosenv.2005.12.062, 2006.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Eder, B., Kang, D., Mathur, R., Pleim, J., Yu, S., Otte, T. and Pouliot, G.: A performance evaluation of the National Air Quality Forecast Capability for the summer of 2007, Atmos. Environ., 43(14), 2312–2320, doi:10.1016/j.atmosenv.2009.01.033, 2009.

Emery, C., Jung, J., Koo, B., Yarwood, G.: Improvements to CAMx Snow Cover Treatments and Carbon Bond Chemical Mechanism for Winter Ozone. Final report for Utah DAQ, project UDAQ PO 480 52000000001, 2015.

Emery, C., Liu, Z., Russell, A. G., Odman, M. T., Yarwood, G. and Kumar, N.: Recommendations on statistics and benchmarks to assess photochemical model performance, J. Air Waste Manag. Assoc., 67(5), 582–598, doi:10.1080/10962247.2016.1265027, 2017.

Foster, K. L., Plastridge, R. A., Bottenheim, J. W., Shepson, P. B., Finlayson-Pitts, B. J. and Spicer, C. W.: The role of Br2 and Brcl in surface ozone destruction at polar sunrise, Science (80-.)., 291(5503), 471–474, doi:10.1126/science.291.5503.471, 2001.

Gantt, B., Sarwar, G., Xing, J., Simon, H., Schwede, D., Hutzell, W. T., Mathur, R. and Saiz-Lopez, A.: The Impact of Iodide-Mediated Ozone Deposition and Halogen Chemistry on Surface Ozone Concentrations Across the Continental United States, Environ. Sci. Technol., 51(3), 1458–1466, doi:10.1021/acs.est.6b03556, 2017.

Grell, G. A.: Prognostic Evaluation of Assumptions Used by Cumulus Parameterizations,

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development
Discussions

Mon. Weather Rev., 121(3), 764–787, doi:10.1175/1520-0493(1993)121<0764:PEOAUB>2.0.CO;2, 1993.

He, J., He, R. and Zhang, Y.: Impacts of Air-sea Interactions on Regional Air Quality Predictions Using a Coupled Atmosphere-ocean Model in Southeastern U.S., Aerosol Air Qual. Res., 18(4), 1044–1067, doi:10.4209/aaqr.2016.12.0570, 2018.

He, P., Bian, L., Zheng, X., Yu, J., Sun, C., Ye, P. and Xie, Z.: Observation of surface ozone in the marine boundary layer along a cruise through the Arctic Ocean: From offshore to remote, Atmos. Res., 169, 191–198, doi:10.1016/j.atmosres.2015.10.009, 2016.

Hou, D., Charles, M., Luo, Y., Toth, Z., Zhu, Y., Krzysztofowicz, R., Lin, Y., Xie, P., Seo, D. J., Pena, M. and Cui, B.: Climatology-calibrated precipitation analysis at fine scales: Statistical adjustment of stage IV toward CPC gauge-based analysis, J. Hydrometeorol., 15(6), 2542–2557, doi:10.1175/JHM-D-11-0140.1, 2014.

Hu, X. M., Klein, P. M. and Xue, M.: Evaluation of the updated YSU planetary boundary layer scheme within WRF for wind resource and air quality assessments, J. Geophys. Res. Atmos., 118(18), 10,490-10,505, doi:10.1002/jgrd.50823, 2013.

Huang, J., McQueen, J., Wilczak, J., Djalalova, I., Stajner, I., Shafran, P., Allured, D., Lee, P., Pan, L., Tong, D., Huang, H.-C., DiMego, G., Upadhayay, S. and Delle Monache, L.: Improving NOAA NAQFC PM 2.5 Predictions with a Bias Correction

Approach, Weather Forecast., 32(2), 407–421, doi:10.1175/WAF-D-16-0118.1, 2017.

Huang, J., McQueen, J., Shafran, P., Huang, H., Kain, J., Tang, Y., Lee, P., Stajner, I. and Tirado-Delgado, J.: Development and evaluation of offline coupling of FV3-based GFS with CMAQ at NOAA, the 17th CMAS Conference, UNC-Chapel Hill, NC, 22-24 October 2018, 2018.

Huang, J., McQueen, J., Yang, B., Shafran, P., Pan, L., Huang, H., Bhattacharjee, P., Tang, Y., Campbell, P., Tong, D., Lee, P., Stajner, I., Kain, J., Tirado-Delgado, J. and Koch, D.: Impact of global scale FV3 versus regional scale NAM meteorological driver model predictions on regional air quality forecasting. The 100th AGU Fall Meeting, San Francisco, CA, 9-13 December 2019, 2019.

Iacono, M. J., Mlawer, E. J., Clough, S. A. and Morcrette, J.-J.: Impact of an improved longwave radiation model, RRTM, on the energy budget and thermodynamic properties of the NCAR community climate model, CCM3, J. Geophys. Res. Atmos., 105(D11), 14873–14890, doi:10.1029/2000JD900091, 2000.

Kang, D., Eder, B. K., Stein, A. F., Grell, G. A., Peckham, S. E. and Mc Henry, J.: The New England Air Quality Forecasting Pilot Program: Development of an Evaluation Protocol and Performance Benchmark, J. Air Waste Manag. Assoc., 55(12), 1782–1796, doi:10.1080/10473289.2005.10464775, 2005.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Kang, D., Mathur, R., Rao, S. T. and Yu, S.: Bias adjustment techniques for improving ozone air quality forecasts, J. Geophys. Res., 113(D23), D23308, doi:10.1029/2008JD010151, 2008.

Kang, D., Mathur, R. and Trivikrama Rao, S.: Assessment of bias-adjusted $PM_{2.5}$ air quality forecasts over the continental United States during 2007, Geosci. Model Dev., 3(1), 309–320, doi:10.5194/gmd-3-309-2010, 2010a.

Kang, D., Mathur, R. and Trivikrama Rao, S.: Real-time bias-adjusted O3 and PM2.5 air quality index forecasts and their performance evaluations over the continental United States, Atmos. Environ., 44(18), 2203–2212, doi:10.1016/j.atmosenv.2010.03.017, 2010b.

Lee, P., Ngan, F., Kim, H., Tong, D., Tang, Y., Chai, T., Saylor, R., Stein, A., Byun, D., Tsidulko, M., McQueen, J. and Stajner, I.: Incremental Development of Air Quality Forecasting System with Off-Line/On-Line Capability: Coupling CMAQ to NCEP National Mesoscale Model, in Air Pollution Modeling and its Application XXI, pp. 187–192, Springer, Dordrecht., 2011.

Lee, P., McQueen, J., Stajner, I., Huang, J., Pan, L., Tong, D., Kim, H., Tang, Y., Kondragunta, S., Ruminski, M., Lu, S., Rogers, E., Saylor, R., Shafran, P., Huang, H.-C., Gorline, J., Upadhayay, S. and Artz, R.: NAQFC Developmental Forecast Guidance for Fine Particulate Matter (PM 2.5) , Weather Forecast., 32(1), 343–360,

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

doi:10.1175/waf-d-15-0163.1, 2017.

Levy, R. and Hsu, C.: MODIS Atmosphere L2 Aerosol Product. NASA MODIS Adaptive Processing System, Goddard Space Flight Center, USA: http://dx.doi.org/10.5067/MODIS/MOD04_L2.006, 2015.

Liu, Y., Fan, Q., Chen, X., Zhao, J., Ling, Z., Hong, Y., Li, W., Chen, X., Wang, M. and Wei, X.: Modeling the impact of chlorine emissions from coal combustion and prescribed waste incineration on tropospheric ozone formation in China, Atmos. Chem. Phys., 18(4), 2709–2724, doi:10.5194/acp-18-2709-2018, 2018.

Lu, C.-H., da Silva, A., Wang, J., Moorthi, S., Chin, M., Colarco, P., Tang, Y., Bhattacharjee, P. S., Chen, S.-P., Chuang, H.-Y., Juang, H.-M. H., McQueen, J. and Iredell, M.: The implementation of NEMS GFS Aerosol Component (NGAC) Version 1.0 for global dust forecasting at NOAA/NCEP, Geosci. Model Dev., 9(5), 1905–1919, doi:10.5194/gmd-9-1905-2016, 2016.

Mathur, R., Yu, S., Kang, D. and Schere, K. L.: Assessment of the wintertime performance of developmental particulate matter forecasts with the Eta-Community Multiscale Air Quality modeling system, J. Geophys. Res., 113(D2), D02303, doi:10.1029/2007JD008580, 2008.

McHenry, J. N., Ryan, W. F., Seamn, N. L., Coats, C. J., Pudykiewicz, J., Arunachalam, S. and Vukovich, J. M.: A real-time eulerian photochemical model forecast system,

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Bull. Am. Meteorol. Soc., 85(4), 525–548, doi:10.1175/BAMS-85-4-525, 2004.

McKeen, S., Wilczak, J., Grell, G., Djalalova, I., Peckham, S., Hsie, E.-Y., Gong, W., Bouchet, V., Menard, S., Moffet, R., McHenry, J., McQueen, J., Tang, Y., Carmichael, G. R., Pagowski, M., Chan, A., Dye, T., Frost, G., Lee, P. and Mathur, R.: Assessment of an ensemble of seven real-time ozone forecasts over eastern North America during the summer of 2004, J. Geophys. Res., 110(D21), D21307, doi:10.1029/2005JD005858, 2005.

McKeen, S., Chung, S. H., Wilczak, J., Grell, G., Djalalova, I., Peckham, S., Gong, W., Bouchet, V., Moffet, R., Tang, Y., Carmichael, G. R., Mathur, R. and Yu, S.: Evaluation of several $PM_{2.5}$ forecast models using data collected during the ICARTT/NEAQS 2004 field study, J. Geophys. Res. Atmos., 112(D10), doi:10.1029/2006JD007608, 2007.

McKeen, S., Grell, G., Peckham, S., Wilczak, J., Djalalova, I., Hsie, E.-Y., Frost, G., Peischl, J., Schwarz, J., Spackman, R., Holloway, J., de Gouw, J., Warneke, C., Gong, W., Bouchet, V., Gaudreault, S., Racine, J., McHenry, J., McQueen, J., Lee, P., Tang, Y., Carmichael, G. R. and Mathur, R.: An evaluation of real-time air quality forecasts and their urban emissions over eastern Texas during the summer of 2006 Second Texas Air Quality Study field study, J. Geophys. Res., 114(12), D00F11, doi:10.1029/2008JD011697, 2009.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Mlawer, E. J., Taubman, S. J., Brown, P. D., Iacono, M. J. and Clough, S. A.: Radiative transfer for inhomogeneous atmospheres: RRTM, a validated correlated-k model for the longwave, J. Geophys. Res. D Atmos., 102(14), 16663–16682, doi:10.1029/97jd00237, 1997.

Murphy, B. N., Woody, M. C., Jimenez, J. L., Carlton, A. M. G., Hayes, P. L., Liu, S., Ng, N. L., Russell, L. M., Setyan, A., Xu, L., Young, J., Zaveri, R. A., Zhang, Q. and Pye, H. O. T.: Semivolatile POA and parameterized total combustion SOA in CMAQv5.2: Impacts on source strength and partitioning, Atmos. Chem. Phys., 17(18), 11107–11133, doi:10.5194/acp-17-11107-2017, 2017.

National Centers for Environmental Prediction: The Global Forecast System (GFS) - Global Spectral Model (GSM). Retrieved from https://www.emc.ncep.noaa.gov/emc/pages/numerical_forecast_systems/gfs/documentation.php, last access: May 2020, 2019a.

National Centers for Environmental Prediction: FV3: The GFDL Finite-Volume Cubed-Sphere Dynamical Core, Retrieved from https://vlab.ncep.noaa.gov/web/fv3gfs, last access: May 2020, 2019b.

Otte, T. L., Pouliot, G., Pleim, J. E., Young, J. O., Schere, K. L., Wong, D. C., Lee, P. C. S., Tsidulko, M., McQueen, J. T., Davidson, P., Mathur, R., Chuang, H.-Y., DiMego, G. and Seaman, N. L.: Linking the Eta Model with the Community Multiscale Air

Quality (CMAQ) Modeling System to Build a National Air Quality Forecasting System, Weather Forecast., 20(3), 367–384, doi:10.1175/WAF855.1, 2005.

Patrick, C., Tang, Y., Lee, P., Baker, B., Tong, D., Saylor, R., Huang, J., Huang, H., McQueen, J. and Stajne, I.: An Improved National Air Quality Forecasting Capability Using the NOAA Global Forecast System Version 16. In preparation, 2020.

Pleim, J., Gilliam, R., Appel, W. and Ran, L.: Recent Advances in Modeling of the Atmospheric Boundary Layer and Land Surface in the Coupled WRF-CMAQ Model BT - Air Pollution Modeling and its Application XXIV, in Air Pollution Modeling and its Application XXIV, edited by D. G. Steyn and N. Chaumerliac, pp. 391–396, Springer International Publishing, Cham., 2016.

Pleim, J. E., Bash, J. O., Walker, J. T. and Cooter, E. J.: Development and evaluation of an ammonia bidirectional flux parameterization for air quality models, J. Geophys. Res. Atmos., 118(9), 3794–3806, doi:10.1002/jgrd.50262, 2013.

Pleim, J. E., Ran, L., Appel, W., Shephard, M. W. and Cady-Pereira, K.: New Bidirectional Ammonia Flux Model in an Air Quality Model Coupled With an Agricultural Model, J. Adv. Model. Earth Syst., 11(9), 2934–2957, doi:10.1029/2019MS001728, 2019.

Putman, W. M. and Lin, S. J.: Finite-volume transport on various cubed-sphere grids, J.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

Comput. Phys., 227(1), 55–78, doi:10.1016/j.jcp.2007.07.022, 2007.

Pye, H. O., Luecken, D. J., Xu, L., Boyd, C. M., Ng, N. L., Baker, K. R., Ayres, B. R., Bash, J. O., Baumann, K., Carter, W. P., Edgerton, E., Fry, J. L., Hutzell, W. T., Schwede, D. B. and Shepson, P. B.: Modeling the Current and Future Roles of Particulate Organic Nitrates in the Southeastern United States, Env. Sci Technol, 49(24), 14195–14203, doi:10.1021/acs.est.5b03738, 2015.

Pye, H. O. T., Pinder, R. W., Piletic, I. R., Xie, Y., Capps, S. L., Lin, Y. H., Surratt, J. D., Zhang, Z. F., Gold, A., Luecken, D. J., Hutzell, W. T., Jaoui, M., Offenberg, J. H., Kleindienst, T. E., Lewandowski, M. and Edney, E. O.: Epoxide Pathways Improve Model Predictions of Isoprene Markers and Reveal Key Role of Acidity in Aerosol Formation, Env. Sci Technol, 47(19), 11056–11064, doi:10.1021/es402106h, 2013.

Pye, H. O. T., Murphy, B. N., Xu, L., Ng, N. L., Carlton, A. G., Guo, H., Weber, R., Vasilakos, P., Wyat Appel, K., Hapsari Budisulistiorini, S., Surratt, J. D., Nenes, A., Hu, W., Jimenez, J. L., Isaacman-Vanwertz, G., Misztal, P. K. and Goldstein, A. H.: On the implications of aerosol liquid water and phase separation for organic aerosol mass, Atmos. Chem. Phys., 17(1), 343–369, doi:10.5194/acp-17-343-2017, 2017.

Pye, H. O. T., Zuend, A., Fry, J. L., Isaacman-VanWertz, G., Capps, S. L., Appel, K. W., Foroutan, H., Xu, L., Ng, N. L. and Goldstein, A. H.: Coupling of organic and inorganic aerosol systems and the effect on gas–particle partitioning in the southeastern US, Atmos. Chem. Phys., 18(1), 357–370, doi:10.5194/acp-18-357-2018, 2018.

Pye, H. O. T., D'Ambro, E. L., Lee, B. H., Schobesberger, S., Takeuchi, M., Zhao, Y., Lopez-Hilfiker, F., Liu, J., Shilling, J. E., Xing, J., Mathur, R., Middlebrook, A. M., Liao, J., Welti, A., Graus, M., Warneke, C., de Gouw, J. A., Holloway, J. S., Ryerson, T. B., Pollack, I. B. and Thornton, J. A.: Anthropogenic enhancements to production of highly oxygenated molecules from autoxidation, Proc. Natl. Acad. Sci. U. S. A., 116(14), 6641–6646, doi:10.1073/pnas.1810774116, 2019.

Ryan, W. F.: The air quality forecast rote: Recent changes and future challenges, J. Air Waste Manage. Assoc., 66(6), 576–596, doi:10.1080/10962247.2016.1151469, 2016.

Sarwar, G., Fahey, K., Napelenok, S., Roselle, S. and Mathur, R.: Examining the impact of CMAQ model updates on aerosol sulfate predictions, the 10th Annual CMAS Models-3 User's Conference, Chapel Hill, NC, October 2011, 2011.

Sarwar, G., Simon, H., Bhave, P. and Yarwood, G.: Examining the impact of heterogeneous nitryl chloride production on air quality across the United States, Atmos. Chem. Phys., 12(14), 6455–6473, doi:10.5194/acp-12-6455-2012, 2012.

Sarwar, G., Gantt, B., Schwede, D., Foley, K., Mathur, R. and Saiz-Lopez, A.: Impact of Enhanced Ozone Deposition and Halogen Chemistry on Tropospheric Ozone over the Northern Hemisphere, Environ. Sci. Technol., 49(15), 9203–9211, doi:10.1021/acs.est.5b01657, 2015.

Schwede, D., Pouliot, G. and Pierce, T.: CHANGES TO THE BIOGENIC EMISSIONS INVENTORY SYSTEM VERSION 3 (BEIS3). [online] Available from: https://www.cmascenter.org/conference/2005/abstracts/2_7.pdf (Accessed 28 June 2020), 2005.

Shen, L., Mickley, L. J. and Gilleland, E.: Impact of increasing heat waves on U.S. ozone episodes in the 2050s: Results from a multimodel analysis using extreme value theory, Geophys. Res. Lett., 43(8), 4017–4025, doi:10.1002/2016GL068432, 2016.

Sillman, S.: The relation between ozone, NO(x) and hydrocarbons in urban and polluted rural environments, Atmos. Environ., 33(12), 1821–1845, doi:10.1016/S1352-2310(98)00345-8, 1999.

Sillman, S. and Samson, P. J.: Impact of temperature on oxidant photochemistry in urban polluted rural and remote environments, J. Geophys. Res., 100(D6), 11497–11508, doi:10.1029/94jd02146, 1995.

Simon, H., and Bhave, P. V.: Simulating the degree of oxidation in atmospheric organic particles. Environmental Science and Technology, 46(1), 331–339. https://doi.org/10.1021/es202361w, 2012.

Stajner, I., Davidson, P., Byun, D., McQueen, J., Draxler, R., Dickerson, P. and Meagher, J.: US National Air Quality Forecast Capability: Expanding Coverage to Include

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Particulate Matter, in Air Pollution Modeling and its Application XXI, pp. 379–384, Springer, Dordrecht., 2011.

Stein, A. F., Lamb, D. and Draxler, R. R.: Incorporation of detailed chemistry into a three-dimensional Lagrangian-Eulerian hybrid model: Application to regional tropospheric ozone, Atmos. Environ., 34(25), 4361–4372, doi:10.1016/S1352-2310(00)00204-1, 2000.

Taylor, K. E.: Summarizing multiple aspects of model performance in a single diagram, J. Geophys. Res. Atmos., 106(D7), 7183–7192, doi:10.1029/2000JD900719, 2001.

Tegtmeier, S., Ziska, F., Pisso, I., Quack, B., Velders, G. J. M., Yang, X. and Krüger, K.: Oceanic bromoform emissions weighted by their ozone depletion potential, Atmos. Chem. Phys., 15(23), 13647–13663, doi:10.5194/acp-15-13647-2015, 2015.

United States Environmental Protection Agency: CMAQ (Version 5.02) [Software]. Available from https://zenodo.org/record/1079898, 2014.

Wang, K., Yahya, K., Zhang, Y., Hogrefe, C., Pouliot, G., Knote, C., Hodzic, A., San Jose, R., Perez, J. L., Jiménez-Guerrero, P., Baro, R., Makar, P. and Bennartz, R.: A multi-model assessment for the 2006 and 2010 simulations under the Air Quality Model Evaluation International Initiative (AQMEII) Phase 2 over North America: Part II. Evaluation of column variable predictions using satellite data, Atmos. Environ., 115, 587–603, doi:10.1016/j.atmosenv.2014.07.044, 2015.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

Watanabe, K.: Measurements of ozone concentrations on a commercial vessel in the marine boundary layer over the northern North Pacific Ocean, J. Geophys. Res., 110(D11), D11310, doi:10.1029/2004JD005514, 2005.

Xu, L., Pye, H. O. T., He, J., Chen, Y., Murphy, B. N. and Ng, N. L.: Experimental and model estimates of the contributions from biogenic monoterpenes and sesquiterpenes to secondary organic aerosol in the southeastern United States, Atmos. Chem. Phys., 18(17), 12613–12637, doi:10.5194/acp-18-12613-2018, 2018.

Yang, F.: GDAS/GFS V15.0.0 Upgrades for Q2FY2019, Retrieved from https://www.emc.ncep.noaa.gov/users/Alicia.Bentley/fv3gfs/updates/EMC_CCB_FV3GFS_9-24-18.pdf, last access: May 2020, 2019.

Yang, X., Blechschmidt, A.-M., Bognar, K., McClure–Begley, A., Morris, S., Petropavlovskikh, I., Richter, A., Skov, H., Strong, K., Tarasick, D., Uttal, T., Vestenius, M. and Zhao, X.: Pan-Arctic surface ozone: modelling vs measurements, Atmos. Chem. Phys. Discuss., 1–33, doi:10.5194/acp-2019-984, 2020.

Yarwood, G., Rao, S., Yocke, M. and Whitten, G.: Updates to the Carbon Bond Chemical Mechanism: CB05. Final Report to the US EPA, RT-0400675. Yocke and Company, Novato, CA, 2005.

Yarwood, G., Whitten, G.Z., Jung, J., Heo, G. and Allen, D.T.: Development, evaluation and testing of version 6 of the Carbon Bond chemical mechanism (CB6), Final report

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions
Open Access

to the Texas Commission on Environmental Quality, Work Order No. 582-7-84005-FY10-26, 2010.

Žabkar, R., Honzak, L., Skok, G., Forkel, R., Rakovec, J., Ceglar, A. and Žagar, N.: Evaluation of the high resolution WRF-Chem (v3.4.1) air quality forecast and its comparison with statistical ozone predictions, Geosci. Model Dev, 8, 2119–2137, doi:10.5194/gmd-8-2119-2015, 2015.

Zhang, C., Xue, M., Supinie, T. A., Kong, F., Snook, N., Thomas, K. W., Brewster, K., Jung, Y., Harris, L. M. and Lin, S.: How Well Does an FV3-Based Model Predict Precipitation at a Convection-Allowing Resolution? Results From CAPS Forecasts for the 2018 NOAA Hazardous Weather Test Bed With Different Physics Combinations, Geophys. Res. Lett., 46(6), 3523–3531, doi:10.1029/2018GL081702, 2019a.

Zhang, X., Kondragunta, S., Da Silva, A., Lu, S., Ding, H., Li, F. and Zhu, Y.: THE BLENDED GLOBAL BIOMASS BURNING EMISSIONS PRODUCT FROM MODIS AND VIIRS Observations (GBBEPx). [online] Available from: https://www.ospo.noaa.gov/Products/land/gbbepx/docs/GBBEPx_ATBD.pdf (Accessed 28 June 2020b), 2019.

Zhang, Y., Liu, P., Pun, B. and Seigneur, C.: A comprehensive performance evaluation of MM5-CMAQ for the Summer 1999 Southern Oxidants Study episode—Part I:

Evaluation protocols, databases, and meteorological predictions, Atmos. Environ., 40(26), 4825–4838, doi:10.1016/j.atmosenv.2005.12.043, 2006.

Zhang, Y., Vijayaraghavan, K., Wen, X.-Y., Snell, H. E. and Jacobson, M. Z.: Probing into regional ozone and particulate matter pollution in the United States: 1. A 1 year CMAQ simulation and evaluation using surface and satellite data, J. Geophys. Res., 114(D22), D22304, doi:10.1029/2009JD011898, 2009.

Zhang, Y., Bocquet, M., Mallet, V., Seigneur, C. and Baklanov, A.: Real-time air quality forecasting, part I: History, techniques, and current status, Atmos. Environ., 60, 632–655, doi:10.1016/j.atmosenv.2012.06.031, 2012a.

Zhang, Y., Bocquet, M., Mallet, V., Seigneur, C. and Baklanov, A.: Real-time air quality forecasting, Part II: State of the science, current research needs, and future prospects, Atmos. Environ., 60, 656–676, doi:10.1016/j.atmosenv.2012.02.041, 2012b.

Zhang, Y., Hong, C., Yahya, K., Li, Q., Zhang, Q. and He, K.: Comprehensive evaluation of multi-year real-time air quality forecasting using an online-coupled meteorology-chemistry model over southeastern United States, Atmos. Environ., 138, 162–182, doi:10.1016/j.atmosenv.2016.05.006, 2016.

Zhang, Y., Jena, C., Wang, K., Paton-Walsh, C., Guérette, É.-A., Utembe, S., Silver, J. D. and Keywood, and M.: Multiscale Applications of Two Online-Coupled Meteorology-Chemistry Models during Recent Field Campaigns in Australia, Part I:

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions

Model Description and WRF/Chem-ROMS Evaluation Using Surface and Satellite Data and Sensitivity to Spatial Grid Resolutions, Atmosphere (Basel)., 10(4), 189, doi:10.3390/atmos10040189, 2019c.

Zhang, Y., Wang, K., Jena, C., Paton-Walsh, C., Guérette, É. A., Utembe, S., Silver, J. D. and Keywood, M.: Multiscale applications of two online-coupled meteorology-chemistry models during recent field campaigns in Australia, Part II: Comparison of WRF/Chem and WRF/Chem-ROMS and impacts of air-sea interactions and boundary conditions, Atmosphere (Basel)., 10(4), 210, doi:10.3390/ATMOS10040210, 2019d.

Zhu, Y. and Luo, Y.: Precipitation Calibration Based on the Frequency-Matching Method, Weather Forecast., 30(5), 1109–1124, doi:10.1175/WAF-D-13-00049.1, 2015.

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development Discussions Open Access EGU

Tables and Figures

Table 1. Configuration of GFSv15-CMAQv5.0.2 system

Attribute	Model Configuration
Forecast period	Jan.-Dec., 2019
Domain	Continental U.S.
Resolution	Horizontal: 12 km (442×265); Vertical: 35 layers
Physical Options	
Shortwave/longwave radiation	The Rapid Radiative Transfer Method for GCMs
Planetary boundary layer (PBL)	Hybrid eddy-diffusivity mass-flux (EDMF) PBL
Land surface	Noah Land Surface Model (LSM)
Microphysics	A more advanced GFDL microphysics scheme
Cumulus	The Simplified Arakawa-Schubert (SAS) deep convection
Chemical Options	
Photolysis	In-line method (Binkowski et al., 2007)
Gas-phase chemistry	The Carbon Bond mechanism version 5 with active chlorine chemistry and updated toluene mechanism (CB05tucl) (Yarwood et al., 2005; Sarwar et al., 2012)
Aqueous-phase chemistry	AQCHEM (Sarwar et al., 2011)
Aerosol module	AERO6 with nonvolatile POA (Carlton et al., 2010; Simon et al., 2012; Appel et al., 2013)

Table 2. Performance statistics of meteorological forecasts

Datasets		CASTNET							METAR						
Variable	Period	Mean Obs.	Mean Sim.	MB	RMSE	NMB, %	NME, %	Corr	Mean Obs.	Mean Sim.	MB	RMSE	NMB, %	NME, %	Corr
T2, °C	DJF	-0.1	-0.5	-0.4	2.6	-588	-2850	0.96	2.7	2.6	-0.1	2.5	-3.1	69.3	0.97
	MAM	9.9	9.4	-0.5	2.4	-5.2	18.2	0.97	12.3	11.9	-0.4	2.3	-3.0	14.0	0.97
	JJA	21.5	21.4	-0.2	2.4	-0.8	8.6	0.93	23.4	23.1	-0.3	2.3	-1.2	7.5	0.93
	SON	11.5	11.3	-0.2	2.6	-2.0	16.1	0.97	13.8	13.8	0.1	2.3	0.4	12.6	0.98
	Annual	10.9	10.6	-0.3	2.5	-3.0	17.0	0.98	13.2	13.0	-0.2	2.3	-1.3	13.1	0.98
RH2, %	DJF	69.1	71.9	2.8	14.3	4.0	15.1	0.74	74.1	74.4	0.4	13.3	0.5	13.4	0.76
	MAM	62.7	66.1	3.4	14.2	5.4	16.6	0.82	67.4	70.1	2.7	13.8	4.0	15.5	0.81
	JJA	55.0	53.3	-1.7	12.2	-3.2	16.4	0.89	67.0	67.3	0.3	13.1	0.5	14.8	0.84
	SON	59.0	57.6	-1.4	13.0	-2.4	16.1	0.87	68.7	67.0	-1.7	13.2	-2.5	14.5	0.83

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Geoscientific Model Development
Discussions
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	Annual	61.4	62.2	0.8	13.5	1.3	16.0	0.85	68.8	69.3	0.4	13.2	0.8	14.4	0.83
WS10, m s^{-1}	DJF	2.5	3.0	0.5	2.0	18.7	56.7	0.59	3.3	3.7	0.4	2.0	10.8	43.5	0.71
	MAM	2.8	3.4	0.6	2.1	22.2	55.6	0.60	3.6	4.0	0.4	2.0	10.3	42.5	0.71
	JJA	2.4	3.0	0.6	1.9	24.5	60.9	0.51	2.8	3.3	0.5	1.9	17.0	52.6	0.62
	SON	2.6	3.1	0.5	2.0	20.4	58.6	0.57	4.0	4.1	0.2	1.8	4.2	33.1	0.69
	Annual	2.6	3.1	0.6	2.0	21.5	57.9	0.57	3.4	3.7	0.4	1.9	10.7	41.8	0.72
WD10, degree	DJF	187.2	189.4	2.2	69.4	1.2	26.4	0.81	158.0	164.3	6.4	60.7	4.0	25.5	0.90
	MAM	184.6	186.5	1.9	68.1	1.0	26.1	0.81	159.9	163.6	3.7	60.7	2.3	25.4	0.89
	JJA	186.7	188.8	2.1	73.0	1.1	28.5	0.77	146.8	147.8	1.0	69.9	0.7	33.9	0.86
	SON	181.8	183.9	2.1	71.3	1.1	28.1	0.79	190.9	196.6	5.7	42.1	3.0	14.5	0.92
	Annual	185.0	187.1	2.1	70.5	1.1	27.3	0.80	162.5	166.6	4.1	59.1	2.5	23.9	0.89
Precip, mm hr^{-1}	DJF	1.0	0.6	-0.4	1.7	-42.5	86.1	0.26	1.3	0.7	-0.6	3.5	-44.4	77.4	0.15
	MAM	1.1	0.6	-0.6	2.0	-51.1	86.3	0.22	1.8	0.7	-1.0	7.5	-58.6	85.6	0.07
	JJA	2.2	0.5	-1.7	4.7	-77.8	93.9	0.11	2.6	0.7	-1.9	7.6	-74.5	91.6	0.04
	SON	1.3	0.6	-0.7	2.4	-54.4	86.2	0.24	1.8	0.8	-1.0	8.8	-56.4	83.8	0.07
	Annual	1.3	0.6	-0.7	2.5	-55.4	87.9	0.18	1.8	0.7	-1.1	7.0	-59.1	85.0	0.07

T2: temperature at 2-m; RH2: relative humidity at 2-m; WS10: wind speed at 10-m; WD10: wind direction at 10-m; Precip: precipitation; DJF: winter; MAM: spring; JJA: summer; SON: autumn; MB: mean bias; RMSE: root mean square error; NMB: normalized mean bias; NME: normalized mean error; Corr: correlation coefficient; Obs.: Observation; Sim.: Prediction.

Table 3. Performance statistics of chemical variables against AIRNow dataset

			MDA8 O_3, ppb								24-h avg $PM_{2.5}$, μg m^{-3}				
Period	Mean Obs.	Mean Sim.	MB	RMSE	NMB,%	NME,%	Corr	Period	Mean Obs.	Mean Sim.	MB	RMSE	NMB,%	NME,%	Corr
Jan	32.4	32.0	-0.3	7.9	-1.1	18.0	0.52	Jan	8.3	13.8	5.5	11.4	66.4	92.4	0.34
Feb	36.7	35.7	-1.1	8.4	-2.9	17.4	0.53	Feb	8.0	12.5	4.5	10.0	55.9	81.0	0.51
Mar	45.1	40.4	-4.7	8.9	-10.4	16.0	0.55	Mar	7.9	11.0	3.1	9.4	39.6	68.9	0.38
Apr	46.6	43.1	-3.5	8.0	-7.5	13.5	0.61	Apr	6.3	8.0	1.7	6.6	26.5	62.0	0.30
May	44.3	42.7	-1.6	7.9	-3.7	14.0	0.66	May	6.8	6.9	0.2	5.0	2.3	49.8	0.23
Jun	45.9	43.9	-2.0	11.2	-4.4	18.5	0.58	Jun	7.2	6.8	-0.4	5.6	-5.1	47.4	0.20
Jul	44.5	46.6	2.1	9.7	4.7	16.7	0.70	Jul	8.3	8.5	0.1	11.7	1.7	59.9	0.30
Aug	43.9	46.9	3.0	9.5	6.8	16.3	0.73	Aug	7.3	6.9	-0.4	4.1	-5.2	40.4	0.33

Sept	42.7	45.6	2.9	8.1	6.8	14.5	0.78	Sept	7.0	7.6	0.5	4.7	7.6	44.4	0.48
Oct	37.2	40.2	3.1	8.0	8.3	15.8	0.77	Oct	6.7	9.5	2.8	8.6	41.7	71.9	0.35
Nov	34.3	34.8	0.5	8.4	1.6	16.9	0.64	Nov	9.0	13.2	4.2	9.8	46.7	72.0	0.48
Dec	30.7	31.2	0.5	9.0	1.6	20.5	0.49	Dec	8.8	13.8	5.0	11.0	56.6	82.9	0.49
O_3-season	44.3	45.1	0.9	9.4	2.0	16.0	0.67	DJF	8.4	13.4	5.0	10.8	59.7	85.6	0.45
								MAM	7.0	8.6	1.6	7.2	23.5	60.6	0.33
Non O_3-season	38.2	37.4	-0.9	8.4	-2.3	16.4	0.68	JJA	7.6	7.4	-0.2	7.9	-2.6	49.7	0.26
								SON	7.5	10.0	2.5	8.0	33.0	63.4	0.45
Annual	41.1	41.0	-0.1	8.9	-0.1	16.2	0.70	Annual	7.6	9.8	2.2	8.6	29.0	65.3	0.40

MDA8 O_3: maximum daily average 8-h ozone; 24-h avg $PM_{2.5}$: 24-hour average $PM_{2.5}$.

Figures

Figure 1. Spatial distribution of MBs for forecasted seasonal T2 by GFSv15-CMAQv5.0.2 against observations from METAR

Figure 2. Taylor diagram with variance, Corr, and NMB for meteorological variables (T2, RH2, WS10, WD10, and Precip) against CASTNET and METAR dataset

Figure 3. Spatial distribution of forecasted MDA8, MB, and NMB during O_3 and winter season. Observation from AIRNow is shown as filled circles in the overlay plots of concentrations

Figure 4. Forecasted seasonal daily $PM_{2.5}$ by GFSv15-CMAQv5.0.2 overlaid observations from AIRNow and MB against observations from AIRNow

Figure 5. Categorical evaluation of MDA8 and 24-h avg $PM_{2.5}$

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Figure 6. Monthly AOD from MODIS (left), predicted AOD from GFSv15-CMAQv5.0.2 (middle), and predicted surface 24-h avg $PM_{2.5}$ (right)

Figure 7. Monthly average concentrations of $PM_{2.5}$ components

Figure 8. Annual performance of MDA8 in 10 CONUS regions (a); Taylor Diagram for annual performance of MDA8 (b); Annual performance of 24-h avg $PM_{2.5}$ in 10 CONUS regions (c); Taylor Diagram for annual performance of 24-h avg $PM_{2.5}$. Outliers represent regions with NSDs >3.5 (d)

Figure 9. Diurnal $PM_{2.5}$ in: (a) O_3 season for regions 1 to 5; (b) Non-O_3 season for regions 1 to 5; (c) O_3 season for regions 6 to 10; (d) Non-O_3 season for region 6 to 10. Solid curves are observed values and dash curves are predicted values. Average of predicted $PM_{2.5}$ and components of $PM_{2.5}$ within CONUS in: (e) O_3 season, and (f) Non-O_3 season

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Preprint. Discussion started: 2 September 2020

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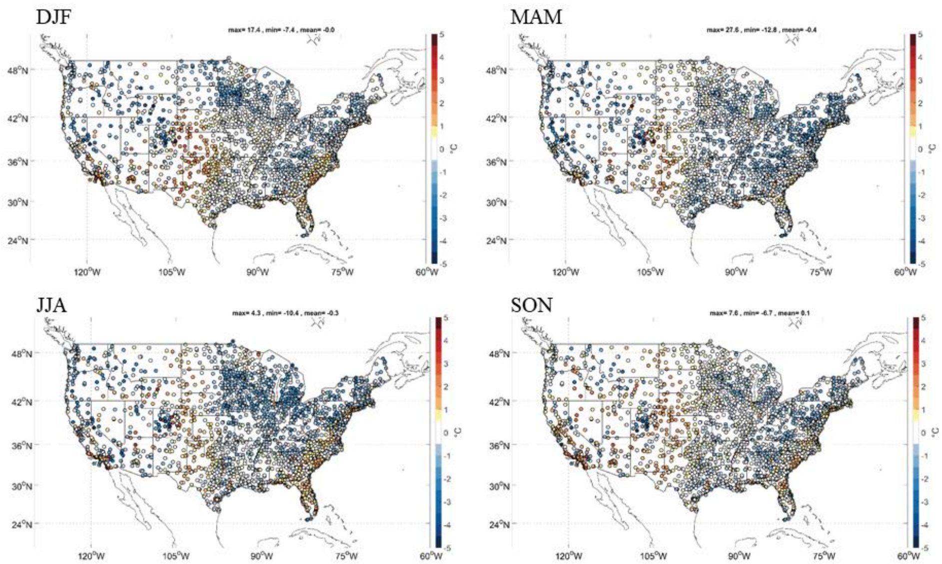

Figure 1. Spatial distribution of MBs for forecasted seasonal mean T2 by GFSv15-CMAQv5.0.2 against observations from METAR

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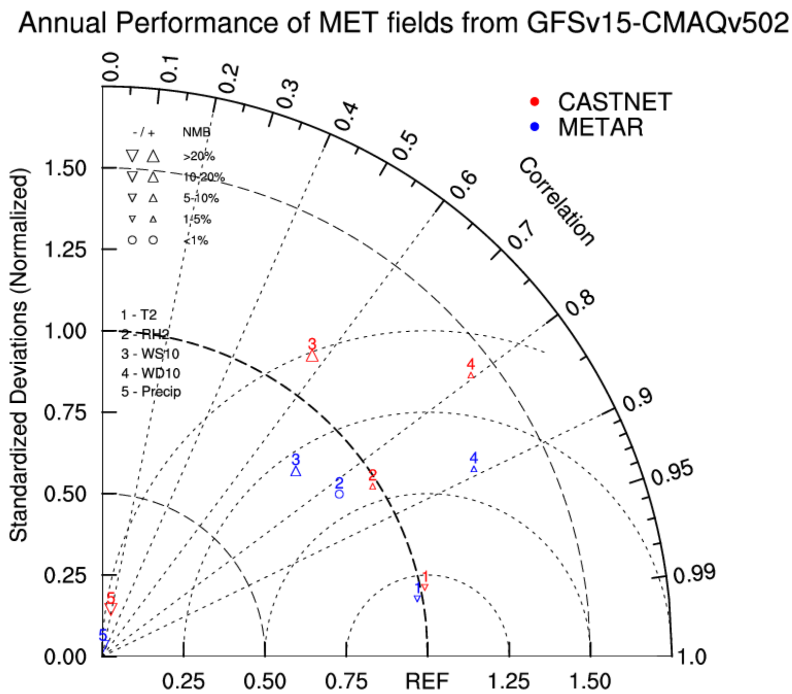

Figure 2. Taylor diagram (Taylor, 2001) with Normalized Standardized Deviations (NSD), Corr, and NMB for meteorological variables (T2, RH2, WS10, WD10, and Precip) against CASTNET and METAR dataset. The REF marker at x-axis represents a referred perfect performance. The closer each variable is to the REF marker, the better performance the forecast system has for that variable

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

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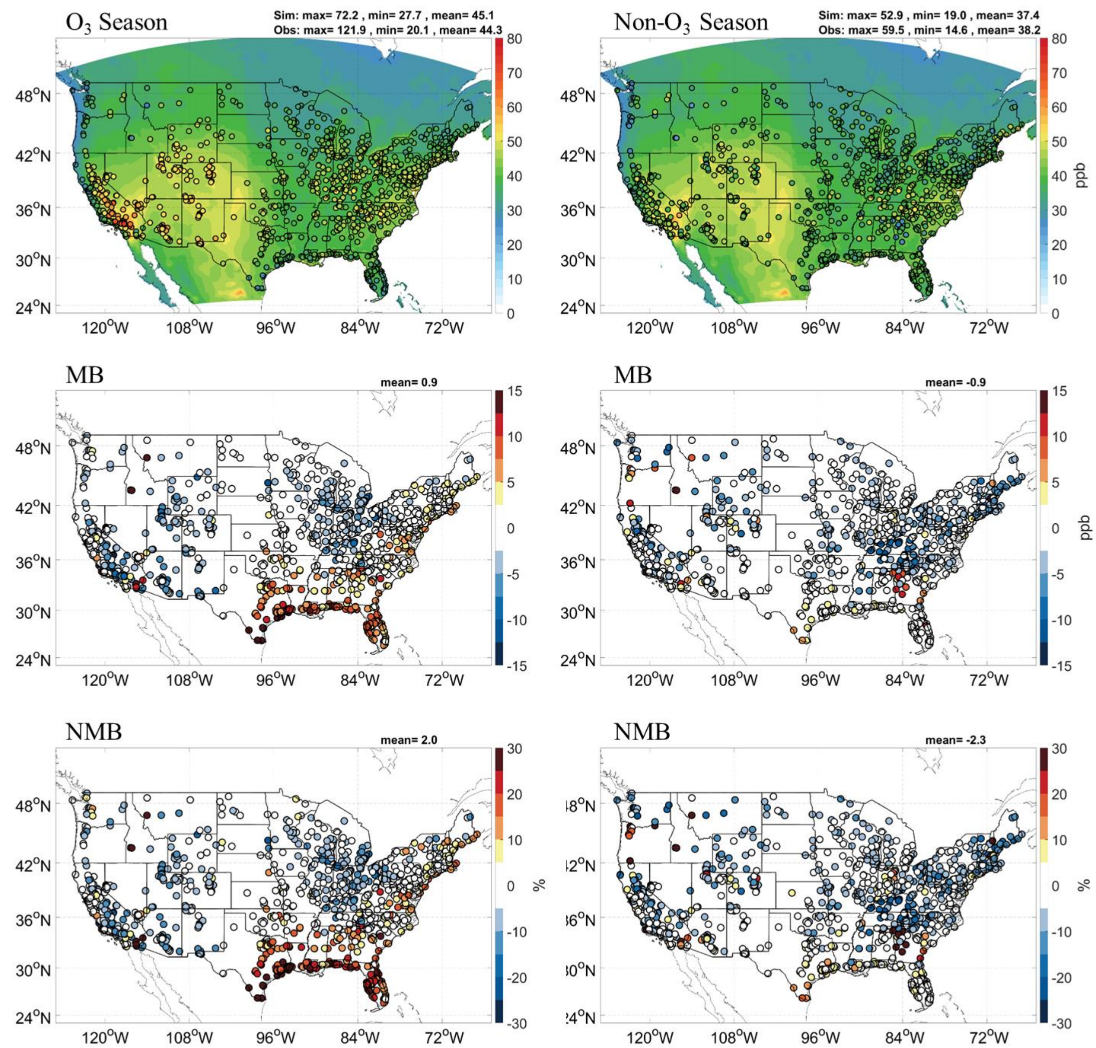

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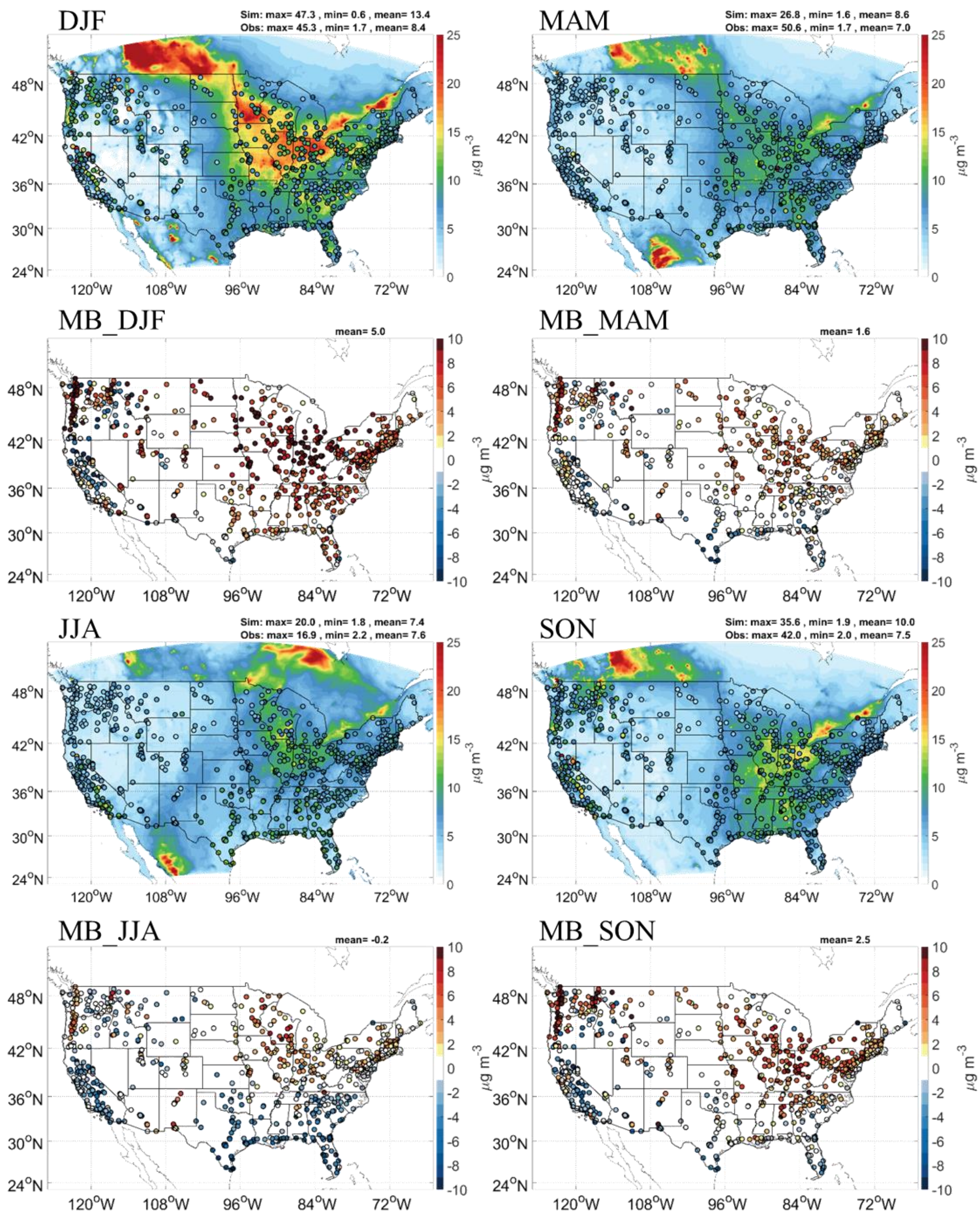
Preprint. Discussion started: 2 September 2020



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Preprint. Discussion started: 2 September 2020

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Discussions

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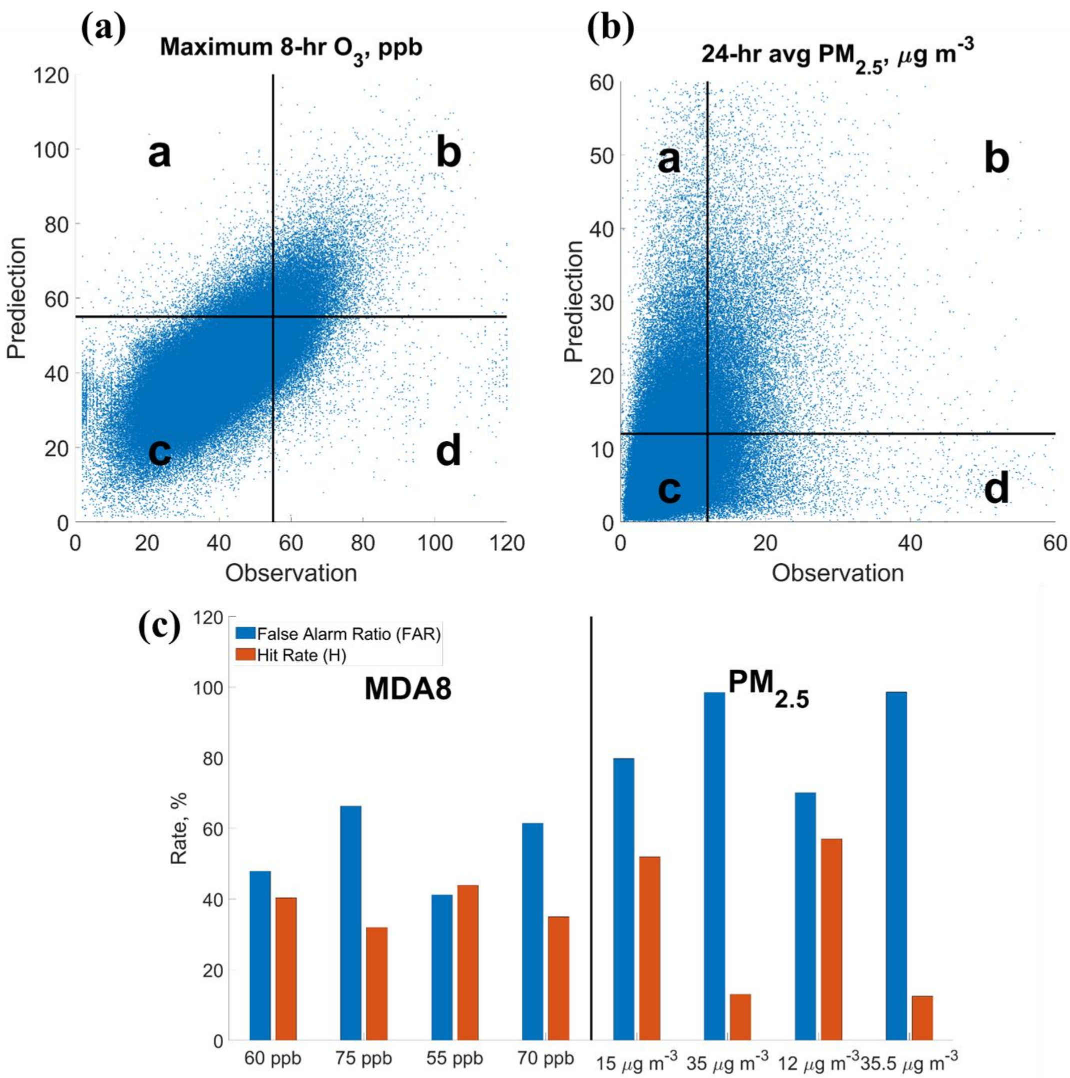

https://doi.org/10.5194/gmd-2020-272
Preprint. Discussion started: 2 September 2020

Figure 5. Categorical evaluation of MDA8 and 24-h avg $PM_{2.5}$: (a) scatter plot of predicted and observed MDA8. The scatters are categorized into 4 areas using the threshold of 55 ppb for both observation and prediction; (b) scatter plot of predicted and observed 24-h avg $PM_{2.5}$. The scatters are categorized into 4 areas using the threshold of 12 μg m^{-3} for both observation and prediction; (c) False Alarm Ratio (FAR) and Hit Rate (H) in 4 categories for forecasts of MDA8 and 24-h avg $PM_{2.5}$.

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Preprint. Discussion started: 2 September 2020

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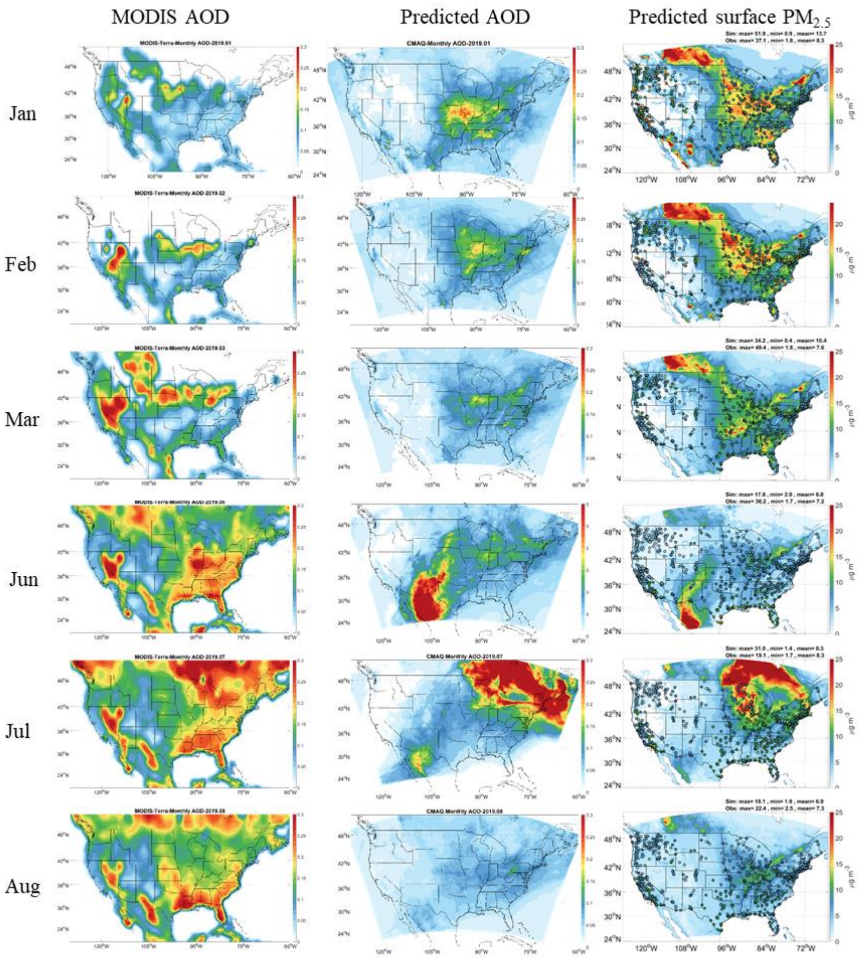

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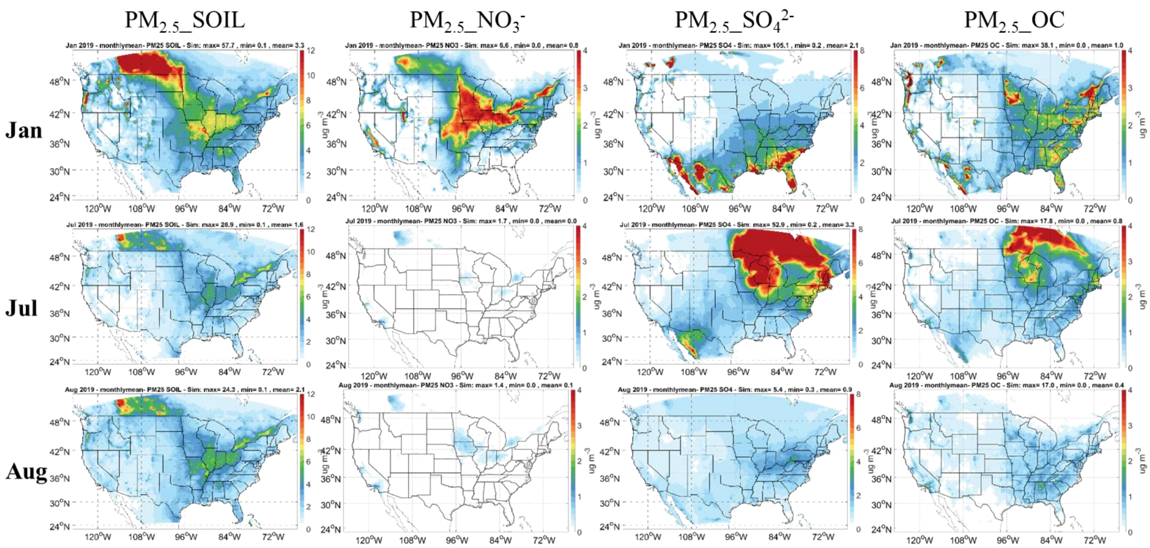

Figure 7. Monthly average concentrations of $PM_{2.5}$ components in Jan, Jul, and Aug. $PM_{2.5}$_SOIL: soil components and unspecified coarse mode components; $PM_{2.5}$_NO_3^-: nitrate components; $PM_{2.5}$_SO_4^{2-}: sulfate components; $PM_{2.5}$_OC: organic carbon components.

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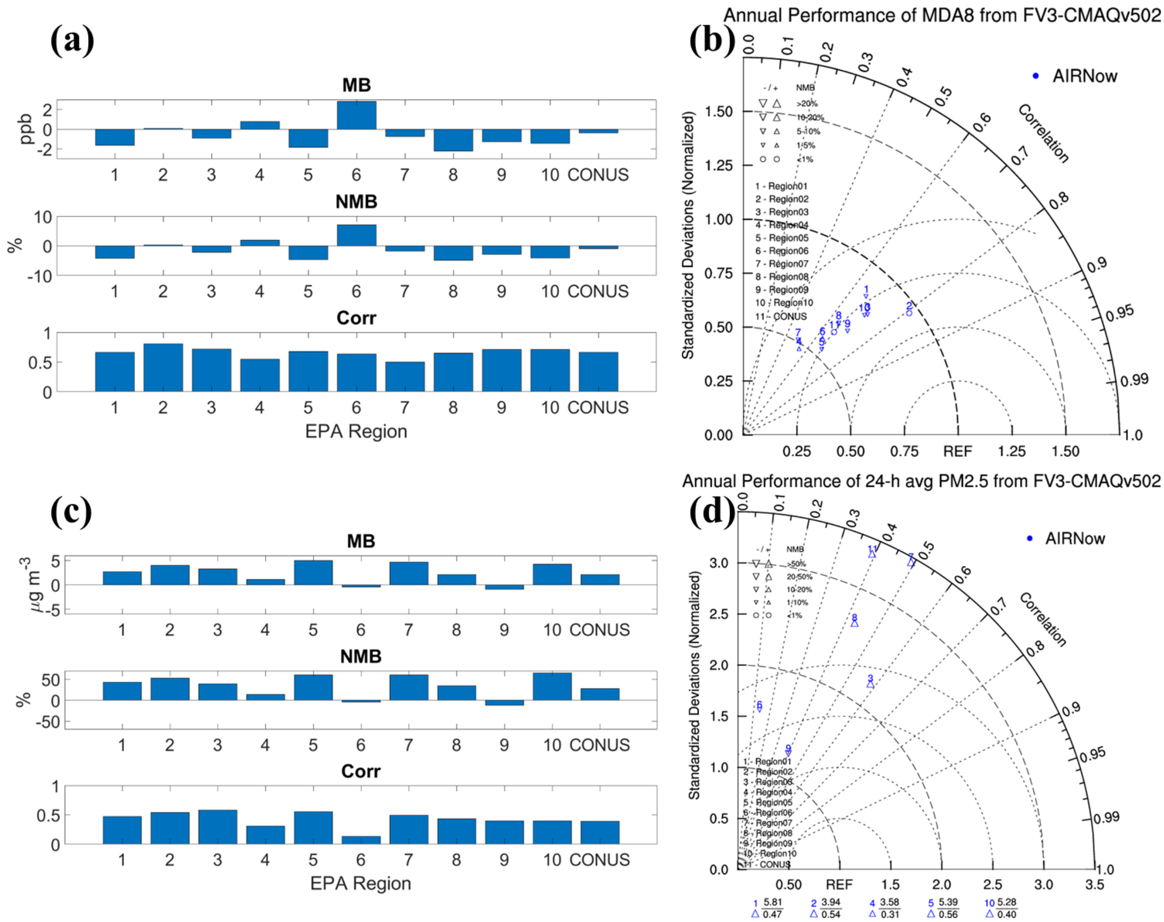
Preprint. Discussion started: 2 September 2020



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Preprint. Discussion started: 2 September 2020

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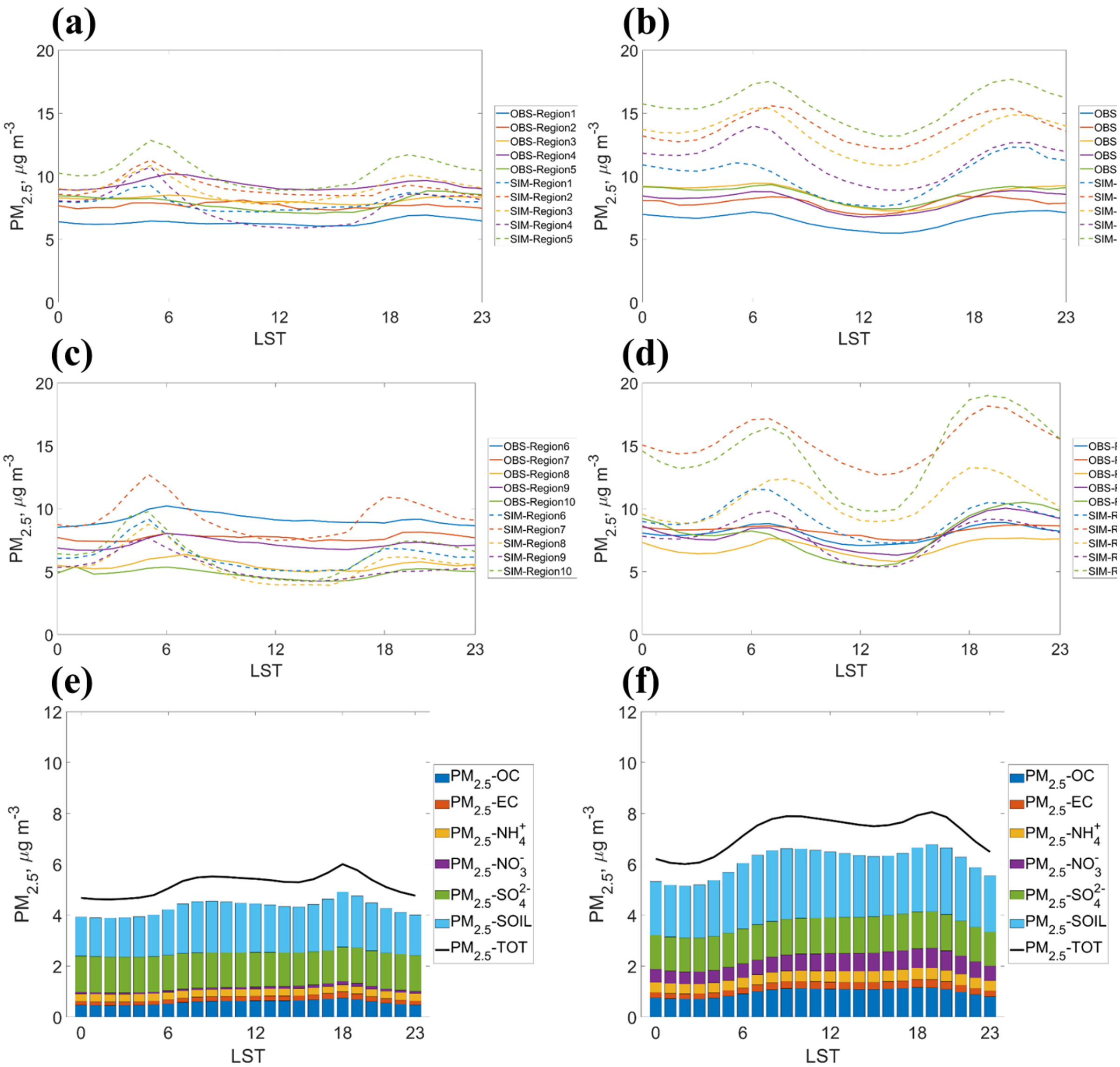

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Preprint. Discussion started: 2 September 2020

predicted $PM_{2.5}$ and components of $PM_{2.5}$ within CONUS in: (e) O_3 season, and (f) Non-O_3 season.