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AN EVALUATION OF PHOTOCHEMICAL MODEL ESTIMATED PM2.5 AND OZONE USING MM5 AND WRF INPUTS FOR THE WESTERN UNITED STATES

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1. INTRODUCTION

Meteorological variables are important inputs to retrospective photochemical modeling applications estimating ozone and particulate matter for regional and local emissions control plans. MM5 has traditionally been used to generate the meteorological inputs critical for appropriately estimating the local and regional formation and transport of ozone and particulate matter. Since support and development for MM5 have ceased it is necessary to transition to an actively developed state of the science prognostic meteorological model.

The WRF-ARW has recently been updated to include features such as four dimensional data assimilation (FDDA), which is important for annual and episodic retrospective applications. MM5 and WRF-ARW using 2 land surface modules are compared for two months (February and August) on a Western United States 12 km model domain. All 3 meteorological model estimates for each month are used as input to the CMAQ photochemical model to estimate ozone and particulate matter performance.

2. METHODS

Each model was applied to a continental scale 36 km domain and a western United States 12 km domain in 5 day blocks (7200 minute simulation) initiated at 12Z with a 90 second time step. Both domains were run for the entire months of February and August 2005.

The continental scale 36 km domain has 165 cells in the X direction and 129 cells in the Y direction. The nested western United States 12 km domain has 229 cells in the X direction and 208 cells in the Y direction. All domains have a Lambert conformal projection centered at coordinates -97, 40 with first and second true latitudes at 33 and 45 degrees.

Vegetative and landuse information is developed based on data released with the MM5 and WRF distributions. Terrain information is based on United States Geographic Survery (USGS) terrain databases. The 36 km domain is based on 5 min (approx. 9 km) and the 12 km domain is based on 2 min (approx. 4 km) Geophysical Data Center global data. Additional options are set in the MM5 TERRAIN processor to allow generation of data to support the Pleim-Xiu land surface module. Variables LSMDATA and IEXTRA are both set equal to TRUE.

ETA/AWIP 3D and surface analyses data (ds609.2) is used to initialize MM5 and WRF. The input analyses data is processed 3 hourly (10,800 seconds). Snow cover is estimated from water equivalent snow depth. Water surface temperature data is based on NCEP RTG global one-half degree analysis for MM5 and WRF.

Objective analysis is applied to enable surface nudging of soil moisture and temperature in the Pleim-Xiu land surface module in the MM5 simulation. NCEP ADP surface (ds 464.0) and upper air (ds 353.1 and ds 353.4) data are input to RAWINS. No objective analysis is applied to the WRF input analysis fields.

The top of the model domain is 100 millibars, which is approximately 15 kilometers above ground level. The vertical atmosphere is resolved to 34 layers, with thinner layers in the planetary boundary layer (PBL). The surface layer is approximately 38 meters in height. The layer configuration is selected to capture the important diurnal variations in the boundary layer while also having layers in the upper troposphere to resolve deep cloud formation.

Important physics options used in the MM5 simulation are listed below.

- Pleim-Xiu PBL and land surface schemes
- Kain-Fritsh 2 cumulus parameterization
- Reisner 2 mixed phase moisture scheme
- RRTM longwave radiation scheme
- Dudhia shortwave radiation scheme

Important physics options used in each of the WRF simulations are listed below.

- YSU PBL
- Janjic Eta Surface Layer scheme
- Kain-Fritsh (new Eta) cumulus parameterization
- Thompson Graupel moisture scheme
- RRTM longwave radiation scheme
- Dudhia shortwave radiation scheme

The land surface models are the only difference between the 2 WRF simulations. The NOAH and Pleim-Xiu land surface schemes are each applied with a WRF simulation.

The Community Multi-scale Air Quality (CMAQ) model v4.7 is a state of the science three-dimensional Eularian "one-atmosphere" photochemical transport model (Aiyyer et al, 2007; Byun and Schere, 2006). CMAQ is applied with the AERO4 aerosol module, which includes the ISORROPIA inorganic chemistry (Nenes et al., 1998) and a semi-volatile secondary organic aerosol module. The CMAQ model is applied with RADM aqueous phase chemistr and the CB05 gas-phase chemistry module. The 34 vertical layers were collapsed to 14 to improve model efficiency, keeping the most resolution in the boundary layer to capture diurnal variations in mixing height.

The observation database for temperature, wind speed, wind direction, and mixing ratio is based on measurements made at United States and Canada airports. The observation data (ds472) is available from NCAR. Shortwave downward radiation measurements are taken at SURFRAD and ISIS monitor locations. The SURFRAD and ISIS networks each have 4 sites in the model domain.

Rainfall observation analysis data (~40 km resolution) is available from the National Weather Service Climate Prediction Center (CPC) on an hourly basis for the Continental United States. Rainfall analysis estimated by the PRISM model (~2-4 km resolution) is also compared with model rainfall estimates (PRISM, 2004). Neither analysis data include any area outside the continental United States.

Model performance is described using quantitative metrics: mean bias (prediction-observation) and mean error (abs[mean bias]) (Boylan et al, 2006). These metrics are useful because they describe model performance in the measured units of a variable. Performance is best when these metrics approach 0.

The models output predictions approximately 15 meters above the surface while observations are at 10 meters. This should be considered when interpreting model performance metrics.

3. RESULTS

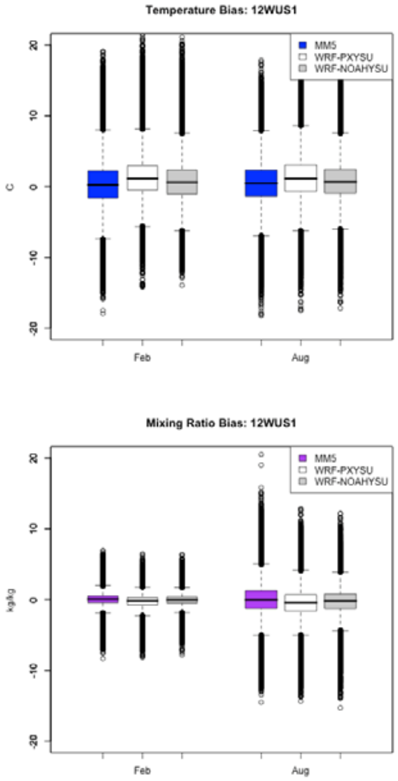

Figure 1. Temperature and Mixing Ratio bias by model and month.

Figures 1 and 2 illustrate the entire distribution of the bias performance metric by month and model for temperature, mixing ratio, and wind speed. The error metric is shown for wind direction.

For temperature, mixing ratio, wind speed, and wind direction the performance is similar for all 3 meteorological model simulations. In general the bias distributions are near zero, but the areas of degraded model performance do not seem substantively improved by any meteorological model configuration.

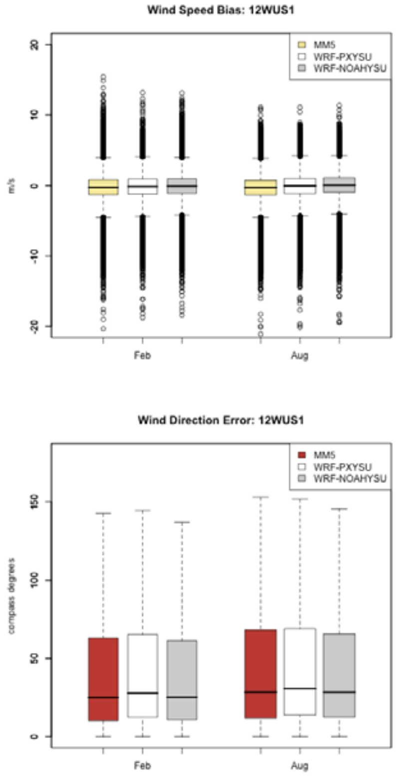

Figure 2. Wind Speed and Wind Direction bias by model and month.

Figure 3 shows the bias metric for shortwave downward radiation by hour of the day for the August 2005 month.

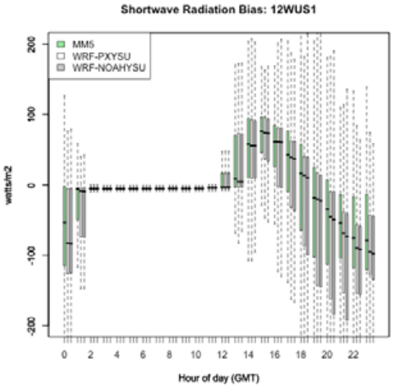

Figure 3. Shortwave radiation bias by hour of the day during August 2005.

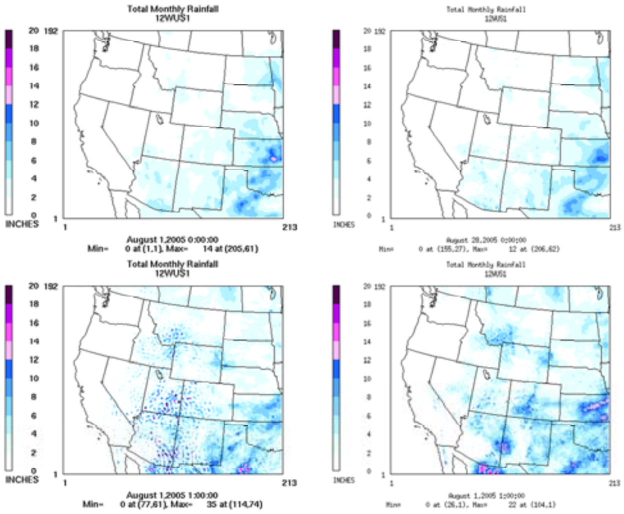

Figure 4. August monthly total rainfall: CPC analysis (top left), PRISM analysis (top right), MM5 estimates (bottom left), and WRF-NOAH estimates (bottom right).

Figure 4 shows August 2005 monthly total rainfall for each of the observation analysis datasets (top row) and MM5 and WRF-NOAH (bottom row). Modeled spatial patterns are in fair agreement with observations, particularly in the southern part of the domain. Ozone bias is shown in Figure 5 by bins of observed ozone concentration to show how the model performs with the different meteorological inputs at high and low concentrations. Clearly, the modeling system in general tends to over-predict low ozone and under-predict high ozone concentrations.

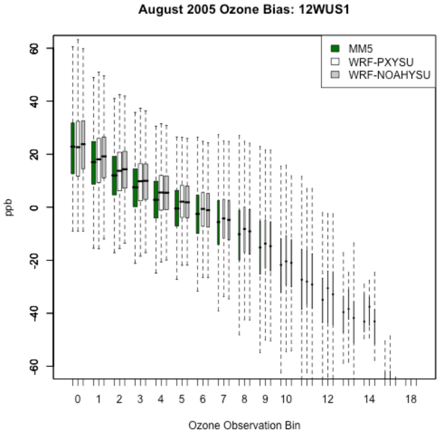

Figure 5. Ozone bias by observation bin

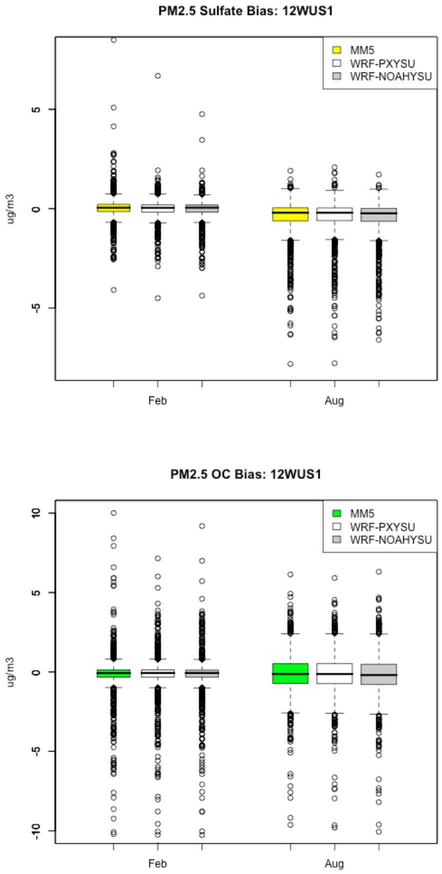

Figure 6. PM2.5 sulfate (top) and organic carbon (bottom) bias by month.

The bias for PM2.5 sulfate ion and PM2.5 organic carbon are shown in Figure 6. CMAQ model performance tendencies are similar for all PM2.5 species over the entire domain regardless of which meteorological data is used as input.

4. DISCUSSION

Each of the simulations similarly predict temperature, relative humidity, wind speed, wind direction, and shortwave downward radiation. CMAQ similarly predicts ozone and PM2.5 in the summer and winter month regardless of which simulation is used to supply meteorological inputs. This large-scale model response may vary for specific monitor locations. Monthly total precipitation estimated by the WRF-ARW simulations tends to better match the magnitudes and spatial patterns seen in precipitation analysis fields. WRF-ARW precipitation estimates in the higher elevation sections of the modeling domain compare better to the PRISM precipitation analysis than the analysis prepared by the National Weather Service Climate Prediction Center. All 3 meteorological model simulations tended to under-estimate summer shortwave downward radiation, particularly in the afternoon and evening hours. The comparability in photochemical model estimates using WRF-ARW compared to MM5 for meteorological inputs increase confidence that WRF is suitable for retrospective regulatory photochemical modeling applications.

5. ACKNOWLEDGEMENTS

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