

Comparisons of the CMAQ and WRF/Chem Models for a 2006 Eastern U.S. Case Study

Introduction

The Community Multiscale Air Quality modeling system (CMAQ; Byun and Schere, 2006) is an offline chemical transport model driven by stored meteorological dynamics from regional to continental scale weather prediction models such as the Fifth-Generation NCAR / Penn State Mesoscale Model (MM5) or the Weather Research and Forecasting model (WRF). A new Carbon Bond chemical mechanism developed in 2005, called CB05 (Yarwood et al., 2005), superseded the Carbon Bond version IV (CB4) mechanism used in the CMAQ model. With around 60 additional reactions, CB05 provides a more detailed representation of urban chemistry while improving the treatment of biogenics, toxics, and species key to the formation of particulate matter and acid deposition (Sarwar et al., 2008).

The Weather Research and Forecasting with Chemistry model (WRF/Chem; Grell et al., 2005) has online coupled chemistry and meteorology, useful for examining two-way interactions between chemistry, aerosols, meteorology, and radiation. The CB05 chemical mechanism was recently implemented in WRF/Chem via its Kinetic PreProcessor (KPP; Sandu and Sander, 2006) modules.

Objective

The object of this study is to conduct a model intercomparison between WRF/Chem Ver. 2.2 with CB05 and the latest CMAQ model (Ver. 4.7), with a focus on ground-level ozone (O_3) predictions.

Approach

• Run WRF/Chem with CB05 for a 10-day period with an O_3 episode, coincident with existing CMAQ simulations that were driven by WRFgenerated meteorology

• Use same emissions for both WRF/Chem and CMAQ simulations

 Conduct comparison of results using air quality forecasting statistical analysis techniques utilizing AIRNow observational data; Statistical metrics include root mean square error (RMSE), mean bias (MB), normalized mean error (NME), normalized mean bias (NMB), and correlation coefficient (r) (refer to Kang et al., 2005, formulations)

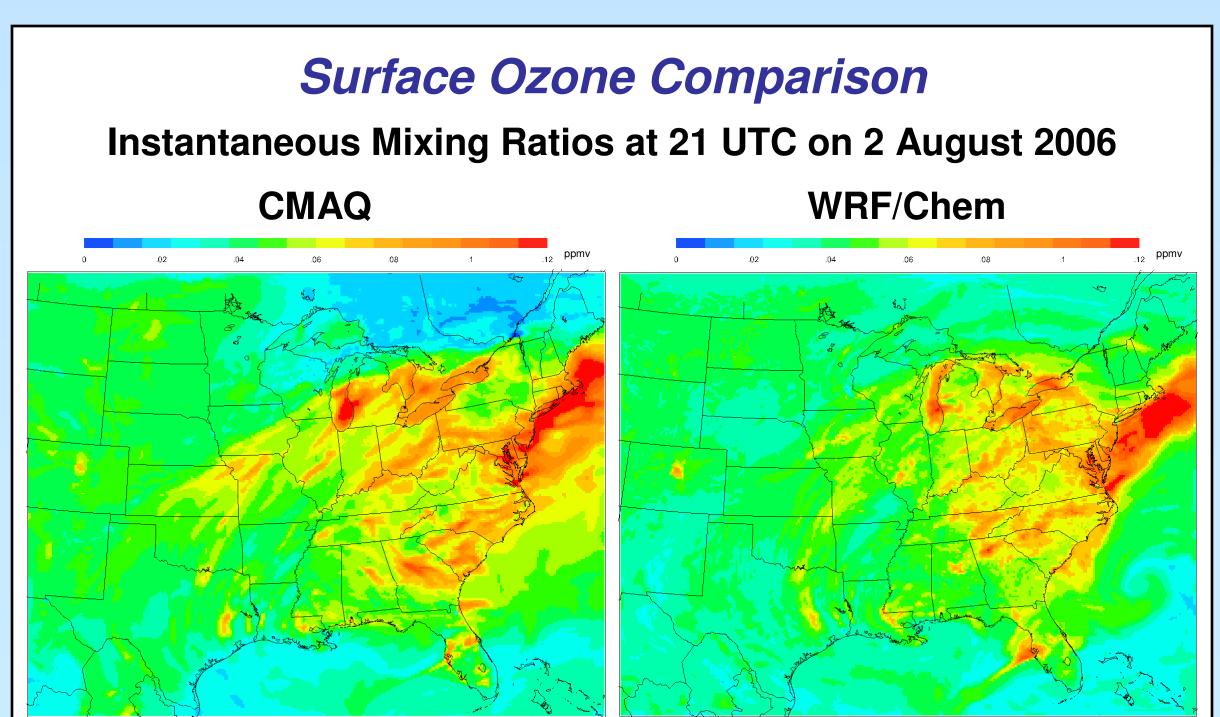
CMAQ and WRF/Chem 29 July – 7 Aug. 2006 Simulation Details

Run Specification Similarities:

WRF-ARW-generated meteorology, CB05 chemical mechanism, same emissions, same E. US 12 km grid with 34 layers

Run Specification Differences:

CMAQ – included aerosol processes; IC/BCs from larger 36 km grid parent domain; data assimilation and nudging; Pleim-Xiu; ACM2 WRF/Chem – no aerosol processes; idealized IC/BCs ("cold" start); no data assimilation or nudging; Monin-Obukhov; Noah LSM; YSU



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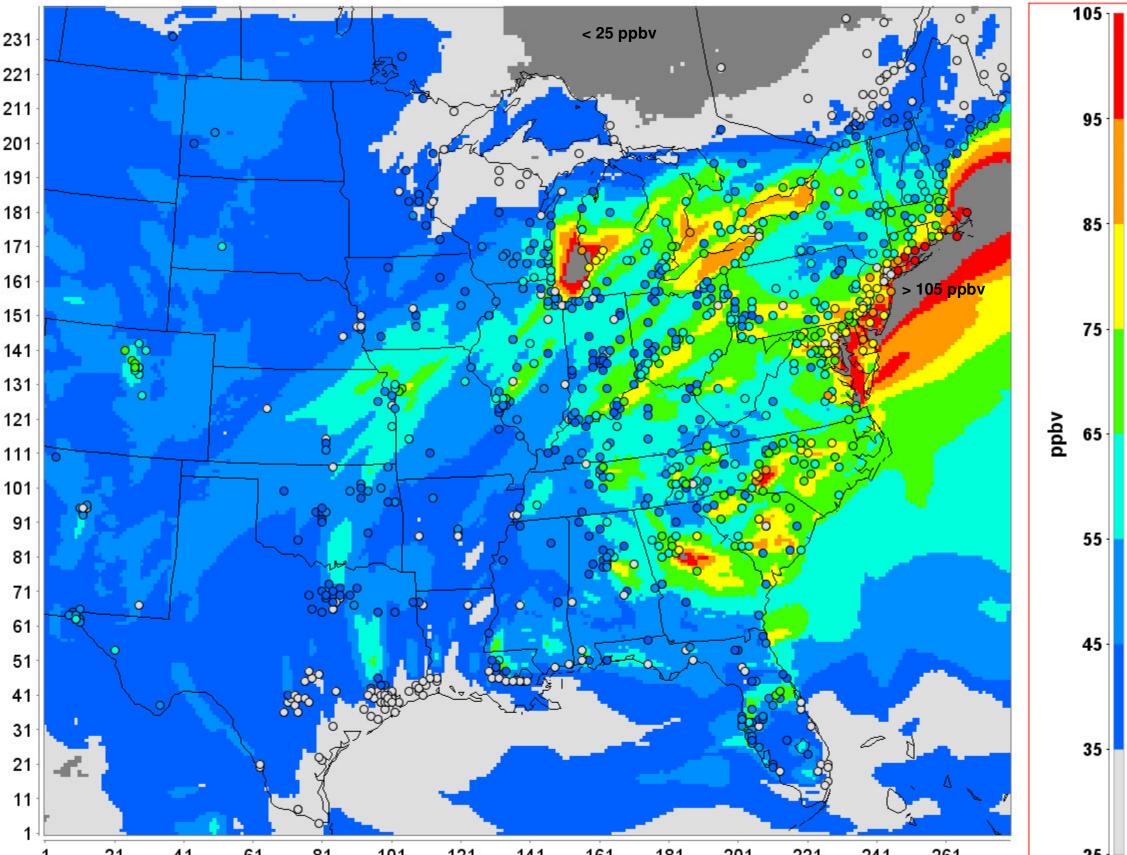
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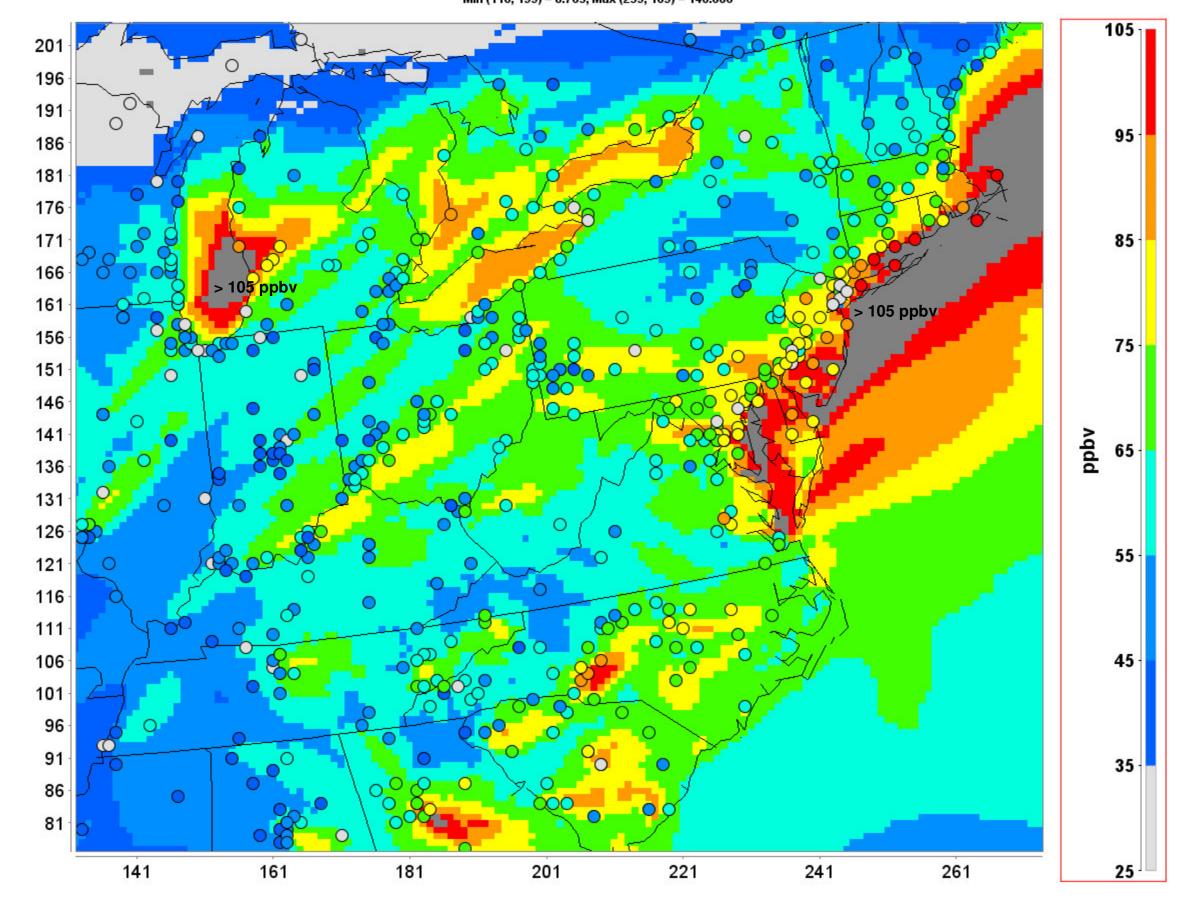
²on assignment from Science and Technology Corporation, Hampton, Virginia

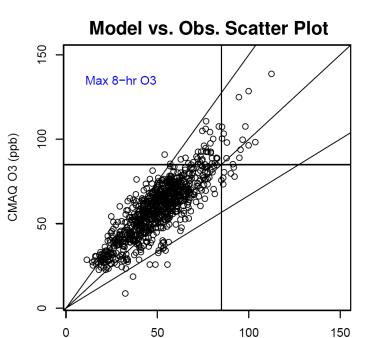
CMAQ Evaluation with AIRNow, 2 Aug. 2006

All based on maximum 8-hour average surface ozone values

WRF-driven CMAQ Maximum 8-h Averaged Surface O3 with AIRNow Data

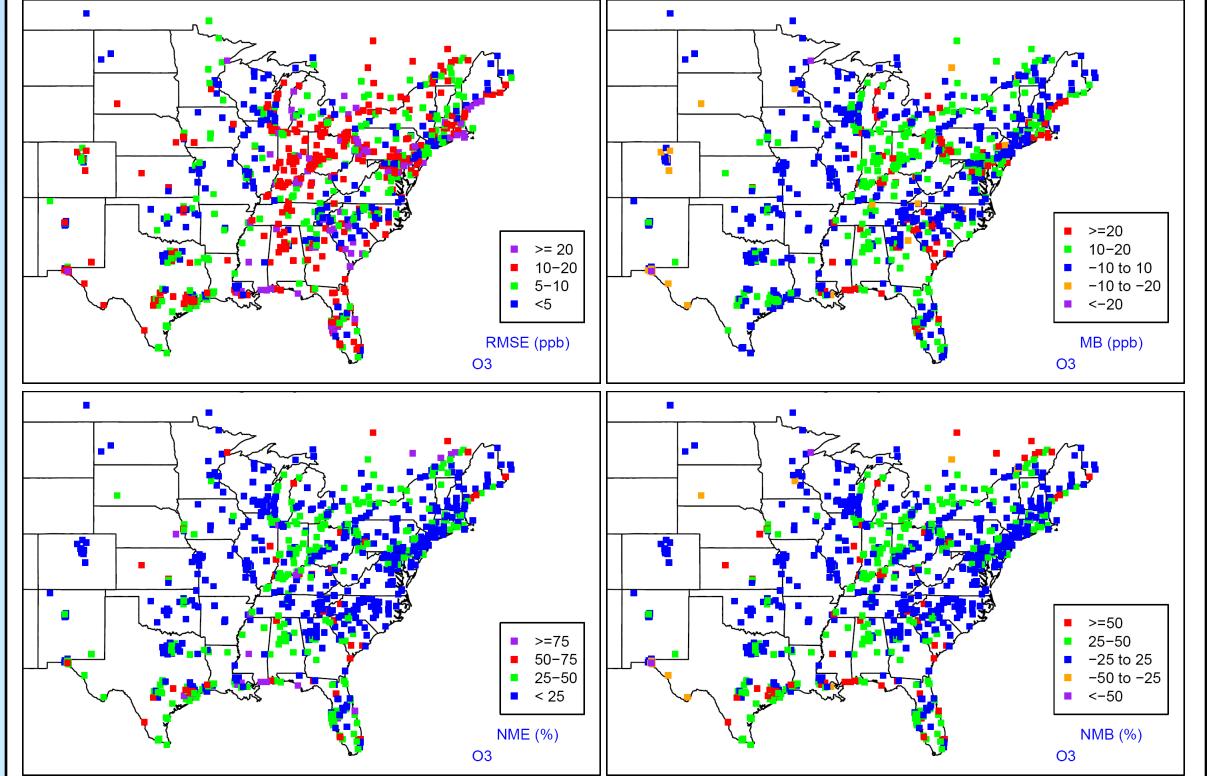






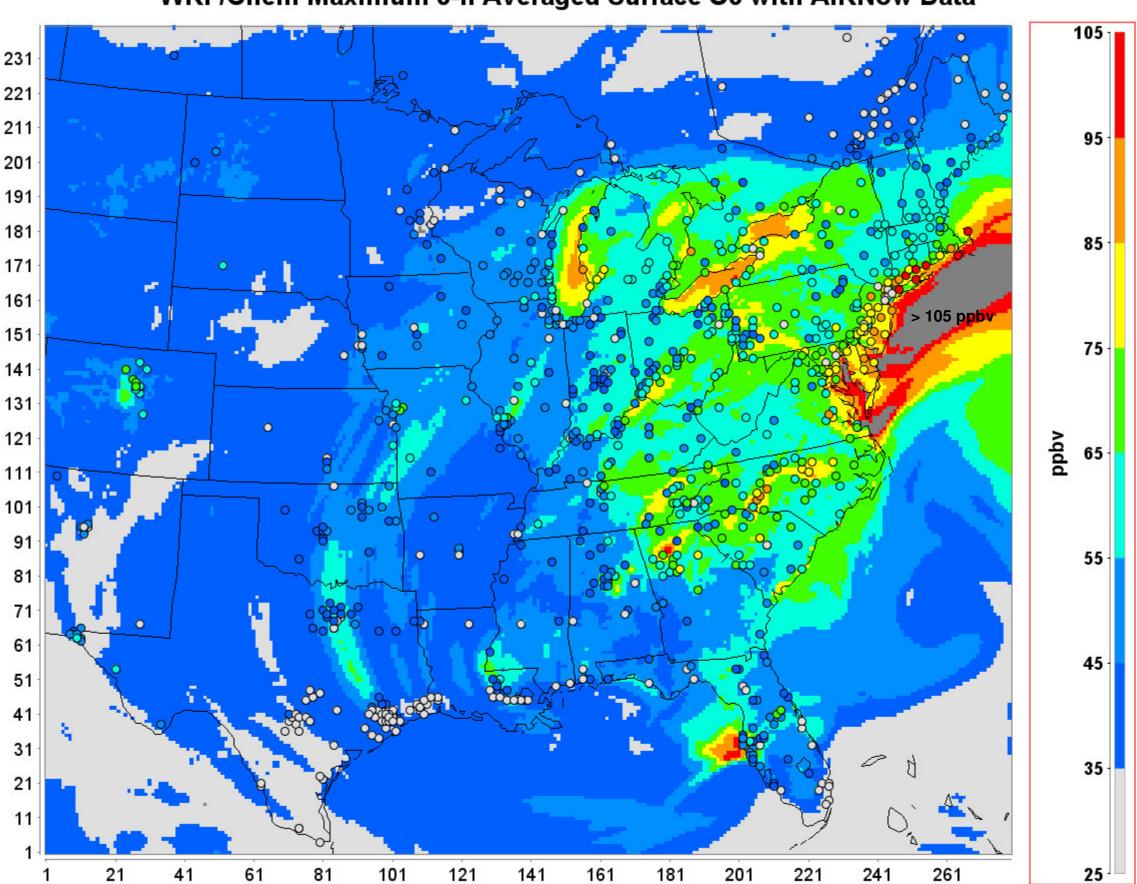
CMAQ Max8h O_3 Statistical Metrics for 2 Aug. 2006												
CMAQ	N	Obs Mean (ppbv)	Model Mean (ppbv)	RMSE (ppbv)	NME (%)	MB (ppbv)	NMB (%)	r				
E U.S.	844	50.38	58.99	12.63	20.94	8.61	17.10	0.85				

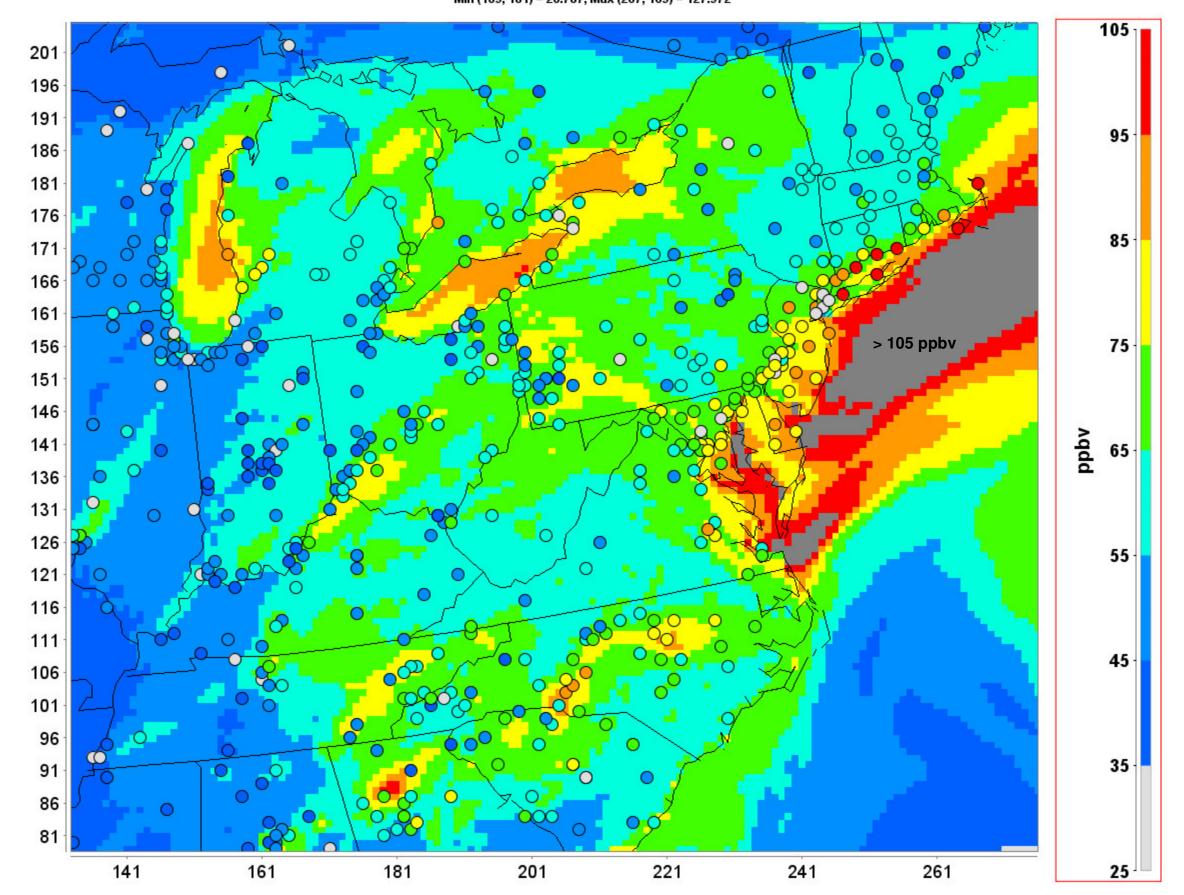
CMAQ Max8h O₃ Statistical Metrics by Monitor Location for 2 Aug. 2006



WRF/Chem Evaluation with AIRNow, 2 Aug. 2006 All based on maximum 8-hour average surface ozone values

WRF/Chem Maximum 8-h Averaged Surface O3 with AIRNow Data

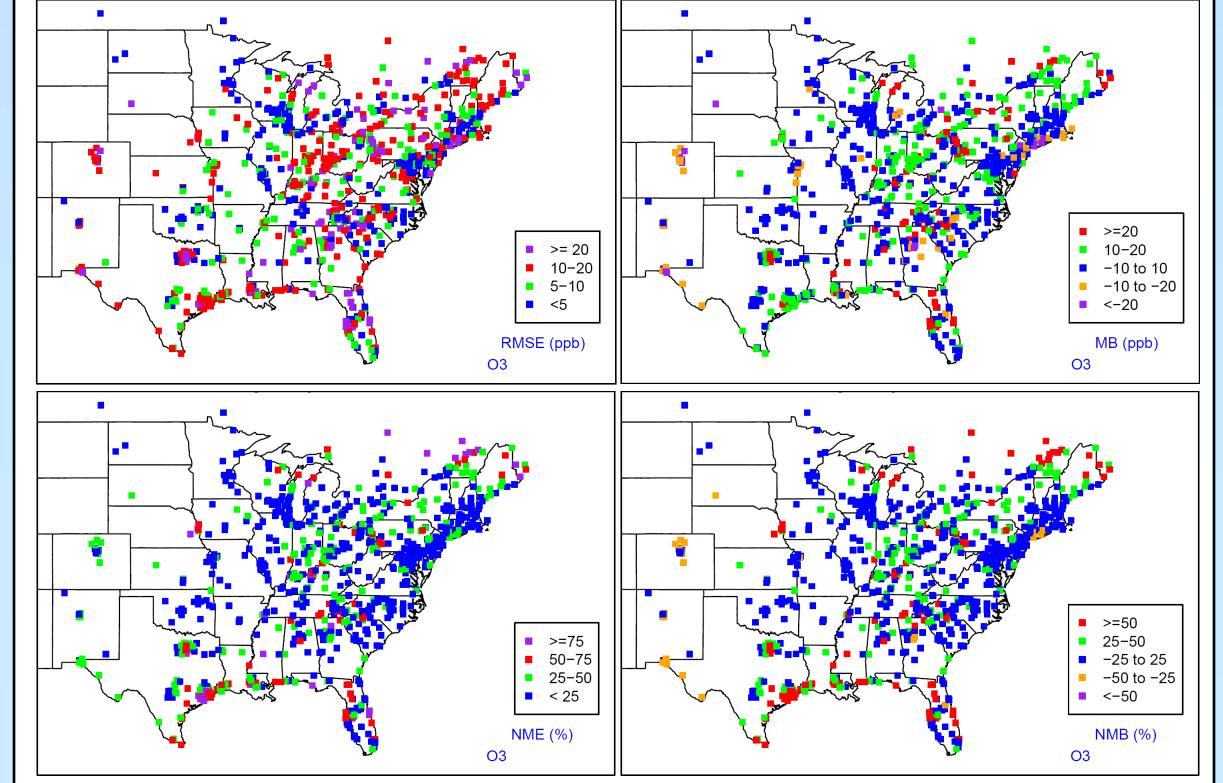




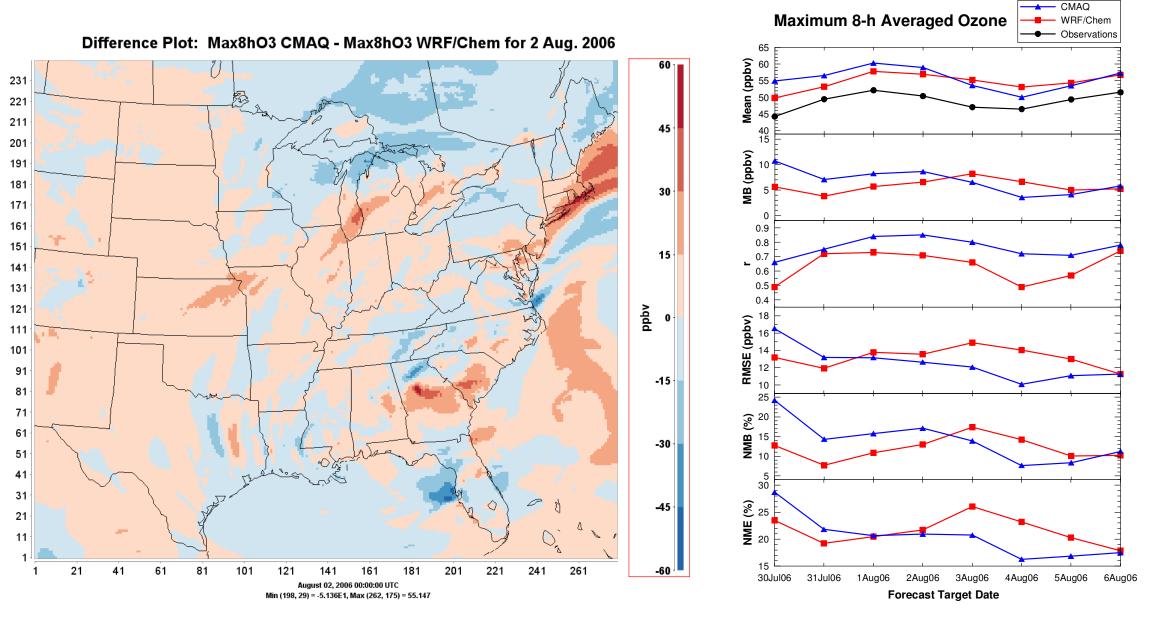
Iodel vs. Obs. Scatter Pl Max 8-hr O3

WRF/Chem Max8h O_3 Statistical Metrics for 2 Aug. 2006											
WRF/ Chem	N	Obs Mean (ppbv)	Model Mean (ppbv)	RMSE (ppbv)	NME (%)	MB (ppbv)	NMB (%)	r			
E U.S.	844	50.38	56.92	13.53	21.72	6.54	12.98	0.71			

WRF/Chem Max8h O₃ Statistical Metrics by Monitor Location for 2 Aug. 2006



Max. 8-h Avg. O₃ Differences and More Statistics



Conclusions

After examination of the maximum 8-hour average ground-level ozone from both the CMAQ and WRF/Chem model simulations for the 29 July – 7 August 2006 study period, we find:

- Both models are biased high by 5-10 ppbv, or 5-20%, using CB05
- CMAQ correlates better with observations than WRF/Chem
- CMAQ shows a greater range of values, for both high and low extremes, than WRF/Chem

• Without direct and indirect feedbacks from aerosol processes, the significance of whether an air quality model is offline or online is mostly irrelevant at these scales

Future Plans

The CB05 chemical mechanism has just been implemented in WRF/Chem V3.0.1.1, which will now allow a rerun of the study period using the same physics options as used in the WRF-ARW that drives the CMAQ model. The 36 km domain IC/BCs and FDDA will also be applied to the WRF/Chem rerun, resulting in a better chemistry model comparison. The CB05 mechanism could also be coupled to one of the available aerosol schemes (such as MADE/SORGAM or MOSAIC) already included in the WRF/Chem model in order to take full advantage of the two-way feedbacks and online framework.

References

Byun, D., and K. L. Schere, 2006: 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, 51-77.

Grell, G. A., S. E. Peckham, R. Schmitz, S. A. McKeen, G. Frost, W. C. Skamarock, and B. Eder, 2005: Fully coupled "online" chemistry within the WRF model. Atmos. Environ., 39, 6957-6975. Kang, D., B. K. Eder, A. Stein, G. A. Grell, S. E. Peckham, and J. McHenry, 2005: The New England Air Quality Forecasting Pilot Program: Development of an evaluation protocol and performance benchmark. J. Air & Waste Manage. Assoc., 55, 1782-1796.

Sandu, A., and R. Sander, 2006: Technical Note: Simulating chemical systems in Fortran90 and Matlab with the kinetic preprocessor KPP-2.1. Atmos. Chem. Phys., 6, 187-195.

Sarwar, G., D. Luecken, G. Yarwood, G. Z. Whitten, and W. P. L. Carter, 2008: Impact of an updated carbon bond mechanism on predictions from the CMAQ modeling system: Preliminary assessment. J. Appl. Meteor. Clim., 47, 3-14.

Yarwood, G., S. Rao, M. Yocke, and G. Whitten, 2005: Updates to the carbon bond chemical mechanism: CB05. Final report to the U.S. EPA, RT-0400675. [Available online at http://www.camx.com.]

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Disclaimer

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