Simulating Ozone: A Comparative Analysis of CMAQ and WRF/Chem

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Introduction

The interaction of meteorology and chemistry is a fundamental part of any air quality (AQ) modeling system. The Community Multiscale Air Quality modeling system (CMAQ) is an offline chemical transport model driven by stored meteorological dynamics from weather prediction models such as the Weather Research and Forecasting model (WRF). In contrast, the WRF with Chemistry model (WRF/Chem) is online-coupled, solving the meteorology and chemistry together each time step, thereby allowing bidirectional feedbacks between the chemistry, aerosols, radiation, cloud microphysics, and meteorology during the simulation.

Objective

The purpose of this study is to conduct a comparative analysis between CMAQ and a modified version of WRF/Chem, focusing on simulated ozone (O_3) and selected processes responsible for any differences between the model predictions.

Approach

- To increase compatibility of the models for intercomparison, the CB05 chemical mechanism was implemented into WRF/Chem v3.0.1.1 and coupled to the MADE/SORGAM aerosol scheme.
- Additional model compatibility was achieved by converting CMAQ-ready emissions, initial and boundary conditions for WRF/Chem use.
- Ran a one-month simulation (August 2006, with July 29-31 spin-up) using the modified WRF/Chem for comparison with an available WRF-driven CMAQ v4.7 air quality simulation of the same period.

Simulation configuration similarities:
Eastern U.S. domain with 12 km grid spacing and 34 layers up to 100 hPa; initial/boundary conditions from NAM (for meteorology) and a CMAQ 36 km simulation (for chemistry); CB05; emissions based on 2001 NEI projected to 2006, BEIS Ver. 3.13, and Mobile6; RRTM longwave radiation; grid (analysis) FDDA; surface updates to SST, albedo, and vegetative fraction; USGS land use; effects of topographic slope and shading on radiation; horizontal Smagorinsky first-order closure; and subgrid convective chemistry transport.
Simulation configuration differences:

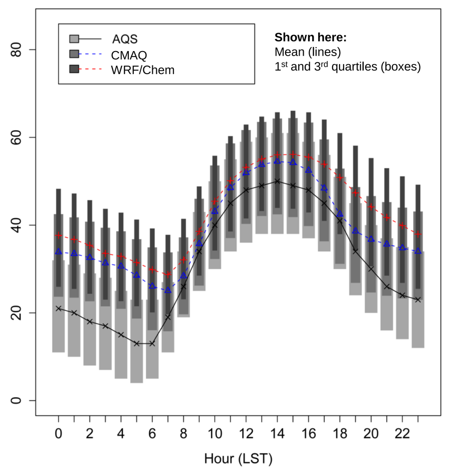
Model Feature	WRF and CMAQ	WRF/Chem
Microphysics	WSM 6-class	Lin et al.
Shortwave Radiation	Dudhia	Goddard
Sfc. Layer Physics	Pleim-Xiu (P-X)	Monin-Obukhov
Land Surface Model	Pleim-Xiu	Noah
Boundary Layer	ACM2	YSU
Cumulus Parm.	Kain-Fritsch	Grell-Devenyi
w-damping	no	yes
Positive-Def. Adv.	moisture, chemistry	moisture, scalars, chemistry
Photolysis	JPROC	Fast-J
Aerosols	AE4 with updated N_2O_5 gamma parm.	MADE/SORGAM

Note: P-X and ACM2 are currently incompatible with WRF/Chem, so recommended alternatives were chosen. Other option differences in WRF/Chem were chosen to allow feedbacks from the aerosols and convective parameterization to the radiation and photolysis schemes. Also, WRF/Chem in this configuration had only a partial, experimental scheme for aqueous phase chemistry.

- Conducted statistical analyses of the month-long WRF/Chem and WRF-driven CMAQ simulations using the Atmospheric Model Evaluation Tool (AMET) and additional custom-built analysis tools.

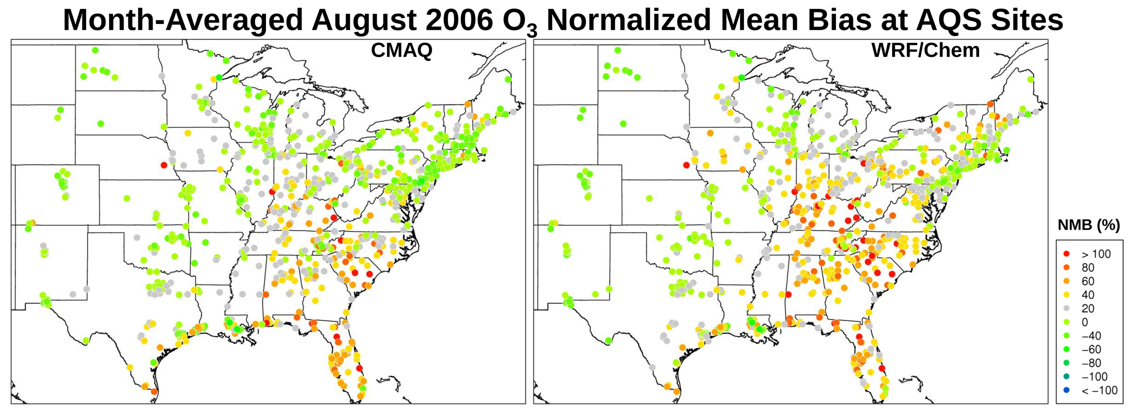
Evaluation of Simulated Ozone

Max. 8-h Avg. O_3 Statistic	CMAQ	WRF/Chem
RMSE (ppbv)	11.52	13.57
NME (%)	18.2	21.5
MB (ppbv)	3.62	6.18
NMB (%)	7.4	12.7
r	0.72	0.66

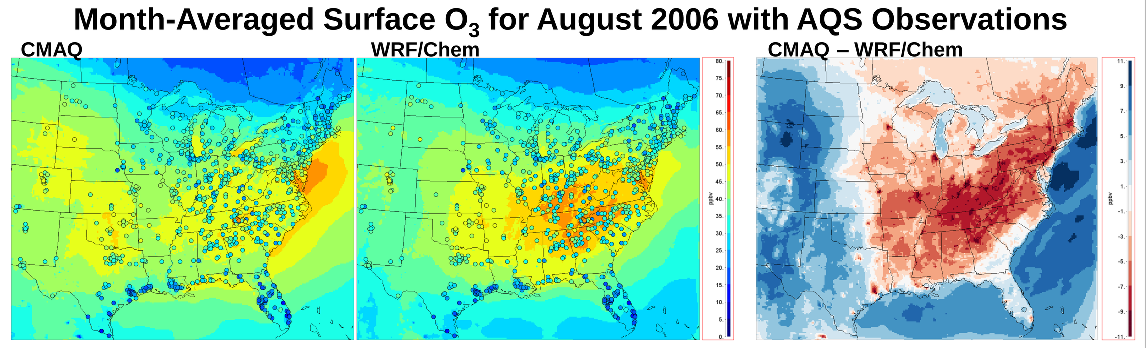


Max. 8-h avgd. statistics and hourly boxplot for O_3 reveal both models have a positive bias, especially at night. WRF/Chem is more biased, and it has slightly larger error and lower correlation to AQS observations than CMAQ.

Month-Averaged August 2006 O_3 Normalized Mean Bias at AQS Sites

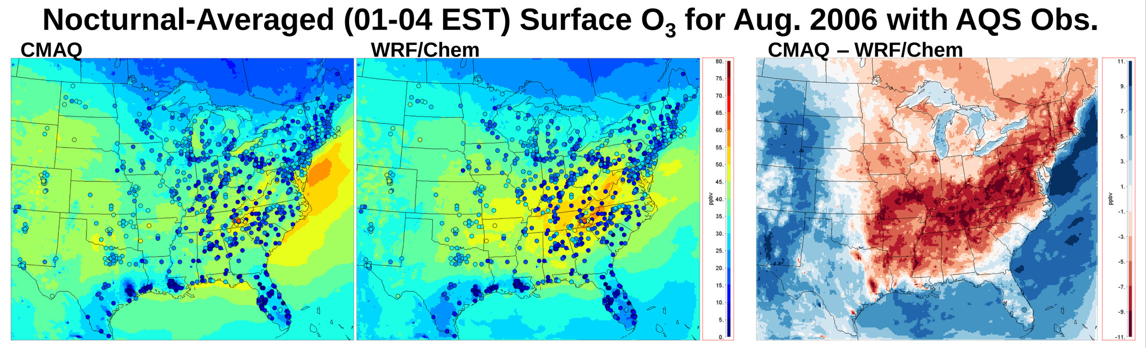


Month-Averaged Surface O_3 for August 2006 with AQS Observations

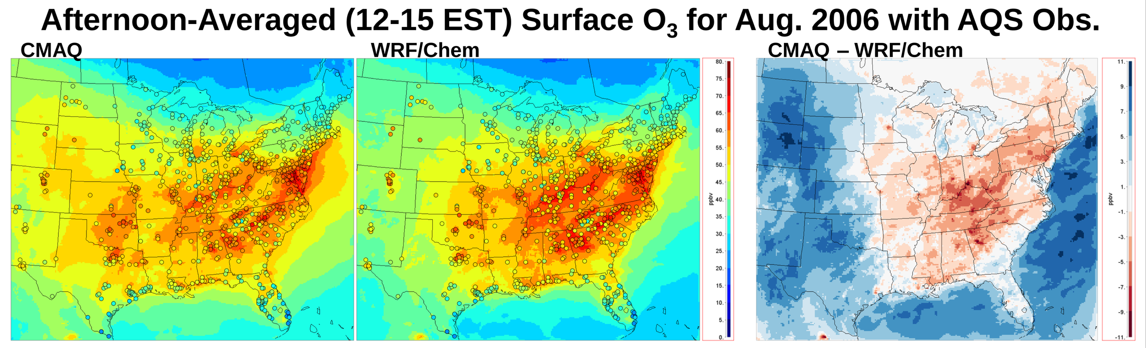


These spatial plots show that both models overestimate O_3, mainly in the South and Ohio River Valley where WRF/Chem bias is greater.

Nocturnal-Averaged (01-04 EST) Surface O_3 for Aug. 2006 with AQS Obs.

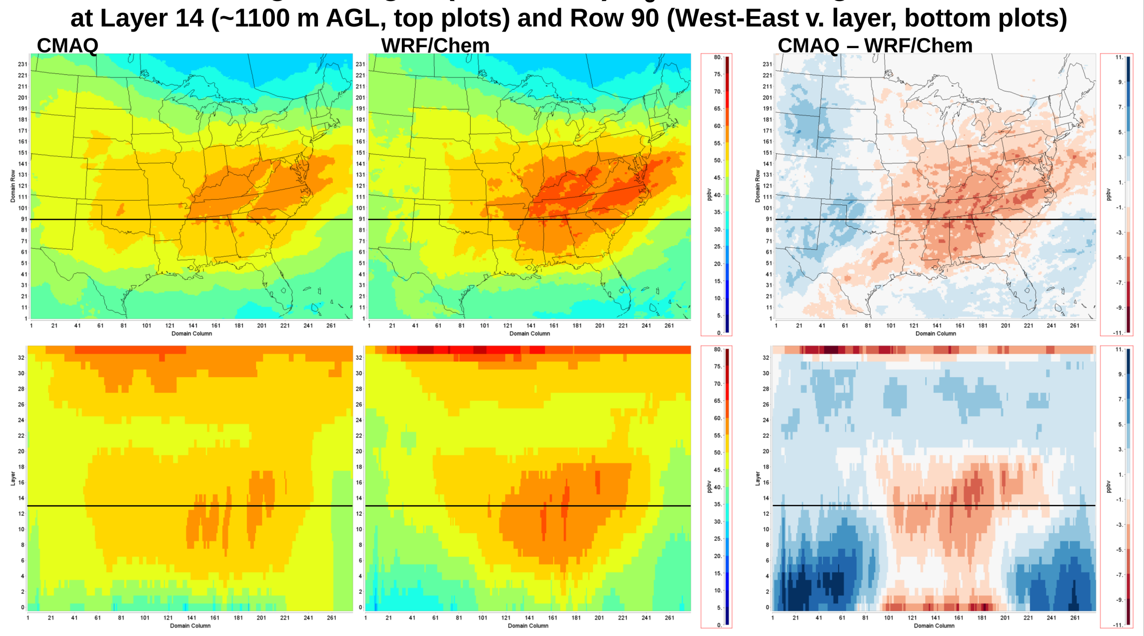


Afternoon-Averaged (12-15 EST) Surface O_3 for Aug. 2006 with AQS Obs.



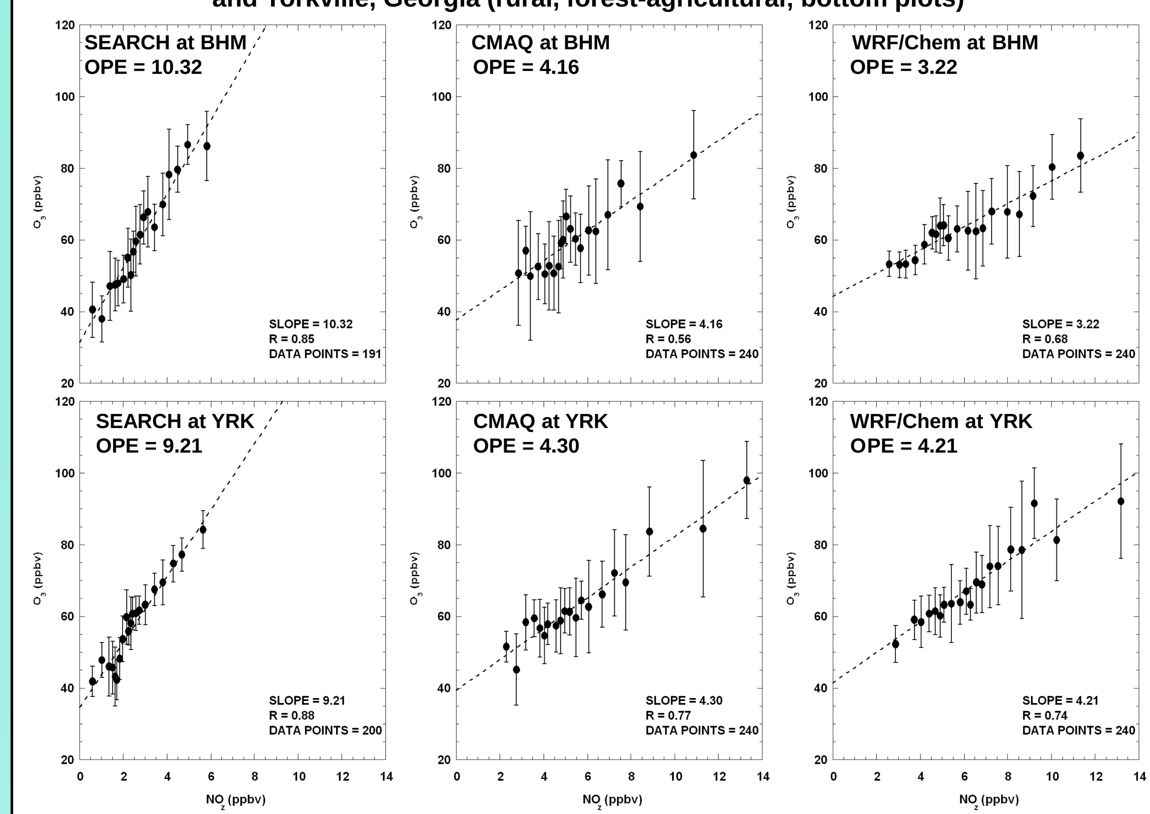
Examining month averages over different periods of the diurnal cycle show the pronounced nocturnal positive bias; less so in the afternoon.

Morning-Averaged (06-09 EST) O_3 Aloft for August 2006
at Layer 14 (~1100 m AGL, top plots) and Row 90 (West-East v. layer, bottom plots)

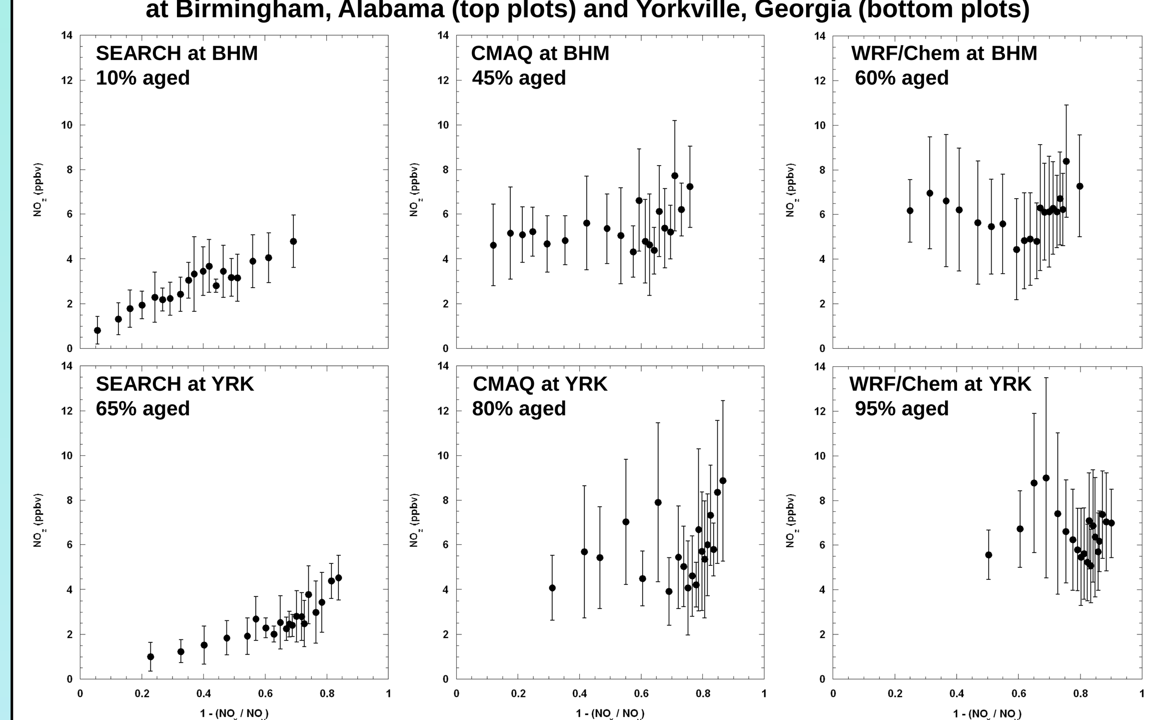


WRF/Chem has more O_3 available in the residual layer on average.

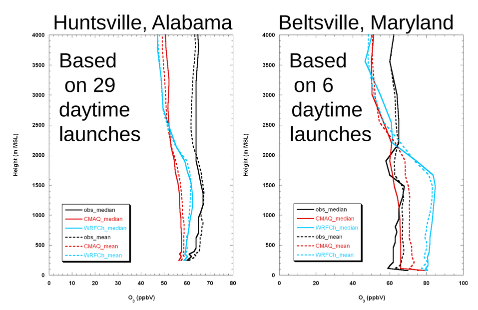
Ozone Production Efficiency (OPE) (10-17 LST) for August 2006
at Birmingham, Alabama (urban, industrial-residential; top plots) and Yorkville, Georgia (rural, forest-agricultural; bottom plots)



Airmass Photochemical Age (10-17 LST) for August 2006
at Birmingham, Alabama (top plots) and Yorkville, Georgia (bottom plots)

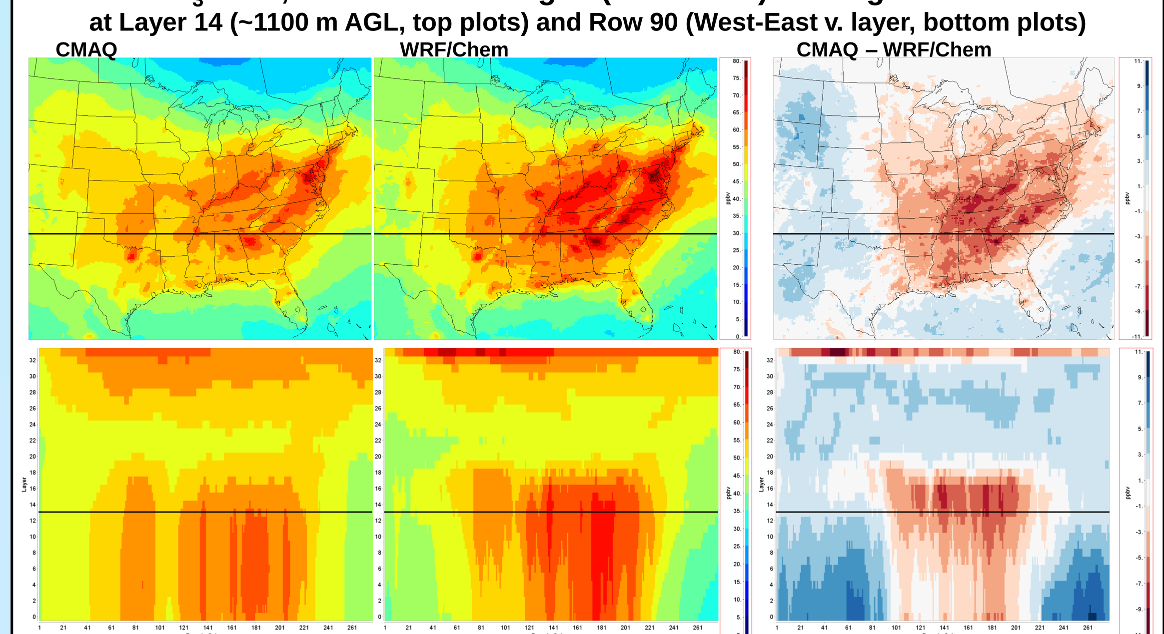


OPE and airmass photochemical age computed from SEARCH data and model results at two sites illustrate that modeled air in grid cell volumes is more aged and has less potential for ozone production.



A comparison of IONS06 ozonesonde observations with corresponding simulated O_3 profiles averaged over available daylight launch times during August 2006 (shown at right) show that both models underestimate O_3 above the PBL and can be either positively or negatively biased within the PBL. At these two IONS06 sites, WRF/Chem has noticeably more O_3 within the boundary layer than CMAQ, though this is not always the case (per other IONS06 sites).

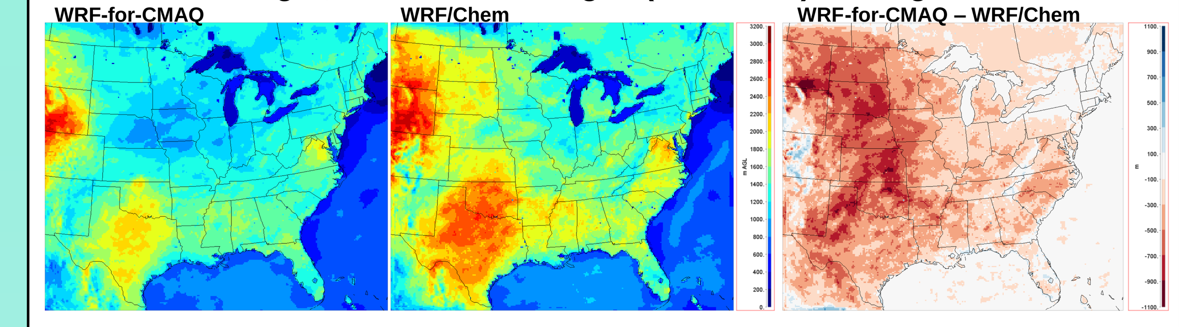
O_3 Aloft, Afternoon-Averaged (12-15 EST) for August 2006
at Layer 14 (~1100 m AGL, top plots) and Row 90 (West-East v. layer, bottom plots)



WRF/Chem also has more O_3 aloft in the afternoon than CMAQ over the eastern half of the U.S., suggesting a persistent O_3 accumulation.

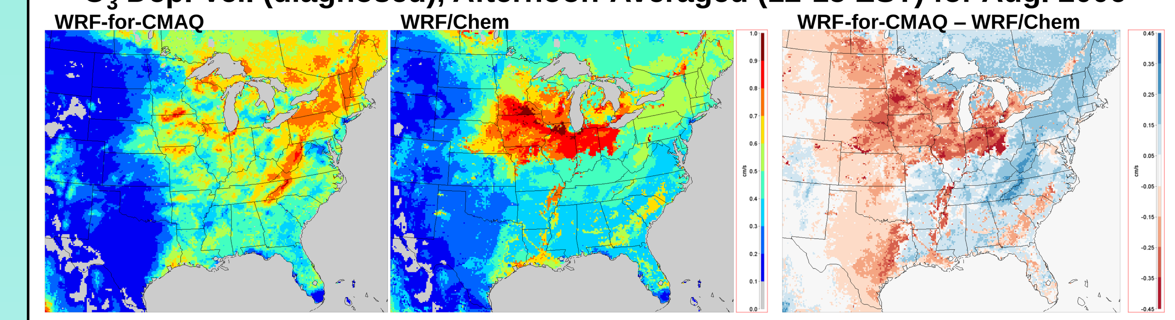
Examination of Associated Processes

PBL Height, Afternoon-Averaged (12-15 EST) for August 2006



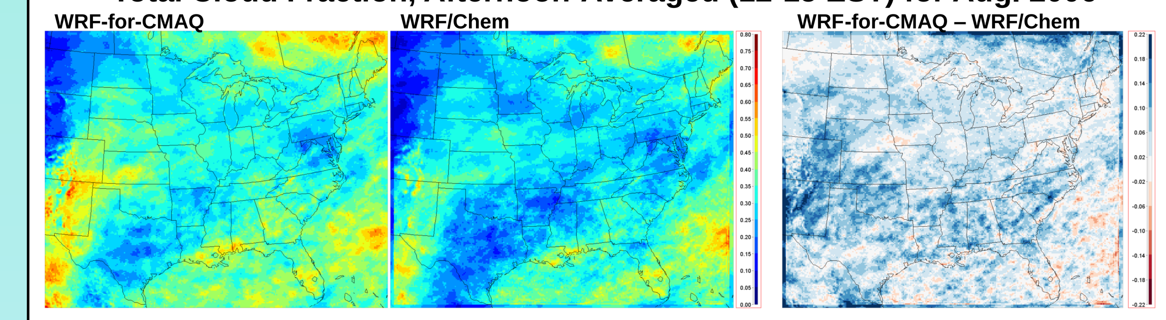
WRF/Chem has a deeper PBL; remarkable considering its greater O_3.

O_3 Dep. Vel. (diagnosed), Afternoon-Averaged (12-15 EST) for Aug. 2006

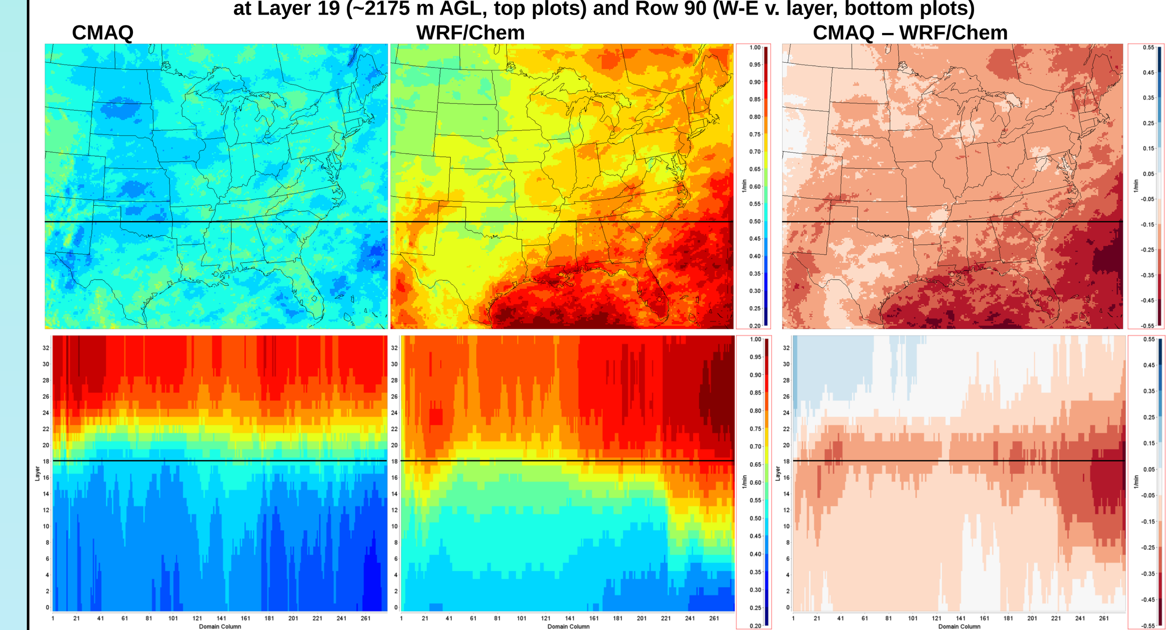


Differences in O_3 deposition partially explain simulated O_3 differences.

Total Cloud Fraction, Afternoon-Averaged (12-15 EST) for Aug. 2006



J_{NO2} Photolysis Rate Aloft, Afternoon-Avgd. (12-15 EST) for Aug. 2006
at Layer 19 (~2175 m AGL, top plots) and Row 90 (W-E v. layer, bottom plots)



Cloudier conditions would reduce photolysis in CMAQ, but differences in J_{NO2} aloft (e.g., shown above) reveal differences in the way CMAQ's JPROC treats cloud effects compared to WRF/Chem's Fast-J.

Conclusions

- Both CMAQ and WRF/Chem overestimate surface ozone during August 2006, mainly in the South and Ohio River Valley.
- WRF/Chem produces more ozone than CMAQ despite having the same chemical mechanism, emissions, and initial/boundary conditions, plus a generally deeper boundary layer of more aged air.
- Over regions where simulated ozone is biased high, WRF/Chem builds and maintains a 10% greater reservoir of O_3 aloft than CMAQ.
- Differences in land surface model and boundary layer physics, dry deposition, clouds, and especially photolysis rates contribute to the presence of more ozone in WRF/Chem than in CMAQ; Chosen model options are important factors in determining AQ simulation results.

Acknowledgements

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