Analysis of a summertime air pollution episode with a new dry deposition velocity scheme

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1. INTRODUCTION

M3DRY is a state of the science gaseous dry deposition velocity scheme used in the Meteorology-Chemistry Interface Processor (MCIP) and Community Multiscale Air Quality (CMAQ) models. The implementation of M3DRY into WRF-chem will be presented and compared to the Wesely scheme, which is WRF-chem's default dry deposition velocity routine. WRF-chem simulations with the M3DRY and Wesely dry deposition velocity schemes will be presented for an air quality episode on July 9, 2007, in which 8-hour maximum ozone and 24-hour average $PM_{2.5}$ concentrations in northeastern Maryland reached 125ppbv and 40μg/m^3 respectively.

WRF-chem simulations are being used as a tool for satellite verification and planning for the development of future satellite instruments that observe trace gases and aerosols in the troposphere. The WRF-chem simulations will be presented and compared with ground-based measurements and satellite observations from the Ozone Monitoring Instrument (OMI) and the Tropospheric Emissions Spectrometer (TES) onboard the Aura satellite. Also, the use of WRF-chem in an Observing System Simulation Experiment for the Geostationary Coastal and Air Pollution Events (GEO-CAPE) mission will be discussed. One of the goals of the GEO-CAPE satellite is to provide hourly daytime maps of air pollution that can be used in air quality analyses and forecasting. Air quality observations from a geostationary satellite have the potential to be a great asset to the air quality field.

2. IMPLEMENTATION OF M3DRY

M3DRY was implemented in WRF-Chem in order to investigate the causes of large differences in ammonia and in dry deposition velocities between WRF-Chem simulations with the Wesely scheme and CMAQ simulations with M3DRY. Simulations with WRF-chem Version 2.2 with both the RADM2 and CBMZ chemical mechanisms show higher ammonia concentrations than CMAQ simulated concentrations (Figure 1) (Yegorova et al., 2008). M3DRY, described in Pleim et al., (2001) and Byun and Ching (1999), has superseded the Wesely dry deposition velocity routine in CMAQ and MCIP. M3DRY is continuously updated at the Community Modeling and Analysis System Center within MCIP and CMAQ as science evolves.

WRF-chem simulations with the M3DRY and the Wesely dry deposition schemes are compared to investigate the differences between the two schemes. Nested 36km and 12km horizontal resolution simulations were performed from July 6 to July 12, 2007 with the CBMZ chemical mechanism and 8 bin MOSAIC aerosols. The 36km domain has dimensions of 170 (east-west) by 103 (north-south) mass points covering the continental US, while the 12km domain has 169 by 169 mass points covering the eastern half of the US. Both domains have 32 vertical levels. Emissions were processed with the Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System with projected 2009 emissions from US Regional Planning Offices and 2007 Continuous Emissions Monitoring Systems measurements.

Figure 2 shows a comparison of CO, O_3, H_2O_2, NH_3, HNO_3, PAN, $PM_{2.5}$, Nitrate, and Ammonium between the two simulations at Maryland ozone monitoring sites. Also included in Figure 2 are the ozone observations. CO concentrations are lower with the M3DRY deposition velocity scheme by an average of 28 ppbv due to Wesely scheme setting CO dry deposition velocity to zero. Ozone concentrations are slightly lower in Maryland with the M3DRY scheme which produces faster dry deposition velocity over Maryland as shown in Figure 3, which displays dry deposition velocities of O_3, H_2O_2, and NH_3. The Wesely scheme produces deposition velocities around 0.1 cm/s over water while the M3DRY scheme calculates velocities around 0.001cm/s. Observed deposition velocities of ozone over water range from 0.01 to 0.12 cm/s (Fairall et al., 2007). Figure 4 shows 8-hour maximum ozone concentrations on July 9, 2007 from ground observations and the M3DRY and Wesely WRF-chem simulations. The M3DRY simulation

calculates less ozone over most of the land and more ozone over the water. The lower H_2O_2 and NH_3 concentrations with the M3DRY scheme shown in Figure 2 correspond with faster deposition velocities as seen in Figure 3. The lower ammonia concentrations correspond with the lower ammonium nitrate aerosol concentrations in Figure 2.

Table 1: WRF-chem configuration options

Atmospheric Processes	**WRF-chem**
Radiation	LW: RRTM SW: Goddard
Surface Layer	MM5 similarity Monin-Obukov
Land Surface Model	Noah
Boundary Layer	YSU
Cumulus	Grell 3D ensemble
Microphysics	Lin et al.
Photolysis	Fast-J
Meteorological initial and boundary conditions	NARR
Chemical initial and boundary conditions	MOZART

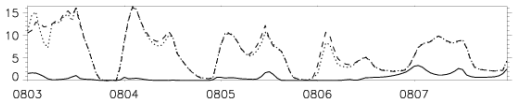

Fig. 1: Surface layer NH_3 concentrations (ppbv) for CMAQ simulation (solid line) WRF-chem Version 2.2 with CBMZ chemical mechanism (dotted line), and WRF-chem Version 2.2 with RADM2 chemical mechanism (dashed line) (Yegorova et al., 2008).

3. WRF-CHEM AS A TOOL FOR SATELLITE VERIFICATION

A WRF-chem simulation is used to investigate if Ozone Monitoring Instrument (OMI) and Troposphere Emission Spectrometer (TES) products can capture a high air pollution episode. A WRF-chem simulation with the RADM2 chemical mechanism, MADE-SORGAM aerosols, and the M3DRY dry deposition velocity was performed for the same July 2007 episode and the same configuration options as shown in Table 1. The simulation consisted of a single domain at 12km horizontal resolution, 173 by 173 mass points, and 23 vertical levels. WRF-chem output is compared with OMI total ozone column subtracted by Microwave Limb Sounder stratospheric ozone column (OMI/MLS) from Mark Schoeberl, OMI level 2 tropospheric ozone observations from Xiong Liu, MOZART model output, and TES Step and Stare Special observations tropospheric ozone.

Tropospheric ozone column from OMI/MLS, WRF-chem, OMI, MOZART, and TES Step and Stare at 18 UTC July 9, 2007 are shown in Figure 5. Along the TES Step and Stare track, TES tropospheric O3 column is greatest, followed by WRF/Chem, OMI, and OMI/MLS column. The lower OMI/MLS tropospheric O3 column values are partially explained by lower tropopause heights and the low detection efficiency of OMI in the PBL. Model calculated and satellite observed tropospheric ozone columns are greater off the coast illustrating continental outflow of pollution. Figure 6 compares WRF-chem with TES and OMI column ozone in the surface to 800 hPa layer, 800 to 600 hPa layer, and tropospheric column along the TES Step and Stare track. OMI measured higher ozone column in the lower troposphere (surface to 800 hPa) even though OMI has fewer points than TES in the column. OMI and TES have better agreement in the residual layer and tropospheric column ozone.

4. WRF-CHEM AS A TOOL FOR DEVELOPING FUTURE SATELLITES

The WRF-chem simulation with M3DRY and CBMZ chemical mechanism described above is being used to help plan for the Geostationary Coastal and Air Pollution Events mission. An Observing System Simulation Experiment (OSSE) is underway using WRF-chem and GEOS 5 model output, radiative transfer codes, and retrieval algorithms. Tropospheric chemical and meteorological information from WRF-chem is being combined with middle and upper atmosphere output from the Geos 5 model during the first step of the OSSE. The OSSE will help determine the spatial and temporal scales the Geo-Cape satellite needs to observe air pollution from space.

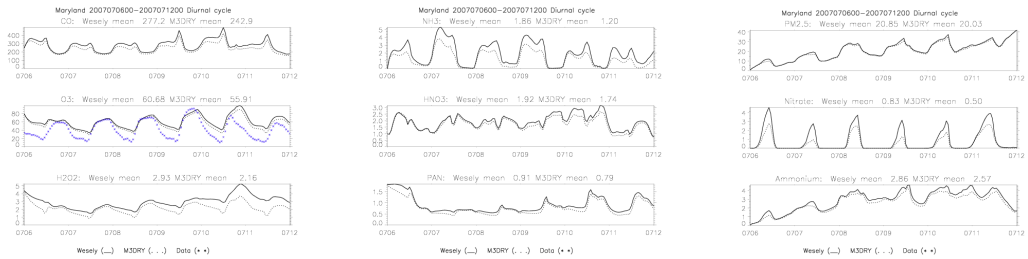

Fig. 2: Time-series of average concentrations in ppbv of CO, O_3, H_2O_2, NH_3, HNO_3, and PAN and in ug/m^3 of $PM_{2.5}$, Nitrate, and Ammonium at all surface ozone monitoring sites in Maryland. The ozone time-series includes observed ozone.

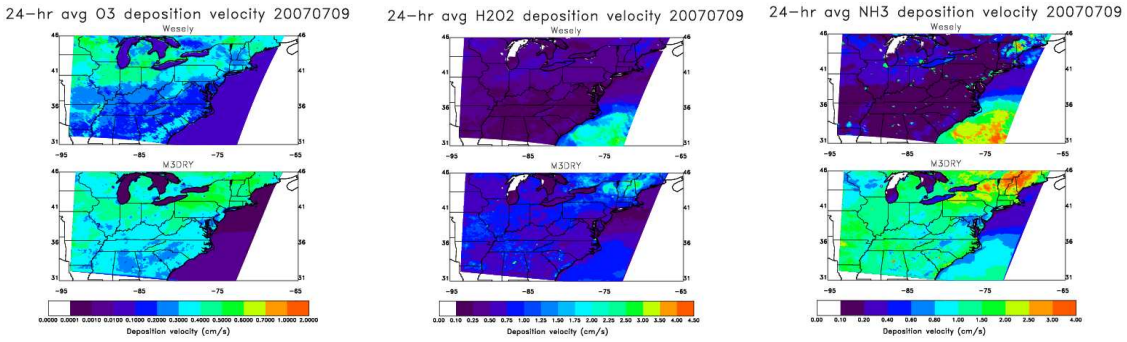

Fig. 3: 24-hour average O_3, H_2O_2, and NH_3 dry deposition velocity with the Wesely and M3DRY schemes on July 9, 2007.

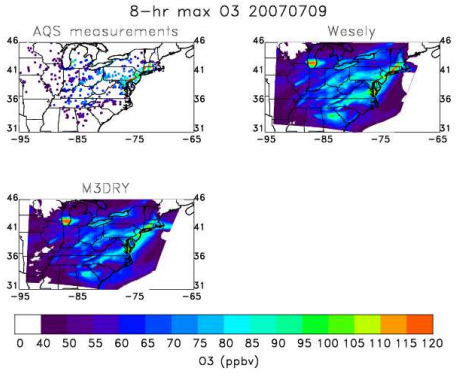

Fig 4: Surface layer 8-hour maximum O_3 concentrations from ground observations and the Wesely and M3DRY WRF-chem simulations with the CBMZ chemical mechanism on July 9, 2007.

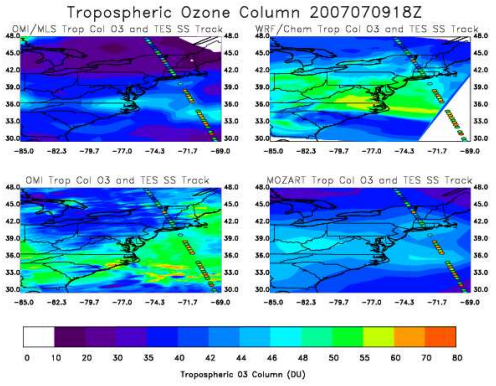

Fig 5: TES Step and Stare tropospheric column ozone overlaid on OMI/MLS, WRF-chem, OMI, and MOZART tropospheric column ozone at 18 UTC July 9, 2007.

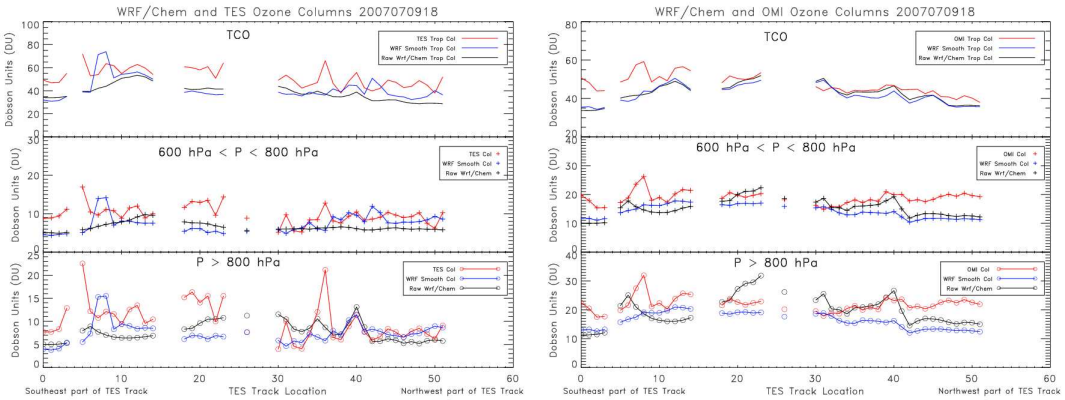

Fig 6: A comparison of WRF-chem, TES, and OMI tropospheric column ozone, 800-600 hPa layer ozone, and surface-800 hPa layer ozone. Raw WRF-chem stands for WRF-chem before model output is processed through the TES or OMI averaging kernel and WRF smooth stands for WRF-chem output after being processed with the averaging kernel.

4. CONCLUSIONS

WRF-chem simulations with a new dry deposition velocity scheme, M3DRY, during an air pollution episode in July 2007 are compared with ground and satellite observations. Comparisons between the M3DRY and Wesely schemes reveal differences in CO, NH_3, O_3, and H_2O_2 dry deposition velocities. WRF-chem and satellite observations revealed continental pollution outflow over the Atlantic. In addition to using WRF-chem to validate satellite retrievals, WRF-chem is also being used to plan for the development of the Geo-Cape satellite which will improve air quality observations from space.

5. REFERENCES

Byun, D.W. and J.K.S. Ching, 1999: Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System, NERL, Research Triangle Park, NC, EPA/600/R-99/030.

Fairall, C.W., D. Helmig, L. Ganzeveld, and J. Hare, 2007: Water-side turbulence enhancement of ozone deposition to the ocean. Atmospheric Chemistry and Physics, vol7, 443-451.

Pleim, J.E., A. Xiu, P.L. Finkleston, and T.L. Otte, 2001: A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. Water, Air, and Soil Pollution: Focus, vol 1, 243-252.

Yegorova, E.A., D. Allen, C.P. Loughner, K. Pickering, 2008: WRF-chem simulations of Mid-Atlantic air quality. 9th Annual WRF User's Workshop.