WRF-Chem modeling of an eastern U.S. pollution event: Comparison with measurements and evaluation of M3DRY dry deposition scheme

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Goals of today’s talk

- Analyze a July 2007 east coast of the U.S. air pollution event using observations and WRF-Chem output.
- Evaluate how well the OMI & TES instruments aboard the Aura satellite detect air pollution.
- Assess sensitivity of WRF-calculated trace gases to the dry deposition algorithm: M3DRY vs. Wesely.
- Show how WRF-CHEM results are being used in support of the upcoming GEO-CAPE mission (2018-2020).
Air quality on July 9, 2007 was Code Red (very bad) in the Mid-Atlantic. 8-hr max O₃ of 131 ppbv within Baltimore NAA.

Baltimore, MD visibility during a clear day

Baltimore, MD visibility At 6:45 PM July 9, 2007

Images obtained from the U.S. Air Quality Smog Blog (http://alg.umbc.edu/usaq).
### WRF-Chem Configuration

<table>
<thead>
<tr>
<th>Atmospheric Processes</th>
<th>WRF/Chem</th>
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<tbody>
<tr>
<td>Radiation</td>
<td>LW: RRTM SW: Goddard</td>
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<tr>
<td>Surface Layer</td>
<td>Monin-Obukhov</td>
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<td>Land Surface Model</td>
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<td>Boundary Layer</td>
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<td>Cumulus</td>
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<td>Microphysics</td>
<td>Lin et al.</td>
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<td>Gas-phase chemistry</td>
<td>RADM2 CBMZ</td>
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<td>Aerosol chemistry</td>
<td>MADE/SORGAM MOSAIC</td>
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<td>Photolysis</td>
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- **Domain**: Eastern U.S.
  - 36/12 km hor res, 32 vertical layers
- **MOZART-4 chemical IC/BC**
- **Meteorology**: driven by the North American Regional Reanalysis (NARR) model with grid nudging (FDDA).
- **Emissions**:
  - Points sources from July 2007 CEMS data.
  - Area sources are projected 2009 emissions used in SIP modeling. Grown from 2002 U.S. inventory.
  - Emissions processed using SMOKE modeling system
- **M3DRY dry dep scheme implemented**
- **No lightning NOx or stratospheric chemistry**
Ozone distribution over eastern United States on day preceding event

Note: No measurements over water. High values over water from MOZART IC
Observed ozone increases rapidly over Great Lakes and Ohio River Valley
Event marches eastward
High ozone seen over urban corridor. Note high-bias over southeast.
Ozone amounts decrease except over northeast U.S.
How well is ozone profile captured by WRF and OMI aboard Aura satellite?

Satellite-retrieved ozone profile from OMI (Xiong Liu) has high-bias but agreement is encouraging and some vertical info

Vertical extent of high ozone is well simulated at eastern U.S. site

WRF-calculated PBL ozone is too low at time of sonde but agrees better 5 hours later.
Pollution event is visible in satellite-retrieved and WRF-calc tropospheric ozone columns (TOC) although column varies considerably.

NOTE: TES level 2 orbit is shown by ovals.

OMI/MLS TOC
OMI total column - stratospheric col from Microwave Limb Sounder (M.Schoeberl)

OMI TOC

WRF-CHEM TOC

MOZART TOC
How does the TES-retrieved TOC in the pollutant outflow region compare to columns observed on other days?

- Analyzed TES TCO in the grid box [75W to 69W], [30N to 38N] for:
  - All 2005-2008 V4 L2 Nadir Step and Stare Observations
  - June-August 2005-2008 V2 L2 Nadir Global Observations
TES measured TCO values $\geq 60$ DU in the pollutant outflow region are at the 95th percentile of all Step and Stare measurements made in July (2005-2008). Note: Boxes show 25th and 75th%. Whiskers show 5th and 95th%.
**Results shown before applying TES and OMI averaging kernels**

- TES measured the highest TCO values; OMI/MLS measured the lowest TCO values

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<tr>
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<th>TES</th>
<th>WRF/Chem</th>
<th>MOZART</th>
<th>OMI/MLS</th>
<th>OMI</th>
</tr>
</thead>
<tbody>
<tr>
<td>AVG TCO (DU)</td>
<td>42.8</td>
<td>36.8</td>
<td>38.0</td>
<td>26.4</td>
<td>37.6</td>
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Comparison of dry deposition velocities between Wesely (top) and M3DRY (bottom)

Ozone          H2O2          NH3

24-hr avg O3 deposition velocity 20070709

24-hr avg H2O2 deposition velocity 20070709

24-hr avg NH3 deposition velocity 20070709
Time series of CO, O3, and H2O2 (upper left) PM2.5, nitrate, and ammonium (upper right) NH3, HNO3, and PAN (lower left) for M3DRY (dotted line) and Wesely (solid line) O3 observations in blue.

RADM2 O3 usually exceeds CBMZ O3

Replacement of Wesely dry dep scheme with M3DRY decreased O3 over land but increased O3 over water. PM species improved.
WRF-calculated 8-hr ozone in southeastern U.S. is too high with both the CBMZ and RADM2 mechanism. CMAQ calculated ozone does not display this high-bias. Is this related to treatment of organic nitrates?
GEO-CAPE (Geostationary Coastal and Air Pollution Events) is a future satellite for atmospheric chemistry measurements proposed by the NRC Decadal Survey.

Early planning activities are underway by NASA. WRF-Chem output is being used in two of these investigations: test retrievals and studies of spatial and temporal variability.

Output from a 12-km WRF-Chem simulation using the CBM-Z mechanism is shown for the July 9, 2007 East Coast ozone episode. Column ozone amount for Surface to 800 hPa is shown in the top panel and for 800 to 600 hPa is in the bottom panel. Three locations have been selected with differing tropospheric ozone structure (asterisks on map) have been chosen for further study.

- Upstate NY – relatively clean
- Central NJ – high ozone in BL
- Eastern NC – enhanced ozone in residual layer
Daytime profiles extracted from WRF-Chem, and stratospheric O$_3$ appended from NASA Goddard GEOS-5 assimilated data.

In addition, profiles extracted for NO$_2$, CO, SO$_2$, HCHO, H$_2$O, AOD, other aerosol parameters, cloud optical depths, temperature

Profiles being used in radiance calculations. Radiances will be input to satellite instrument retrieval algorithms and resulting profiles/columns will be tested against the original model data.

Can the instruments capture the spatial and temporal variability seen in the model?
Can boundary layer ozone be detected?

4-km horizontal resolution simulation will be run; statistics on horiz. variability will be computed and compared with those from 12-km run.
Conclusions

- Spatial pattern and vertical extent of July 9-11 air quality event is captured by WRF/Chem. High-bias is seen in southeastern U.S. possibly due to treatment of organic nitrates.
- Both TES and OMI show elevated ozone off of the coast, in agreement with WRF-Chem and MOZART-4 models, illustrating continental outflow of pollutants.
- M3DRY has been implemented in WRF-Chem. Resulting change in deposition velocities led to less ozone over land and more over water. Nitrate/ammonium more realistic.
- Vertical profiles and partial columns of trace gases and aerosols from regional models such as WRF-Chem are being used in preparation for GEO-CAPE.

*Acknowledgements: Gregory Osterman, Mark Schoeberl, Dylan Jones, George Grell, Steven Peckham, Xiong Liu, Louisa Emmons.
Origin of the Elevated Ozone Air Mass

- **HYSPLIT 72 hr back trajectories from TES profiles with high TCO values:** starting at 2km (left), 4km (center), 7km (right)
- At all levels air mass passed over the Great Lakes and Ohio River Valley within the previous 48 hours.
On July 7, 8, and 9, 2007 surface 8-hr max O3 was above 70 ppb in the Great Lakes Region and Ohio River Valley.
Sensitivity of tropospheric ozone column to BC/IC, mechanism, dep scheme
8–hr max 03 20070709

WRF/Chem RM3Moz

WRF/Chem RM3

WRF/Chem RMoz

WRF/Chem CM3Moz

AIRNOW measurements

0 20 30 40 45 50 55 60 65 70 75 80 90 100 110 125
O3 (ppbv)
- TES and OMI have the greatest sensitivity in the 850 mb – 600 mb range
- Capable of detecting pollution in the lower troposphere, but with greatly diminishing sensitivity below 800 mb
TES measured TCO values are \( \geq 60 \) DU in the pollutant outflow region and are at \( \approx \) the 75\textsuperscript{th} percentile of all Level 2 measurements made in June-August (2005-2008).
TES and OMI

Tropospheric Column Ozone – 20070709 18UTC

- TES measured elevated Tropospheric Column Ozone (TCO) in the pollutant outflow region
Build-up to July 9, 2007 Air Pollution Episode: Comparison to ground stations

- WRF/Chem simulation: 00 UT July 6, 2007 – 00 UT July 12, 2007
- Good agreement along the I-95 corridor.
- High-bias present over the Appalachian Range (northern GA to se VA)
- Note: After these simulations were made, a patch was added to M3DRY. This patch increases deposition over water.