Regional Chemistry and Transport Modeling for DISCOVER-AQ

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Planned DISCOVER-AQ Modeling Activities

- **Run the WRF-Chem model with 4-km resolution over the field mission region (nested in 12-km and 36-km resolution domains) using best possible source emission data.**

- **Perform comparisons with ground-based data (Pandora spectrometer, sun photometer, ozonesonde, and in-situ) and aircraft data (ACAM, HSRL, and in-situ) to evaluate various model components (e.g., photolysis scheme, chemical mechanism, aerosol module etc.) of WRF-Chem. Perform sensitivity simulations to bring the model calculation in close conformity to the measurements spatially and temporally.**

- **Use the regional meteorology from WRF to drive the CMAQ model. Compare model output with the ground-based and airborne data sets and run sensitivity calculations to reach good agreement with observations in a manner similar to the above.**

- **Evaluate boundary layer depths in the WRF model using aerosol lidar, sounding, profiler, and aircraft observations.**

Modeling Activities (continued)

- **Use the model output to interpret the observations. For example, examine the spatial and temporal variation of observed trace gases at the surface and in the tropospheric column in both the models and observations.**

- **Compute local (grid-cell) scaling factors between tropospheric column amounts and surface mixing ratios from the model. Compare these factors with those derived from observations and determine if the scaling factors can be related to meteorology (e.g., boundary layer depth), transport, proximity to major emission sources, time of day, etc.**

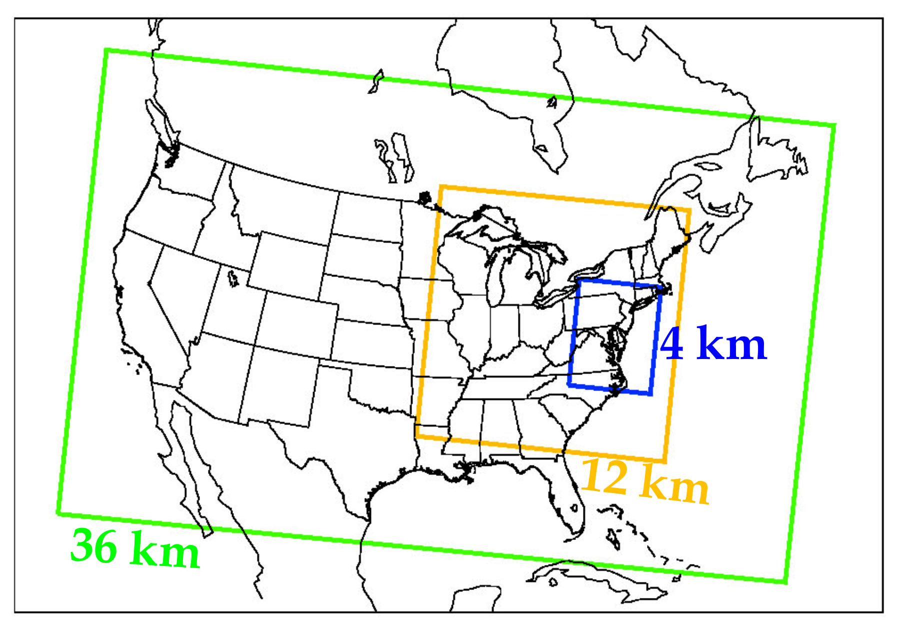
- **Employ transport feature information from the model to explain inconsistencies between surface and column observations.**

- **Examine the horizontal and temporal variability of trace gases and aerosols in the observations to determine how much of this variability is captured by the model at 4 km resolution.**

- **Perform finer-resolution WRF and CMAQ simulations to examine effects of fair weather cumulus and bay breeze.**

Weather Research & Forecasting Model (WRF)

- **Advanced Research WRF (ARW) core V3.2**
  - 32 levels in the vertical, up to 100 hPa
  - Initial and boundary conditions based on NARR (GEOS-5 possible)
- **Online Chemistry Module – V3.2**
  - CBMZ chemical mechanism and MOSAIC aerosol parameterization including some aqueous reactions
  - Initial and boundary conditions for trace gases and aerosols based on MOZART (NASA GMI possible)
  - Anthropogenic emissions generated by (Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system using annual emissions from US Regional Planning Offices and hourly Contiguous Emissions Monitoring data from the EPA
  - Biogenic emissions from Biogenic Emissions Inventory System (BEIS) V3.12



MOSAIC 8-bin Aerosol Variables

- 8 aerosol mass size bins* (µg/kg dry air):
  - SO_4, NH_4, NO_3, Cl, Na, organic carbon, black carbon, other inorganics , water
- 8 aerosol in cloud mass size bins* (µg/kg dry air):
  - SO_4, NH_4, NO_3, Cl, Na, organic carbon, black carbon, and other inorganics
- PM2.5 dry mass (µg/m^3)
- PM10 dry mass (µg/m^3)

- Backscatter coefficient
- Single scattering albedo
- Asymmetry parameter
- Extinction coefficient
  - All at 4 wavelengths (300, 400, 600, and 999 nm)

* Size bins range from 0.039 to 10 µm

Community Multiscale Air Quality Model (CMAQ)

- Developed by EPA (Ching and Byun, 1999; Byun and Schere, 2006)

- Applications:

  By state air quality agencies for regulatory modeling as part of State Implementation Plan process

  By EPA for national air quality assessments

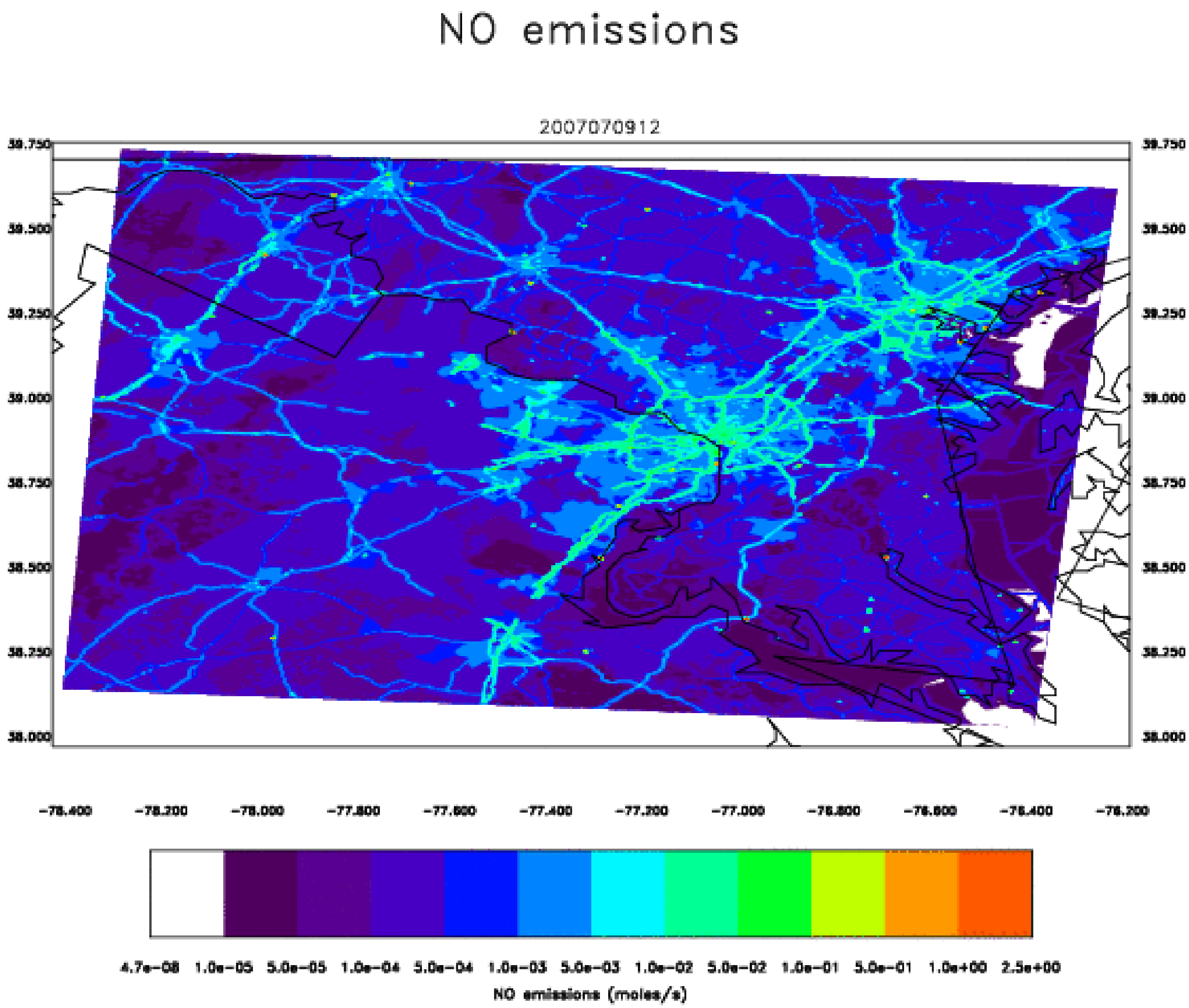
  By NOAA for operational air quality forecast guidance

- Current version: 4.7.1 (June 2010)

  Contains CB05 chemical mechanism; AE-5 aerosol module

- WRF meteorological data processed by MCIP (Meteorology and Chemistry Interface Processor)

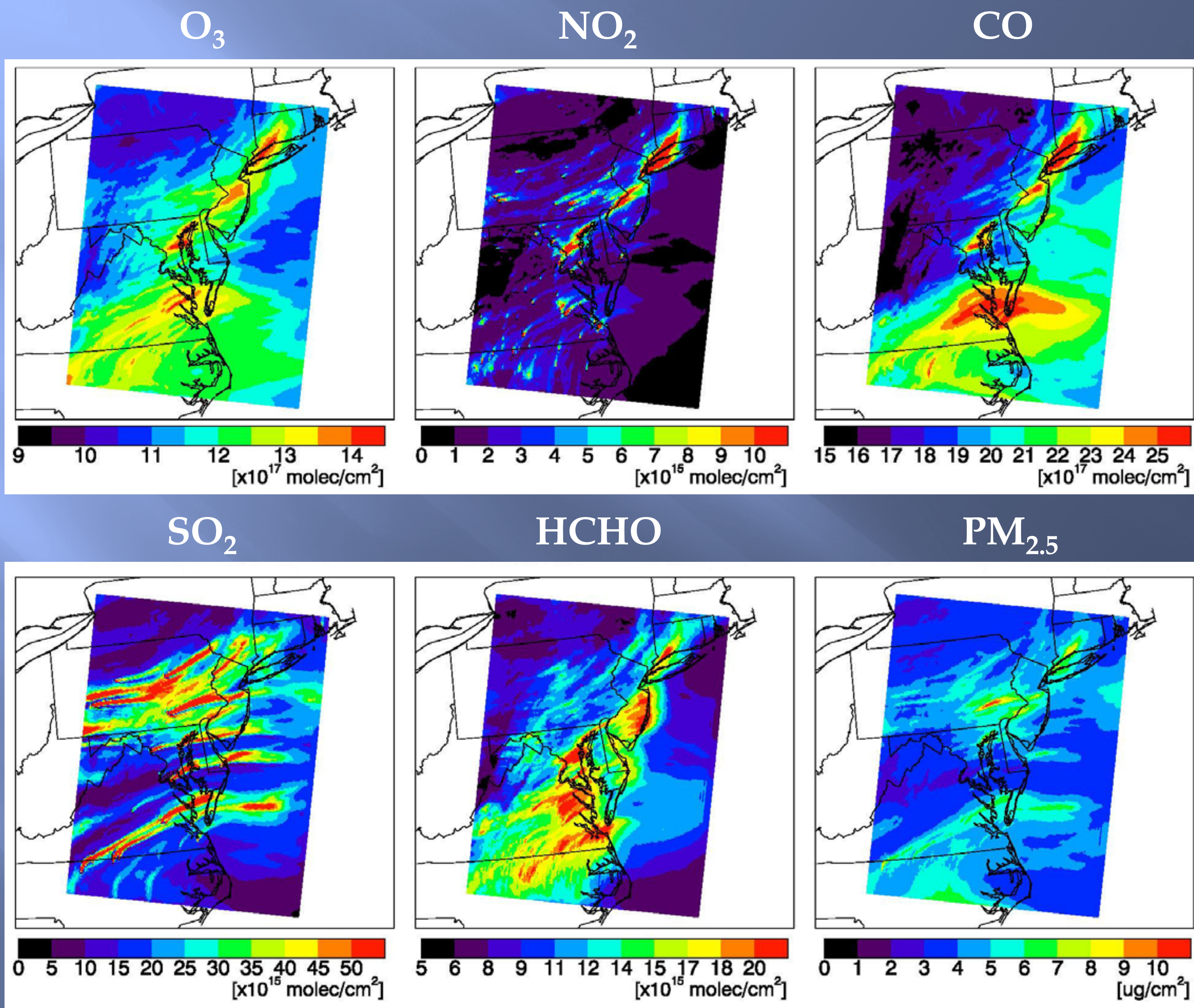
- Emissions data sets developed using SMOKE



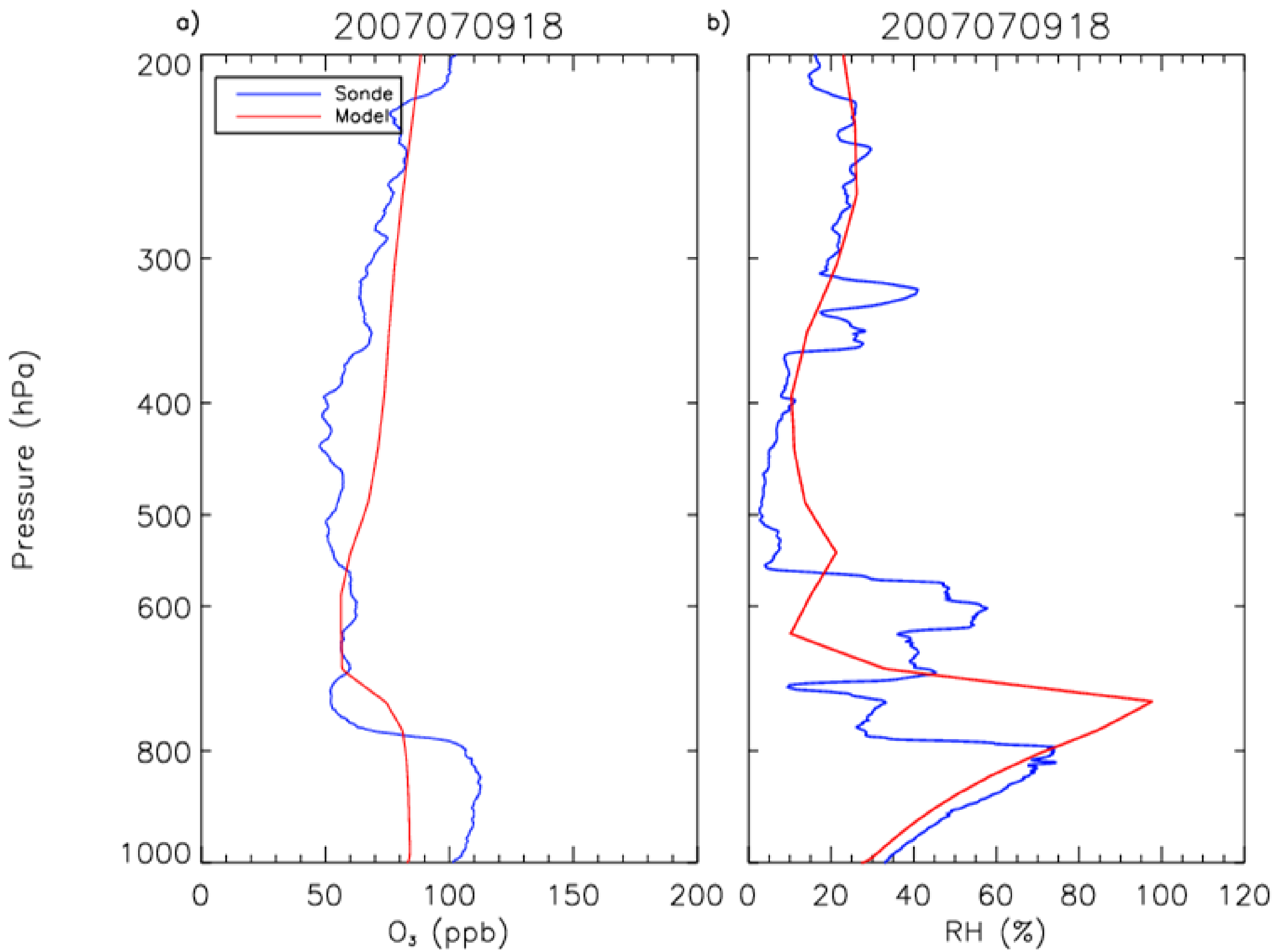
Emissions from SMOKE at 0.5-km resolution for Monday 8 AM

Trace Gas Species & Aerosols

July 9, 2007 – 18 UTC **Trop Column (sfc – 200 hPa)**



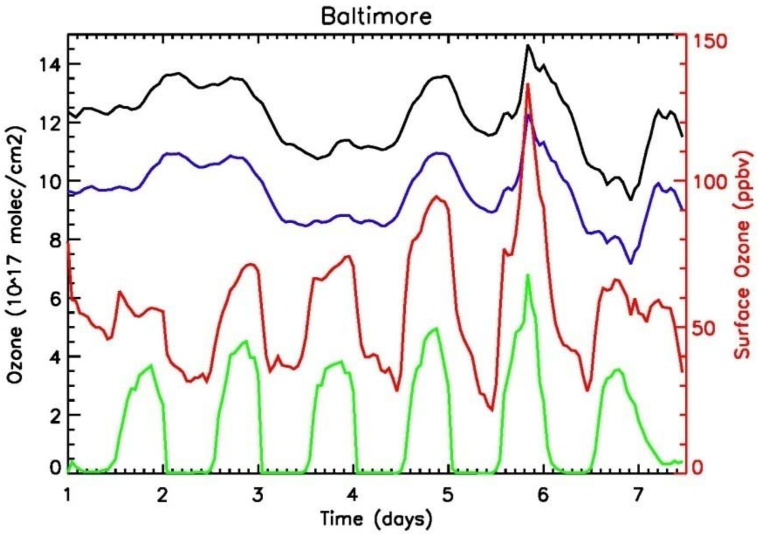
WRF-Chem (12-km res.) vs. Beltsville, MD Ozonesonde Profiles

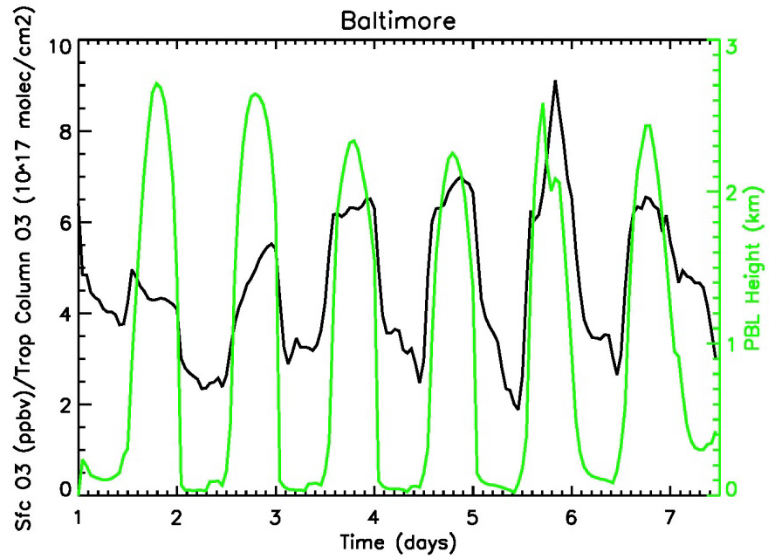


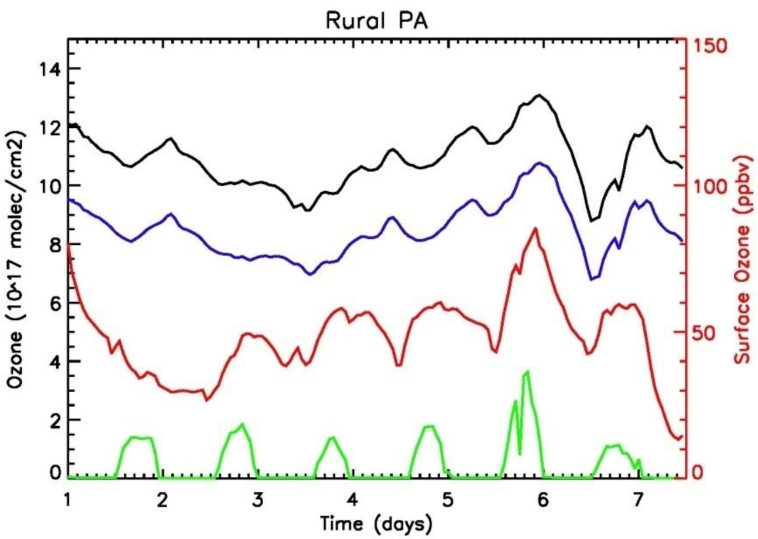
Yegorova et al., JGR, subm., 2010

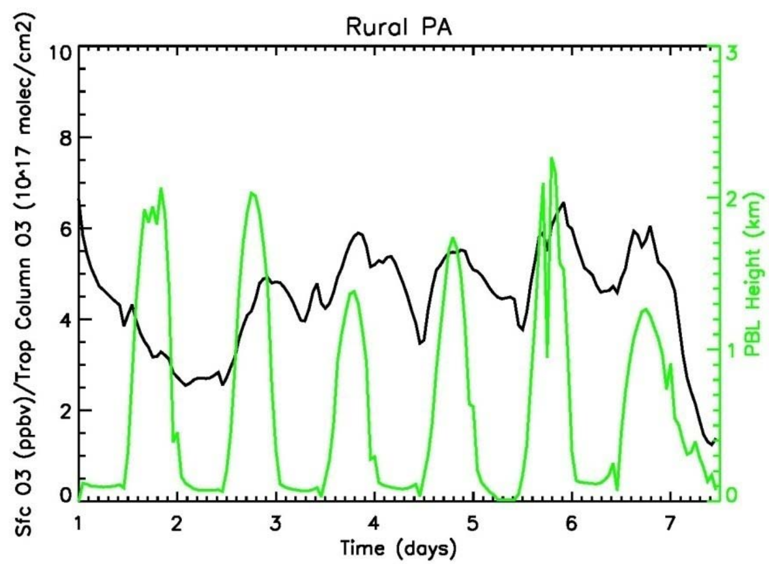
Trop. Column (sfc – 200 hPa)
ACAM Column (sfc – 330 hPa)
PBL Column
Surface mixing ratio

Sfc. O_3 (ppbv) / Trop Col. O_3 (10^{17} molec / cm^2)
Trop Column = sfc – 200 hPa



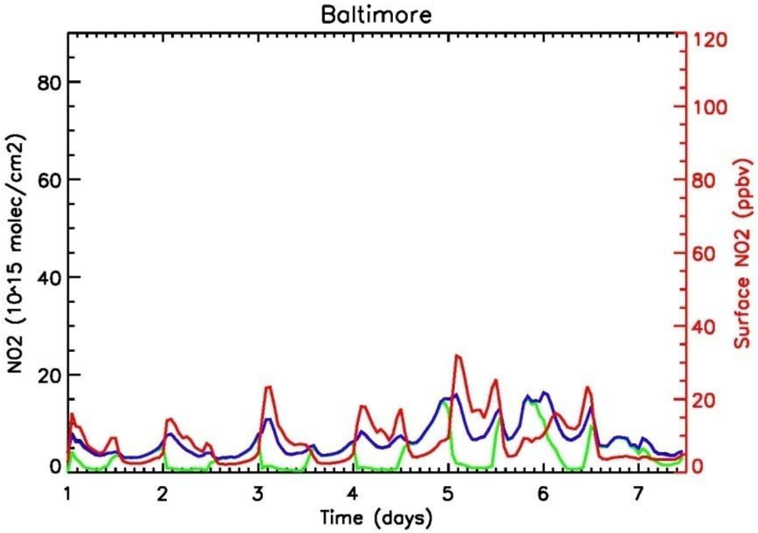


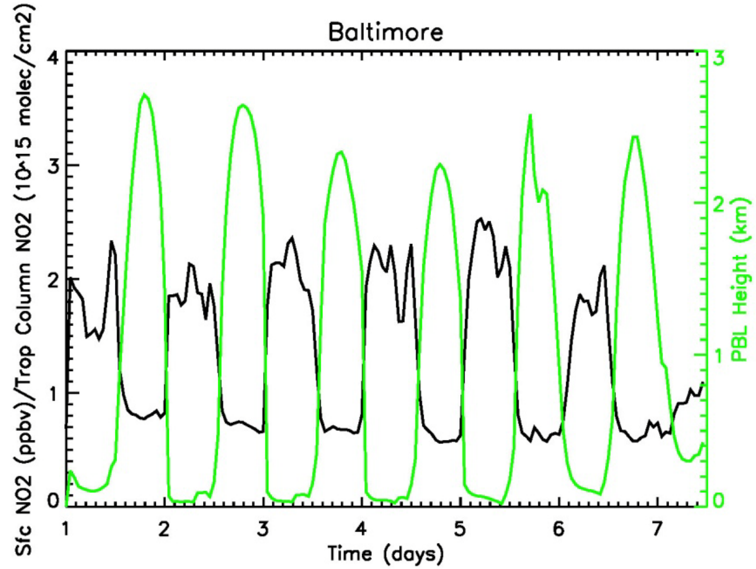


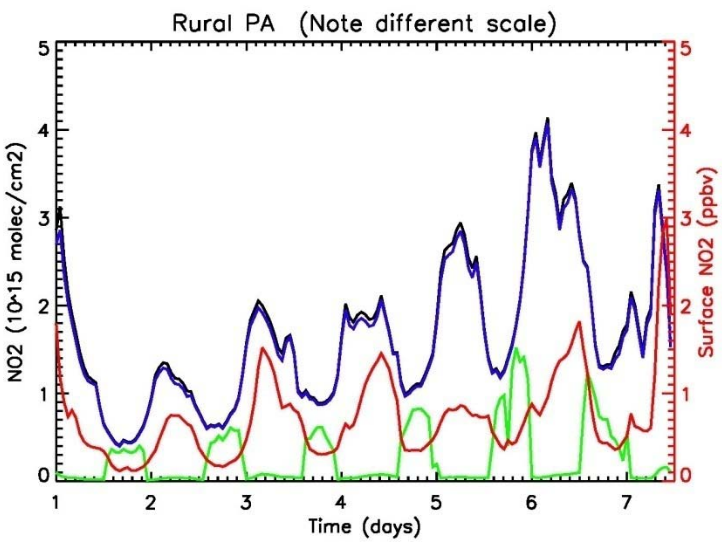


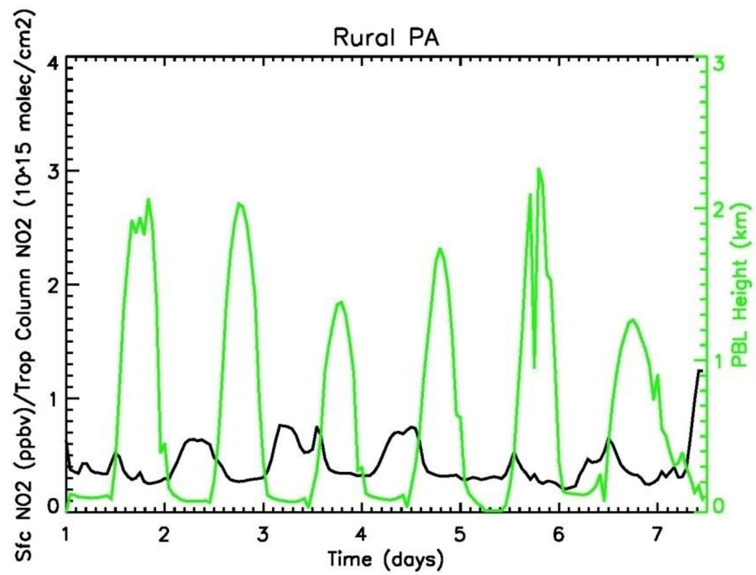
Trop. Column (sfc – 200 hPa)
ACAM Column (sfc – 330 hPa)
PBL Column
Surface mixing ratio

Sfc. NO_2 (ppbv) / Trop Col. NO_2 (10^{15} molec / cm^2)
Trop Column = sfc – 200 hPa



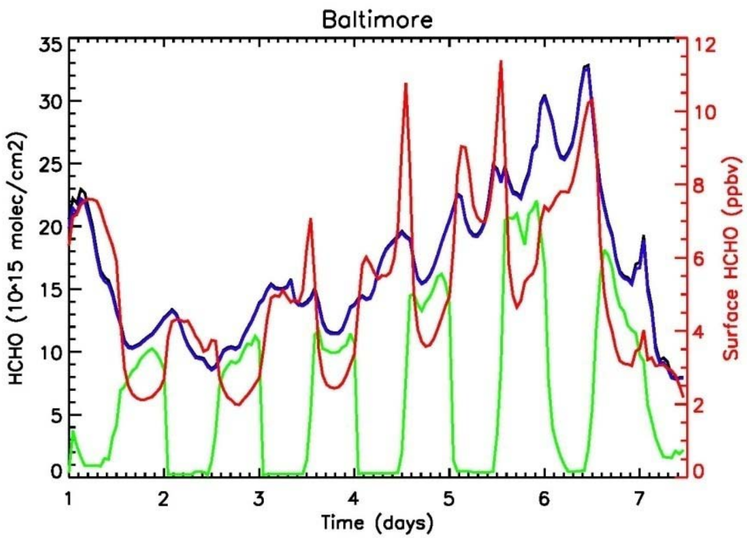


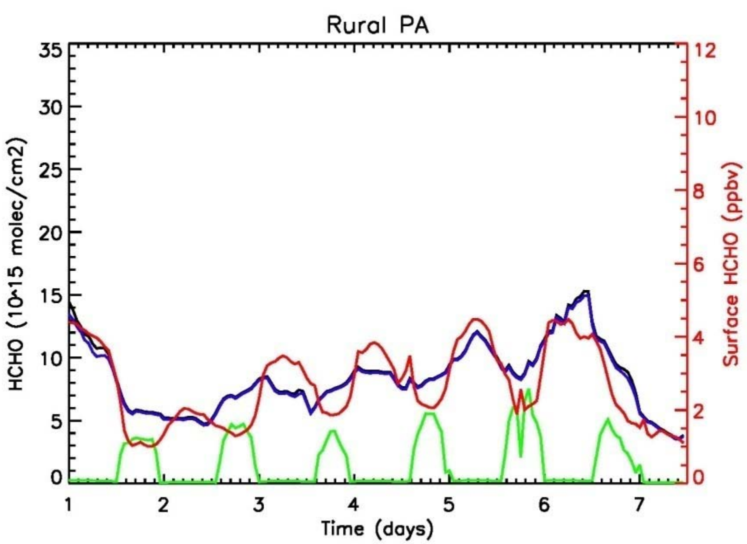


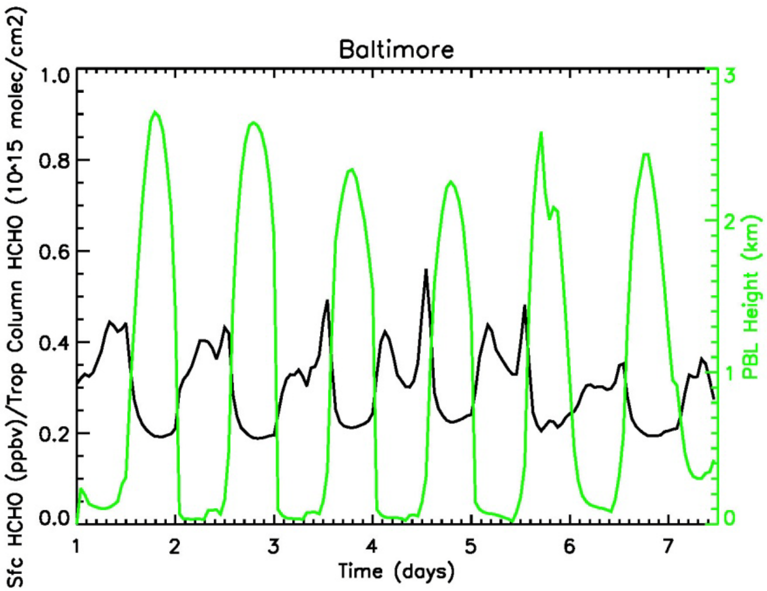


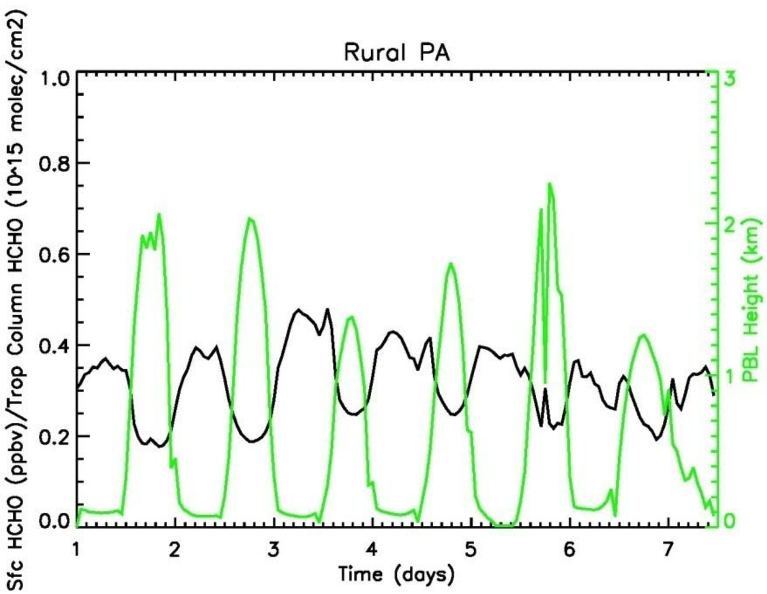
Trop. Column (sfc to 200 hPa)
ACAM Column (sfc to 330 hPa)
PBL Column
Surface mixing ratio

Sfc. HCHO (ppbv) / Trop Col. HCHO (10^{-15} molec / cm^2)
Trop Column = sfc – 200 hPa



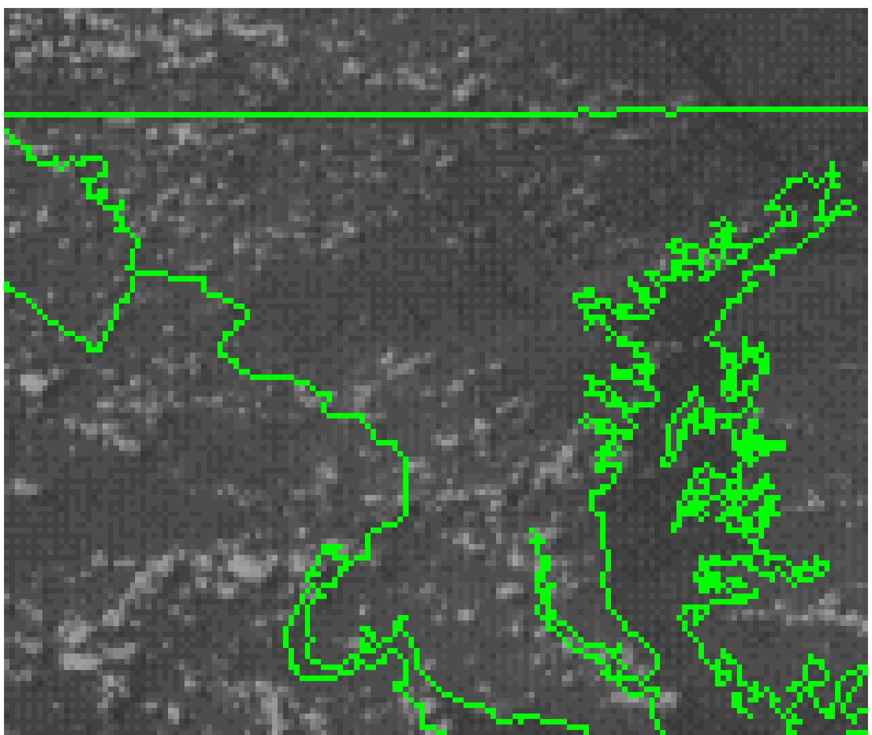


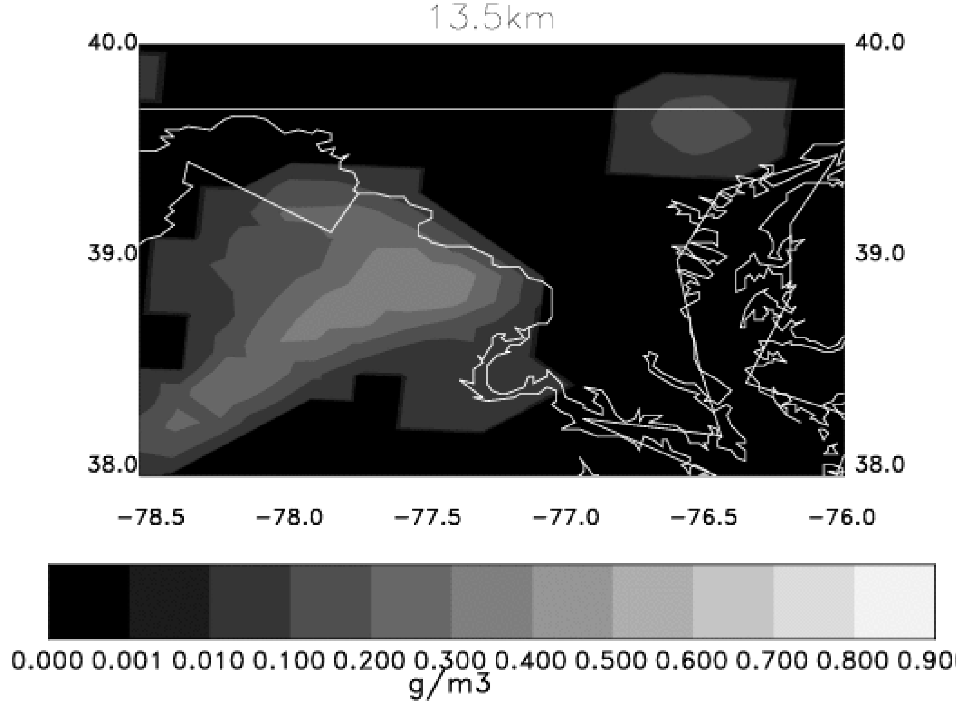


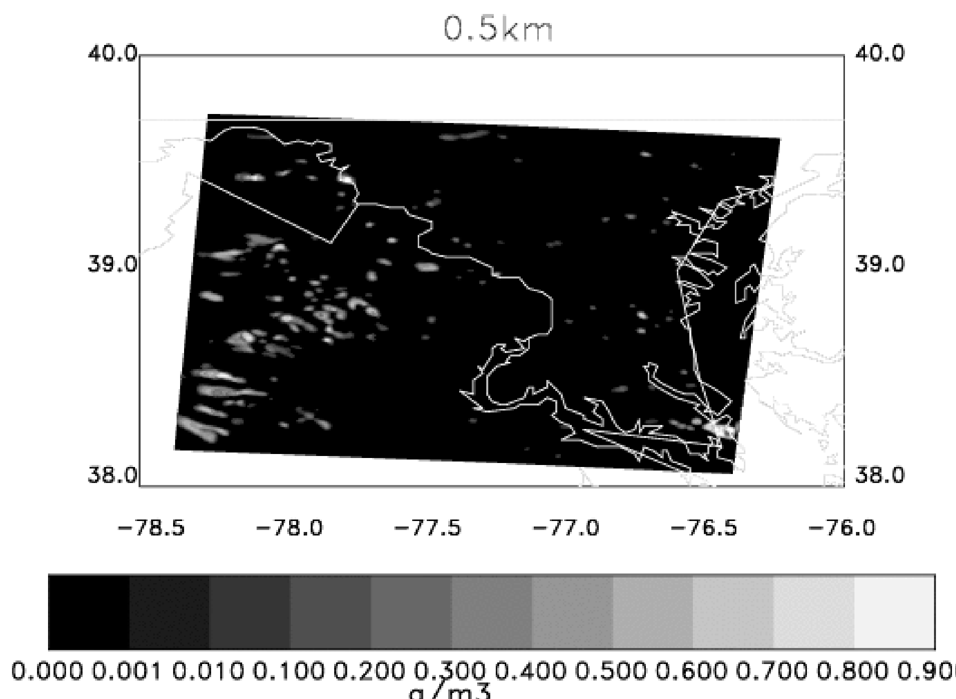


Loughner et al., 2010, in prep.
CMAQ Base – WRF clouds

GOES visible satellite image and average cloud liquid water content from the 13.5 and 0.5km base case simulations at 2000 UTC (3pm EST) July 7, 2007.

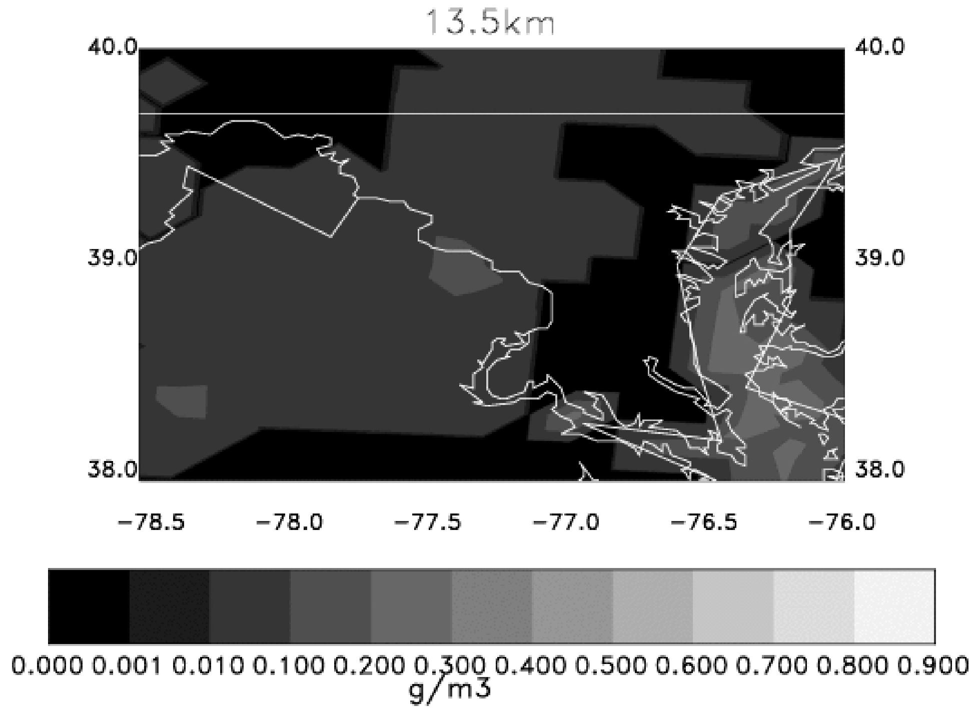


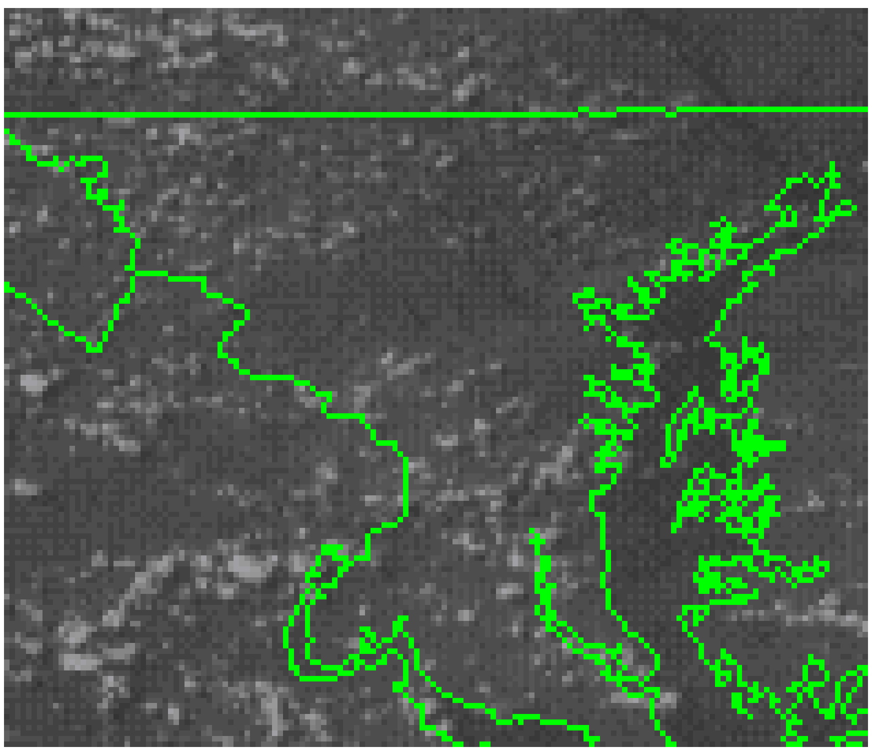


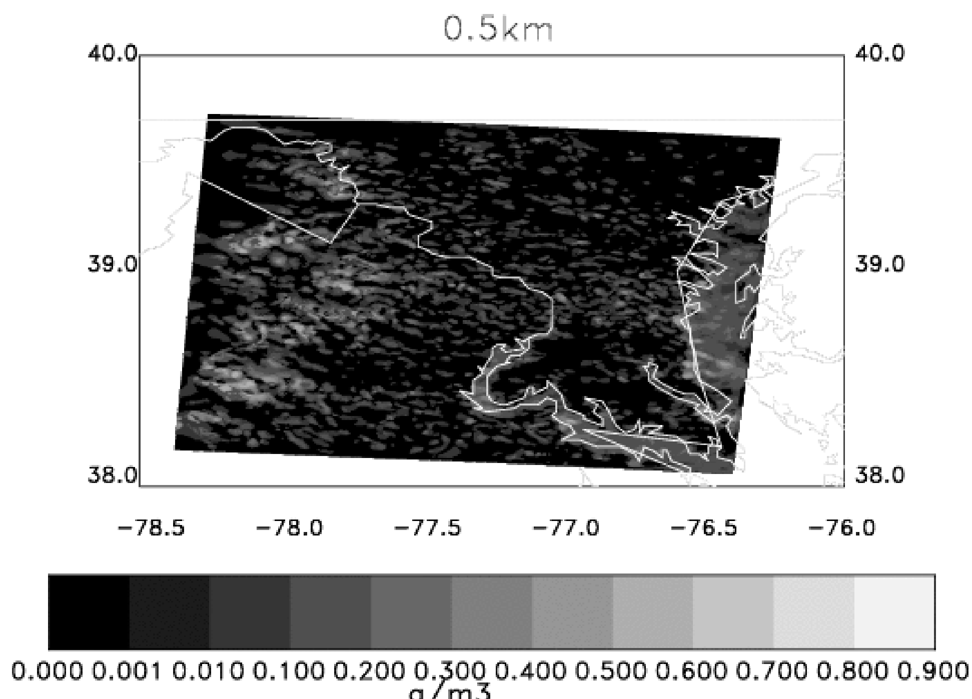


Loughner et al., 2010, in prep.
CMAQ Sensitivity – MCIP clouds

GOES visible satellite image and average cloud liquid water content from the 13.5 and 0.5km sensitivity simulations at 2000 UTC July 7, 2007.



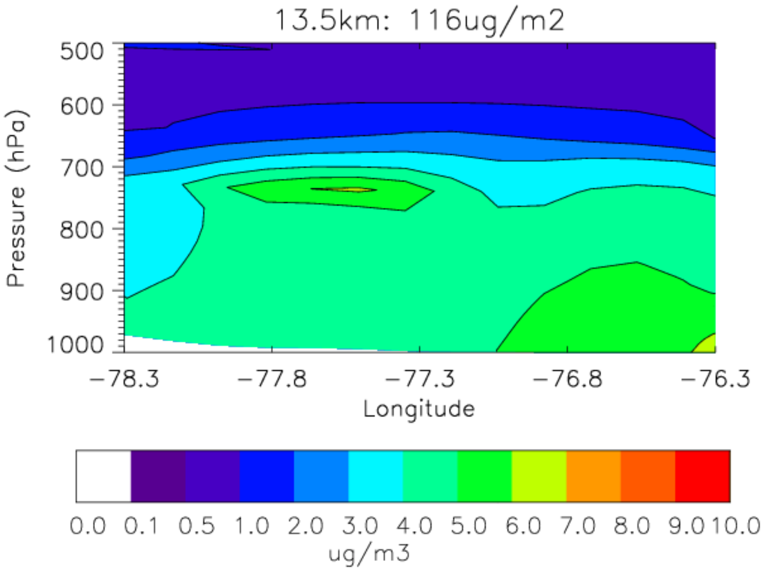


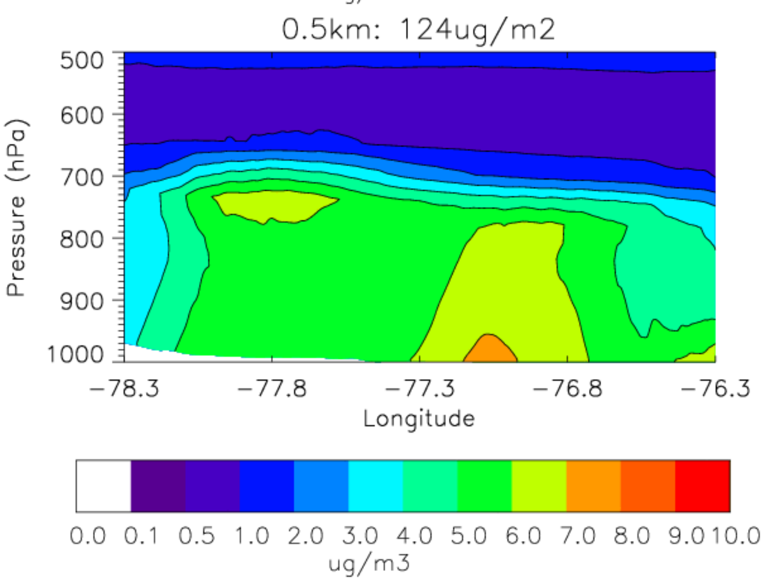


SO_4 cross-sections averaged over inner-most domain at 2000 UTC July 8, 2007

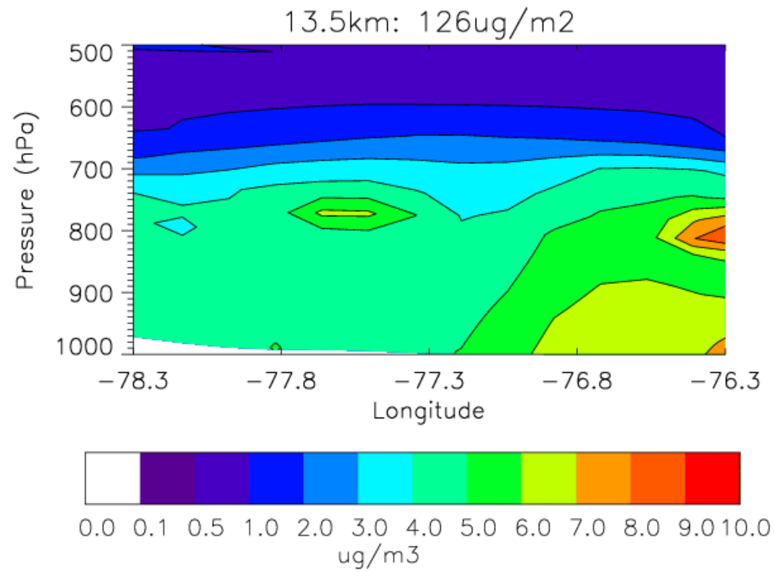
Sfc. SO_4 at Washington DC IMPROVE station better matched with 0.5 km Sensitivity

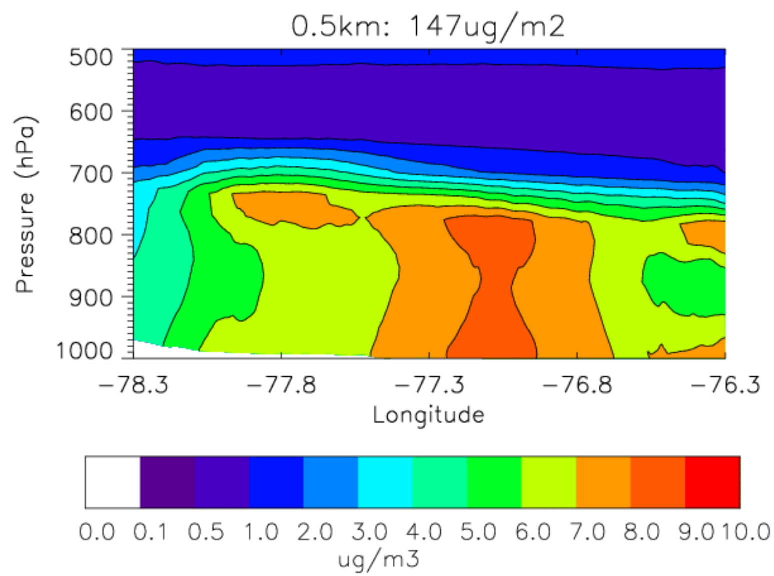
Base Case





Sensitivity Case

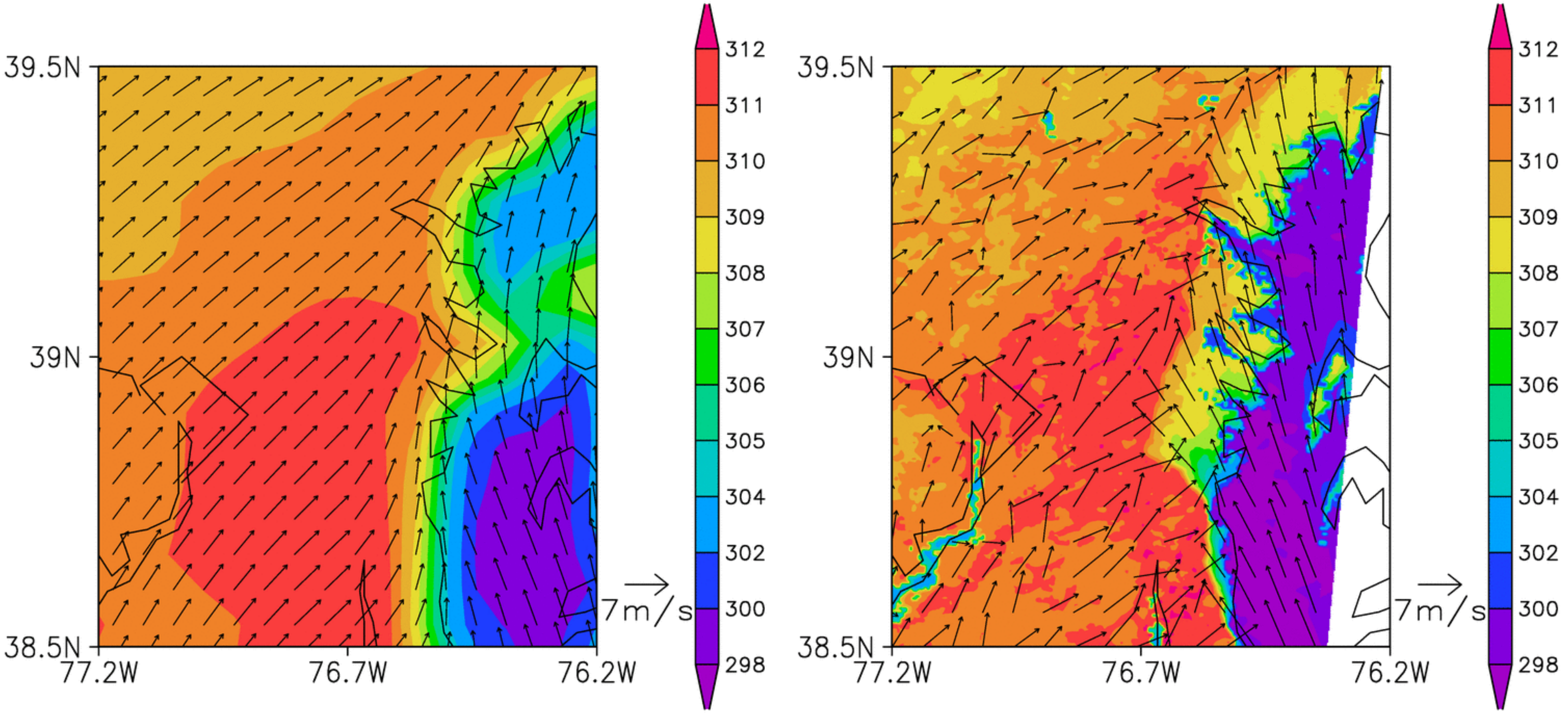




Loughner et al., 2010, in prep.

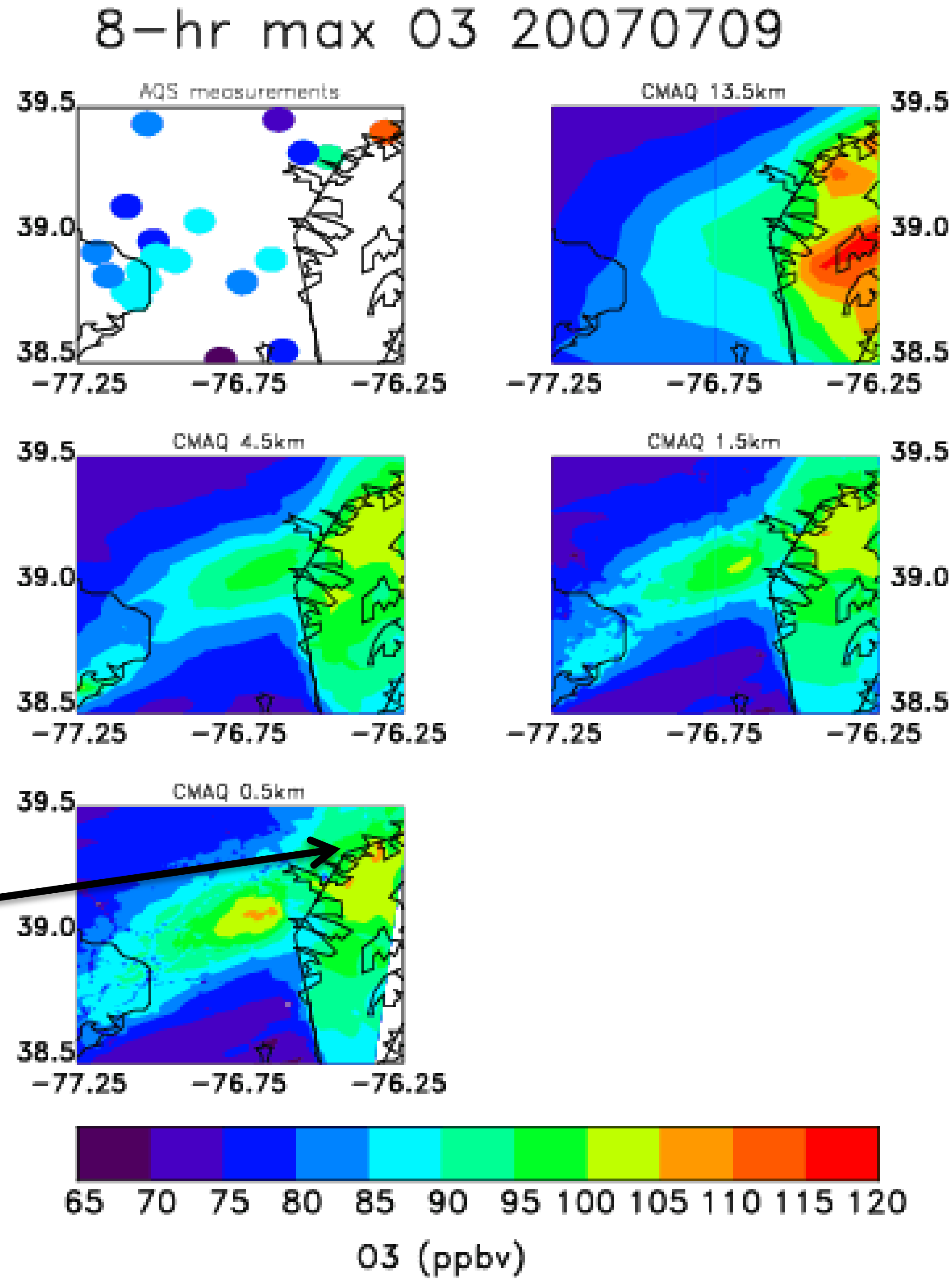
WRF-UCM 2-m temperature and 10-m wind speed at 2000 UTC (3pm EST) July 9, 2007. A stronger temperature gradient along the coastline of the Chesapeake Bay in the 0.5km domain results in a stronger Bay breeze.

13.5km 0.5km



8-hr max O_3 concentrations on July 9, 2007 from measurements and the base case simulation. Less pollutants over the water in the higher resolution simulations due to a stronger bay breeze results in lower ozone concentrations over the water.

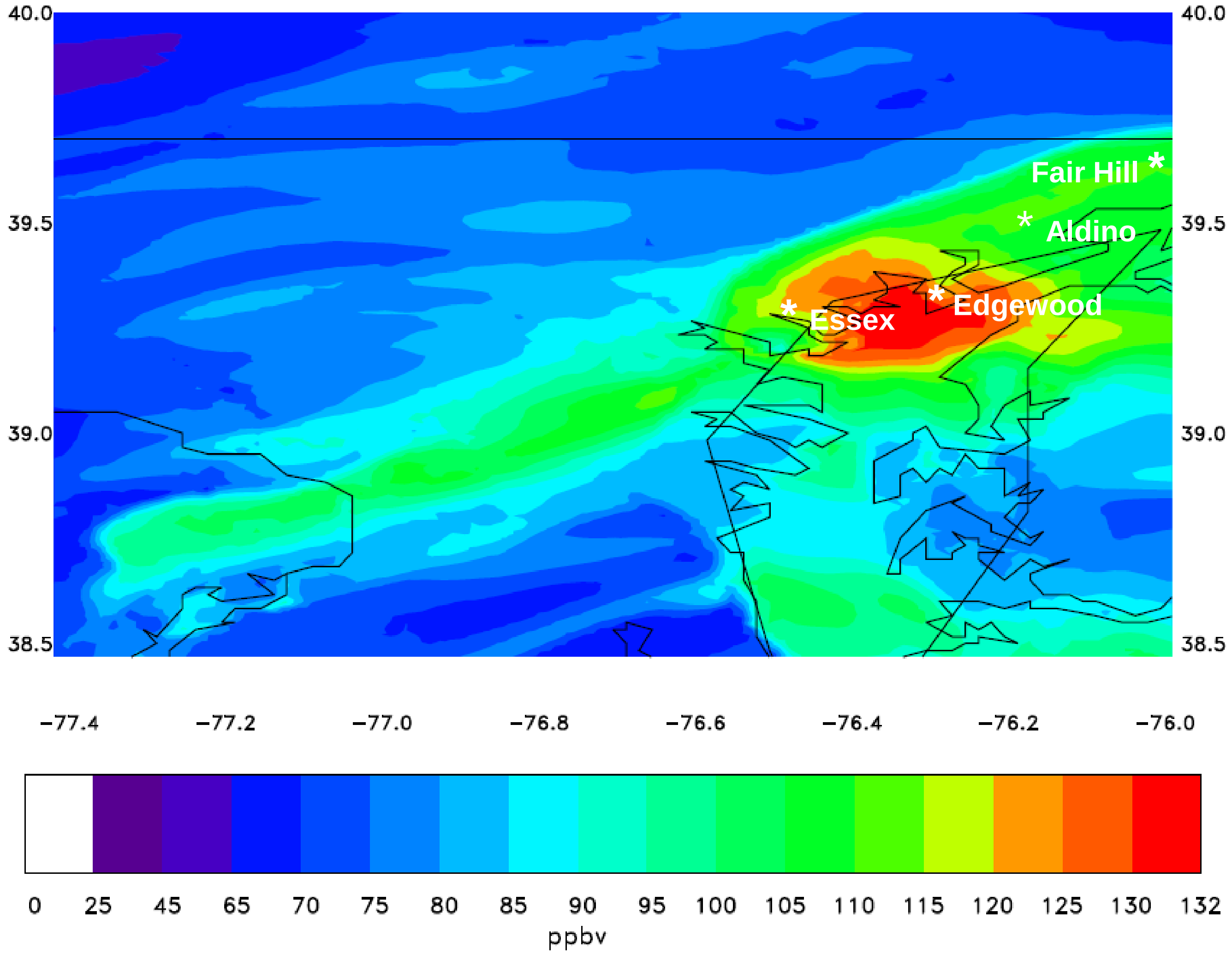
Convergence zone along western shore of bay leads to largest ozone values in that location



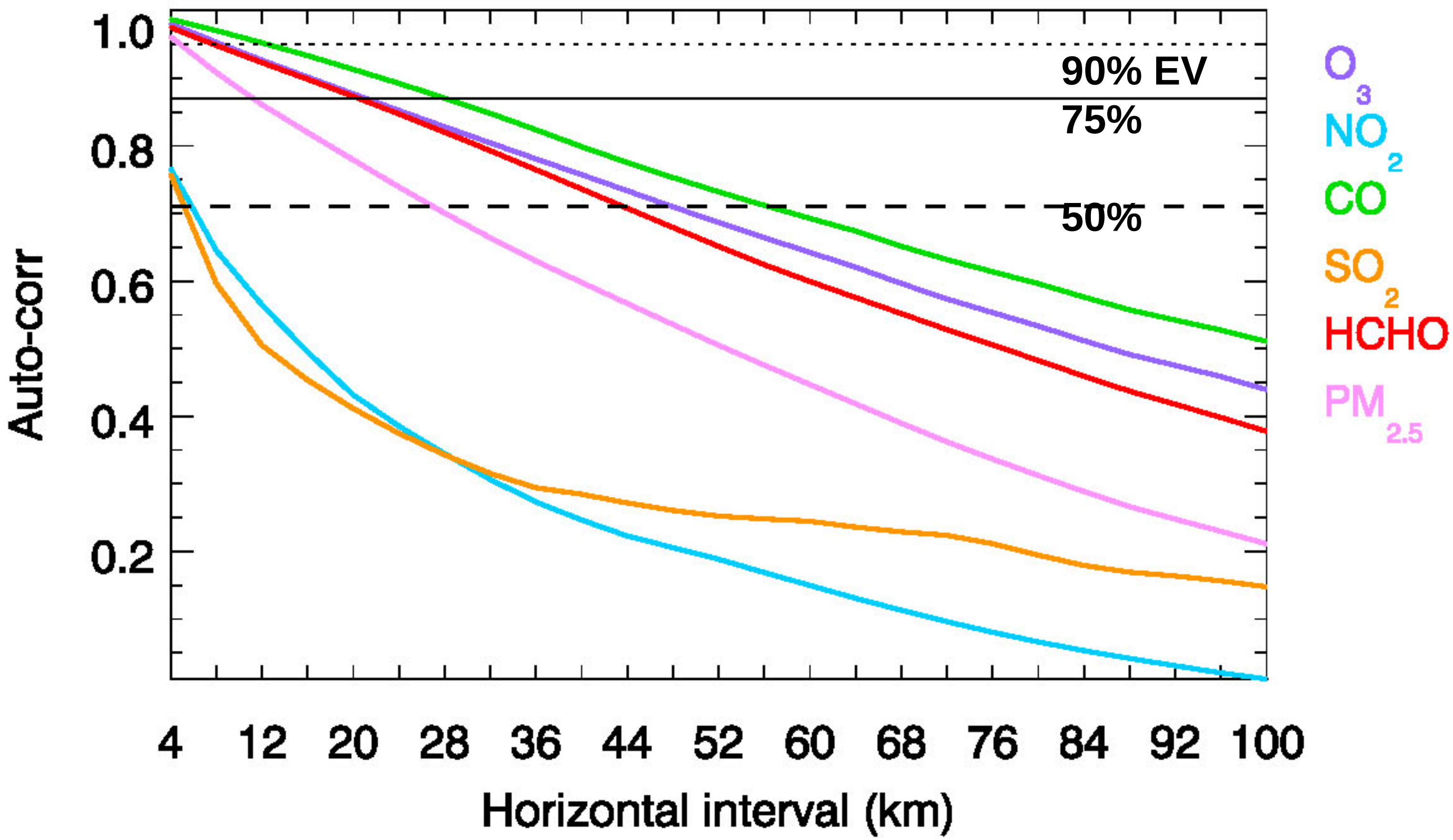
Loughner et al., 2010, in prep.

O3, 2007070919

CMAQ 1.5-km simulation

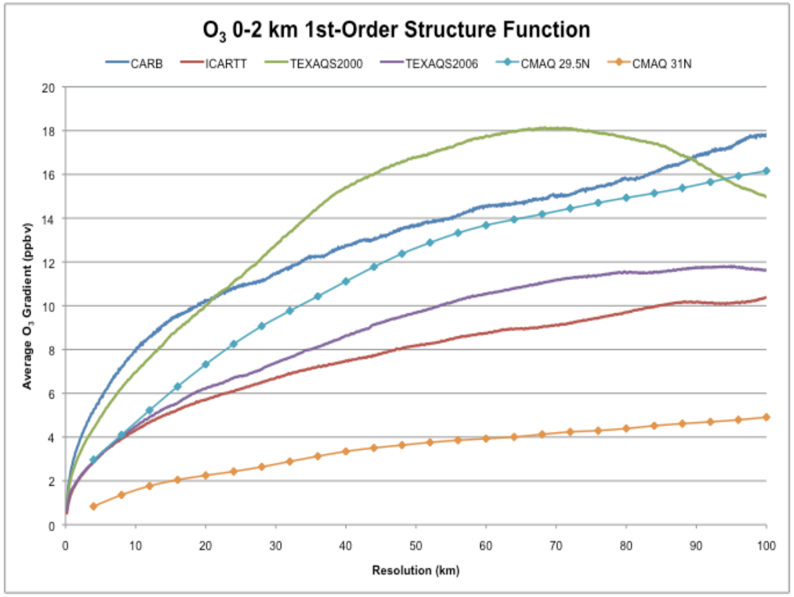


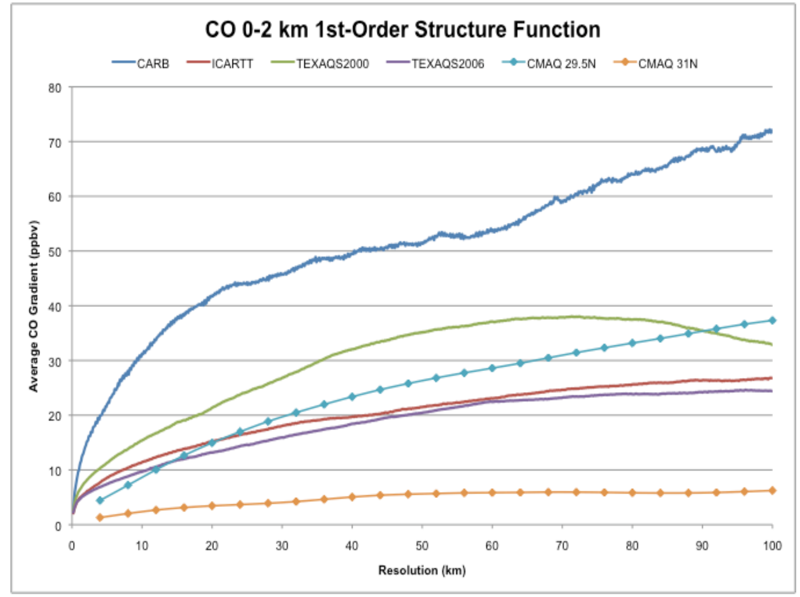
Spatial Variability in 4-km WRF-Chem Simulation

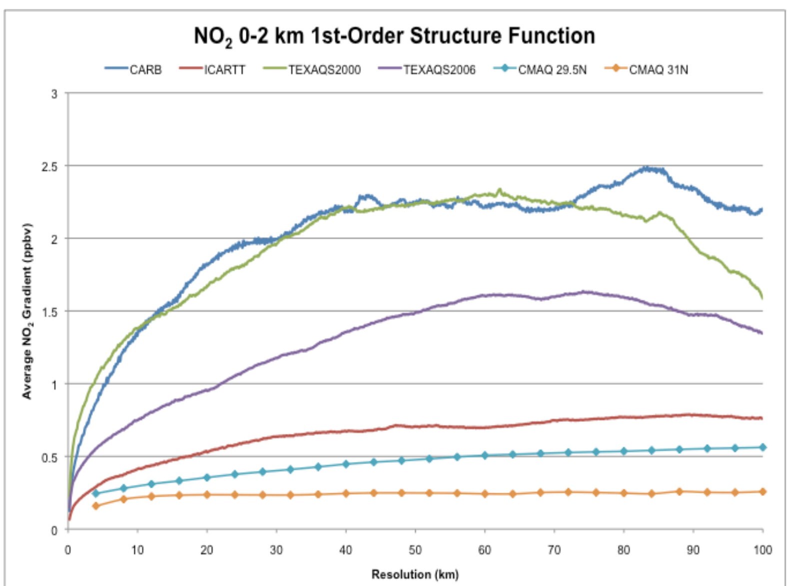


Follette-Cook et al., 2010, in prep.

CMAQ and Aircraft Variograms







First-order structure functions from four aircraft campaigns (CARB, ICARTT, TEXAQS 2000, and TEXAQS 2006) compared with CMAQ-generated data along the two "flight paths" in the Houston area.

For CO and O_3, the urban case in the model lies in between most aircraft data with the exception of the CO measurements for the CARB campaign. For NO_2, the model's variability is much less than the measurements, indicating that the 4-km resolution of the model cannot capture the variability seen in the atmosphere when measured from an aircraft with a 100-m resolution.

Fishman et al. 2010, in prep.