Refined Grid CMAQ Modeling of Acidic and Mercury Deposition over Northeastern US

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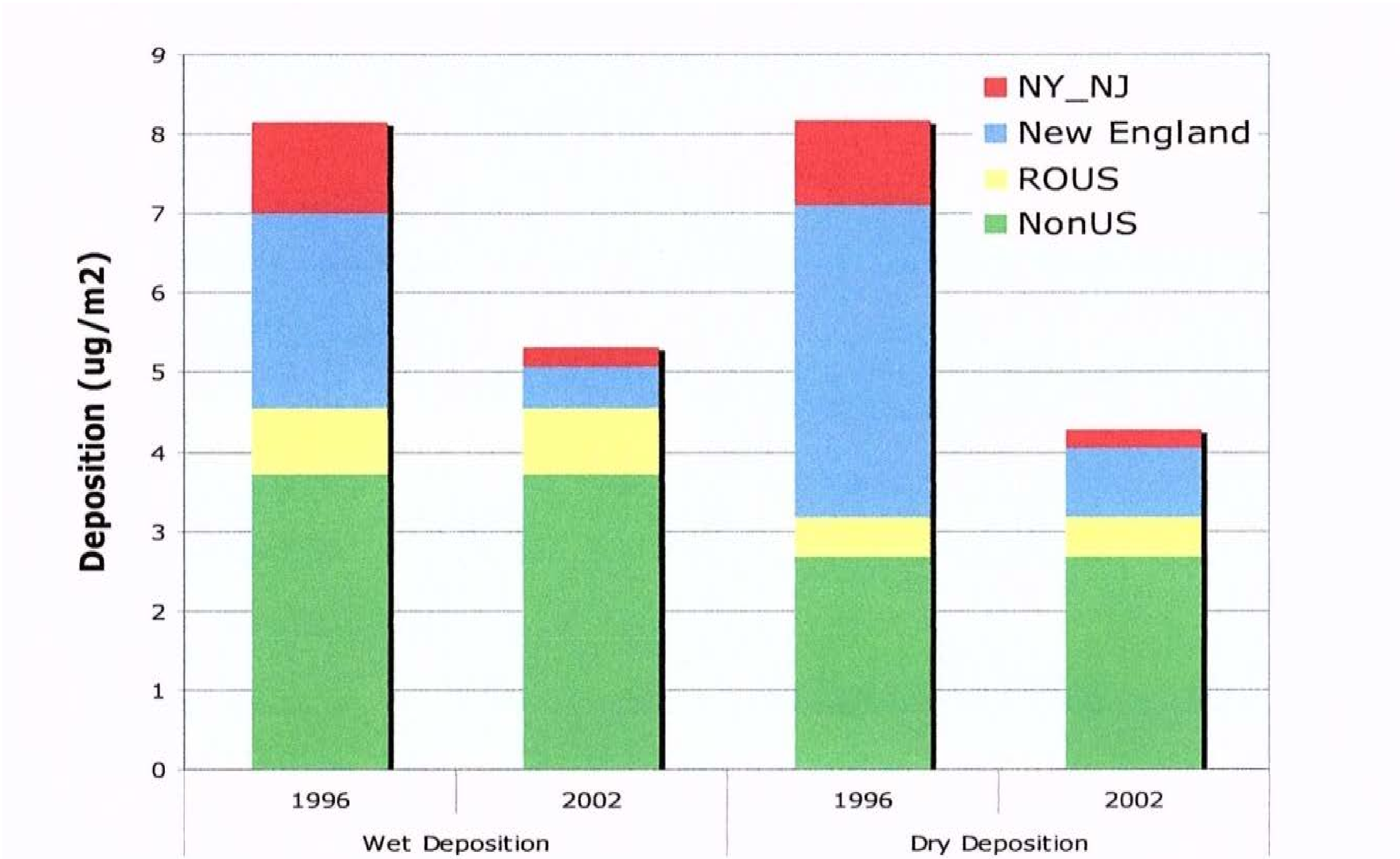
Why carry out the study?

- Resolved the Community Multiscale Air Quality CMAQ model grid to 4km spacing to better characterize terrain in New York State (NYS) and refined acidic and mercury deposition estimates; i.e. resolved the most recently available 2011 National Emissions Inventory (NEI) and meteorological fields by Weather Research Forecast (WRF) processor on the 4km grid.
- Determined the contribution of NYS energy production point sources (i.e. Electric Generation Units (EGUs), Waste to Energy (WTE) facilities) and "other" large mercury (Hg) sources to deposition in NYS.
- Compared the 2011 results to observed wet deposition at National Atmospheric Deposition Program (NADP) monitoring sites.
- Provide a report which can be used for policy decisions such as the EPA secondary standard for SOx and NOx.

Regional contribution to Hg wet and dry deposition in NESCAUM states



* <u>Modeling Mercury in the Northeast United States</u>, NESCAUM 2007

NYS Large Emitting Facility Data Reviewed and used to Revise Unit Based Data

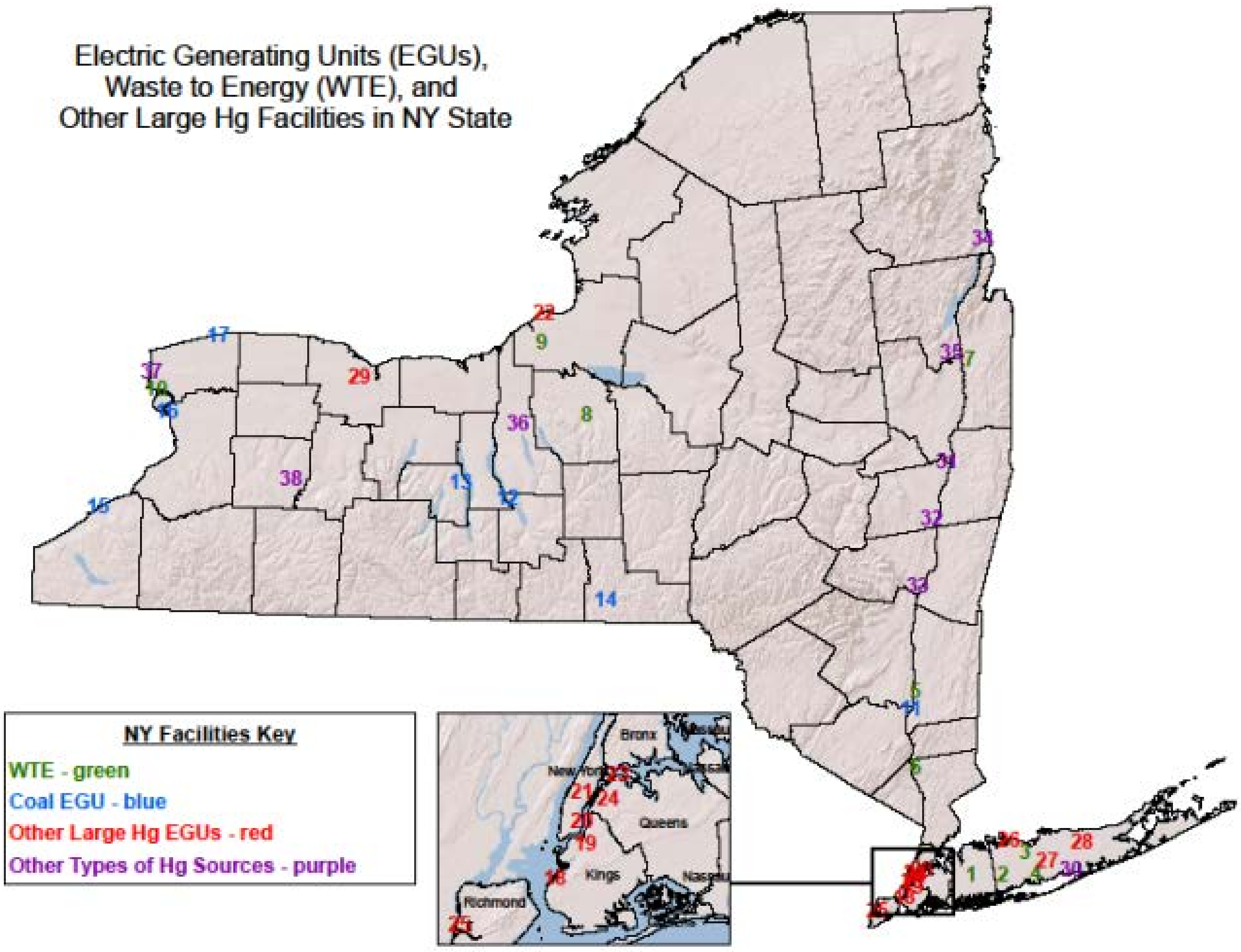
- Of the potential 38 large Hg/SO2/NOx facilities, 26 had large Hg emissions (excluded gas or oil backup EGUs)

- The stack parameters for all 38 were checked and also revised where necessary on a unit basis for 157 units.

- Roughly 1/3 of stack parameters needed revisions of some sort in the potential source set (mostly minor for this study)

- Total Hg emissions reduced by 23% from data base entries. The biggest revision was for the gas/backup oil EGUs, with a <u>factor of 11</u> drop (193 to 17 lb/yr).

Location of Potential Large Point Sources in NY based on 2011NEI data.



Are there any other potential Hg source categories in NYS?

- Found "area" sources with high total Hg emissions in the NYC/Long Island region associated with metals processing and residual oil use: Based on a report on oil Hg specific to NYS, adjusted downwards by a factor of 7.

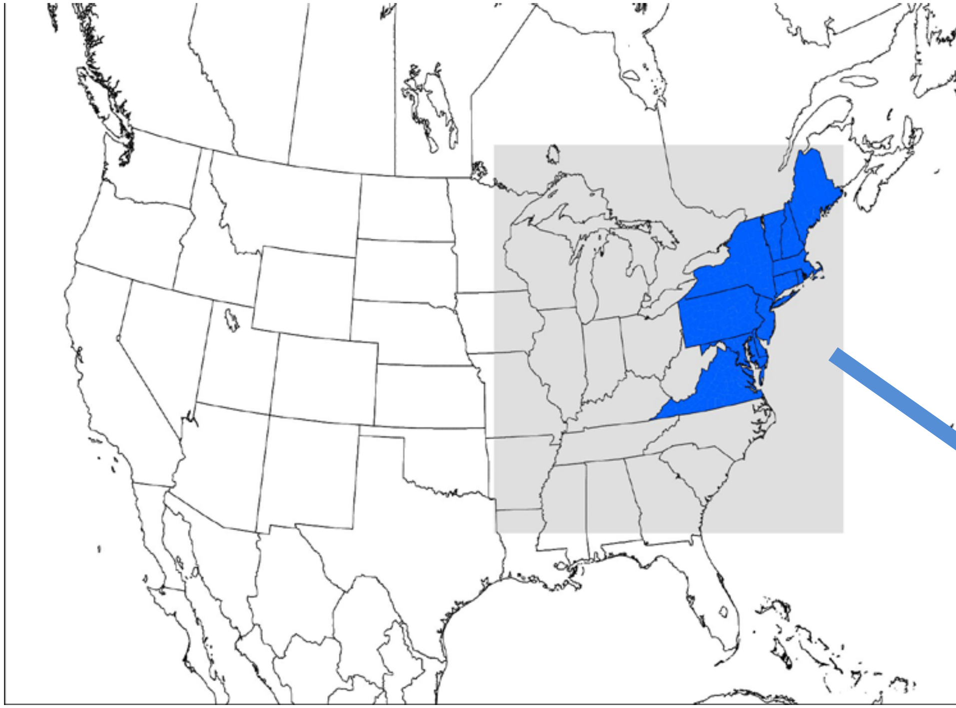
- EPA's factor for Hg in gas revised using a 2010 study for NYSERDA on metal content in NYS. EPA AP42 factor is for untreated gas, while data from treated gas (e.g. in US) is much less.

- Possible wood burning as a source on facility scale dismissed based on a 2013 study for NYSERDA which indicated minimal Hg concentrations.

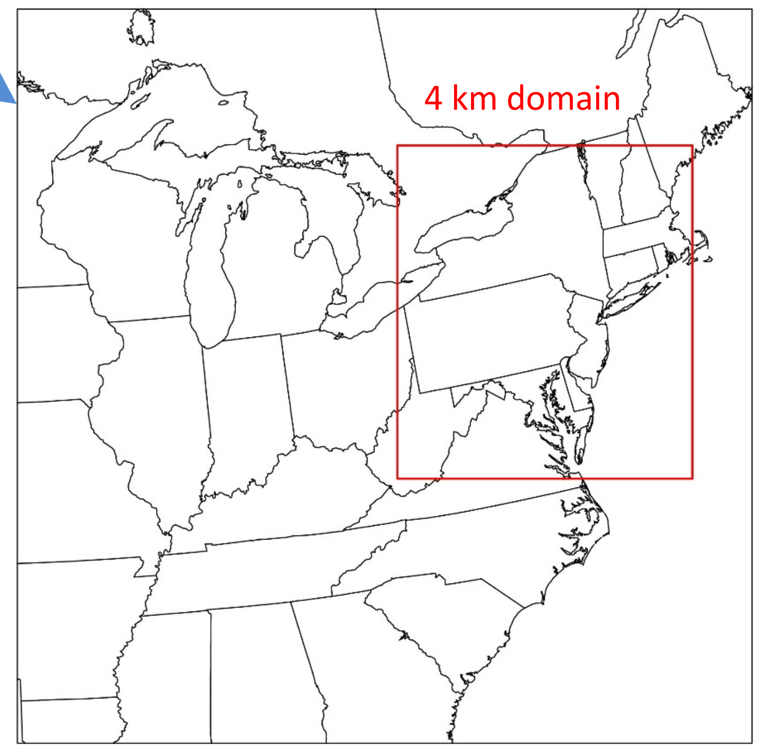
- Another possibility was mobile sources, but a 2011 study for MA estimated almost nil Hg emissions from the mobile sector. (no Hg emission factor from MOVES, the version used in this study).

CMAQ 2011 Modeling Platform

- EPA NEI 2011 version 2
- WRF: Weather Research and Forecasting Model v 3.4 – WRF 12 km data cover CONUS provided by EPA
- WRF data generated on the the 4km grid, except for March due to missing data.
- CMAQ with 35 vertical layers, with 15 between 21m to 1200m (to height of resolved Whiteface mountain elevation).
- Gas chemistry – CB05; PM - AERO6 scheme.
- Cloud Dynamics: with/without sub-grid parameterization.

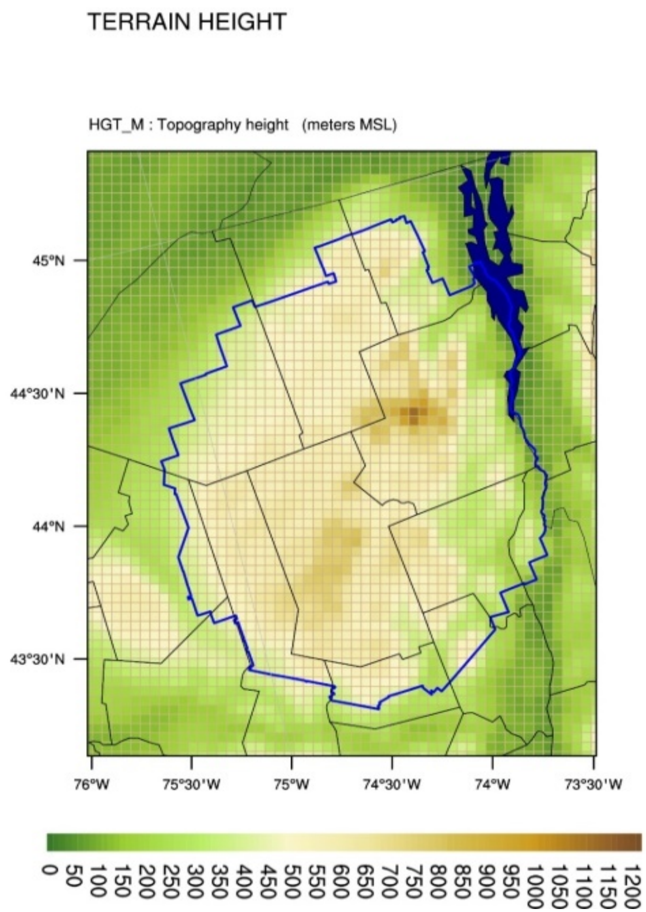


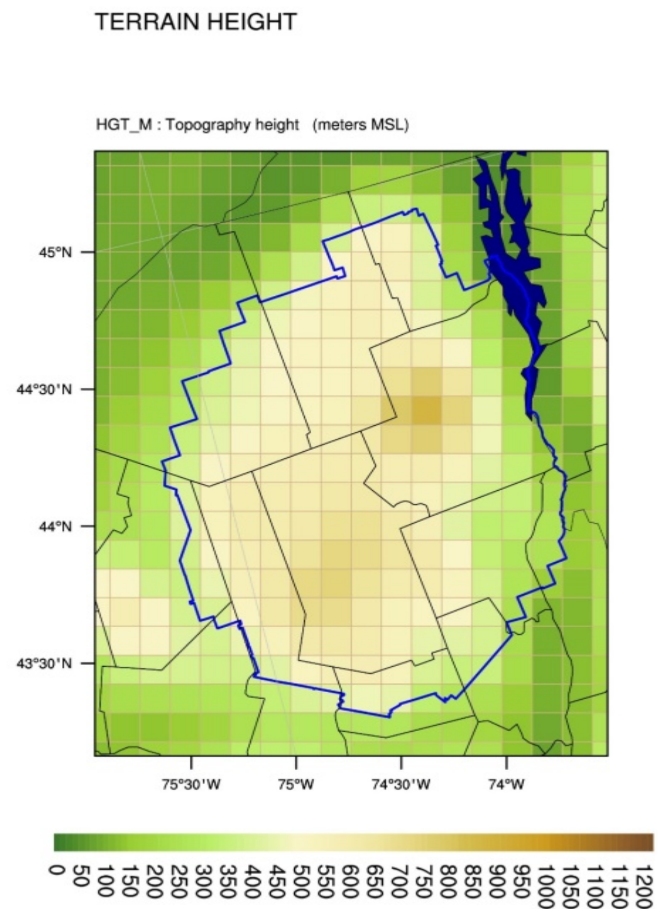
OTC modeling domain:
172 x 172 12km grid
35 vertical layers



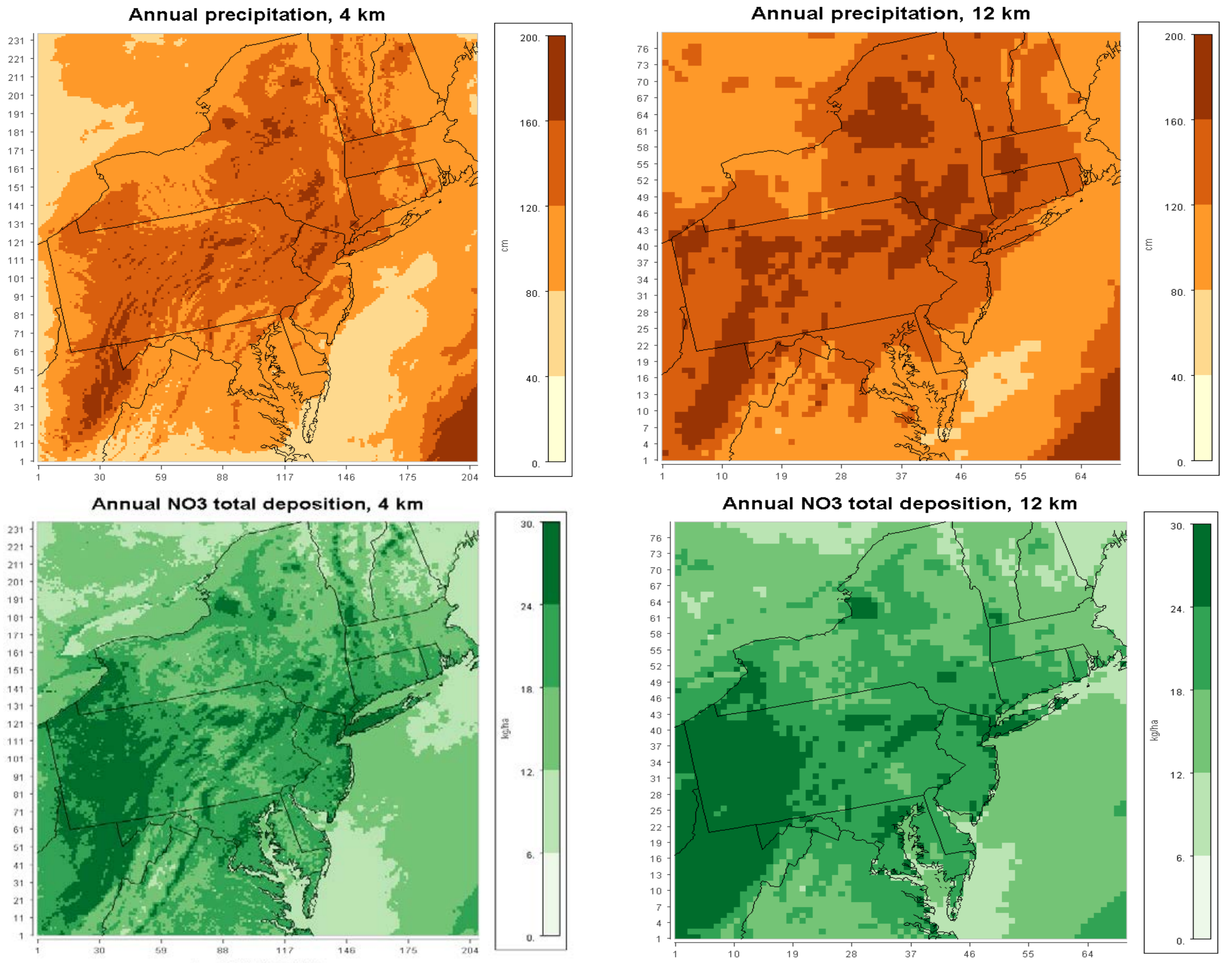
CMAQ terrain resolution for 4km (left) vs 12km grids

Maximum terrain at Whiteface resolved to 1200m by 4km and 800m by 12km grid.





Does the 4km grid provide better resolution of the fields than the 12km grid?



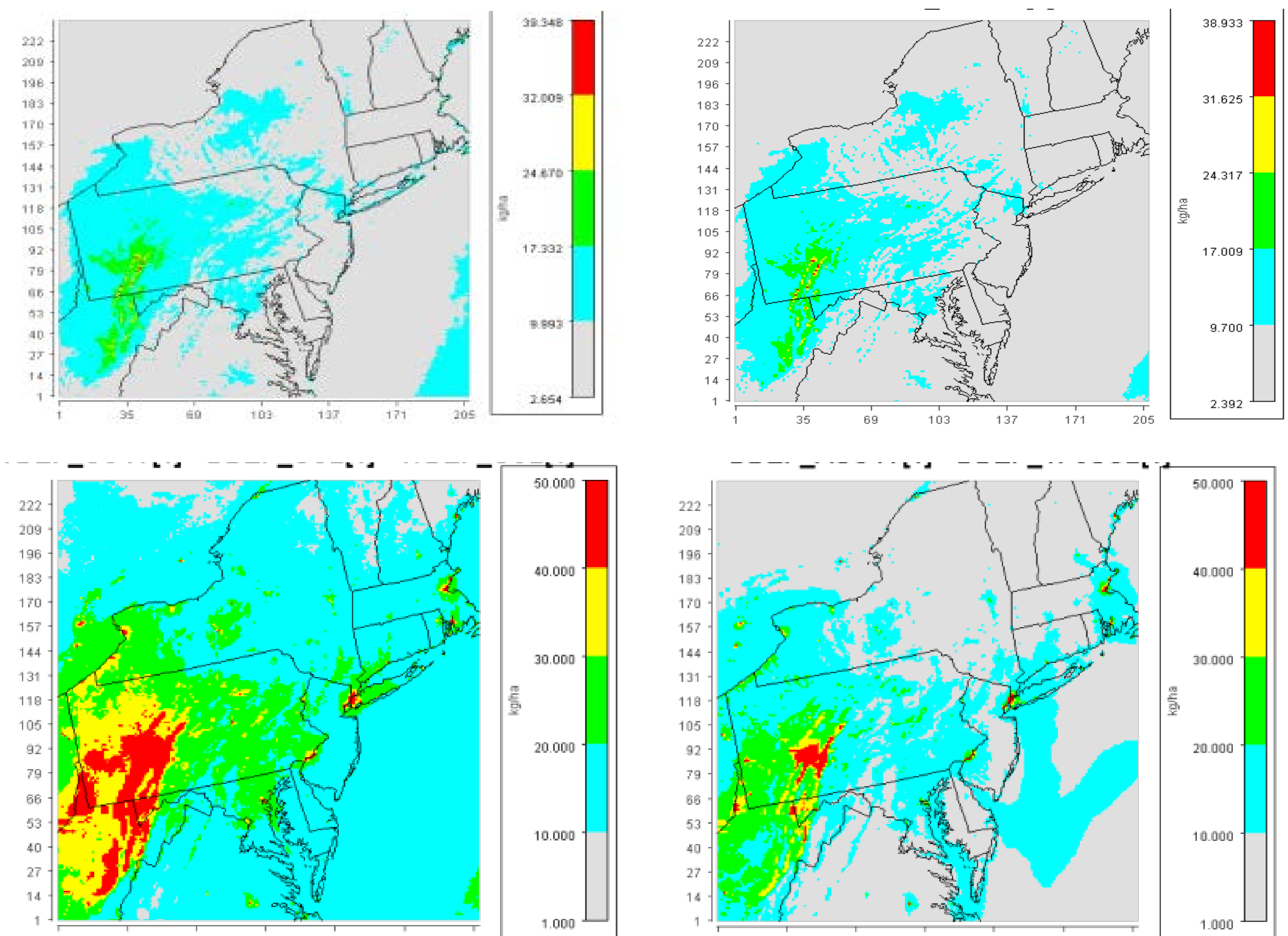
Definitions and terminology

- SO4eq = particulate SO4 + gaseous H2SO4
- Total sulfur (TS) = SO4eq + 1.5*SO2
- NO3eq = particulate NO3 + gaseous HNO3
- NHxeq = particulate NH4 + gaseous NH3
- 2011 base case: CMAQ modeling of the 2011 NEI for all sources in the 4km domain.
- 2011 "zero out" case: same as the 2011 base case, but with all NYS tracked sources (EGUs, WTEs and "other" categories) removed.
- Normalized or relative difference: 2011 base case minus 2011 "zero out" case, the difference divided by base case. This is an indication of the power sector (plus "other" category for Hg) contribution.

Annual acidic species accumulated deposition for <u>base case</u>

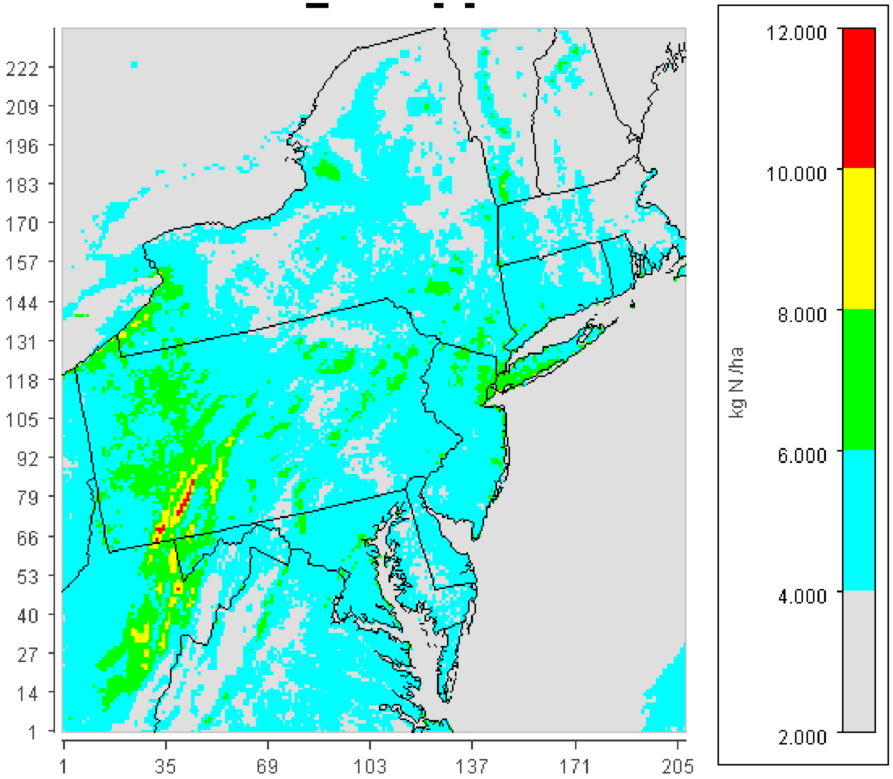
<u>top panels: SO4eq-total (left); SO4eq-wet (right)</u>

<u>bottom panels: TS (left); TS-dry (right)</u>

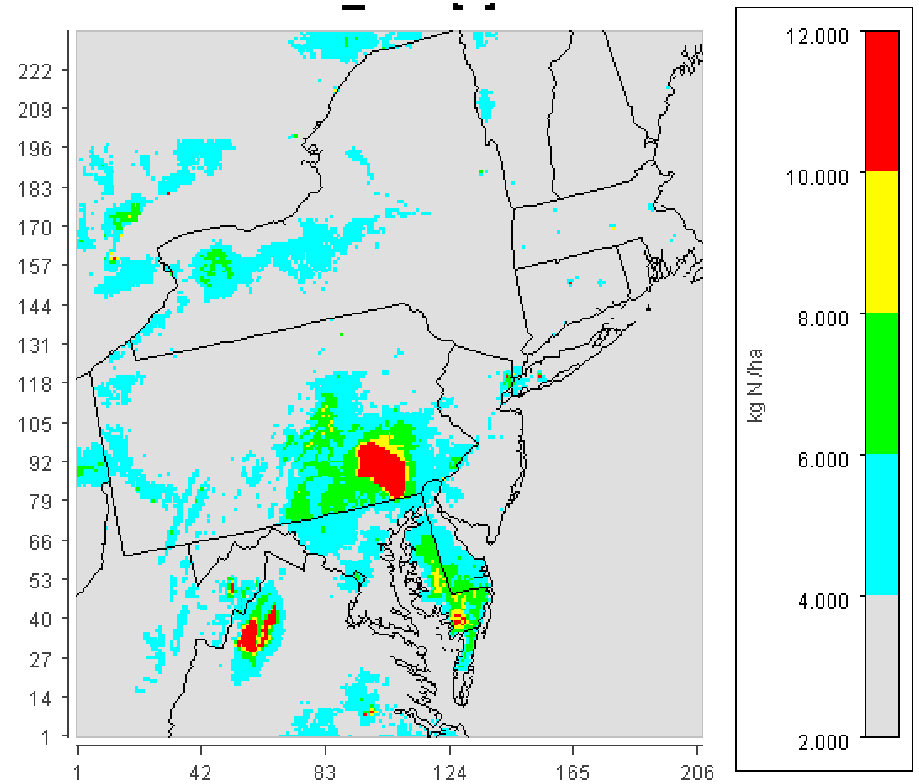


Nitrogen Species in kg N/ha basis. Although absolute deposition for NO3eq is much larger than for NHxeq, the difference in kg N/ ha is much smaller over NYS

Total NO3eq deposition



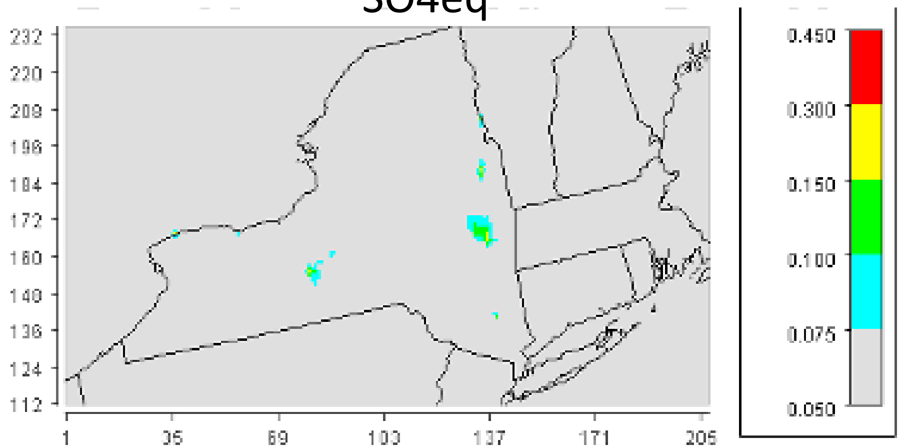
Total NHxeq deposition



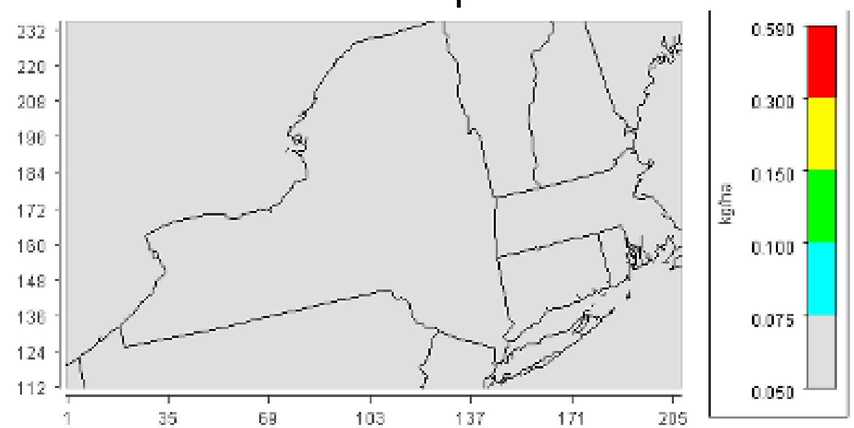
NYS energy production contributions in SO4eq (top left), NO3eq (top right) and TS (bottom)

Reductions in fractions are all “around” the NYS coal plants

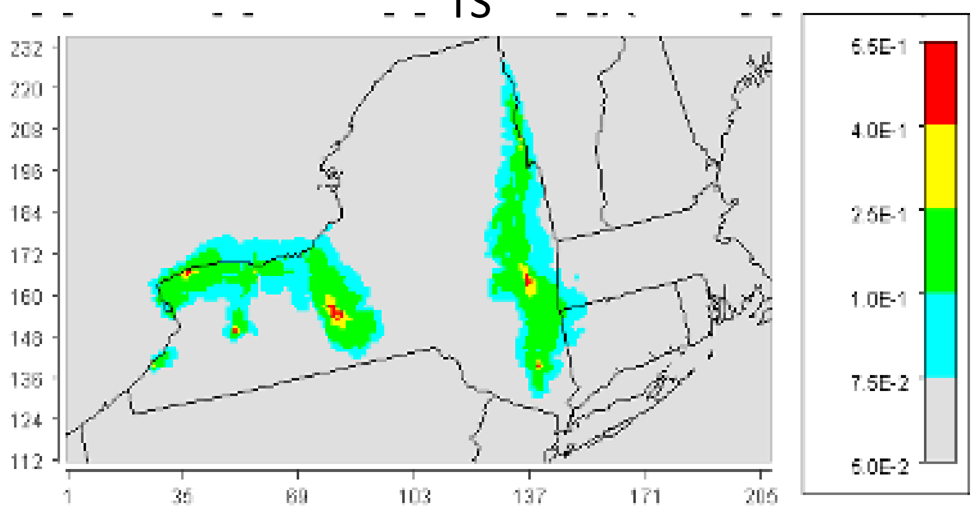
SO4eq



NO3eq



TS



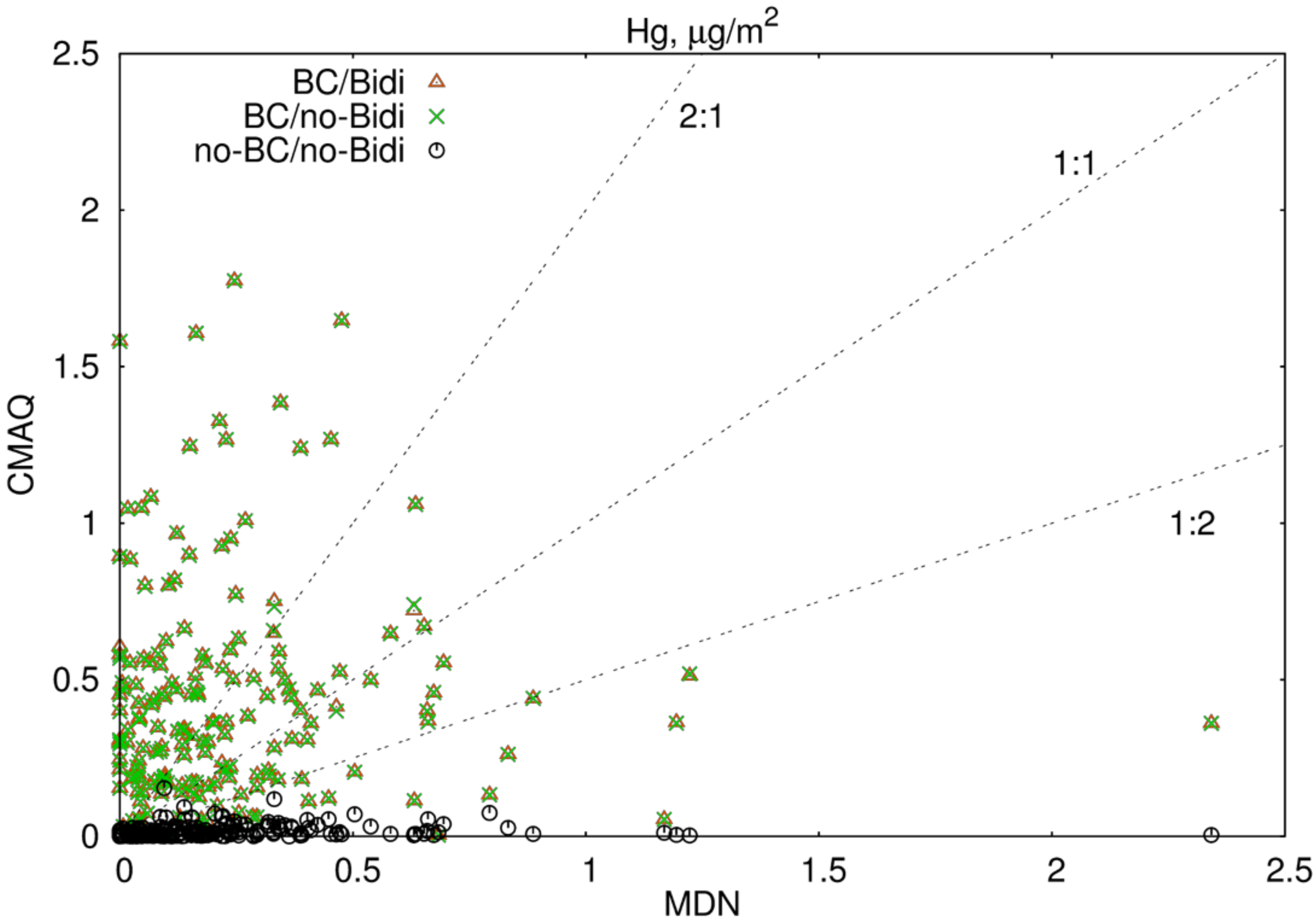
Some of the results for acidic species

- Wet component dominates sulfate deposition.
- Dry component dominates total sulfur, but over NYS the wet portion is as important.
- Fraction of TS due to wet deposition is >50% in the eastern NYS and the reverse in the western part.
- For NO3eq, the dry component more important than for SO4eq.
- Summer SO4eq deposition higher than winter and higher in the Catskills than in the Adirondacks due to precipitation.
- The contributions of NYS energy production sources are around the coal plants.

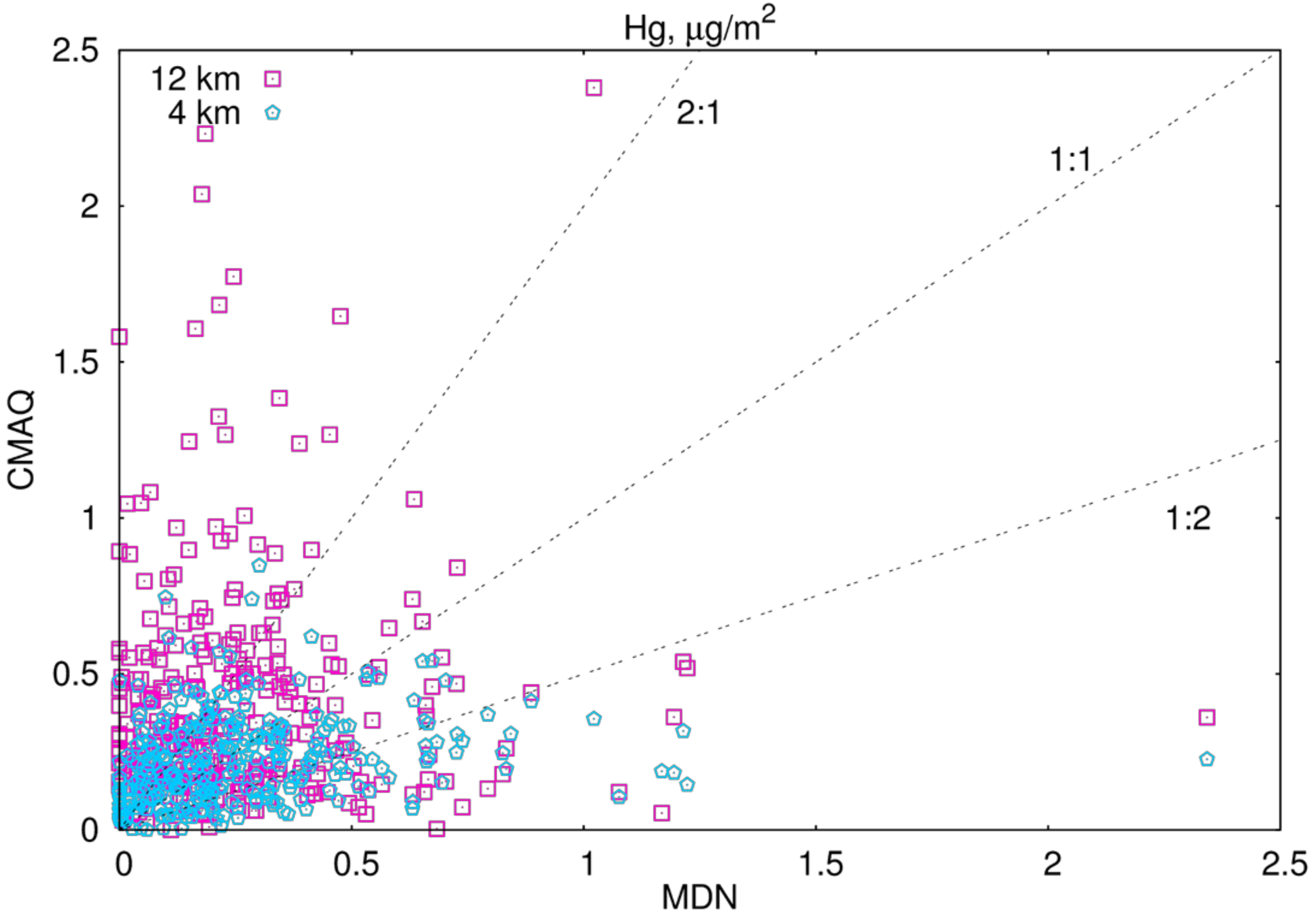
CMAQ Mercury Results

- Initial run with May to July data indicated low impacts relative to observed levels when only in-domain sources modeled. Thus, extracted 12km data as boundary conditions (BC) and also included bi-directional (BiDi) exchange (for Hg0, to and from underlying surface) and redid the same period.
- CMAQ predictions of weekly mercury wet deposition at all MDN sites for mid-May to end of July, 2011 with and without boundary conditions (BC) and bi-directional (BiDi) flux.

Observed and predicted (12 km) weekly wet Hg deposition, June-July 2011 at 27 sites in the model domain; BC/Bidi, BC/no-Bidi, and no-BC/no-Bidi

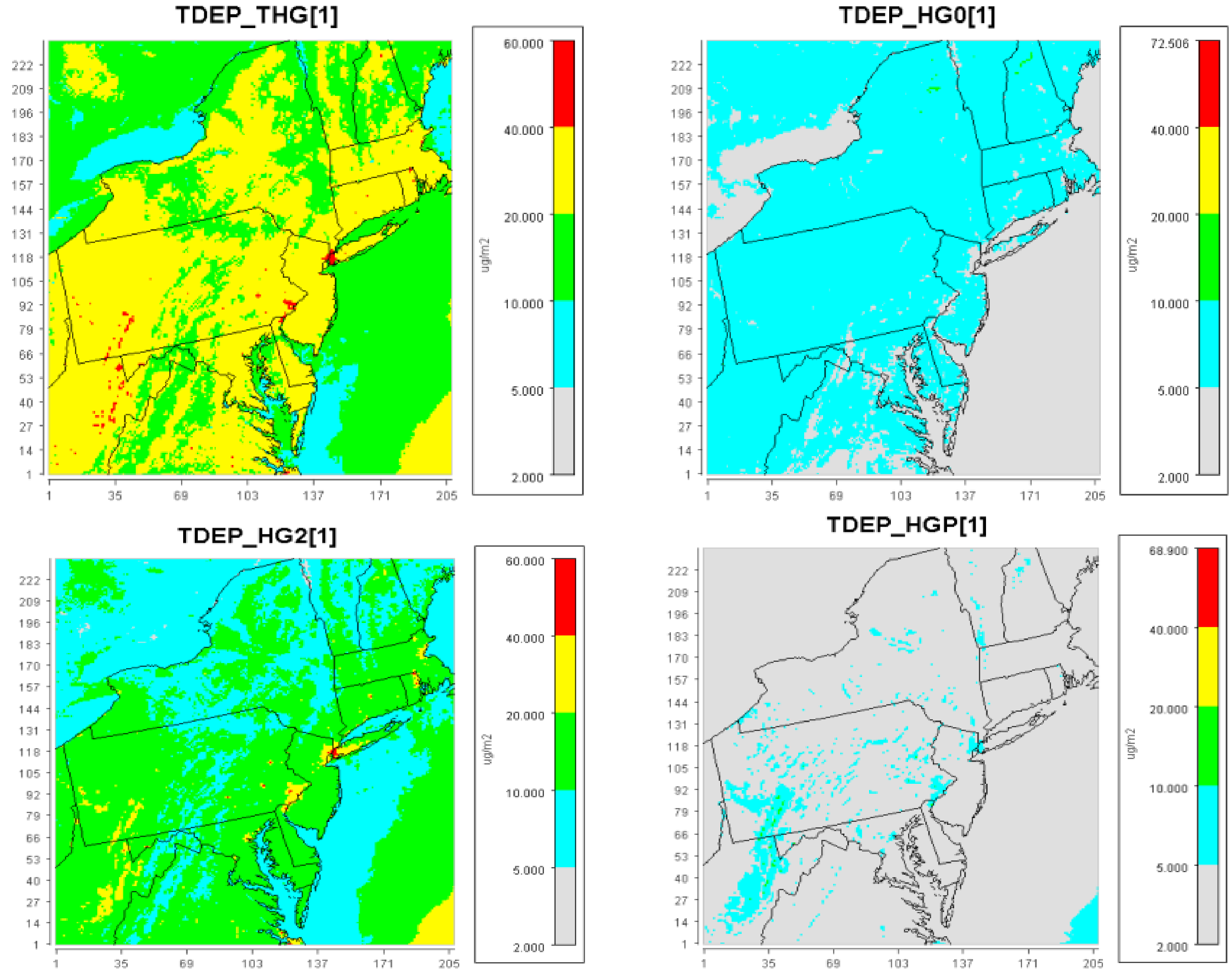


Observed and predicted weekly wet Hg deposition, June-August 2011 at 27 sites in the model domain, BC/no-Bidi; 12 km vs 4 km



Annual Mercury total deposition-Base case

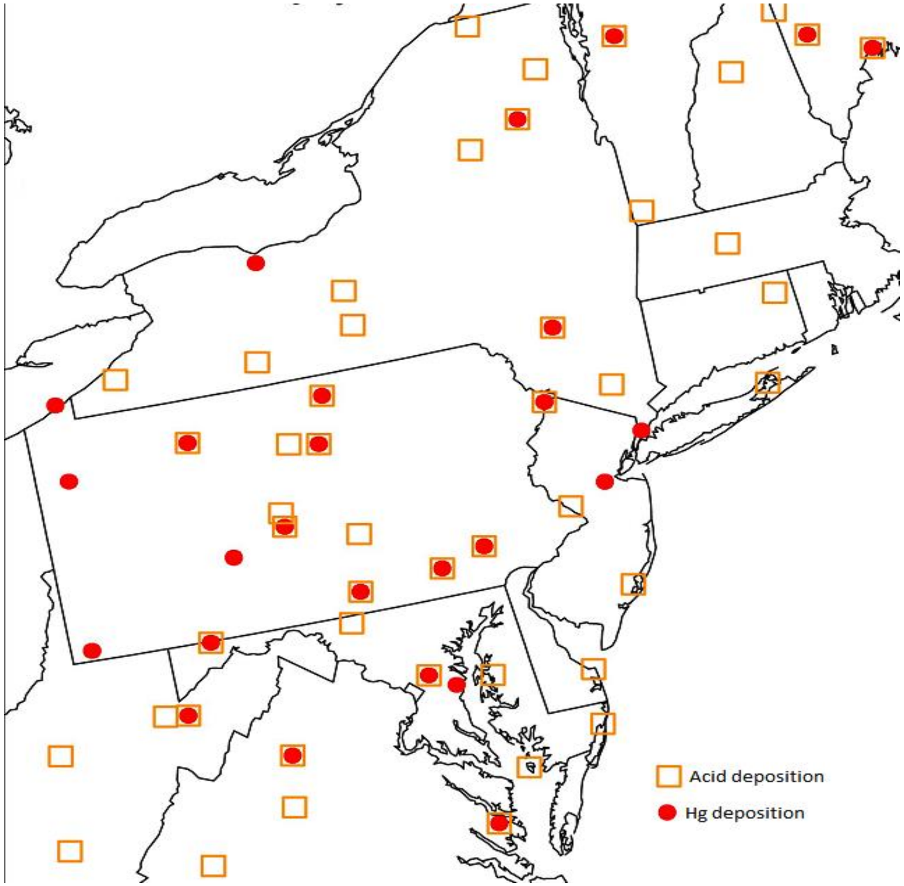
Total (THG), elemental (Hg0), oxidized gas (Hg2), particulate (HgP)



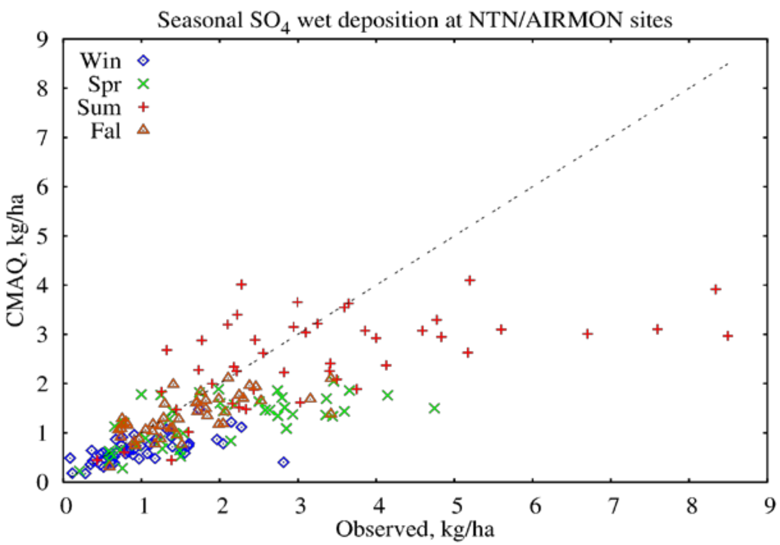
Some CMAQ mercury results

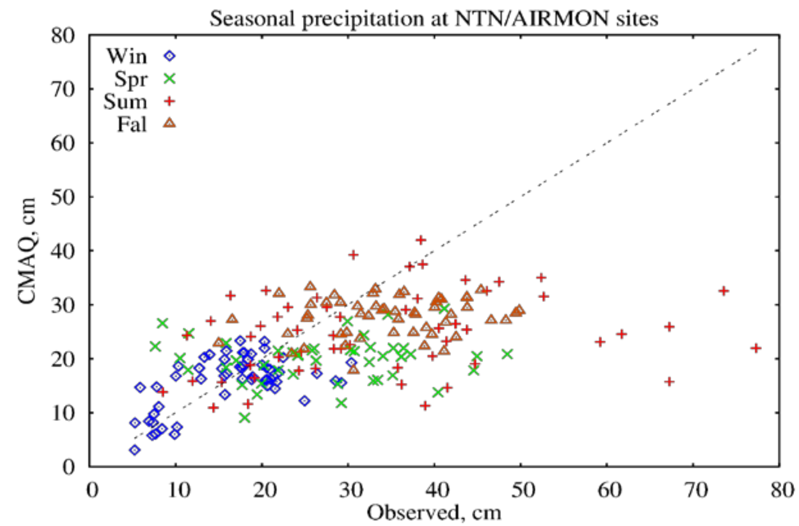
- Hg0 deposition low due to insolubility and low deposition velocity, while Hg2 has relatively higher values. HgP has lower contribution due to low emissions and low wet component.
- No real seasonal difference between summer and winter, with both contributing about ¼ each.
- Summer months have higher wet deposition in Catskills than Adirondacks similar to sulfate.

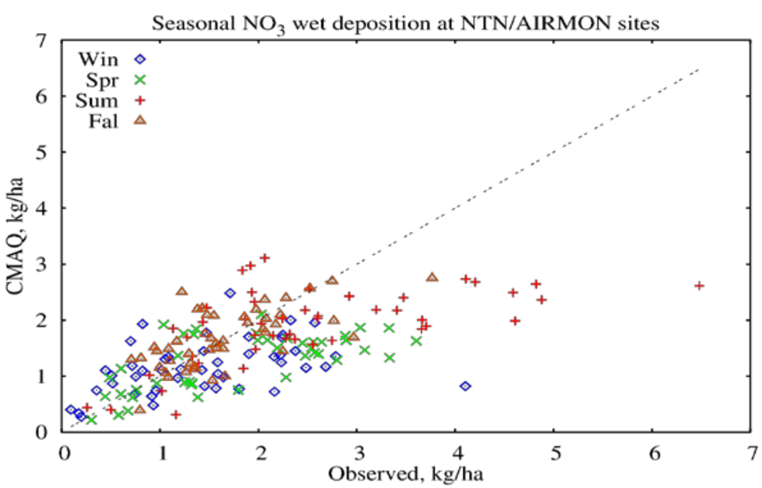
NADP wet deposition sites used for comparisons to CMAQ predictions

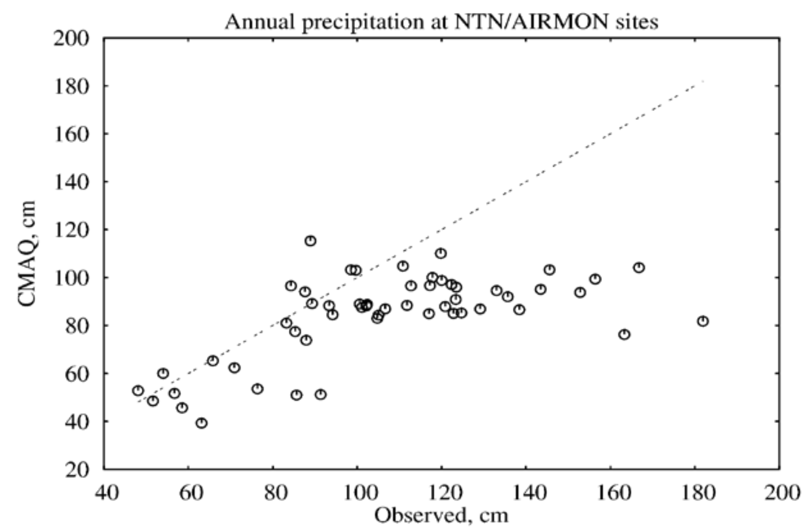


Comparison of CMAQ wet deposition of acidic species and precipitation to NADP observations.









NADP comparisons

- Underestimated the precipitation in summer season, led to underestimated the wet deposition.
- Mean normalized error is about 30%.
- WRF biased dry in 4 Km simulations.

Acknowledgement:

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Final report will be posted in 2017 on the NYSERDA page:
https://www.nyserda.ny.gov/All-Programs/Programs/Environmental-Research/Air-Quality