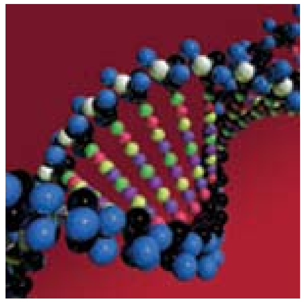
Single Source Ozone and PM Modeling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EPA's 9th Conference on Air Quality Modeling
Non-Guideline Applications
October 10, 2008

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EPA Guidelines/Guidance for Air Quality Modeling Assessments

- AERMOD for near-source (< 50 km) air quality impacts of primary pollutants (EPA, 2005)
- CALPUFF for far-field (> 50 km) air quality impacts of primary pollutants (EPA, 2003)
  - CALPUFF adopted for SO_2 and primary PM PSD increments and NAAQSs, not AQRV analysis
- Photochemical Grid Models (PGMs) recommended for ozone and secondary components of PM (e.g., SO_4 & NO_3) (EPA, 2007)
  - Lagrangian models (e.g., AERMOD and CALPUFF) only suitable for primary components

New Ozone and $PM_{2.5}$ NAAQS

- New 0.075 ppm 8-hour and 35 µg/m^3 24-hr $PM_{2.5}$ NAAQSs will bring many more areas into nonattainment
  - $PM_{2.5}$ NAAQS increases importance of secondary $PM_{2.5}$
- Capability needed to obtain individual contributions to ozone and $PM_{2.5}$ concentrations, deposition and visibility
- Current guideline models have no (AERMOD) or highly simplified (CALPUFF) representation of chemistry
- Photochemical Grid Models (PGMs) have capability to correctly treat chemistry
  - But how can they resolve and correctly simulate near source plume chemistry and dispersion?

Why PGMs Have Not Been Used to Address "Single Source" Impacts

- PGMs can only resolve impacts to the grid resolution
  - Fine grid size needed near the source to resolve near-source plume chemistry and dispersion
    - Need many grid cells to assess downwind impacts
    - High computer resource requirements
- Must account for all emission sources
    - Needed to correctly simulate chemistry
- Databases more costly to develop
    - MM5/WRF applications
    - SMOKE or other emissions model
- More expertise needed in their application

Recent Developments for "Single Source" Modeling using PGMs

- Two-way interactive grid nesting
  - Allows fine grid over sources with coarser grid downwind when plumes are larger
- Flexi-nesting
  - Can specify fine grid to resolve point source plume chemistry and dispersion without providing met and emission inputs
- Full Chemistry Plume-in-Grid Modules
  - Treats unique near-source chemistry of point source plumes
- PM and Ozone Source Apportionment
  - Allows individual source(s) assessments
- Computational advances
- Availability of PGM Databases and model set ups
  - RPOs, AIRPACT, SIPs, etc.

Advanced Grid Nesting

- Two-way interactive grid nesting
  - Allows specification of high resolution grid over sources with coarser grids downwind where plumes are larger
- Flexi-Nesting
  - Interpolate meteorology, emissions and/or other inputs for nested fine grid from coarse grid data
  - Allows fine grid treatment of point source plumes
    - Available within the CAMx model (just specify where fine grid domains are desired in job script)
    - Have developed tool to generate flexi-nest fine grid inputs for CMAQ (for EPA/OAQPS)

Full Chemistry Plume-in-Grid

- Incremental chemistry approach allows full gas-phase, aqueous-phase and aerosol chemistry within Plume-in-Grid modules
  - CAMx Incremental Reactions for Organics and NOx (IRON) Plume-in-Grid (PiG) treatment
  - CMAQ Advanced Plume Treatment (APT)

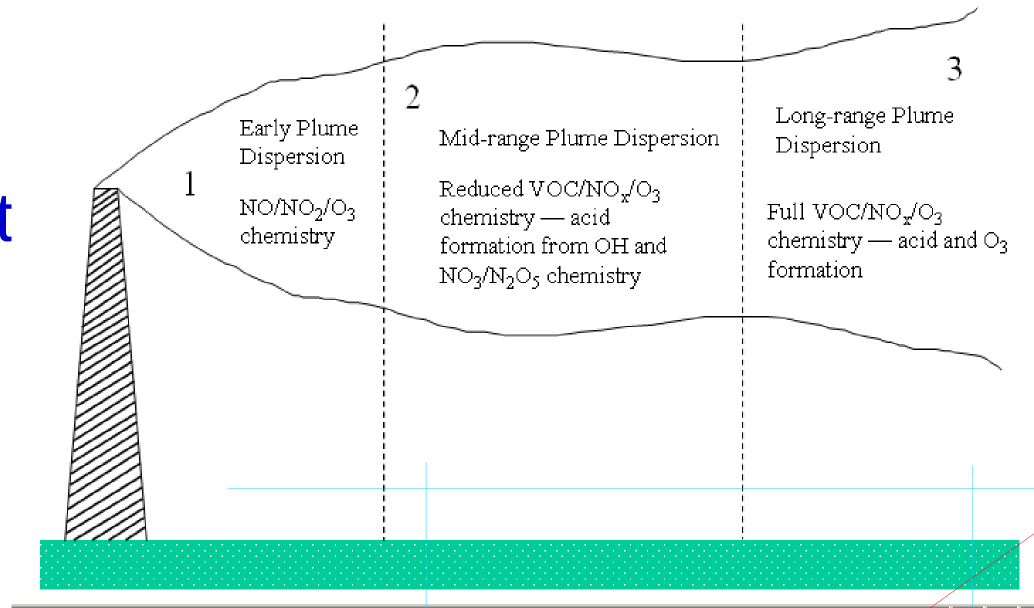
    • Calculate chemical kinetic reaction rates using total concentrations (PiG + Grid)

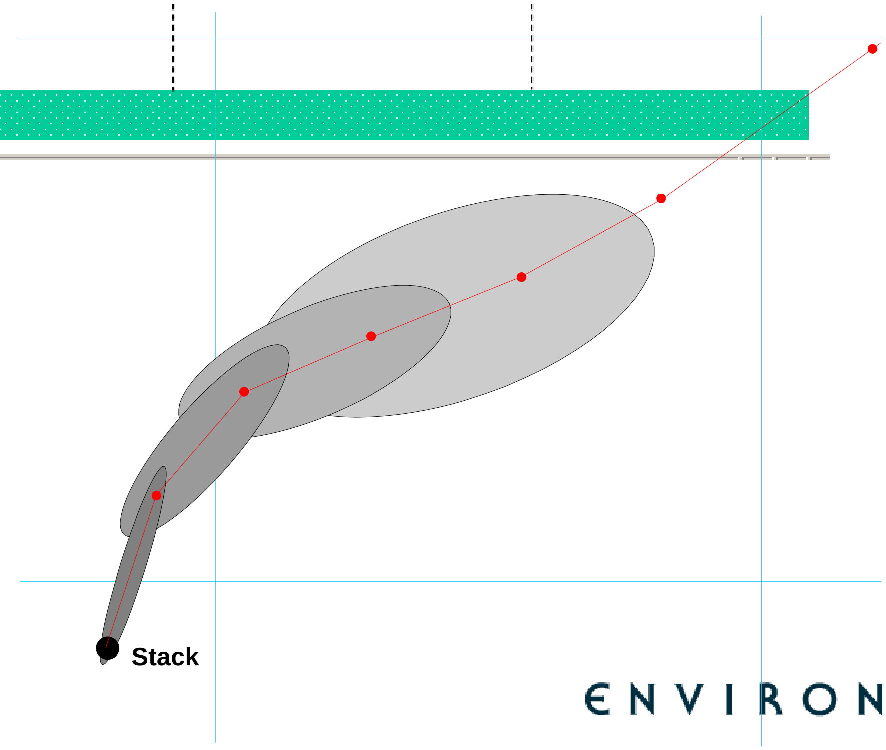
    • Apply chemical rates to incremental concentrations within puffs (PiG alone)

    • When size of plume is commensurate with grid cell size release incremental PiG concentrations to grid model

Full Chemistry Plume-in-Grid

- Important to simulate proper chemistry in early evolution of point source plumes
- Very little if any ozone and secondary $PM_{2.5}$ formed under Stage 1 and 2 plume chemistry conditions for large NOx sources





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PM and Ozone Source Apportionment

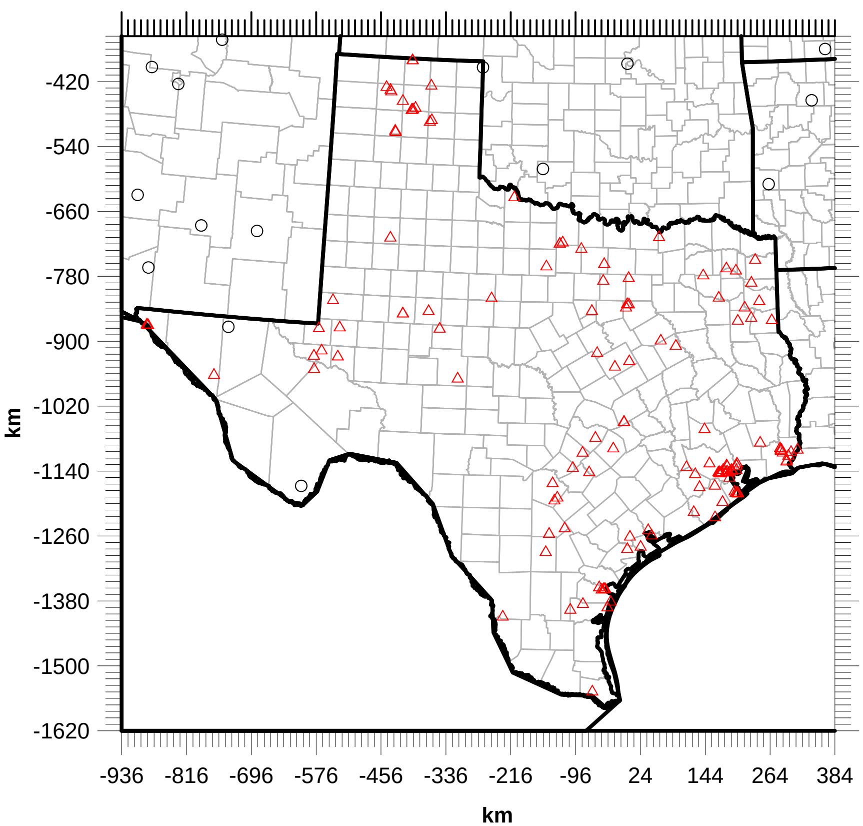
- PM and Ozone Source Apportionment Technology (OSAT/PSAT) available in CAMx
  - Uses reactive tracers that operate in parallel to host model and tracks ozone and PM formation back to emission source regions and categories
  - PSAT has five families of tracers: SO4; NO3/NH4; Primary PM; SOA; and Hg
- Similar approaches in CMAQ (TSSA and PPTM)
- Allows for identification of the ozone and PM impacts from several individual sources or groups of sources in single run

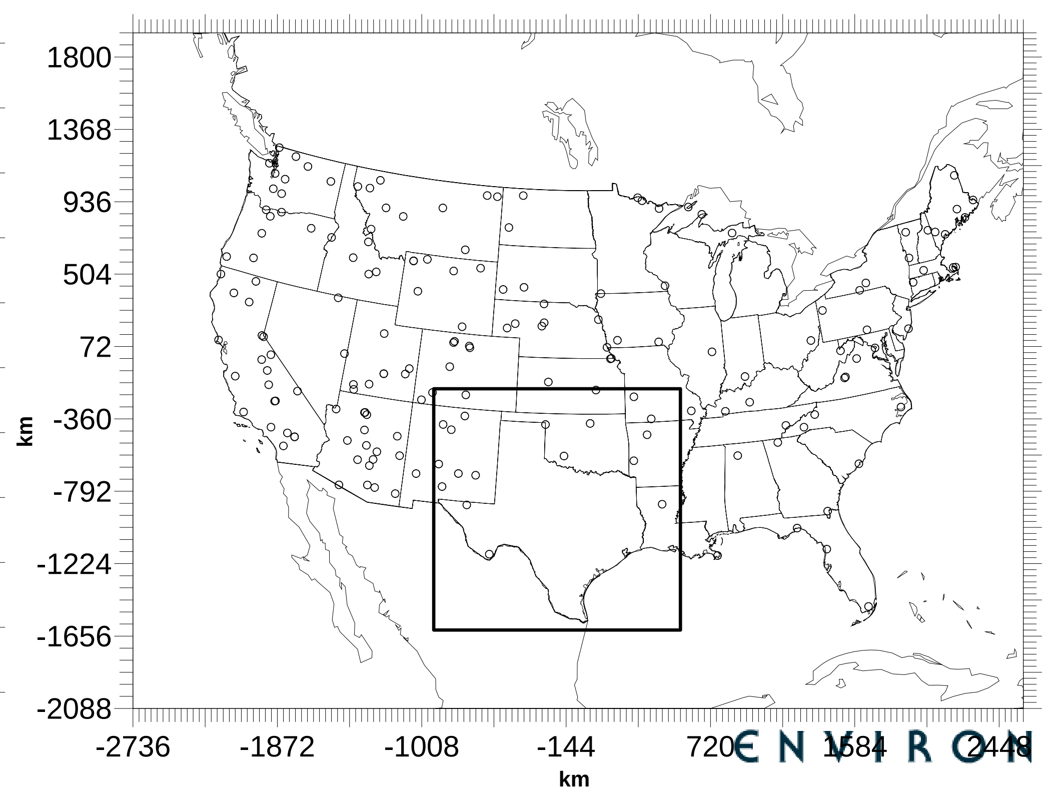
Example "Single Source" PGM Applications

- Texas "Group BART" application
  - CAMx 36/12 km with PiG and PSAT
- Estimation of individual contributions of 31 point sources to annual $PM_{2.5}$ in the eastern U.S.
  - Individual point source contributions to 2009 annual $PM_{2.5}$ concentrations
  - Visibility Improvements for States and Tribal Association of the Southeast (VISTAS) and Association for Integrated Planning of the Southeast (ASIP)
- Annual $PM_{2.5}$ SIP modeling for St. Louis
  - Effects of local sources on $PM_{2.5}$ nonattainment

Texas Group BART Analysis

- CENRAP 2002 36 km modeling CAMx database
  - Add 12 km flexi-nest grid covering Texas and nearby Class I areas
  - Use IRON PiG for Texas BART Source
  - Use PSAT to obtain PM2.5 contributions of groups of Texas BART sources for comparison with 0.5 deciview threshold





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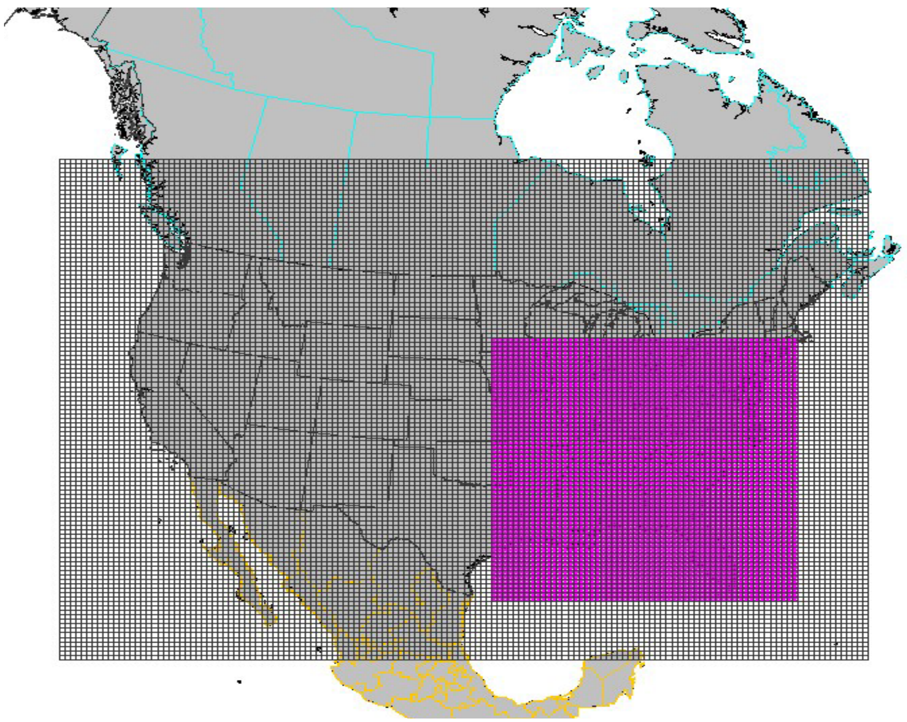
VISTAS/ASIP 36/12 km Domains

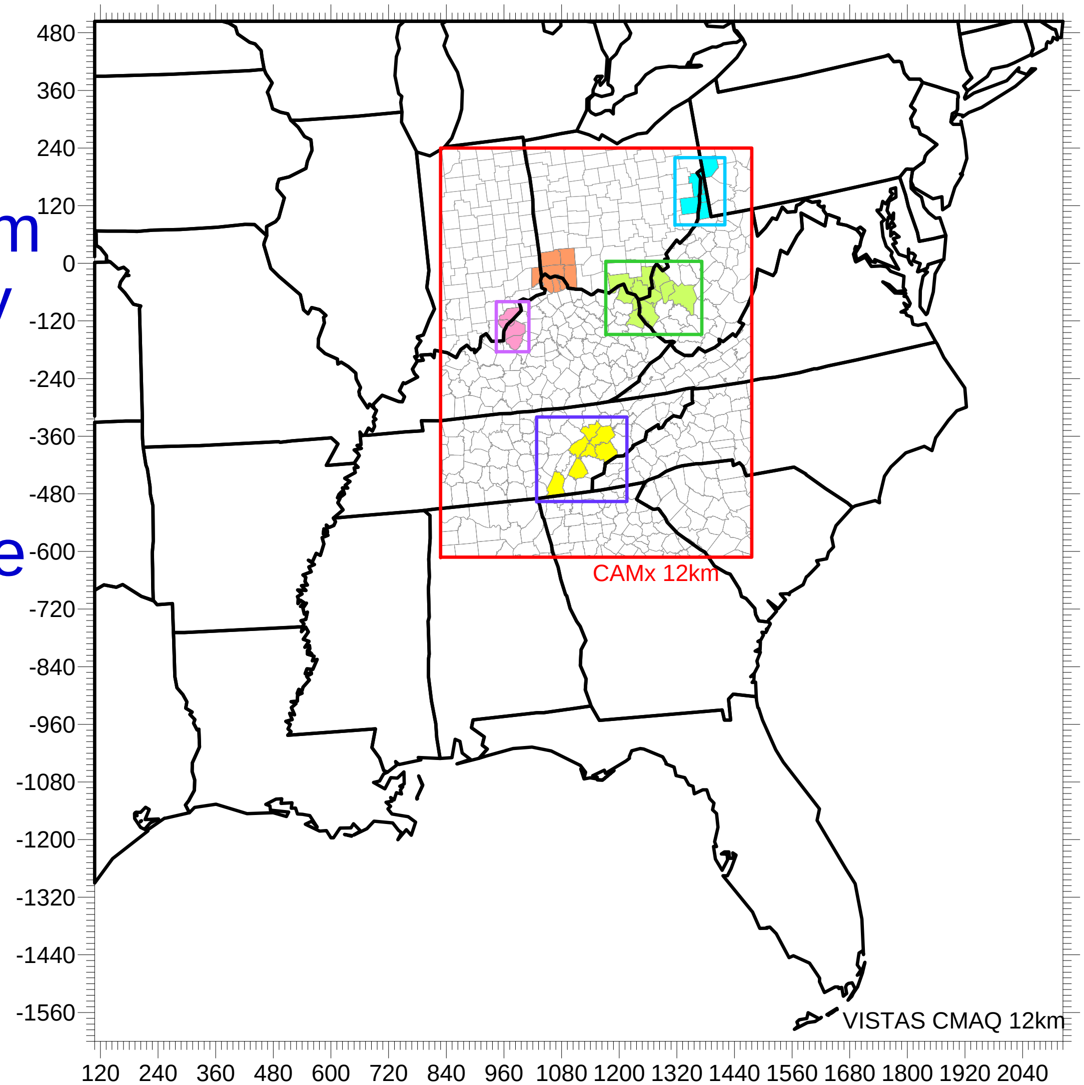


- 2002 Annual Runs
  - 4 Quarters w/ ~15 day spin up
  - MPI w/ 6 CPUs
- 36 km: 148 x 112 (4 days)
- 12 km: 168 x 177 (10 days)
- 19 Vertical Layers
- CMAQ V4.51 w/ SOAmods
  - M3Dry
  - CBM-IV/AE4/SORGAM
  - SOAmods: In 2005 VISTAS enhanced CMAQ to include SOA from sesquiterpenes and isoprene (Morris et al., 2006)

ASIP $PM_{2.5}$ Point Source Contributions

- Some ASIP/VISTAS states wanted to know individual contributions of several point sources to 2009 $PM_{2.5}$ levels
  - 31 individual point sources in 6 states identified
  - Contributions due to SO2 and primary PM emissions requested
- CALPUFF considered for assessment
  - Not consistent with CMAQ full-science chemistry
  - Provide inconsistent source contributions with 2009 $PM_{2.5}$ SIP projections
- ASIP 36/12 km database inappropriate for individual point source modeling
  - 12 km grid cell size too coarse to treat chemistry and dispersion of point source plumes
  - Use of high enough resolution to resolve point source plume would be computationally prohibitive
  - Would need to perform base case and 31 zero-out runs to get individual source contributions
- Elected to develop a new CAMx 2002 database:
  - 12/4 km domain with two-way nested grids
  - Plume-in-Grid to address near-source chemistry and dispersion
  - PM Source Apportionment Technology (PSAT) to obtain individual source contributions

- CAMx 12/4 km domain nested within ASIP 12 km CMAQ domain (one-way nesting)
- CAMx 12/4 modeling using two-way interactive grid nesting
- 2002 base case using standard model
- 2009 base case with PSAT $PM_{2.5}$ source apportionment for 31 point sources



VISTAS CMAQ 12 km: 168 x 177 (108, -1620) to (2124, 504)
CAMx 12km: 54 x 71 (828, -612) to (1476, 240)

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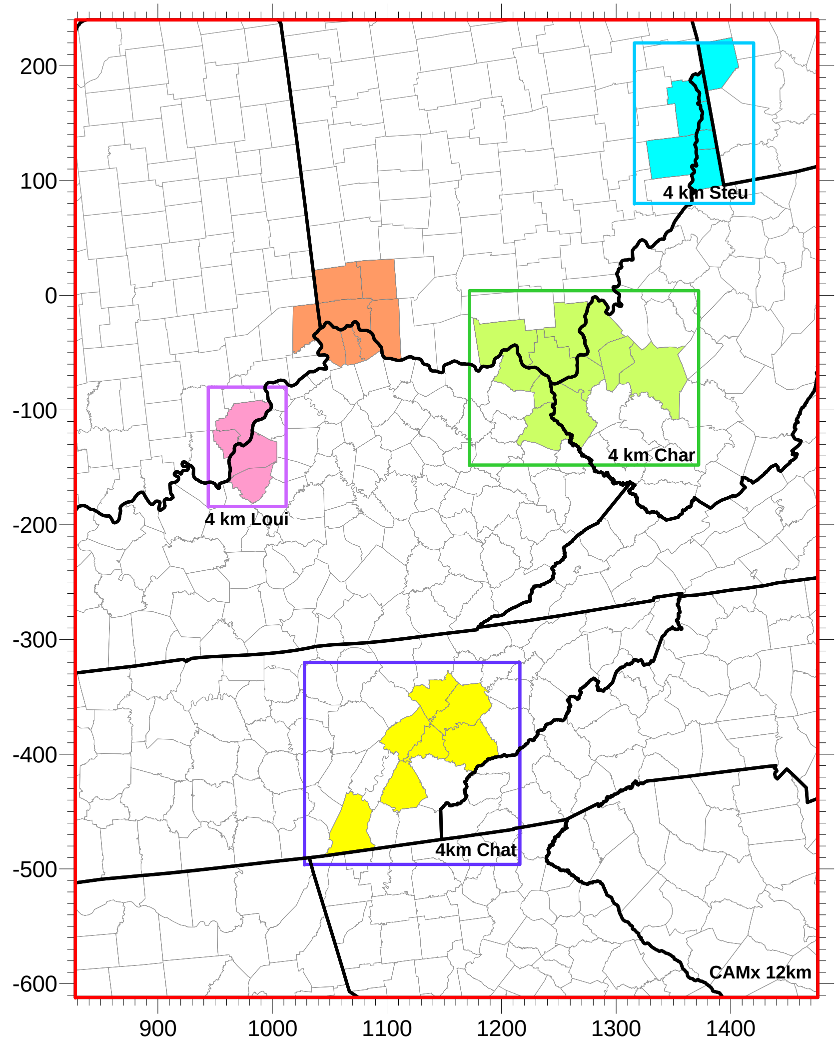
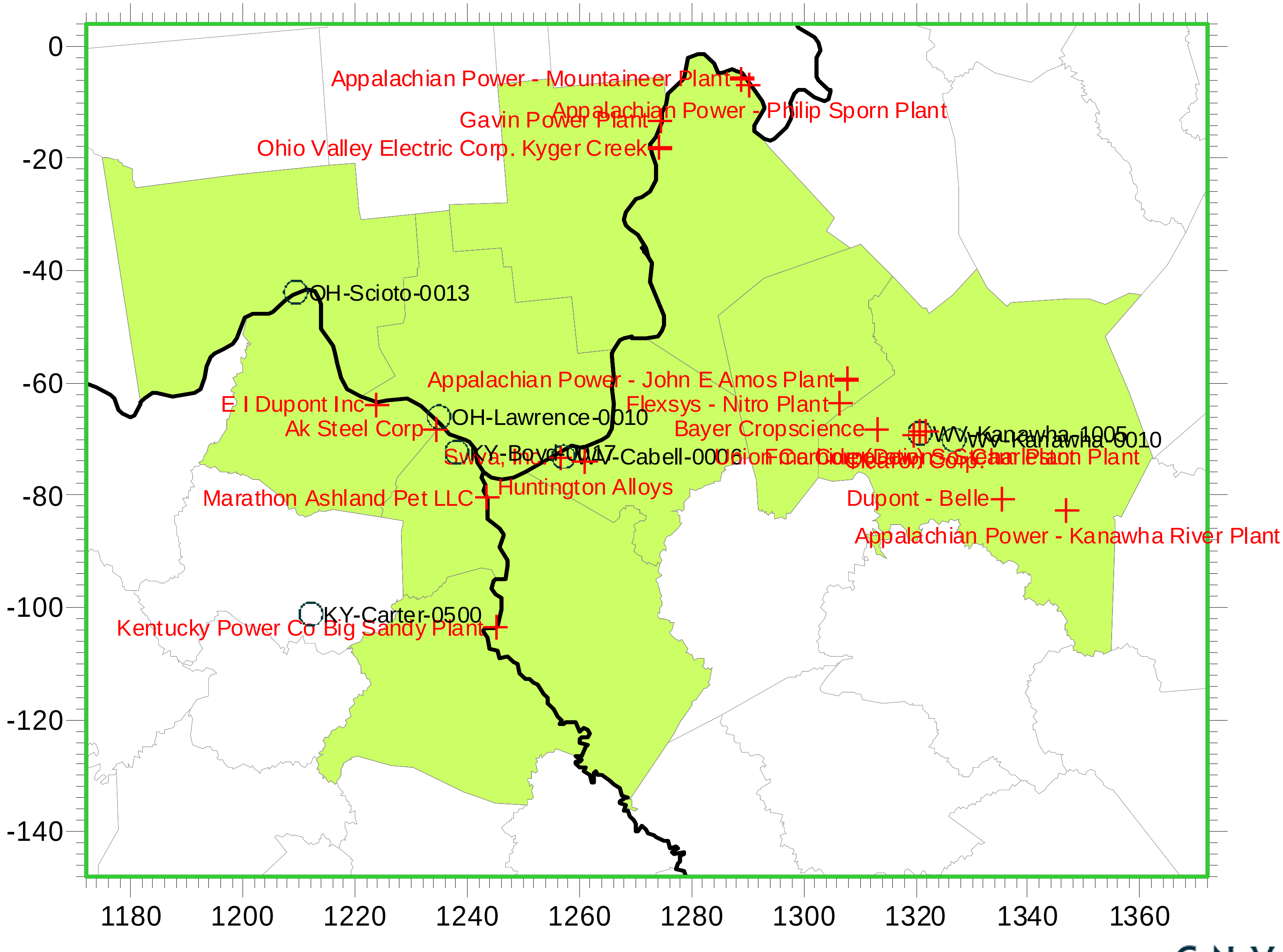
- CAMx 12/4 Domains
- Four 4 km domains:
  - Charleston-Huntington, KY/OH/WV
  - Wheeling-Weirton, OH/PA/WV
  - Louisville, IN/KY
  - Knoxville-Chattanooga, GA/KY/NC
- PSAT to obtain individual $PM_{2.5}$ contributions from 31 point sources
- Plume-in-Grid for 31 plus other large point sources



CAMx 12km:	54 x 71	(828, -612) to (1476, 240)
CAMx 04km (includes buffer cells):		
Steubenville/Wierton	26 x 35	(1316, 80) to (1420, 220)
Charleston	50 x 38	(1172, -148) to (1372, 4)
Louisville	17 x 26	(944, -184) to (1012, -80)
Chattanooga/Knoxville	47 x 44	(1028, -496) to (1216, -320)

Huntington-Ashland and Charleston 4 km Domain Map with FRM sites & Source Locations



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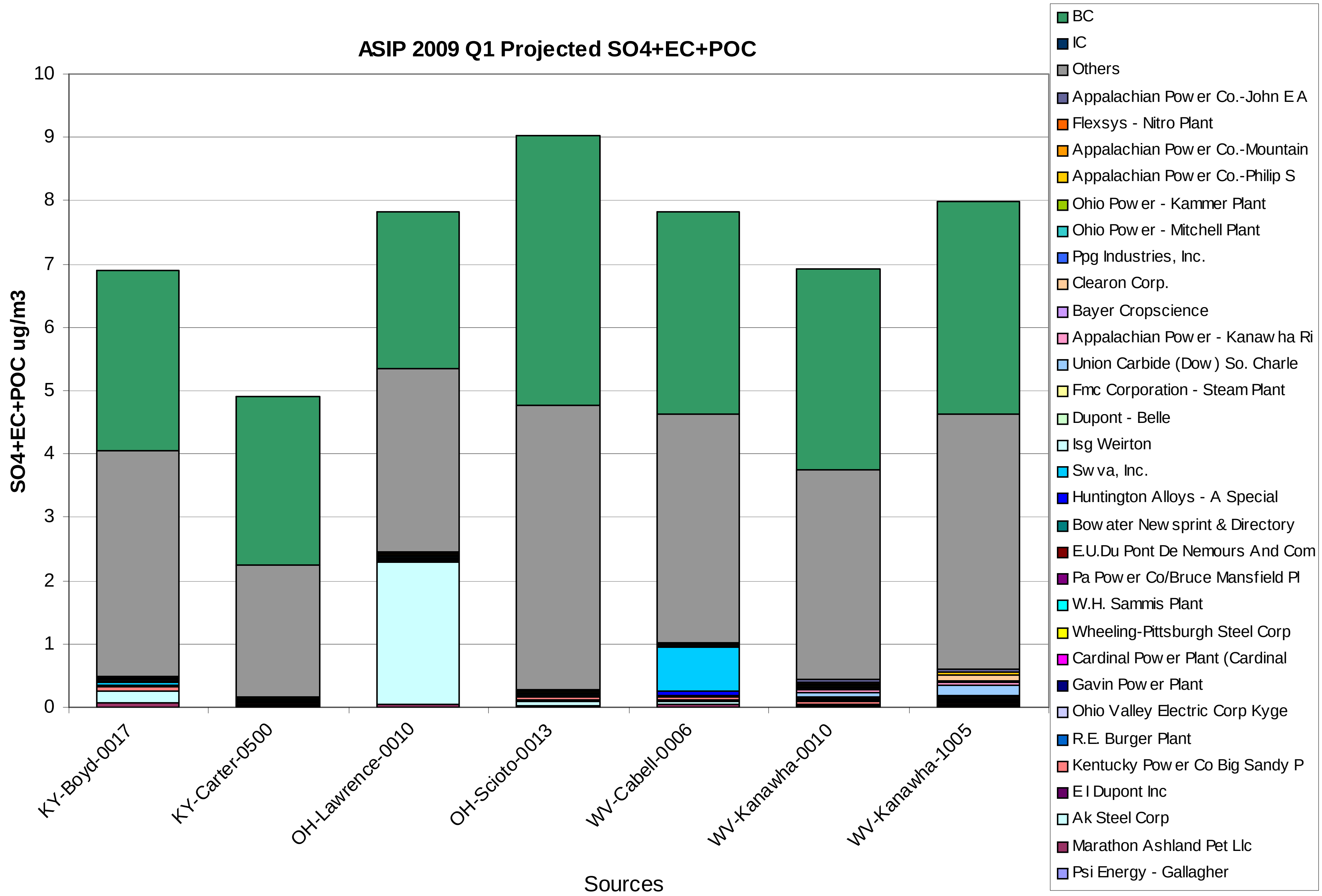
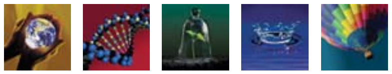
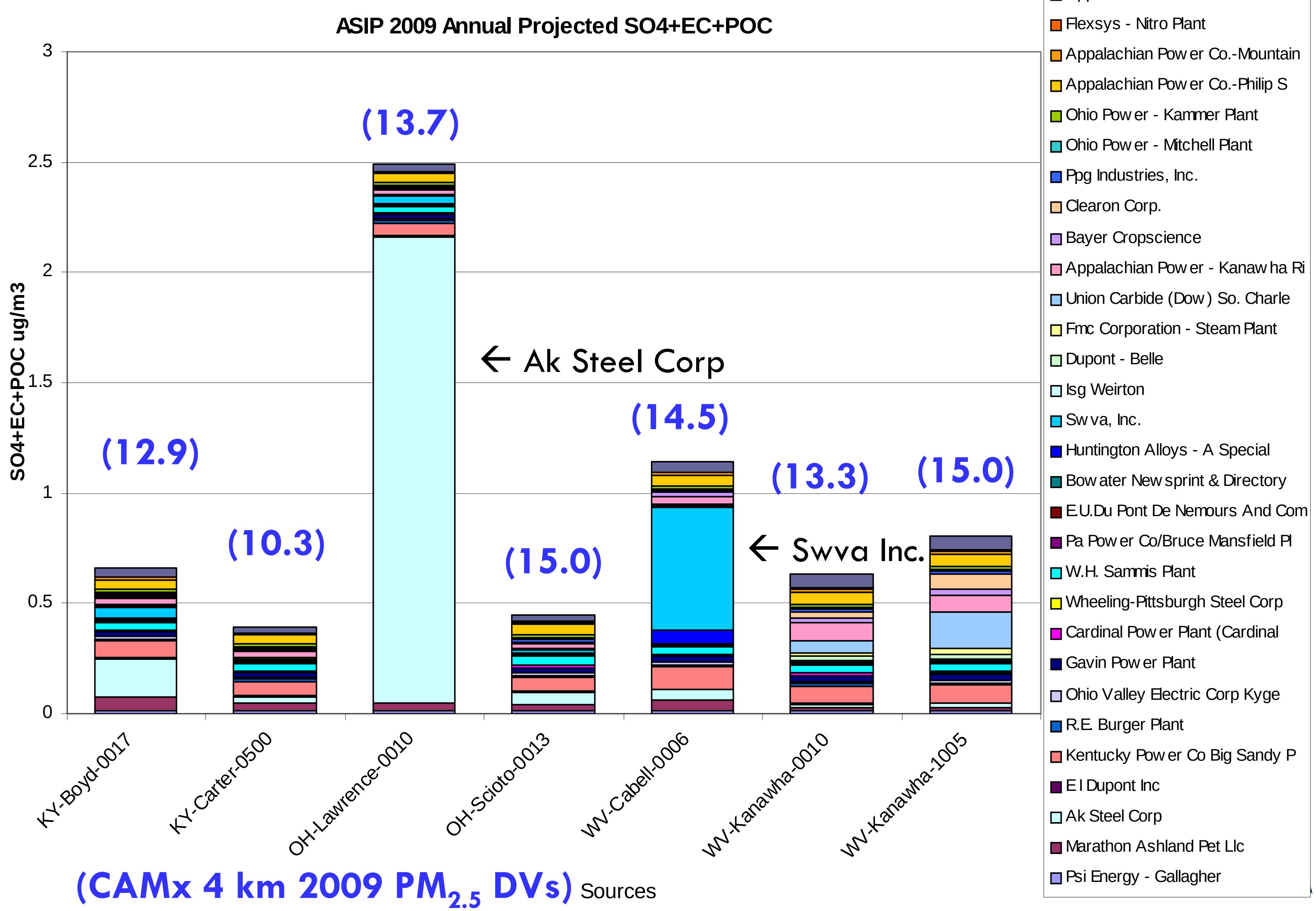
Huntington-Ashland-Charleston: 4 km Grid; All Sources and SO4+Prim-PM

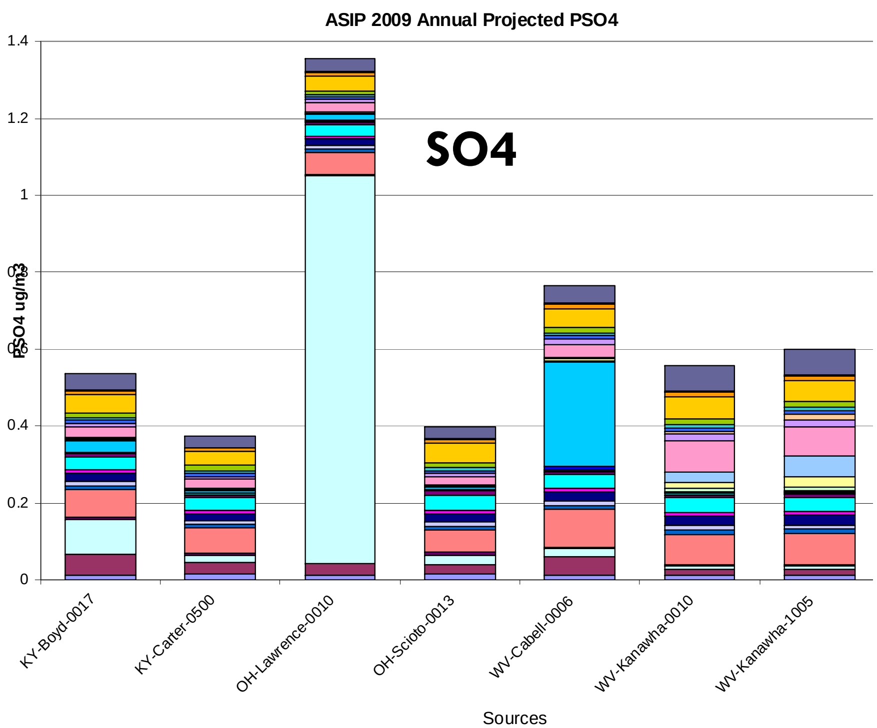


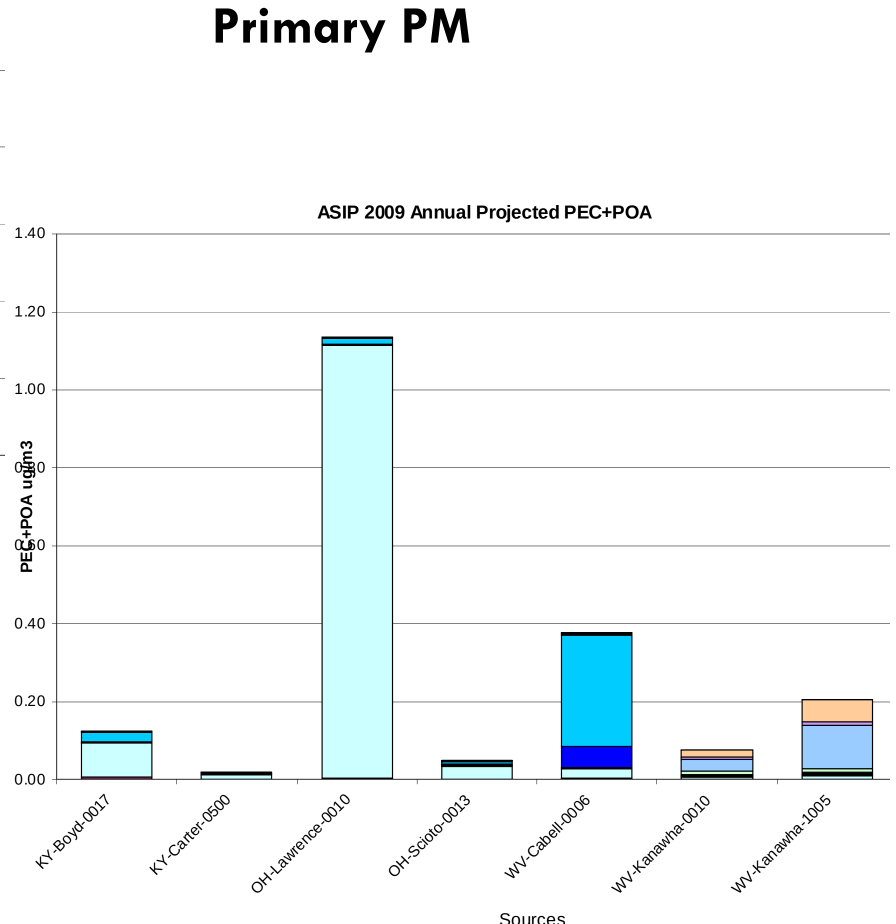


Huntington-Ashland and Charleston: 4 km Grid; 31 Facilities



Huntington- Ashland and Charleston: 31 Facilities; SO4 (left) and Primary PM (right)





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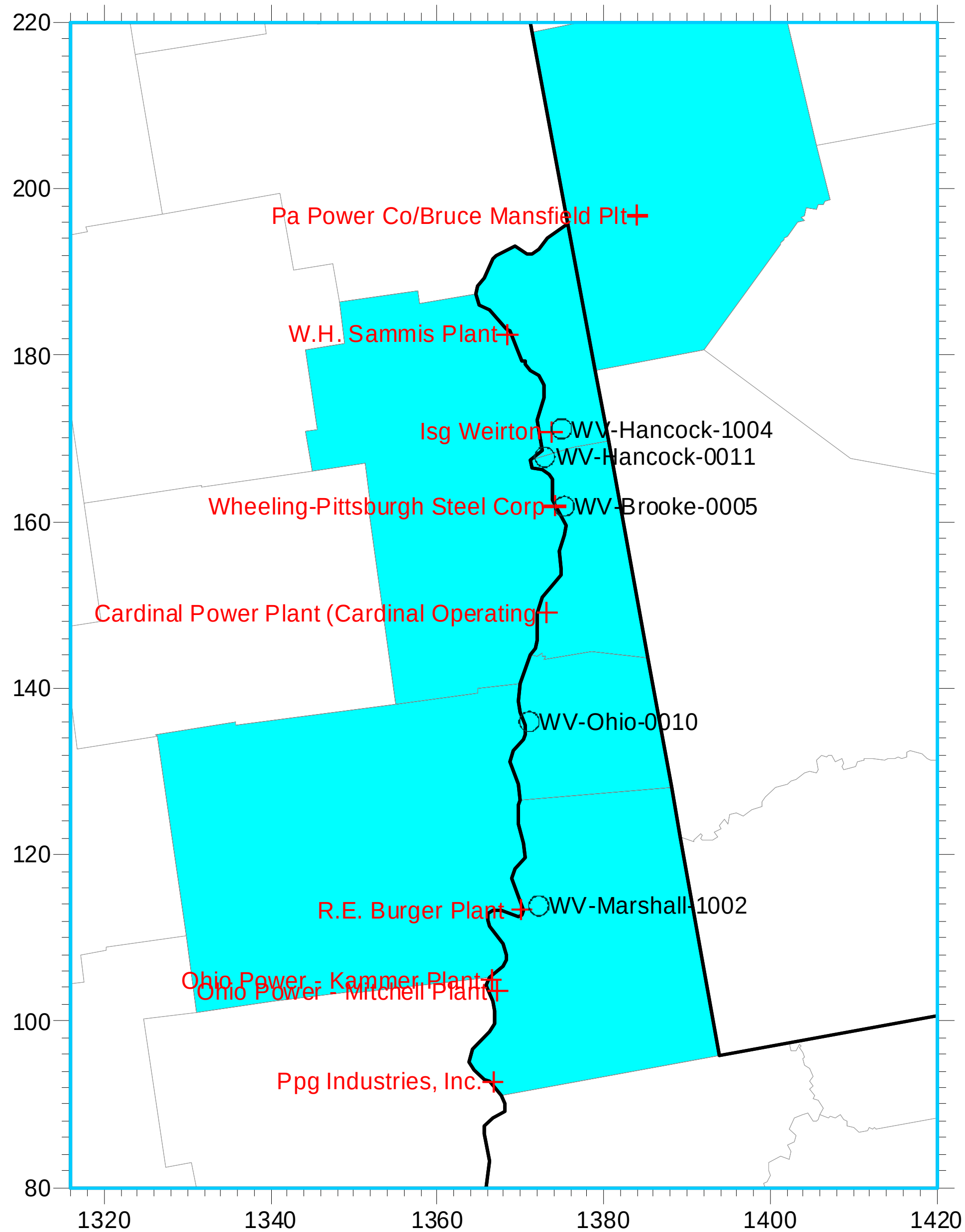
Wheeling 4 km Domain Map with FRM sites and Source Locations



CAMx 04km (includes buffer cells):
Steubenville/Wierton 26 x 35 (1316, 80) to (1420, 220)

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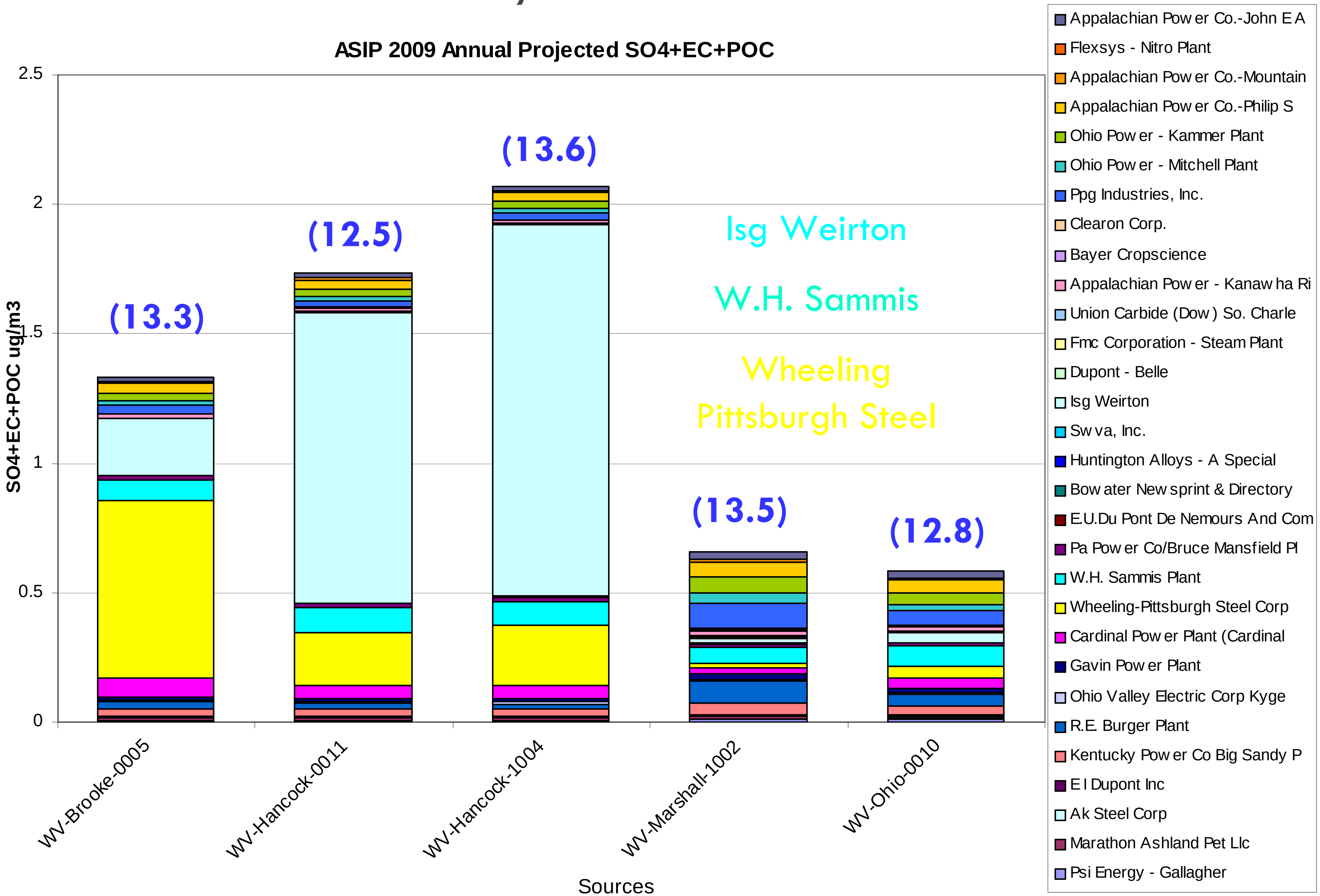
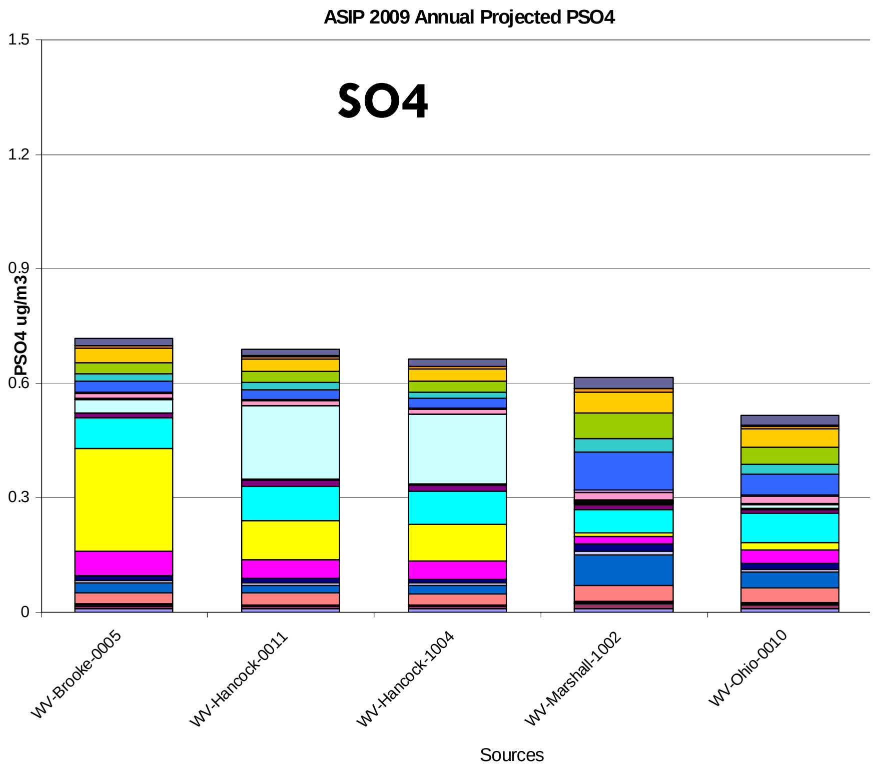
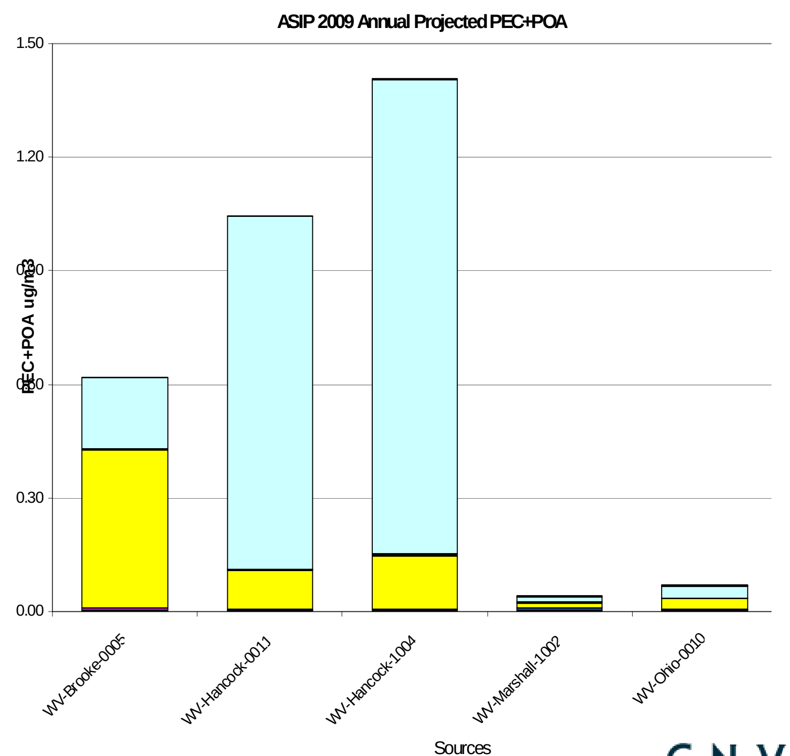
Wheeling and Steubenville-Weirton: 4 km Grid; 31 Facilities and SO4+Prim-PM



Wheeling-Weirton: 31 Facilities; SO4 (left) and Primary PM (right)



Primary PM



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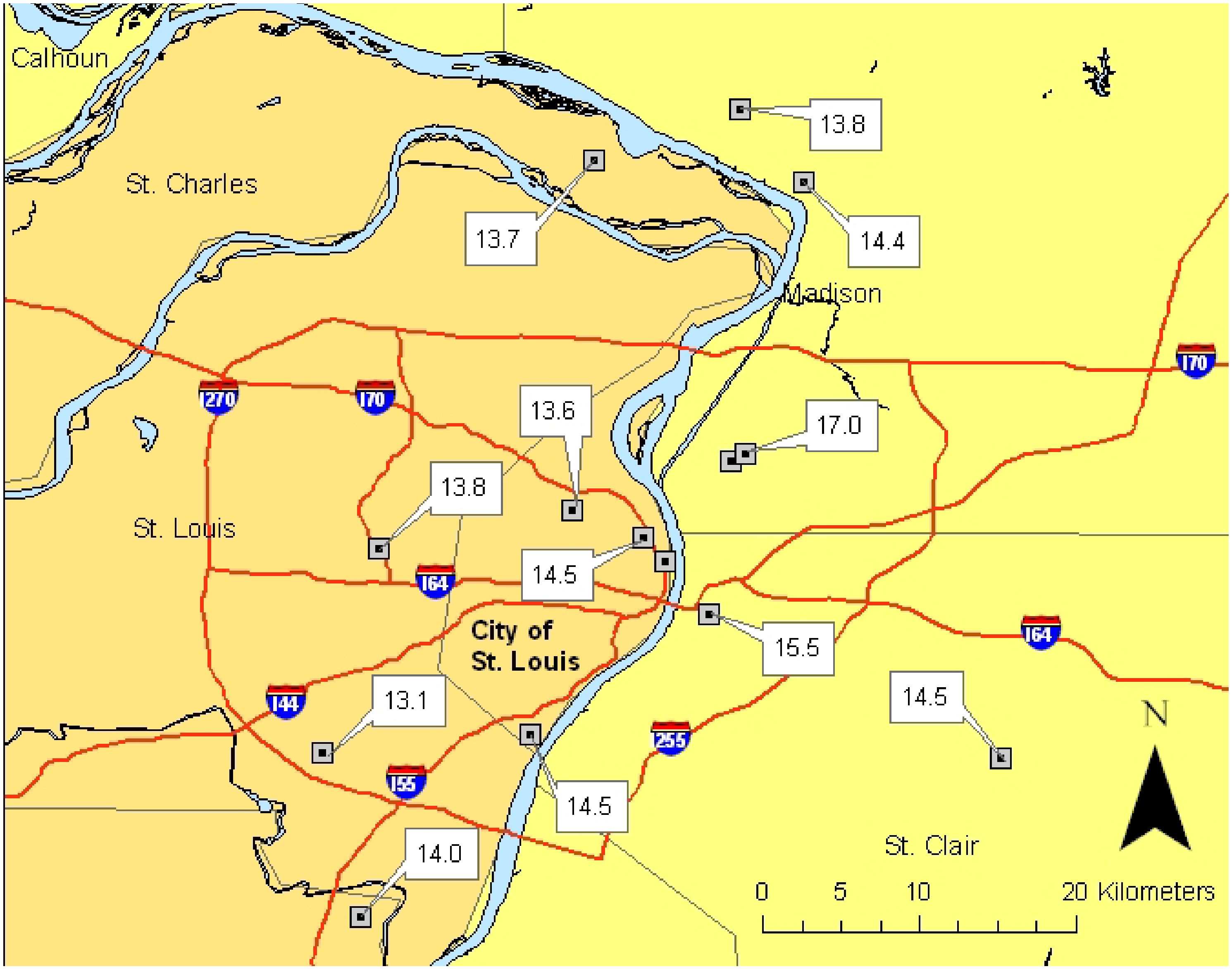
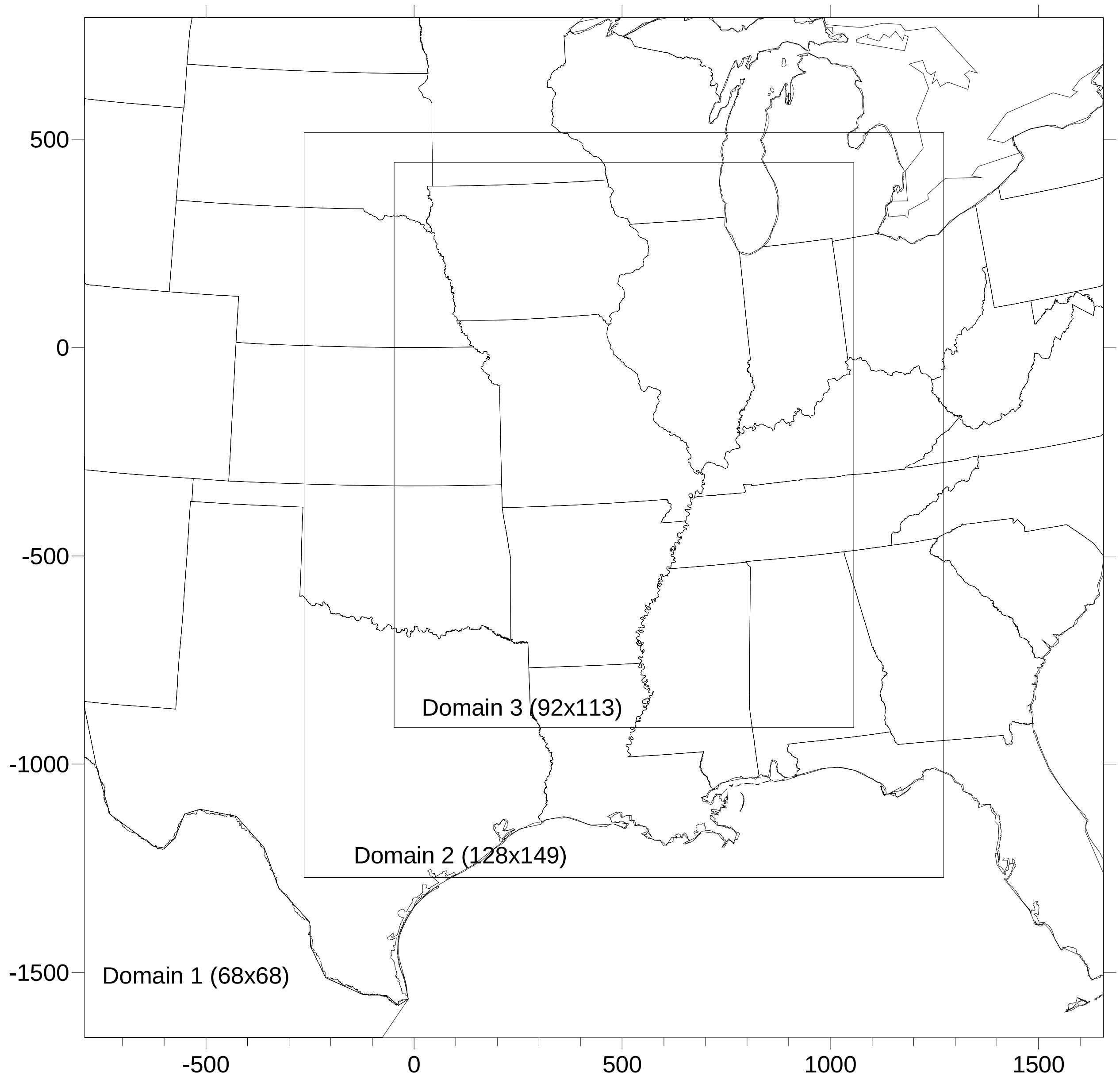
St. Louis 2003-2005 Annual $PM_{2.5}$ Design Values



IRON

St. Louis Regional 36/12 km grid



CMAQ V4.5 SOAmods

Projected 2009 and 2012 PM2.5 Design Values at Granite City and East St. Louis still exceed the annual PM2.5 NAAQS

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Evidence that local sources contribute to PM2.5 nonattainment at Granite City Monitor (B) and Washington St. Monitor (A)

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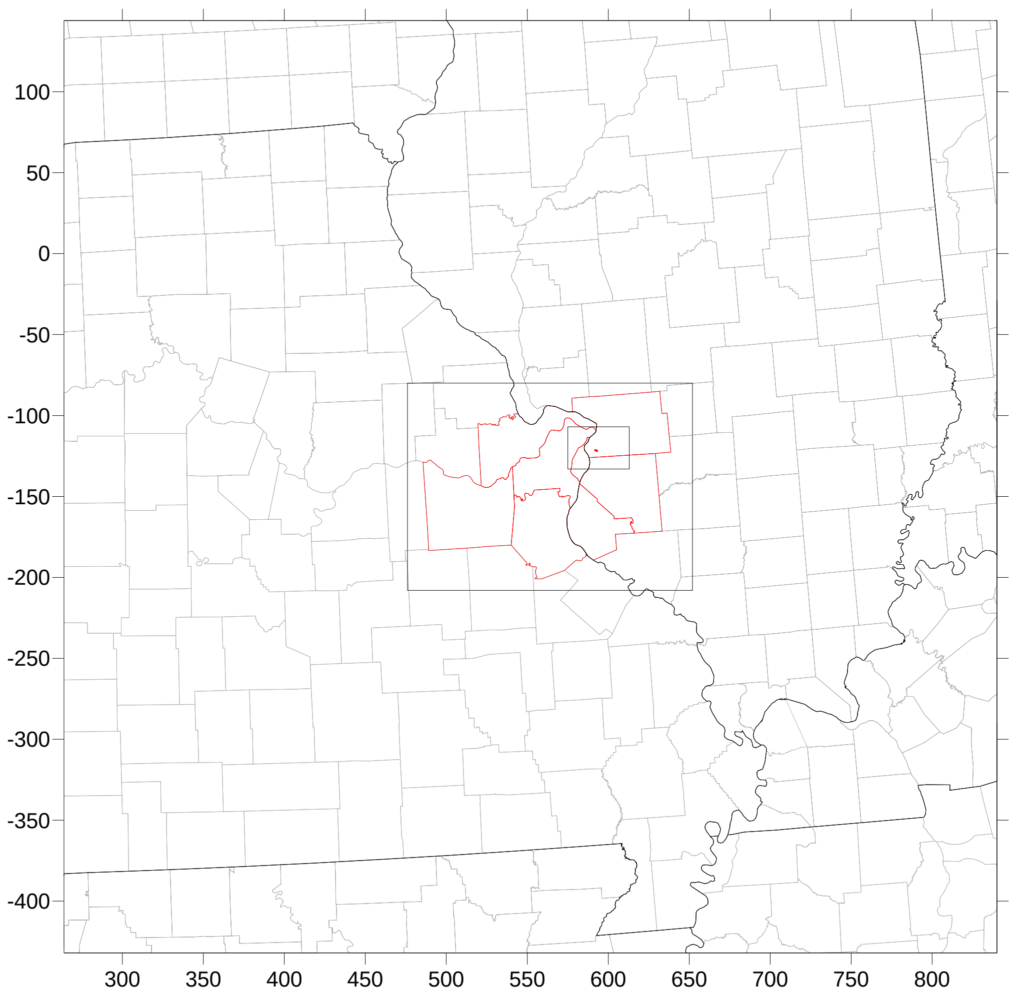
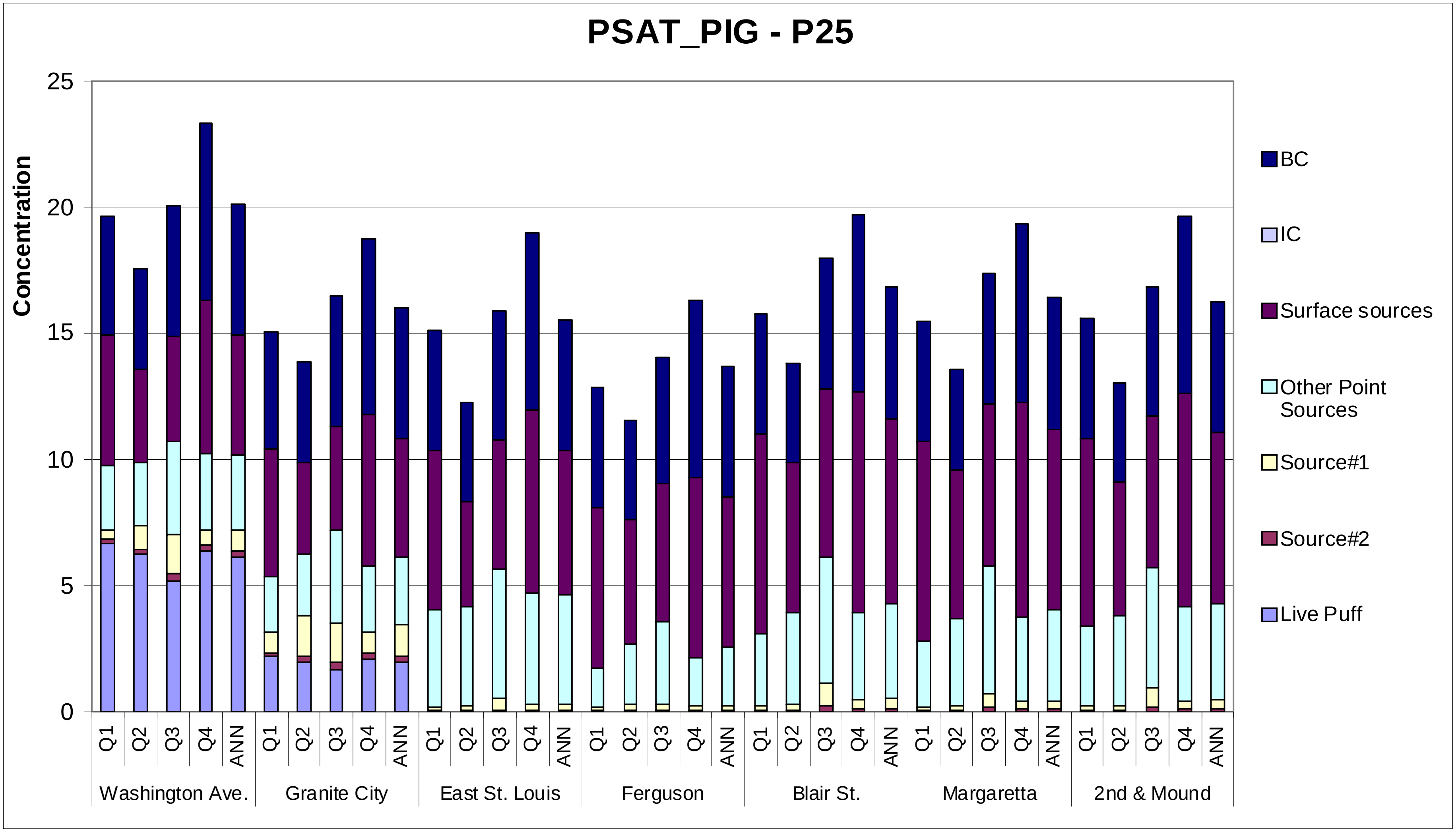
Hybrid CAMx 2002 12/4/1 km Modeling with PiG for Local Sources



- BCs for from CMAQ 36/12 km regional modeling
- 12/4/1 km two-way interactive grid nesting
  - Allows for recirculation of pollutants within domains
- Plume-in-Grid and PSAT used for local sources
  - Subgrid-scale sampling grid use to sample puffs before released to grid
  - Ability for near-source “fence line” impacts

Preliminary Results for Total $PM_{2.5}$



Local Sources contributing ~7 and ~3.4 µg/m^3 to annual average $PM_{2.5}$ at Washington Street and Granite City monitoring sites

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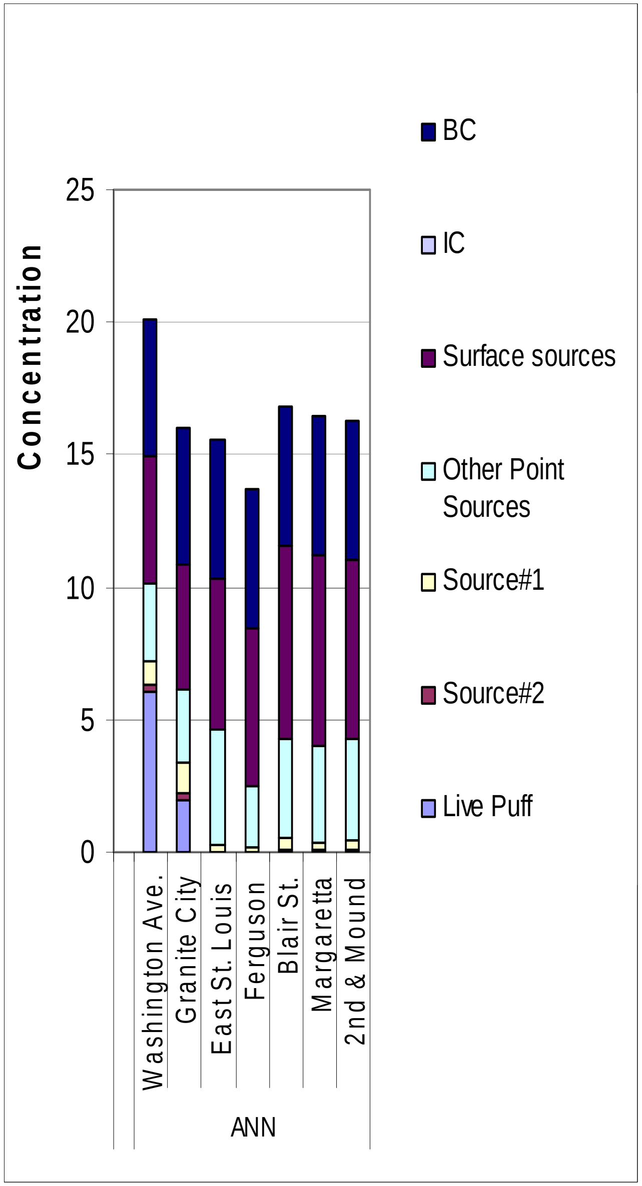
St. Louis Conceptual Model



- Turner and co-workers (2007a,b,c,d) have developed a Conceptual Model for $PM_{2.5}$ exceedances in the St. Louis area
  - They found that local sources contribute ~3.2 μg/m^3 to $PM_{2.5}$ at the Granite City monitor on average
  - The CAMx 12/4/1 km PiG modeling attributes 3.4 μg/m^3 to local sources at Granite City
  - Turner, J.R. and J.L. Garlock. 2007a. A Conceptual Model for Ambient Fine Particulate Matter over the St. Louis Area. Revision 3.0. Washington University, St. Louis, MO. October.
  - Turner, J., J. Garlock, S. Raffuse, J. Rubin, S. Brown, B. Anderson and G. Norris. 2007b. Task#5 Transport Regimes Analysis, Version 1. Technical Memorandum. Washington University, St. Louis, MO. October.
  - Turner, J.R., J. Garlock, J. Jaeckels and J. Schauer. 2007c. Task#2 Fine Particulate Matter Carbon Apportionment, Version 1. Washington University, St. Louis, MO. October.
  - Turner, J. and J. Garlock. 2007d. Task#4 Urban/Regional Contrast and Intraurban Variability, Version 1. Washington University, St. Louis, MO. October.

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Conclusions

- Recent advances in PGMs make them more suitable for assessing "single source" contributions to ozone, $PM_{2.5}$, visibility and deposition
  - Fine resolution grids, two-way grid nesting, and flexi-nesting
  - Full chemistry Plume-in-Grid modules
  - Ozone and PM source apportionment
  - Full gas-phase and aqueous-phase chemistry and aerosol thermodynamic modules
- The use PGM modeling to assess "single source" air quality, visibility and deposition issues has become more routine:
  - ASIP point source $PM_{2.5}$ assessment
  - Oil and gas AQ and AQRV assessments as part of NEPA
  - Texas and Arkansas BART assessment
  - $PM_{2.5}$ SIP modeling