Single Source Modeling with Photochemical Models

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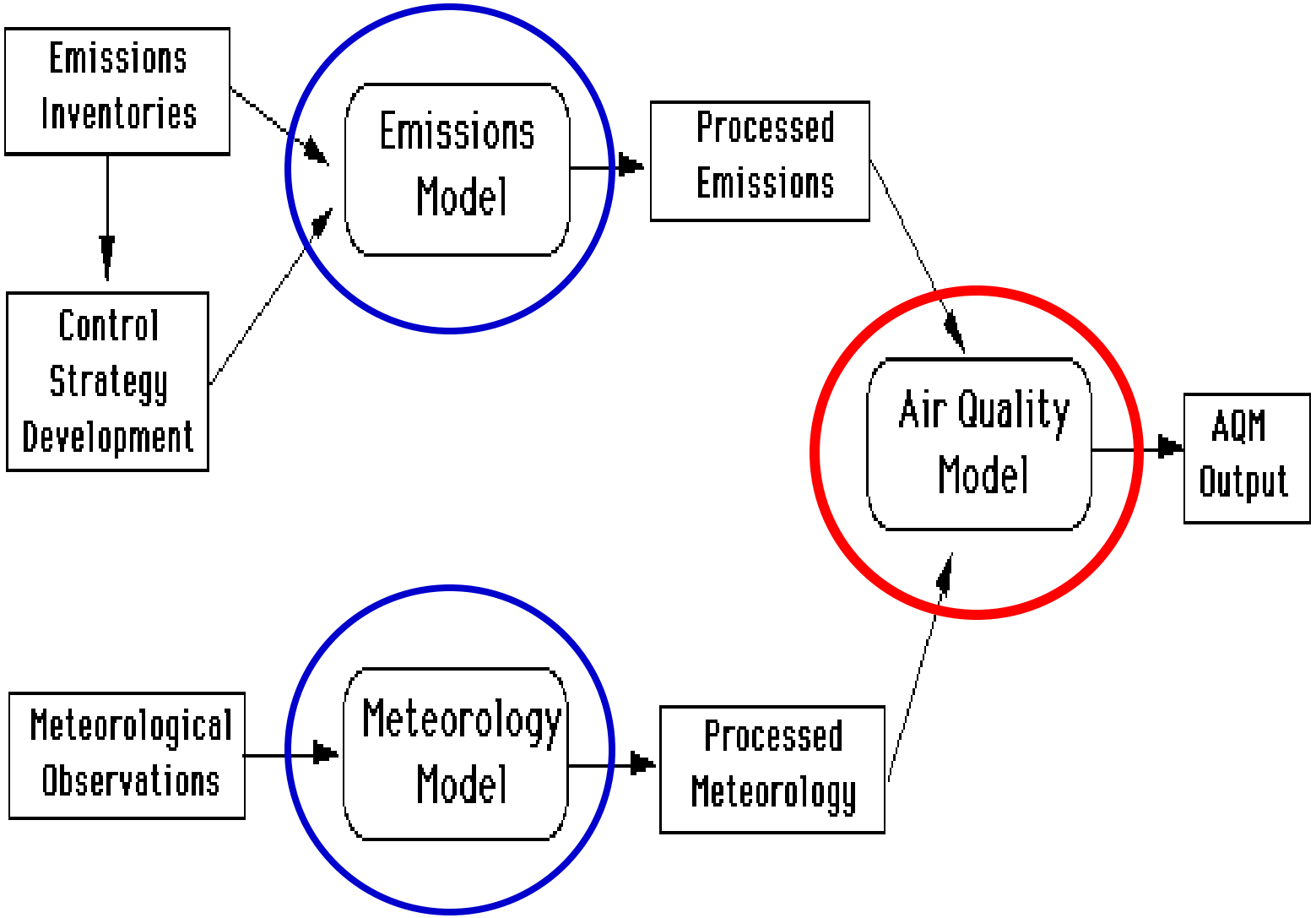
Basic Components of Air Quality Modeling System



Evolution of Air Quality Models

- **1st-generation AQM (1970s - 1980s)**
  - **Dispersion Models (e.g., Gaussian Plume Models)**
  - **Photochemical Box Models (e.g. OZIP/EKMA)**
- **2nd-generation AQM (1980s - 1990s)**
  - **Photochemical grid models (e.g., UAM, REMSAD)**
- **3rd-generation AQM (1990s - 2000s)**
  - **Community-Based "One-Atmosphere" Modeling System (e.g., U.S. EPA's Models-3/CMAQ)**

One-Atmosphere Approach

Mobile Sources

NOx, VOC, PM, Toxics

(Cars, trucks, planes, boats, etc.)

Industrial Sources

NOx, VOC, SOx, PM, Toxics

(Power plants, refineries/ chemical plants, etc.)

Area Sources

NOx, VOC, PM, Toxics

(Residential, farming commercial, biogenic, etc.)

Chemistry

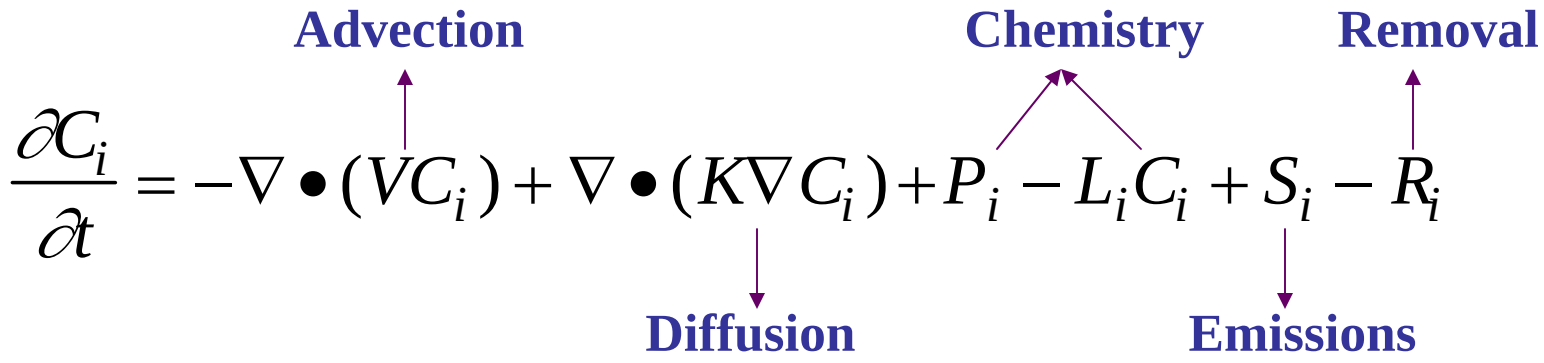
Meteorology

- Ozone
- PM
- Acid Rain
- Visibility
- Air Toxics
- Atmospheric Deposition
- Climate Change

Major Atmospheric Processes Simulated in Air Quality Models

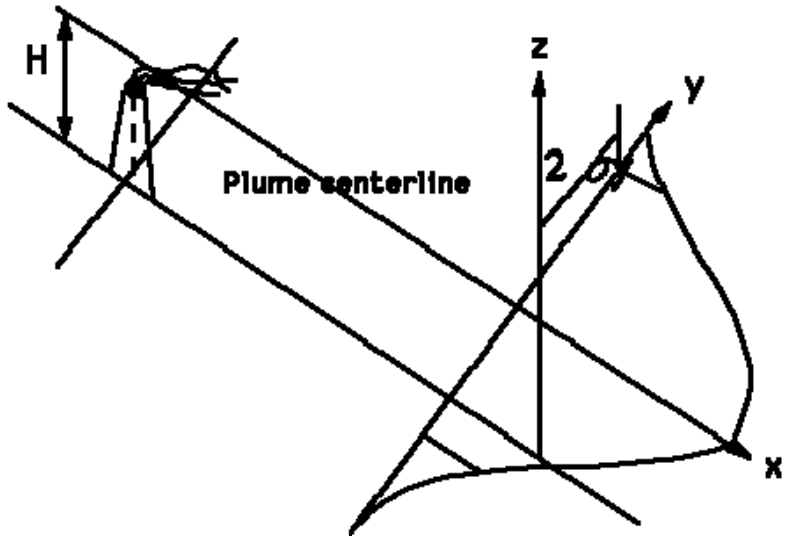
- **Chemical Transformations (Gas- & Aqueous-phase and Heterogeneous Chemistry)**
- **Advection (Horizontal & Vertical)**
- **Diffusion (Horizontal & Vertical)**
- **Removal Processes (Dry & Wet Deposition)**

Species Mass Continuity Equation:



First-Generation Air Quality Models

Gaussian Dispersion Model

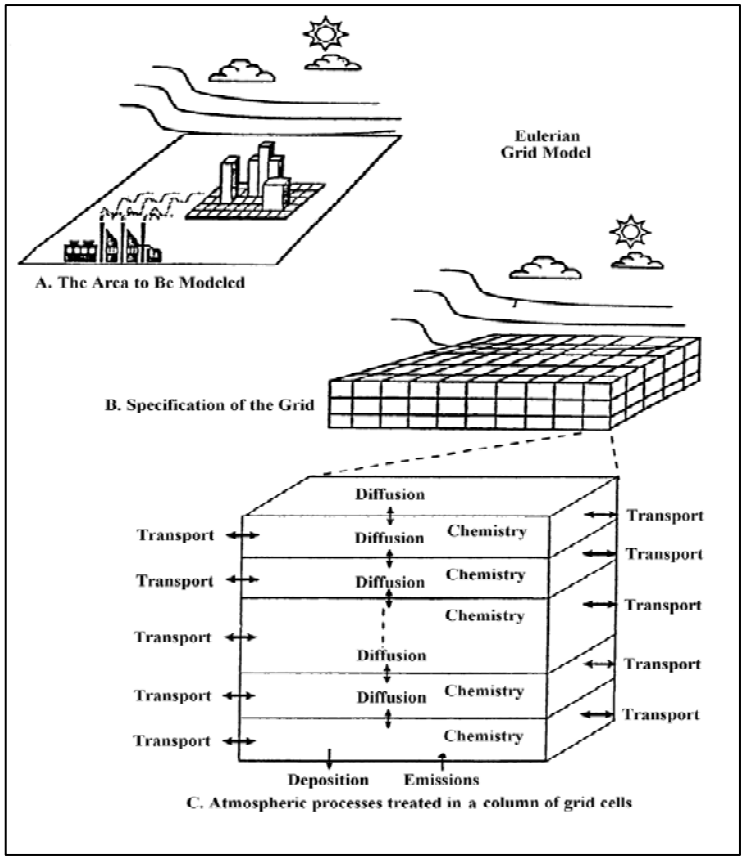


$$C(x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(\frac{-y^2}{2\sigma_y^2}\right)\left(\exp\left(\frac{-(z-h)^2}{2\sigma_z^2}\right) + \exp\left(\frac{-(z+h)^2}{2\sigma_z^2}\right)\right)$$

ISC3, CALPUFF, AERMOD

(for primary pollutant)

Photochemical Grid Model



CMAQ, CAMx

(multi-pollutant one-atmosphere)

PCM/Source Apportionment Advantages

- Full state of the science gas-phase chemistry
  - Ability to estimate realistic ozone concentrations
  - No need for a constant ozone background value for PM
- Advanced aqueous phase chemistry provides realistic sulfate estimates; wet and dry deposition processes included
- Photochemical models generally have good temporal and spatial estimates of ammonia concentrations
- Spatial/temporal representation of ammonia and nitric acid concentrations and state of the science inorganic chemistry (ISORROPIA) allow for realistic nitrate partitioning between gas and particle phase
- Source apportionment tools allow for tracking of single emissions sources or groups of emissions sources

PCM Source Apportionment Background

- Photochemical models estimate [single] source contribution with **source apportionment** routines
- Source apportionment tracks the formation and transport of PM2.5/ozone from emissions sources and allows the calculation of contributions at receptors
- Chemically speciated PM2.5 contribution can be converted to light extinction for visibility applications

- Precursor emissions tracked to chemically speciated PM2.5, ozone, toxics

NOX → $NO3^-$
SOX → $SO4^=$
NH3 → $NH4^+$
Primary OC → POC
Primary EC → PEC
Primary Other → POTH
VOC → SOA

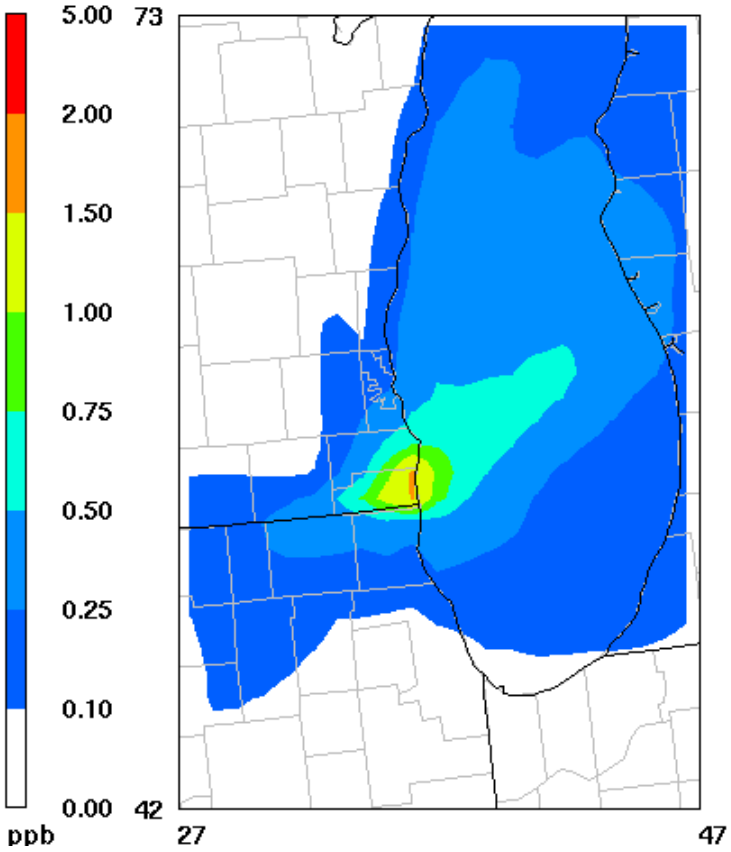
NOX → O3
VOC → O3

Particulate Source Apportionment

- Particle and Precursor Tagging Methodology (PPTM) has been implemented in CMAQ v4.6
- Particulate Source Apportionment Technology (PSAT) has been implemented in CAMx v4.5
- Tracks contribution to mercury and PM sulfate, nitrate, ammonium, secondary organic aerosol, and inert species
- Estimates contributions from emissions source groups, emissions source regions, and initial and boundary conditions to PM2.5 by adding duplicate model species for each contributing source
- These duplicate model species (tags) have the same properties and experience the same atmospheric processes as the bulk chemical species
- The tagged species are calculated using the regular model solver for processes like dry deposition and advection as bulk species
- Non-linear processes like gas and aqueous phase chemistry are solved for bulk species and then apportioned to the tagged species

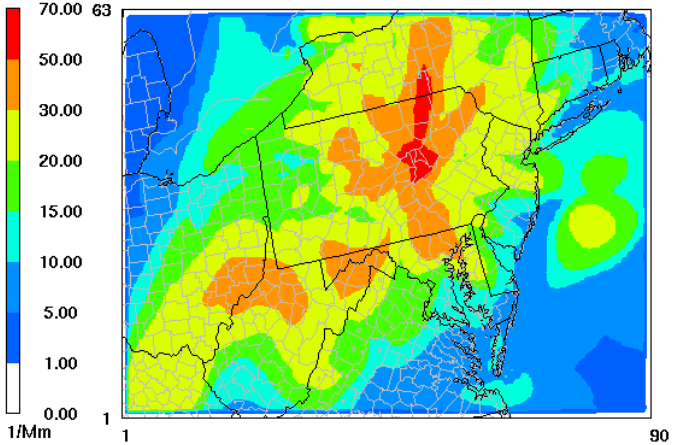
Ozone Source Apportionment

- Ozone source apportionment has been implemented in CAMx v4.5 (OSAT & APCA) and CMAQ v4.6 (OPTM)
- Tracks ozone contribution from sources similarly to PM with reactive tracers
- July maximum ozone contribution from a source shown at right
- OSAT is simulated separately from particulate source apportionment

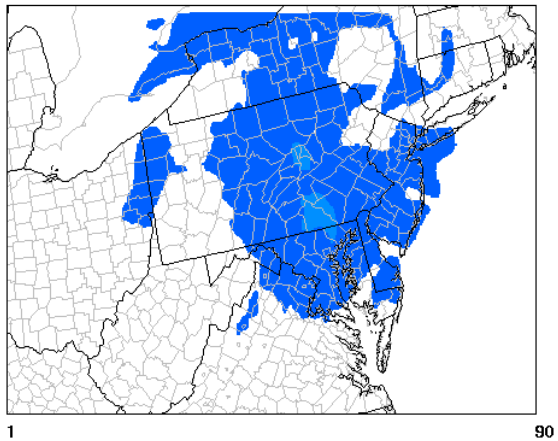


Annual Maximum Light Extinction (1/Mm)

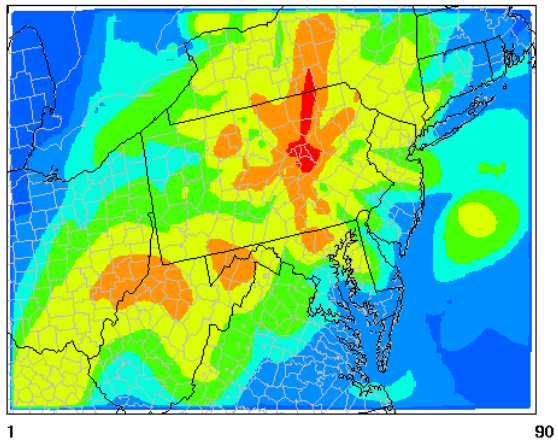
Total Light Extinction



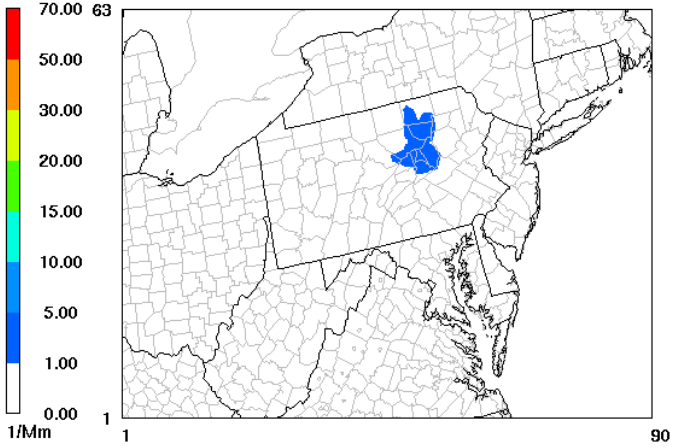
Ammonium Nitrate



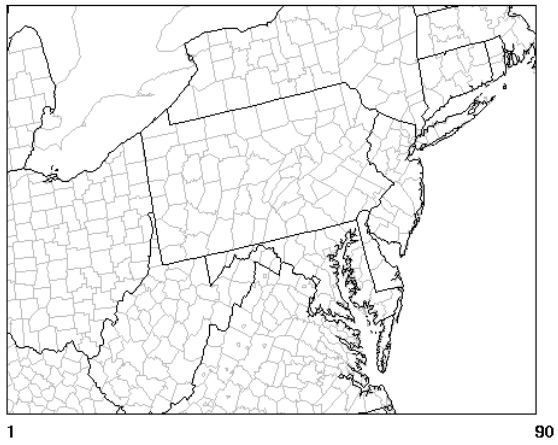
Ammonium Sulfate



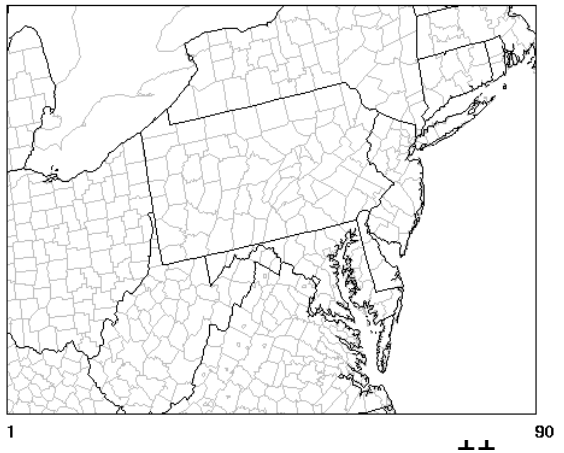
Other: Metals/Soil/Etc



Primary Organic Carbon

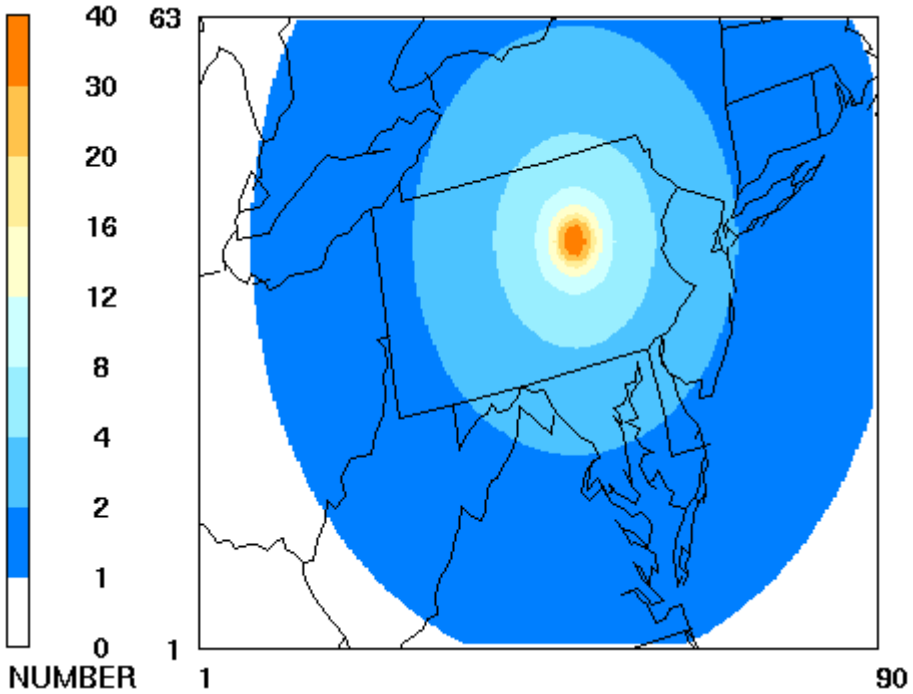


Elemental Carbon

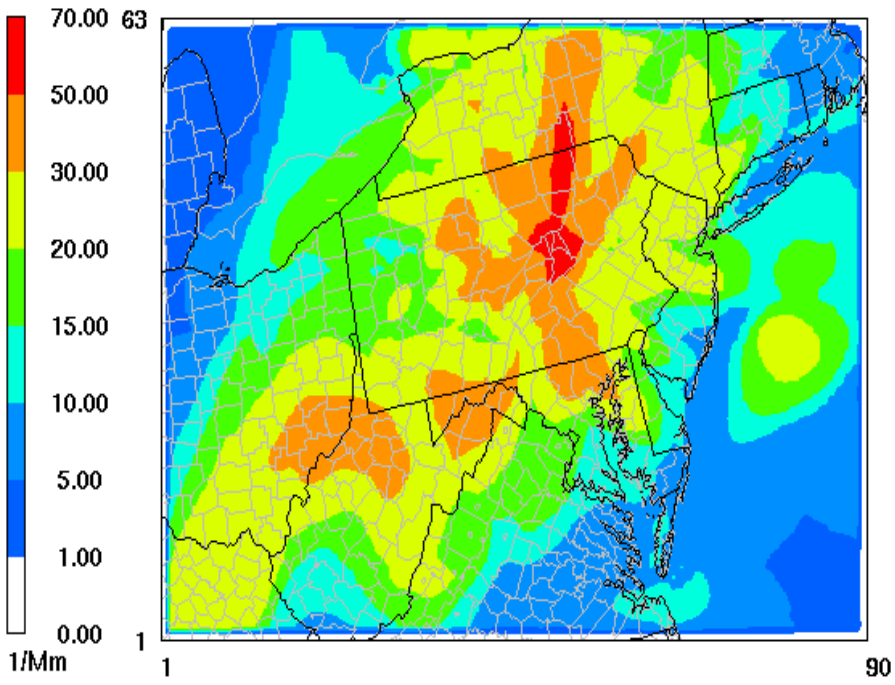


Qualitative comparison to screening metric Emissions/Distance

Emissions/Distance



Total Light Extinction

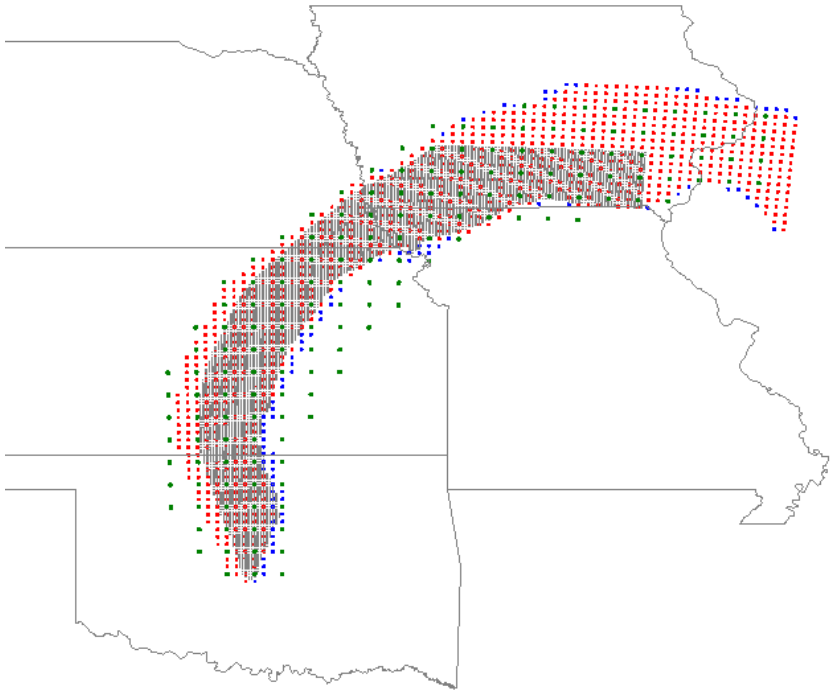


Issues using PCM for Single Source Apps.

- Photochemical models resource intensive (computational, disk space, staff) for multi-year applications, especially at grid resolutions <= 12km
- Additional level of staff expertise
- Existing community emissions inputs (from States, RPOs, etc) for photochemical models are actual emissions and may need to be modified if more conservative emissions estimates are necessary
- Useful for near-field applications?

Near Field & Long Range Transport

- Further research is necessary to determine how useful PCMs are for near-field modeling (<50 km)
- Currently, some photochemical models support full science sub-grid plume treatment, sub-cell receptor locations, and 2-way nesting capability
- Review existing near-field applications using PCMs, evaluate tracer studies



Other Work

- Midwest RPO did some preliminary testing (not an evaluation of CAMx PSAT or CALPUFF) of single source modeling with CAMx PSAT to compare with CALPUFF visibility estimates

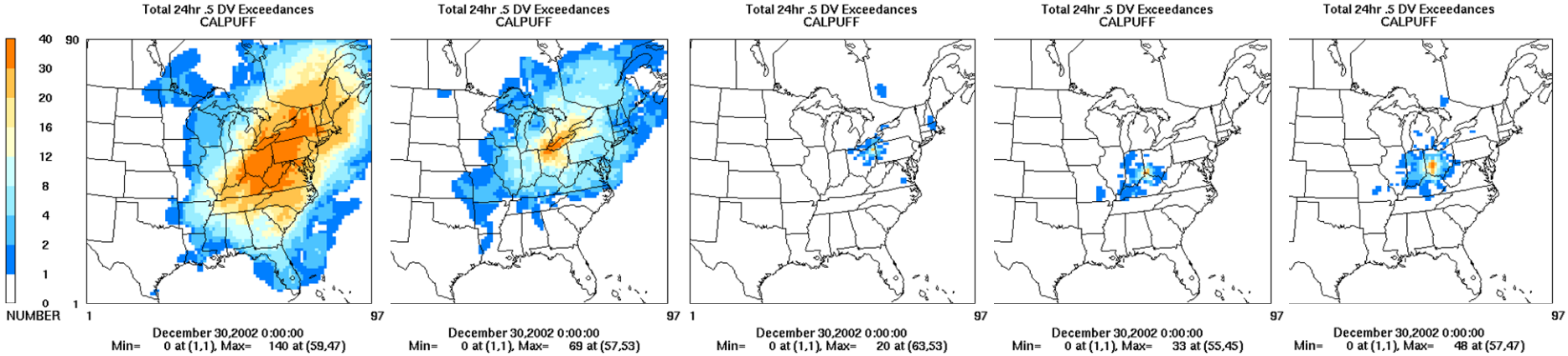
- Several States did single source visibility modeling for sources less than 50 km from Class I areas; used sub-grid plume treatment

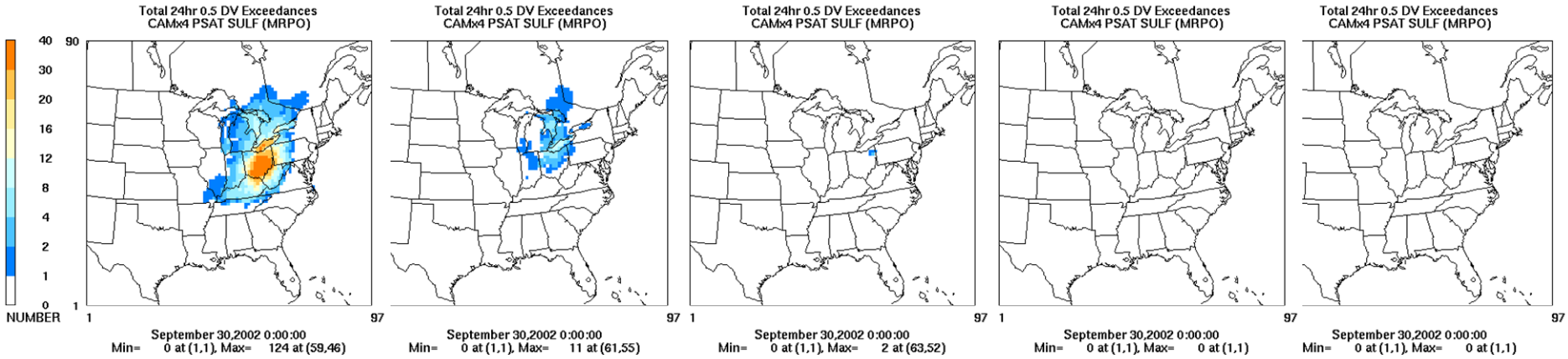
MRPO: CALPUFF (left) and CAMx PSAT (right)

- Annual 2002 Simulations using latest version of CALPUFF (incl. POSTUTIL and CALPOST)
- Meteorological input data is hourly and from an annual 2002 MM5 simulation
- Grid is consistent with photochemical model grid: 97 X 90 x 16 (36km grid cells) over Eastern U.S.
- Results show the number of times each grid cell exceeds the 24hr average .5 DV degradation over "background" visibility
- Results are the combined visibility degradation from sulfate and nitrate
- These runs were facility total actual emissions

- Applied CAMx4 PSAT sulfate for April-Sept 2002
- These results do not show the impact from nitrate; Assume that visibility degradation is dominated by summer sulfate
- Results for each facility are shown similar to CALPUFF results: counts of > .5 DV change over natural background conditions
- fRH values derived using daily average relative humidity in the grid cell as predicted by MM5 and calculated using the exact same look-up table that is used in CALPOST; the maximum daily average RH is 90

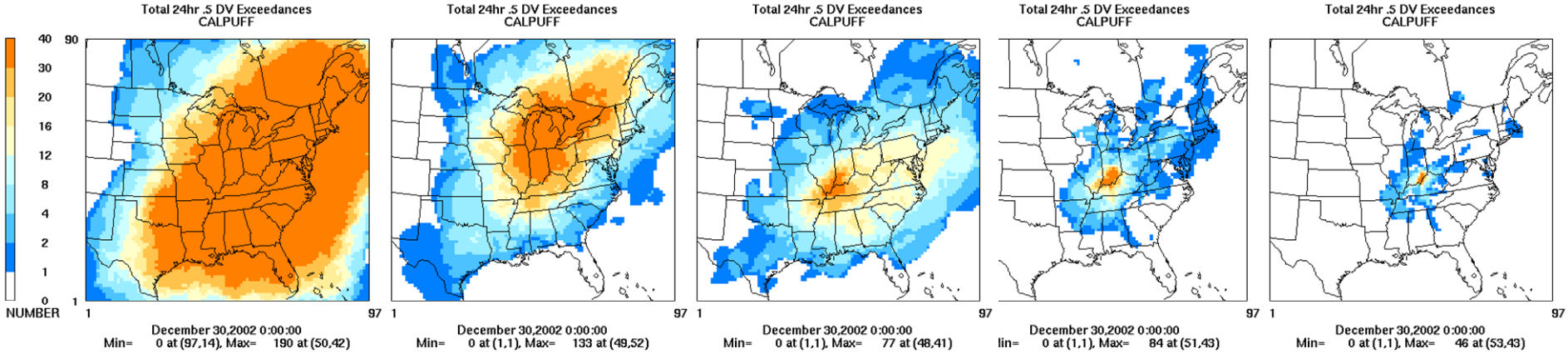
Total 24hr avg .5 DV Exceedances
CALPUFF (top) CAMx4 PSAT (bottom)

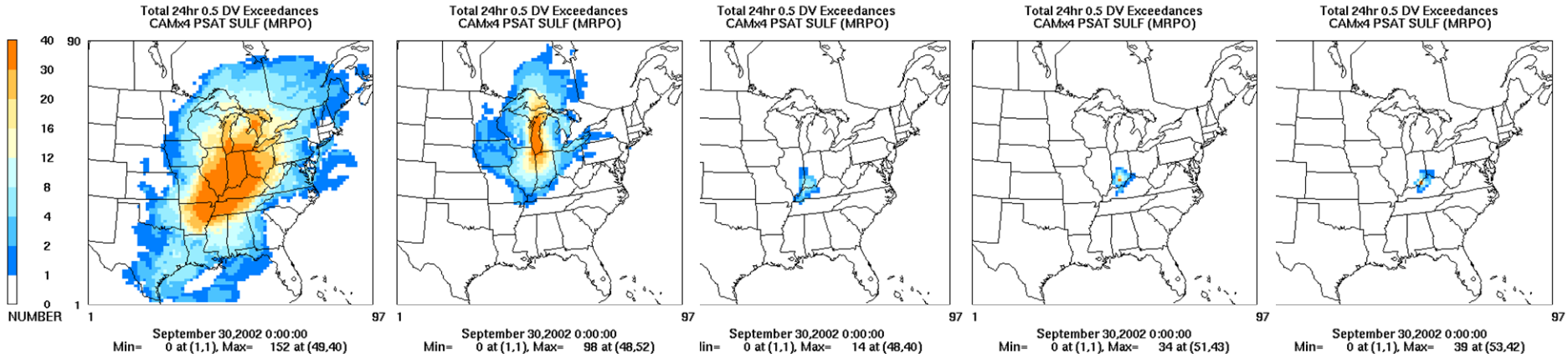




**CALPUFF includes sulfate+nitrate and CAMx4 includes sulfate*

Total 24hr avg .5 DV Exceedances
CALPUFF (top) CAMx4 PSAT (bottom)





**CALPUFF includes sulfate+nitrate and CAMx4 includes sulfate*

MRPO Conclusions

- CAMx4 PSAT results do not show visibility degradation as far downwind as CALPUFF
- Need to consider nitrate PSAT runs for better comparison although visibility degradation is expected to be dominated by summer sulfate
- The tools agree qualitatively for certain facilities but not all of them

Final Remarks

- Photochemical grid models provide an opportunity for credible single source modeling with source apportionment methodology
- These models have the advantage of state of the science chemistry, but that comes with increased resource burden
- These models are routinely used for other regulatory purposes like O3/PM2.5/Regional Haze State Implementation Plans

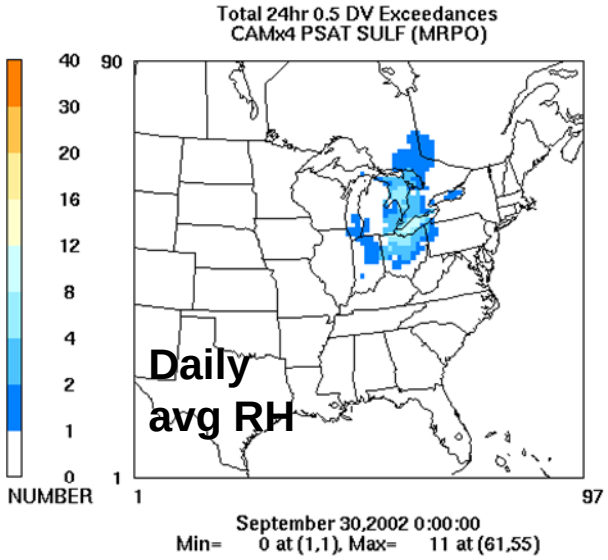
END OF PRESENTATION

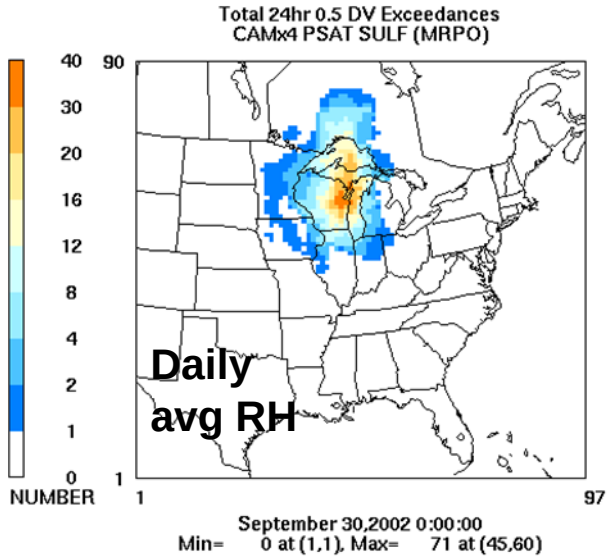
Post-Processing

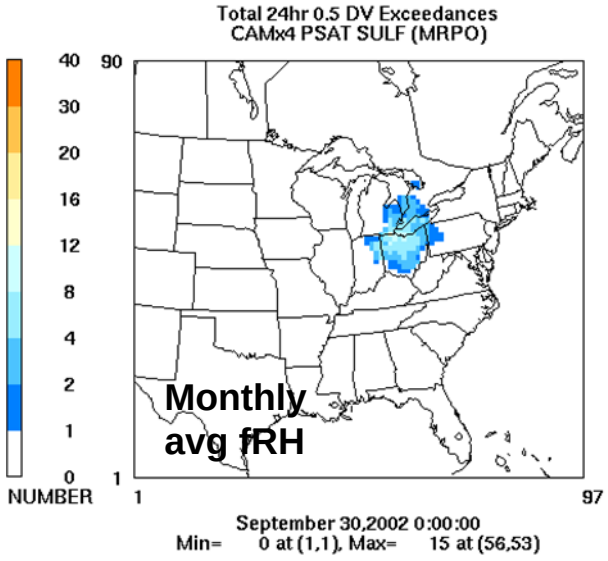
- Estimate .5 DV changes over natural background conditions
- Methodology equivalent to CALPOST visibility post-processing
- A natural background value of 18 1/Mm is used for the Eastern U.S. *(see CALPUFF manual)*
- A count of > .5 DV change over natural background is kept for each grid cell and compared to Class I areas

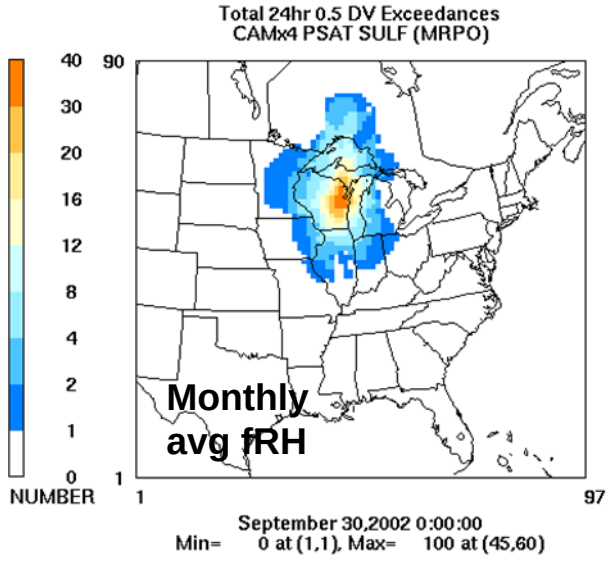
- Bext Total = Bext Modeled + Bext Background
- Delta DV = 10*ln(Bext Total/10) – 10*ln(Bext Background/10)

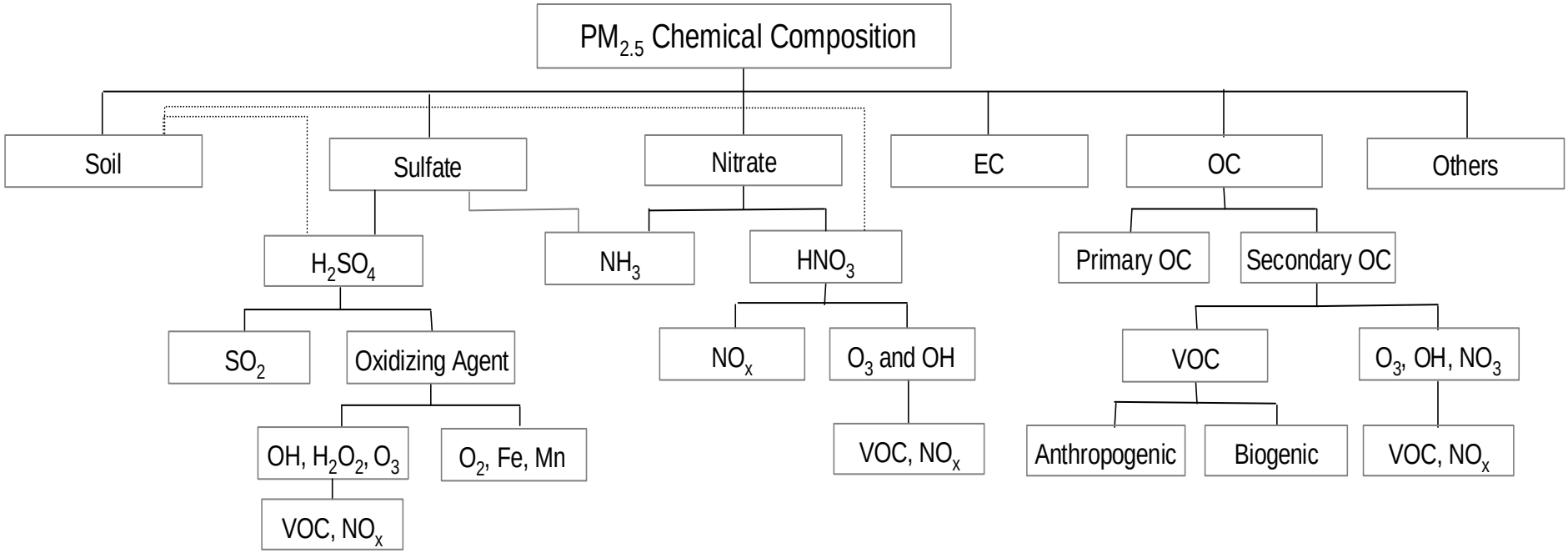
PSAT Results:
fRH calc from 24-hr RH v monthly gridded fRH values









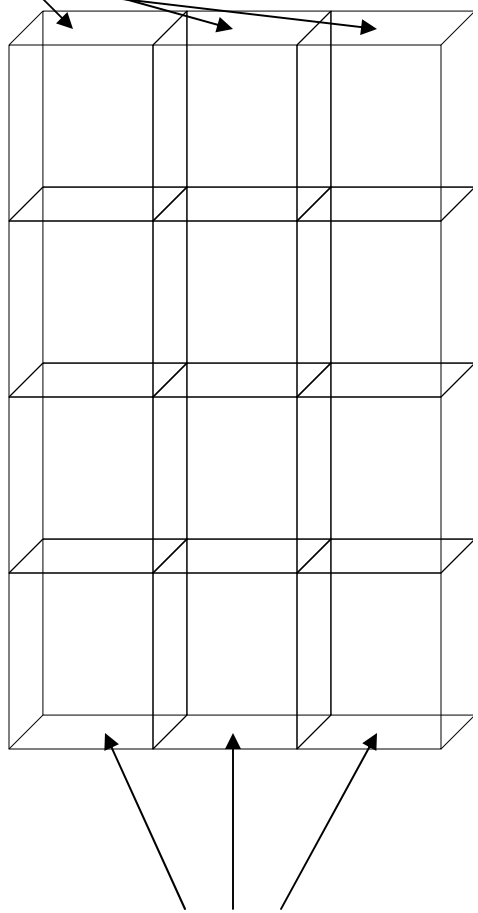


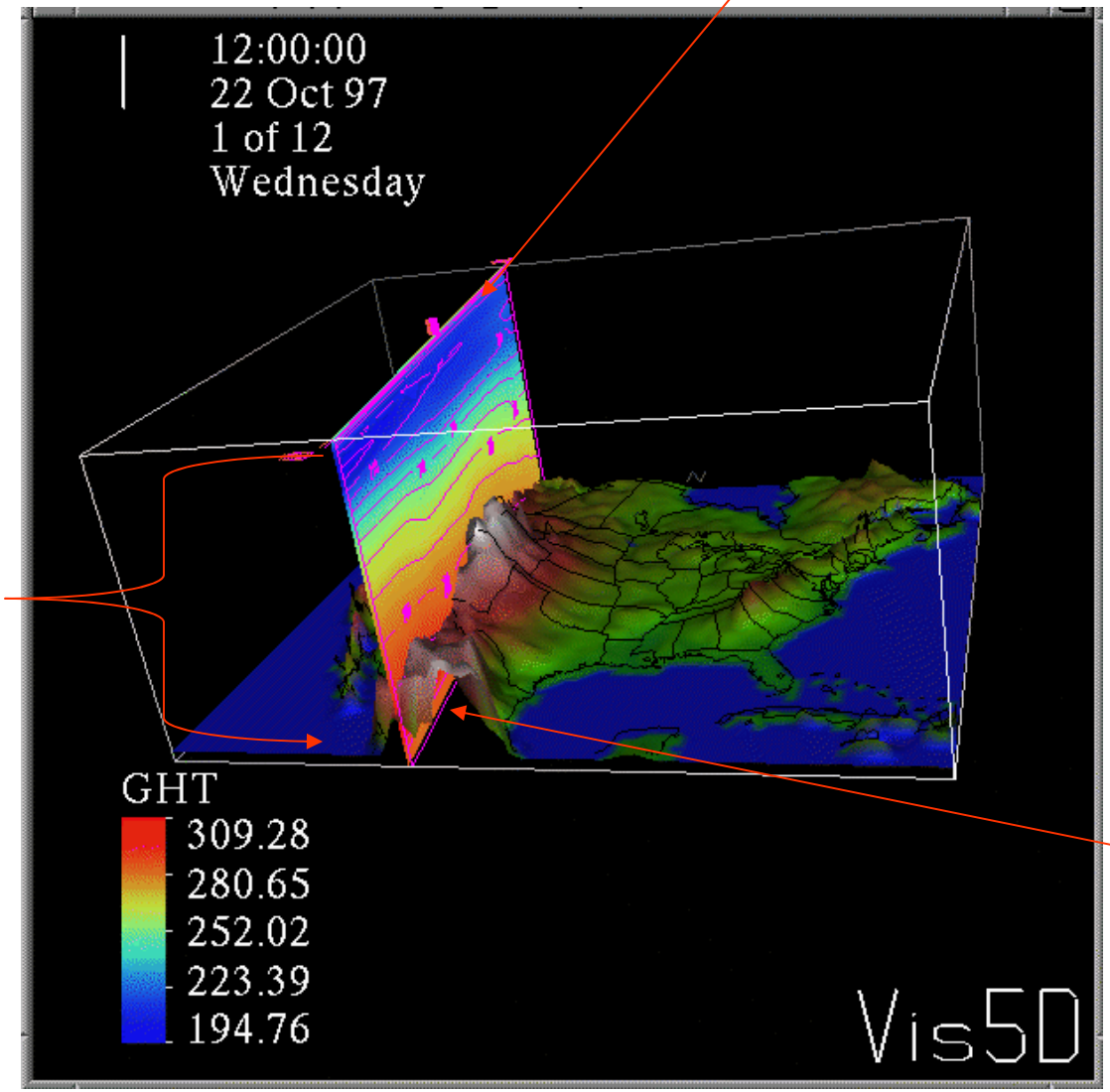
- **PM2.5 Nitrate formation depends on temperature, humidity, and the concentration of other nearby species**
- **PM2.5 Nitrate formation is favored by lower temperatures and higher humidity (winter and night-time)**
- **PM2.5 Sulfate and Organic Carbon is higher during the summer when there is higher availability of by-products of photochemical activity**

Regional Photochemical Models:

Tool for O3, PM2.5 (and Haze)

TOP





~ 9 miles

SURFACE

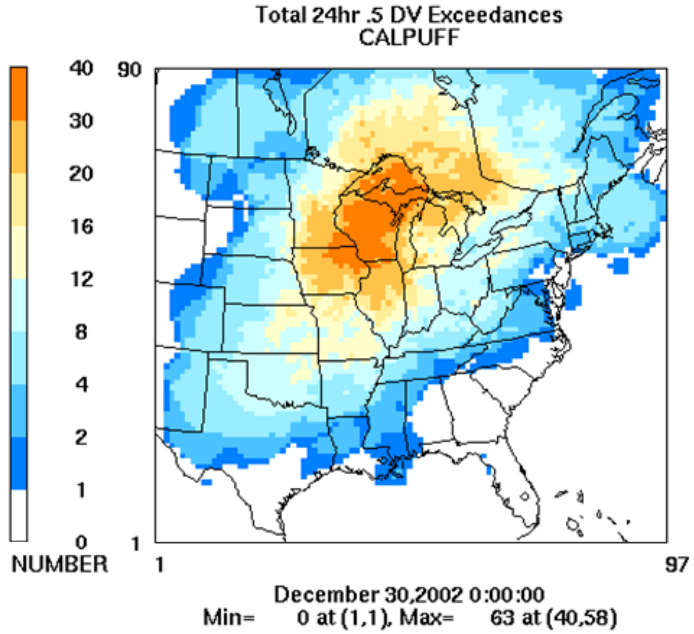
CALPUFF Sensitivity

- Sensitivity simulation for visibility calculation parameter BCKNH3
- Background ammonia concentrations (same value for entire domain for entire year)
- Important parameter in CALPUFF estimation of PM2.5 nitrate

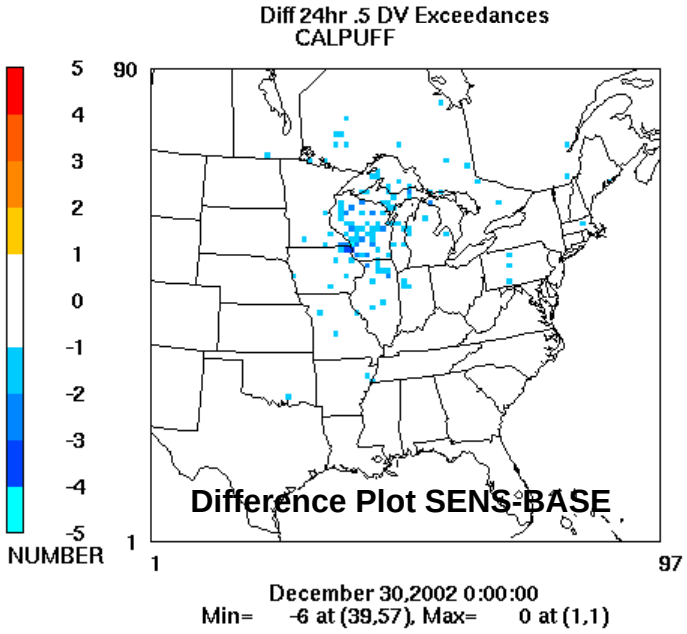
CALPUFF Sensitivity:

BCKNH3 = 1.0 (basecase/default)

BCKNH3 = 0.5 and 1.5



Ammonia Conc SENS (NH3=0.5)



Ammonia Conc SENS (NH3=1.5)