Speciated Modeled Attainment Test (SMAT)
What is it and why do we need it?

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Model Attainment Test- General

- Attainment test methodology uses ambient data (design values) and model output to estimate future year concentrations
  - Relative Reduction Factor = model predicted (%) change in pollutant(s) from base year to future year
  - Base year DV * Relative Reduction Factor = Future year concentration
- Attainment test for ozone is relatively simple- there is only one component

Model Attainment Test- General

- Attainment test for PM2.5 needs to use all of the PM2.5 component species
  - Individual RRFs are calculated for each PM2.5 species
  - Total PM2.5 is reconstructed from the sum of individual components
- The speciated model attainment test methodology was conceived for the PM2.5/Regional Haze modeling attainment guidance
  - The guidance recommends the use of the speciated test for PM2.5 (annual and 24-hour standard) modeled attainment demonstrations and regional haze reasonable progress

What Has SMAT Been Used for?

- Clear Skies modeling
  - Draft guidance version of SMAT
- Clean Air Interstate Rule (CAIR)
  - "Revised" SMAT
    - 2010 nonattainment counties
      - Downwind receptors
    - Downwind impacts
      - Relative impacts from upwind states to downwind receptor areas (zero-out model runs)
    - Nonattainment county counts
    - PM2.5 Air quality health benefits
- BART rule
  - Relative change in regional haze at Class I areas (ongoing)
- Modeled attainment and reasonable progress demonstrations (upcoming)

Applications

- SMAT can be directly applied where speciated PM2.5 data is available
  - Species concentrations are related back to the FRM design values at FRM sites with co-located speciation monitors
    - FRM design values are the only values that can be used to determine attainment/nonattainment
- There are two major obstacles to applying SMAT
  - Speciated data does not exist at most FRM sites
  - The measurements collected at the speciation networks (STN and IMPROVE) are not directly comparable to FRM measurements

Availability of Speciated Data

- There are ~1200 FRM sites across the country
  - There were ~150 STN sites and 58 IMPROVE sites (in the East) with complete data at the end of 2002 (used for the CAIR analysis)
  - There are now ~250 STN sites nationwide and ~165 IMPROVE sites
- Over 75% of the FRM sites do not have a co-located speciation monitor
  - Therefore, interpolation approaches are needed to perform SMAT at all of the FRM sites
  - The SMAT application for CAIR used interpolated species data from the STN and IMPROVE networks
    - Voronoi Neighbor Averaging (VNA) technique contained in the BenMAP software

FRM vs. STN Data

- The species measured at the speciation monitors do not match what is measured on the FRM Teflon filter
- Adjustments were made to the speciation measurements so that they replicated the PM2.5 mass that was retained on the FRM filters (based on our best understanding)
  - We applied the principles of the Neil Frank “SANDWICH” technique

Application of SMAT for CAIR- An Example

- Limited speciation data available
  - Used a single year of STN and IMPROVE data (2002)
    - Multiple years of data are now available
- FRM data was from the period 1999-2003
  - Used 5 year weighted average design values for projections

SMAT Basic Procedures

- Derive quarterly mean concentrations for each component of PM2.5 by multiplying FRM PM2.5 by fractional composition of each species
- Calculate a model derived relative reduction factor for each species
- Multiply each RRF times each ambient PM2.5 component (for each quarter) to get the future concentrations
- Sum the future quarterly average components
- Average the four mean quarterly future PM2.5 concentrations

Draft PM2.5 Guidance

- Current guidance recommends deriving PM2.5 components using the IMPROVE equation
  - Ammonium sulfate
  - Ammonium nitrate
  - Elemental Carbon
  - Organic carbon mass (OC*1.4)
  - Soil (inorganic particulate)
  - Unidentified mass (difference between FRM and reconstructed fine mass)

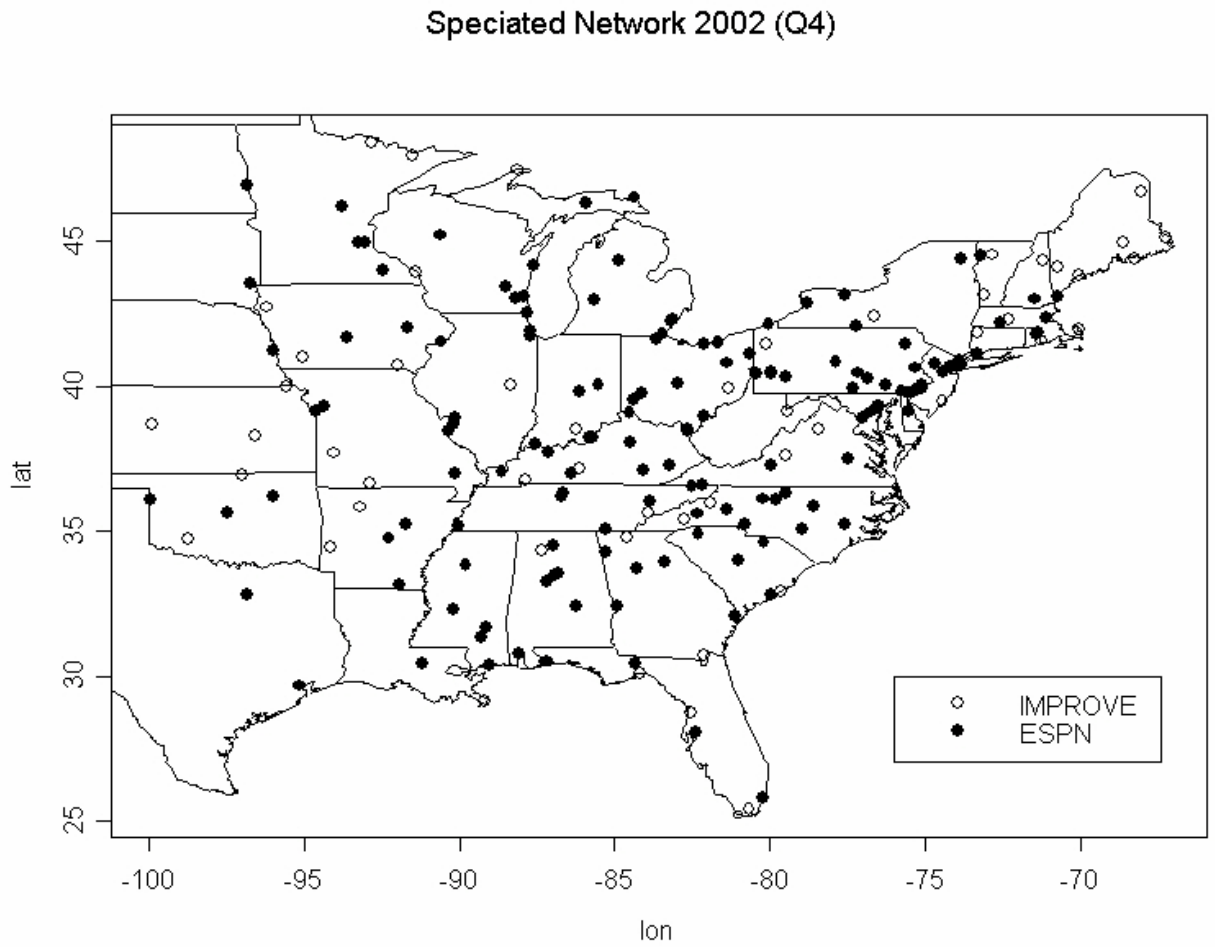
Reconstructed PM2.5 Mass

- From the SANDWICH work, we know that the FRM filters do not retain all mass (negative artifacts) and also have positive artifacts
- “Revised SMAT” calculates
  - Sulfate
  - Nitrate (adjusted)
  - Ammonium
  - Particle bound water
  - Organic carbon (by difference)
  - Elemental carbon
  - Other inorganic particulate (crustal/other)
  - Passive (blank) mass

Data Notes

- Measured organic carbon was used in the analysis to ensure that the OC by difference was not severely underestimated
  - A “floor” was calculated so that OC by difference could not be more than 30% below the measured OC*1.4
  - The quarterly average measured STN OC was blank corrected (monitor specific value which ranged from 0.29-1.42 ug/m3)
- July 6-9th data was thrown out for 10 Northeastern States due to the influence of Quebec wildfires
  - Quarterly data for 2002 needs to be representative of the 1999-2003 period

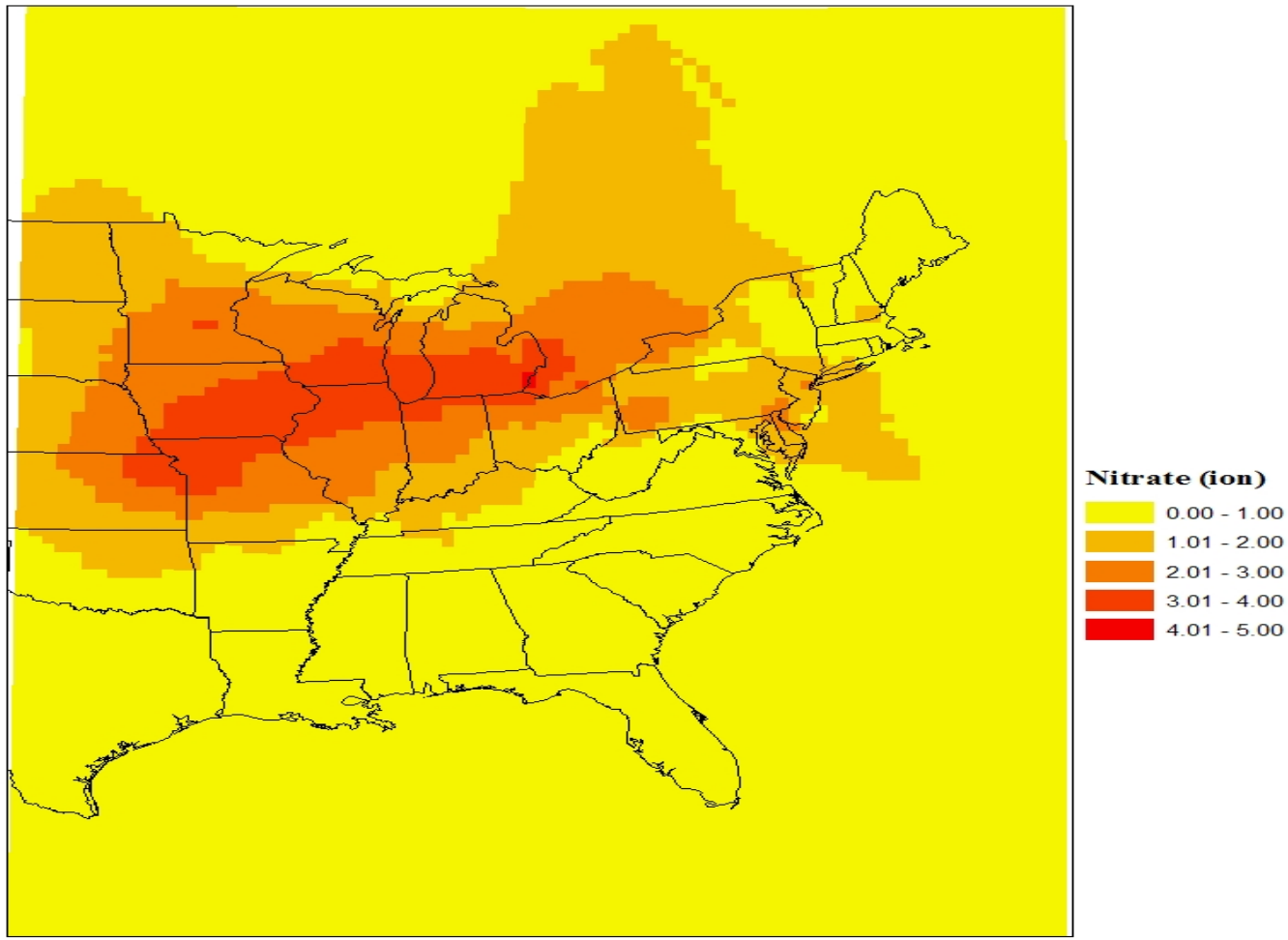
Complete Eastern STN and IMPROVE Sites- 4th Quarter 2002



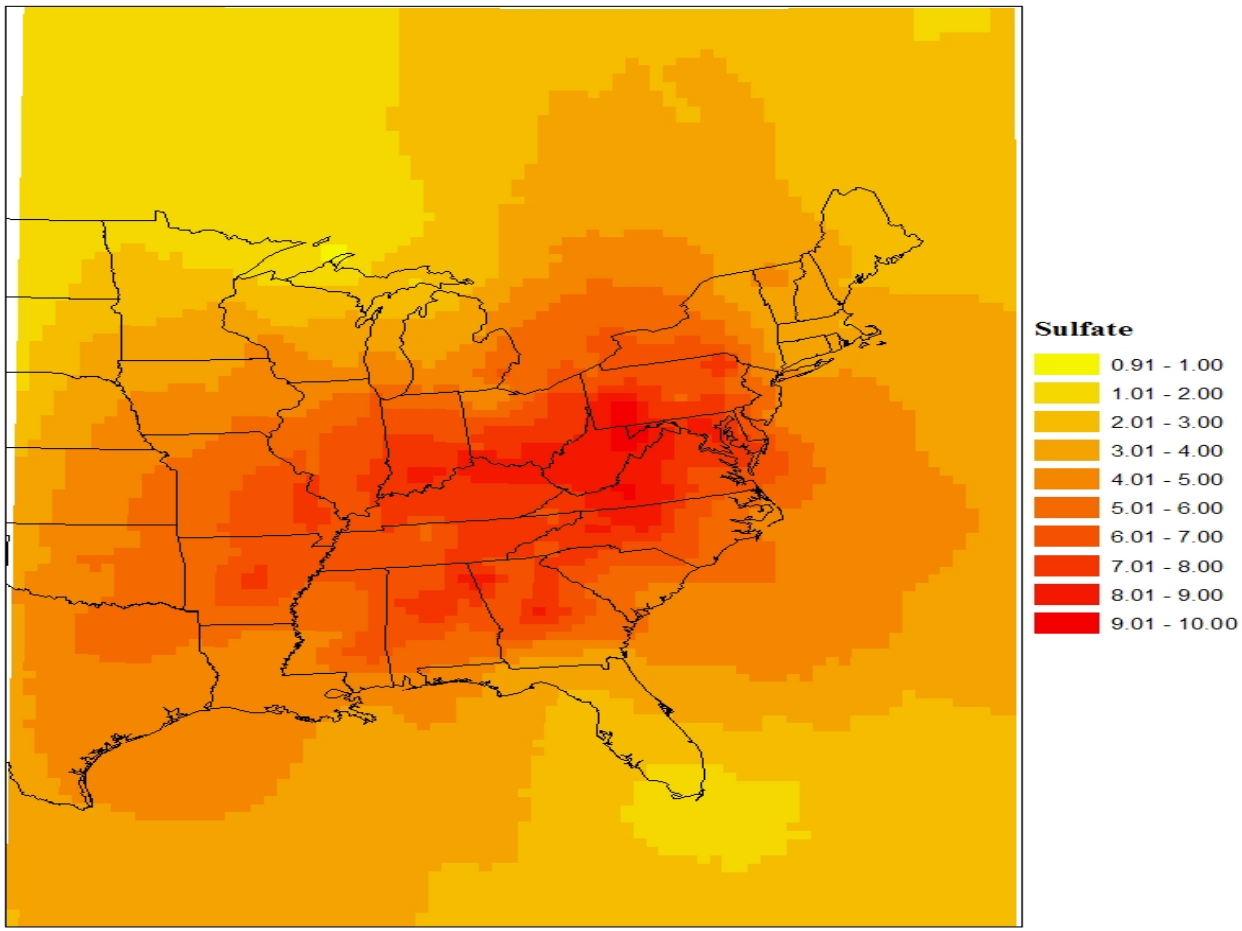
Interpolations

- Interpolations were completed (using VNA) for each quarter for the following species
  - Sulfates
  - Nitrates
  - Organic carbon mass (OC*1.4)
  - Crustal/other
  - Elemental carbon
  - Degree of neutralization (DON) of sulfate (0 to 0.375)

Interpolated Nitrate- Quarter 1



Interpolated Sulfate- Quarter 3



Nitrates

- Nitrate measurements are adjusted using the SANDWICH formulas
  - Used hourly NWS meteorology and 24-hour average nitrate measurements
- Adjusted nitrate concentrations were then interpolated

Ammonium Estimates

- Ammonium is measured at STN sites only
  - Measurement is somewhat uncertain
- It was assumed that when NO3 volatilizes, half of the associated NH4 evaporates with it
  - $NH4_{Adj} = NH4_{STN} - ½ * 0.29 * (NO3_{STN} - NO3_{FRM})$
- DON is calculated using the NH4 associated with SO4 and SO4
  - DON was interpolated to smooth the measured values
- Ammonium is calculated from interpolated DON, sulfate and nitrate (measurements are not used directly)

$\mathbf{NH4_{FRM}}$ =DON*SO4+0.29*$NO3_{FRM}$

Particle Bound Water

- Particle bound water was estimated using the AIM model (Clegg, 1998)
  - Inputs are ammonium, sulfate, and nitrate
    - Used quarterly average values
  - Assumed 35% relative humidity and 22° C
    - Conditions that FRM filters are weighed
- Derived an empirical equation to describe relationship
  - **PBW** =(-0.002618) + (0.980314*nh4) + (-0.260011*no3) + (-0.000784*so4) + (-0.159452*nh4**2) + (-0.356957*no3*nh4) + (0.153894*no3**2) + (0.212891*so4*nh4) + 0.0444366*so4*no3) + (-0.048352*so4**2)
- PBW varies by DON and is not linear
  - Future year change in DON can lead to a non-linear response in PBW (water can go up as sulfate goes down)
  - We held DON constant in the future to avoid non-linearities in an uncertain calculation

Organic Carbon by Difference

- OC is the most uncertain PM component
  - Mass by difference attempts to account for uncertainties associated with positive and negative OC artifacts
    - Multiplier (1.2-2.0)
    - Volatilization of semi-volatile mass
    - Blank mass
    - Large gradients of primary OC
      - If an FRM measures an OC hot spot that is not measured by an STN site, then the OC by difference will likely account for the high OC
  - **Organic carbon mass by difference**

(OCmb) = $PM2.5_{FRM}$ - { [SO4] + [$NO3_{FRM}$] + [$NH4_{FRM}$] + [water] + [crustal material] + [EC] + [0.5] }

Summary of Steps to Derive FRM Speciated Mass

- Adjust nitrate to account for volatilization
- Calculate quarterly average nitrate, sulfate, EC, DON, crustal, and measured OCM
- Calculate quarterly average NH4 from adjusted NO3, SO4, and DON
- Calculate particle bound water from DON, sulfate, and nitrate values
- Calculate OC by difference from PM2.5 mass, adjusted nitrate, ammonium, sulfate, water, EC, crustal, and passive (blank) mass
- **$PM2.5_{FRM}$** = { [OCMmb] + [EC] + [SO4] + [$NO3_{FRM}$] + [$NH4_{FRM}$] + [water] + [crustal material] + [0.5] }

Application of SMAT for CAIR

- Reconstructed mass equation and interpolated species data are used to calculate species mass fractions at each FRM site (2002 data)
  - Species fractions for each quarter
- The species fractions are then multiplied by the 1999-2003 (quarterly) average design value to get the species concentrations at each site
  - The individual species add up to FRM PM2.5 concentration
- RRFs are derived from the model outputs
  - RRFs are calculated for sulfate, nitrate, OC, EC, and crustal mass
  - Water and ammonium are then calculated from the DON and future year sulfate and nitrate concentrations
- The future year (seven) species are summed for each quarter
- The four quarters are averaged to get a future year annual average PM2.5 for each FRM site

SMAT Issues for the Final PM Guidance

- SMAT needs to be updated
  - Should the CAIR example become the default methodology?
  - Are other changes/improvements needed?
  - Is there new science to drive updates?
  - How is SMAT applied for the 24-hour standard?
- Questions:
  - Ammonium measurements
    - How uncertain?
  - Particle bound water estimates
    - Use AIM, empirical equation, linear assumption, or other model?
- Interpolations
  - Revise techniques?
  - Provide flexibility
  - Are interpolations necessary?
    - Are there enough speciation sites to avoid interpolating?

New Orleans Photochemical Modeling Workshop Presentations

- SMAT and SANDWICH presentations (as well as all others) can be found at:

http://www.cleanairinfo.com/modelingworkshop/presentations/PM_RH_O3.htm