

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 PM_{2.5} needs to use all of the PM_{2.5} component species
 - Individual RRFs are calculated for each PM_{2.5} species
 - Total PM_{2.5} is reconstructed from the sum of individual components
- The speciated model attainment test methodology was conceived for the PM_{2.5}/Regional Haze modeling attainment guidance
 - The guidance recommends the use of the speciated test for PM_{2.5} (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 - Draft guidance version of SMAT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 PM_{2.5} 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 PM_{2.5} mass that was retained on the FRM filters
 - We applied the principles of the 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 PM_{2.5} by multiplying FRM PM_{2.5} by fractional composition of each specie
- Calculate a model derived relative reduction factor for each specie
- Multiply each RRF times each ambient PM_{2.5} component (for each quarter) to get the future concentrations
- Sum the future quarterly average components
- Average the four mean quarterly future PM_{2.5} concentrations



Draft PM_{2.5} Guidance

- Current guidance recommends deriving PM_{2.5} 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 PM_{2.5} 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

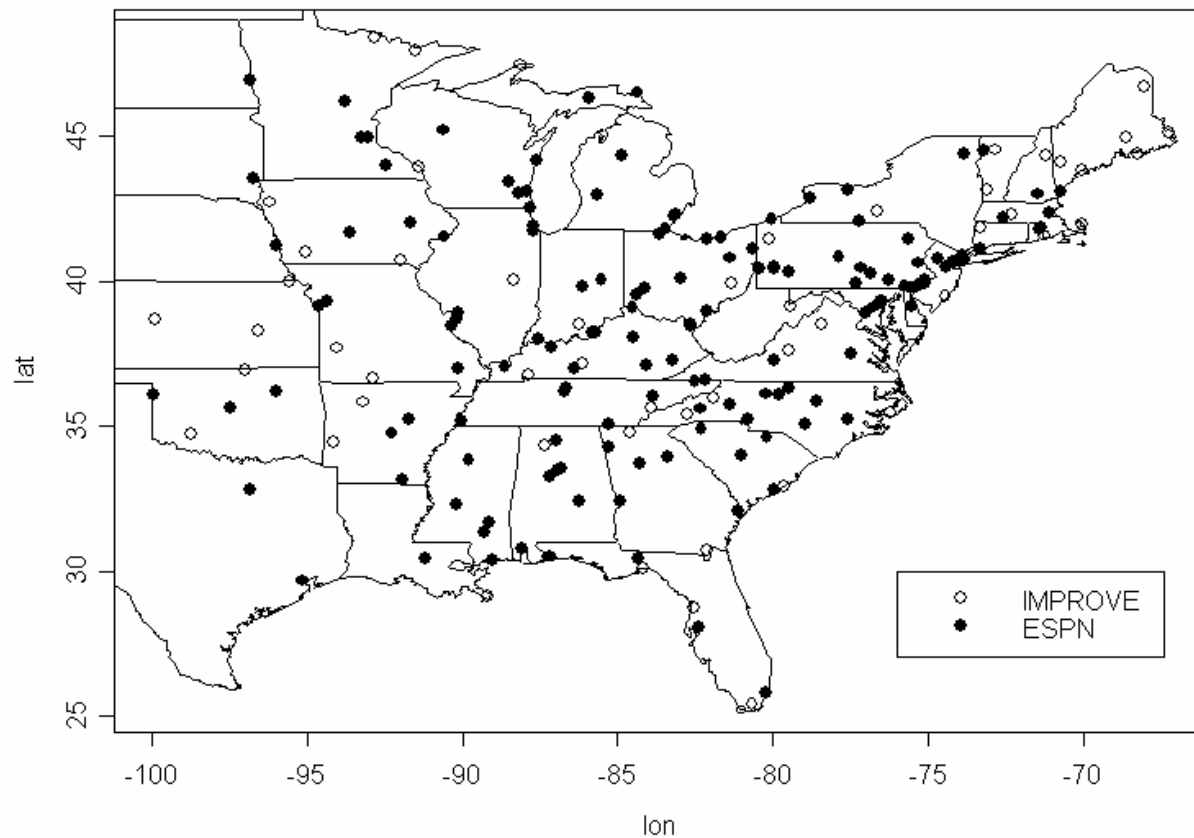


Data Notes

- 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

Speciated Network 2002 (Q4)

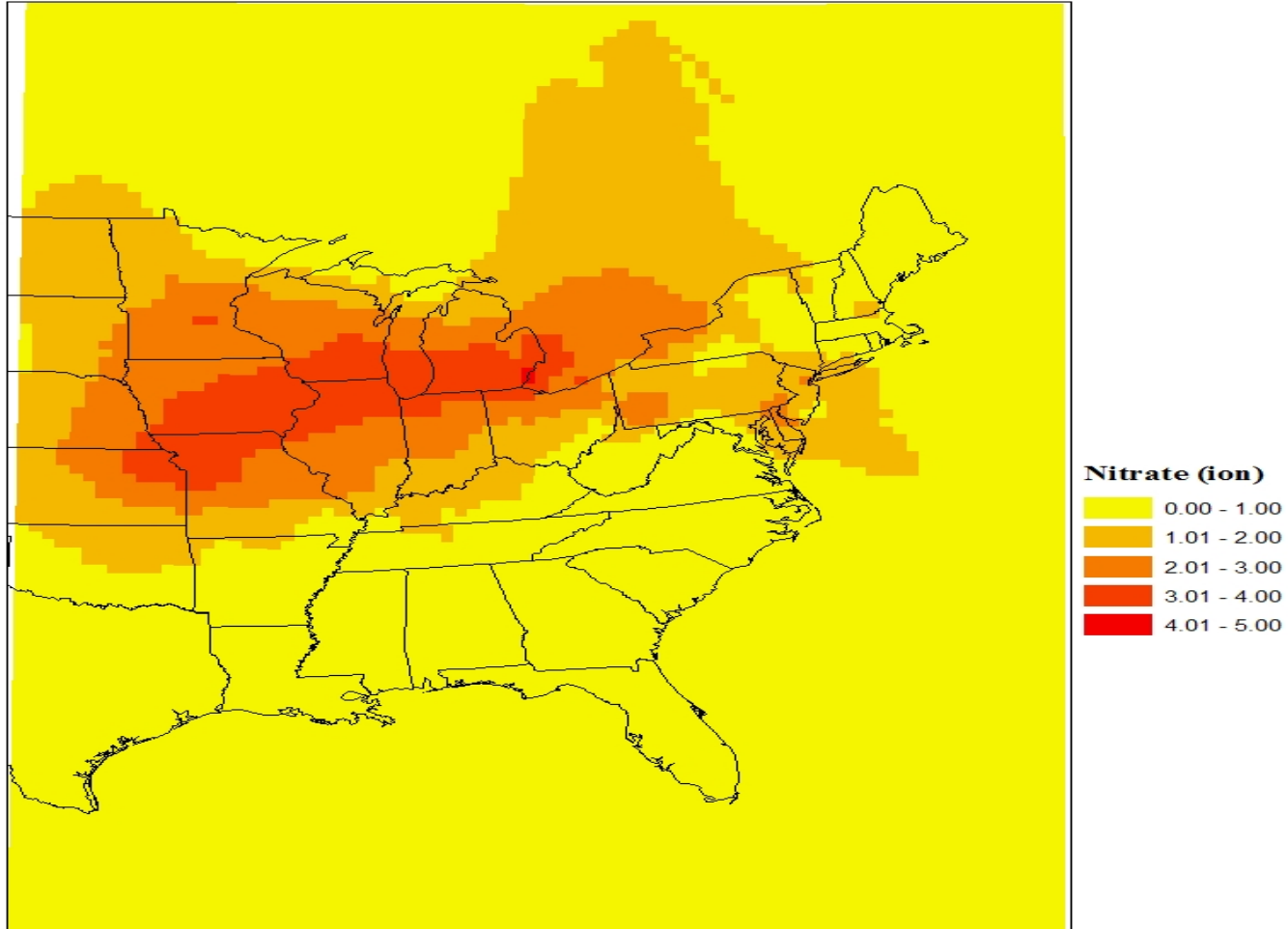




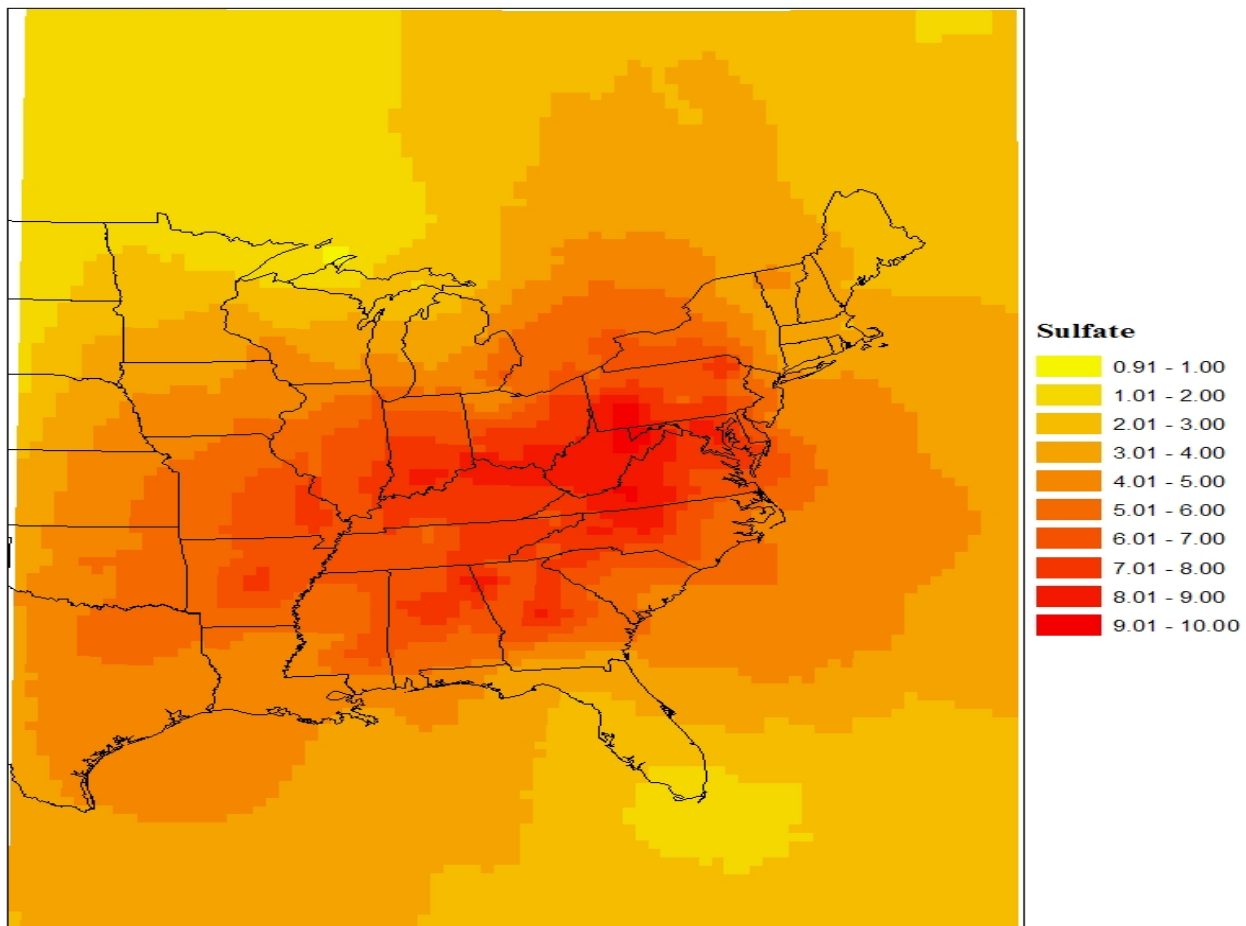
Interpolations

- Interpolations were completed (using VNA) for each quarter for the following species
 - Sulfates
 - Nitrates
 - Organic carbon mass ($OC \times 1.4$)
 - 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
 - $NH4_{Adj} = NH4_{STN} - \frac{1}{2} * 0.29 * (NO3_{STN} - NO3_{FRM})$
- 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)

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

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
 - $$\text{PBW} = (-0.002618) + (0.980314 \cdot \text{nh4}) + (-0.260011 \cdot \text{no3}) + (-0.000784 \cdot \text{so4}) + (-0.159452 \cdot \text{nh4}^2) + (-0.356957 \cdot \text{no3} \cdot \text{nh4}) + (0.153894 \cdot \text{no3}^2) + (0.212891 \cdot \text{so4} \cdot \text{nh4}) + 0.0444366 \cdot \text{so4} \cdot \text{no3} + (-0.048352 \cdot \text{so4}^2)$$
- 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**
- $$(\text{OCmb}) = \text{PM}_{2.5\text{FRM}} - \{ [\text{SO}_4] + [\text{NO}_3]_{\text{FRM}} + [\text{NH}_4]_{\text{FRM}} + [\text{water}] + [\text{crustal material}] + [\text{EC}] + [0.5] \}$$



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 PM_{2.5} mass, adjusted nitrate, ammonium, sulfate, water, EC, crustal, and passive (blank) mass
- $$\text{PM}_{2.5\text{FRM}} = \{ [\text{OCMmb}] + [\text{EC}] + [\text{SO}_4] + [\text{NO}_3\text{FRM}] + [\text{NH}_4\text{FRM}] + [\text{water}] + [\text{crustal material}] + [0.5] \}$$



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?

Other PM/RH Guidance Issues





Other PM/RH Guidance Issues

- Model performance
 - Revise details of model performance evaluation chapter
 - Add recommendations to include “new” plots and metrics
 - “Soccer” plots
 - “Bugle” plots
 - Enhance discussion of diagnostic analyses
 - Greater emphasis on the use of ambient data analysis to help evaluate the performance of various species



Other PM/RH Guidance Issues

- Attainment test for 24-hour PM_{2.5} NAAQS
 - SMAT should also be applied for the 24-hour standard
 - The test becomes more similar to the ozone test
 - Need a minimum number of days in the mean RRF calculation?
 - Many additional issues and uncertainties
 - How reliable are daily measurements and daily model predictions
 - Are daily interpolations needed?
 - Blank mass corrections on a daily basis?
 - Currently only California violates the 24-hour standard
 - If the standard is lowered, many other States will eventually need to apply 24-hour SMAT



Other PM/RH Guidance Issues

- Weight of evidence/Supplemental analyses
 - Expand WOE to below the NAAQS?
 - Additional details for PM_{2.5} and regional haze
 - Revise suggested analyses
 - Enhance data analysis section
 - Accountability and tracking plan?



Other PM/RH Guidance Issues

- Regional Haze test
 - Test needs to be revised to account for differences in the draft modeling guidance and the final regional haze tracking guidance
 - Tracking guidance specifies calculation of daily deciview values which are averaged across the 20% best and 20% worst days
 - The modeling guidance specifies calculation of daily beta extinction values which are averaged across days, then converted to deciviews as the last step
 - Because deciviews is a log function, the values depend on the order of the calculation
 - The modeling guidance should be changed so that it is consistent with tracking guidance



Other PM/RH Guidance Issues

- Regional Haze test
 - There are many potential methods of calculating RRFs
 - Average RRF
 - Quarterly average RRF
 - Day specific RRF
 - etc.
 - VISTAS has identified and tested different options
 - Developed a white paper
 - The options will be discussed in detail at the next RPO meeting in Denver