Attachment C

PM Speciation Data Analysis

General/Background:

This attachment describes the SP PM speciation-related analyses. The PM speciation data were obtained from a variety of sources, including AQS, IMPROVE’s website (VIEWS), and from PM2.5 Supersite Principal Investigators.

Construction of PM2.5 Urban Speciation Database:

PM2.5 speciation data were extracted from the AQS in July 2004. The following post-processing of the extracted data was done to arrive at the final database.

• All event-flagged data were removed.
• Only data from ‘suburban’ or ‘urban’ sites were retained; sites designated ‘RURAL’ in AQS were omitted from the database.
• Completeness was checked to ensure that a minimum of 11 observations were present for all major chemical components for each of the 4 quarters that make up a year. Quarters are defined as: January-March; April-June; July-September; and October-December. Major species include: organic carbon, elemental carbon, ammonium, all components of crustal material (as listed below in the Crustal Material equation), nitrate, and sulfate.
• New variables were computed as follows:
  - \( \text{OCM} = (\text{Measured organic carbon-blank corrected}) \times 1.40 \)
  - Ammonium Sulfate = 1.375 \times \text{Measured Sulfate}
  - Ammonium Nitrate = 1.290 \times \text{Measured Nitrate}
  - Crustal Material = 2.2\times[\text{Al}]+2.48\times[\text{Si}]+1.63\times[\text{Ca}]+2.42\times[\text{Fe}]+1.94\times[\text{Ti}]
  - Total Carbonaceous Mass (TCM) = \text{Organic Carbon Mass (OCM)} + \text{Elemental Carbon (EC)}
• Data were reduced into quarterly and annual averages. Note that annual averages must have four complete quarters of data.
• Excel spreadsheets were developed of the extracted and reduced data.

Construction of PM2.5 Rural Speciation Database:

PM2.5 speciation data were extracted from IMPROVE’s VIEWS website, http://vista.cira.colostate.edu/views/, in October 2004. A methodology similar to that outlined above (for the urban data) were used to reduce the IMPROVE data. It should be noted that VIEWS already does some of the computations outlined above.

• Data were used as reported to VIEWS website
• Only data for rural sites Washington, DC site were retained.
• Completeness was checked to ensure that a minimum of 11 observations were present for all major species for each of the 4 quarters for the year in question. Quarters are defined as before. Major species are also the same as before with the exception of ammonium, which is not routinely measured in the IMPROVE protocol.
• All the variables calculated above are automatically computed by and reported in VIEWS for the IMPROVE data. In addition, the PM10 measured values were retained as an additional parameter for all observations.
• The data were reduced into quarterly and annual averages. Note that annual averages must have four complete quarters of data.
• As before, Excel spreadsheets were developed of all the extracted and reduced data.

Creation of PM Supersite Database:

A summary of speciation data collected at the Los Angeles Supersite (USC site) was sent to EPA by its Principal Investigator, Constantos Sioutas. These data were used as delivered. Mass and speciation data were available for PM$_{1.0}$ (ultrafine), PM$_{2.5}$ (fine), and PM$_{10-2.5}$ (coarse). These data spanned the one year 10/2001 to 9/2002.


Because there aren’t enough urban PM2.5 speciation data to construct a trend line, rural IMPROVE data were used to generate an 11-year trend. Note that the Washington, DC IMPROVE data can only be used to investigate urban trends in that single location.

Goals:
? To show PM2.5 mass and chemical constituent trends by region.
? To better explain how mass and components vary spatially and temporally.

Outputs:
○ See Output C.1.

Methods:
• Using the PM2.5 rural database constructed above, sites that were complete for the entire time period of 1993-2003 (by quarter) were retained and binned into East, West, and DC.
• Annual averages were computed by site for each year then averaged for the entire region. Only one site went into the Washington, DC trend line.
• Line graphs (to represent PM2.5 mass, ammonium sulfate, ammonium nitrate, total carbonaceous mass (TCM), and crustal material) were generated in a spreadsheet (Lotus 1-2-3)

Analysis 2 – Rural PM10-2.5 Trends for 1993-2003

As with Analysis 1 outlined above, IMPROVE data were used to construct a trend line of the difference between PM10 and PM2.5 (which represents the coarse fraction of PM).

Goals:
? To show PM10-PM2.5 trends by Region of the United States.
? To show East, West, and Washington, DC (urban) trends.

Outputs:
○ See Output C.2.

Methods:
• Using the PM2.5 rural database constructed above, sites that were complete for the entire time period of 1993-2003 were retained and binned into East, West, and DC. Only two variables were checked for completeness, PM2.5 and PM10.
• Annual averages were computed by site for each year and then averaged for the entire region. Note that only one site went into the trend line for Washington, DC.
• Line graphs were generated in a spreadsheet (Lotus 1-2-3).

Analysis 3 – 2003 Annual Average urban and rural PM2.5 speciation patterns

Goals:
? To show urban and rural speciation patterns for the year 2003 by Region of the United States. Regions were subdivided into: Northeast, Southeast, Industrial Midwest, Upper Midwest, Southwest, Northwest, and Southern California.

Outputs:
o See Output C.3.

Methods:
• Using the rural and urban PM2.5 speciation databases developed above, site that complete were complete for year 2003 were retained
• Annual averages were computed for each site for the year 2003.
• Sites were binned into each of the Regions mentioned above and regional averages were computed.
• Urban and rural stacked bar charts for each region [using the major species ammonium sulfate, ammonium nitrate, total carbonaceous mass (TCM), and crustal material] were generated in Lotus.

Analysis 4 – 2003 Seasonal urban and rural PM2.5 speciation patterns

Goals:
? To ascertain if there are seasonal variations in regional speciation profiles.

Outputs:
o See Output C.4.

Methods:
• For those sites that were complete for the entire year of 2003, quarterly averages were computed for all the major components and binned by region.
• Urban and rural stacked bar charts (for the major components) for each region, for each of the four seasons were generated via Lotus.


Goals:
? Using one year of available data, as developed above, for the USC Los Angeles supersite, speciation patterns of ultrafine PM, coarse PM, and PM2.5 were evaluated.

Outputs:
o See Output C.5

Methods:
• Using data as directly received from the Los Angeles Supersite’s principal investigator, speciation patterns were depicted (generated in Lotus 1-2-3 spreadsheets) using pie charts for each of the three modes mentioned above. Major species displayed in the pie charts
include ammonium sulfate, ammonium nitrate, organic carbon, elemental carbon, and crustal material.
Average annual average trend in PM$_{2.5}$ mass, ammonium sulfate, ammonium nitrate, total carbonaceous mass, and crustal material at IMPROVE sites, 1993-2003.
Average measured annual average PM$_{10-2.5}$ concentration trend at IMPROVE sites, 1993-2003.
Annual average composition of PM$_{2.5}$ by region, 2003. Rural data (top panel) from IMPROVE network, urban data (bottom panel) from EPA Speciation Network. Components (from top to bottom) are crustal material, total carbonaceous mass (TCM), ammonium nitrate, and ammonium sulfate.
Seasonal average composition of urban PM$_{2.5}$ by region, 2003. Data from EPA Speciation Network. Components (from top to bottom) are crustal material, total carbonaceous mass (TCM), ammonium nitrate, and ammonium sulfate.
Seasonal average composition of rural PM$_{2.5}$ by region, 2003. Data from IMPROVE Network. Components (from top to bottom) are crustal material, total carbonaceous mass (TCM), ammonium nitrate, and ammonium sulfate.
Average PM$_{10-2.5}$, PM$_{2.5}$, and PM$_{0.1}$ (ultrafine) chemical composition at an EPA ‘supersite’ monitor in Los Angeles, CA, 10/2001 to 9/2002. Components shown in clockwise order (starting with ammonium nitrate) as listed in legend from top to bottom.