

## Theme Two: Air Quality Management

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### Introduction

Air quality management and “implementation” research are terms used in this review to categorize research designed to better understand atmospheric concentrations of PM-Ozone, sources that contribute to these levels, and approaches to reduce emissions. The principal focus of the discussion that follows is on PM and its co-pollutants. The Agency has been gradually merging its ozone research program under this topic over the past few years, and will formally combine the two, eliminating separate ozone research beginning in FY06. Atmospheric environmental research addresses the characterization, governing processes, and sources of air pollution (see Table 2.1).

PM and co-pollutant research is organized under several major topics based on NRC classifications; air measurement, emissions characterization, and air quality processes and modeling. Research under these topics serves two principal purposes. One is to provide the environmental characterization inputs to exposure and health assessments that lead to setting national environmental goals. See the Figure 2.1 representation of the risk assessment/risk management paradigm for Federal research. The second is to provide the atmospheric science analysis tools used to inform environmental management strategies and programs to achieve National, Regional, and local air quality goals. See the Figure 2.2 representation of the framework for the role science plays in air quality management.

The overview that follows starts with the state of knowledge when the Agency’s PM program took on highest priority status and doubled in size. It covers the work done over the past six years, what we think we know now, and implications for future research.

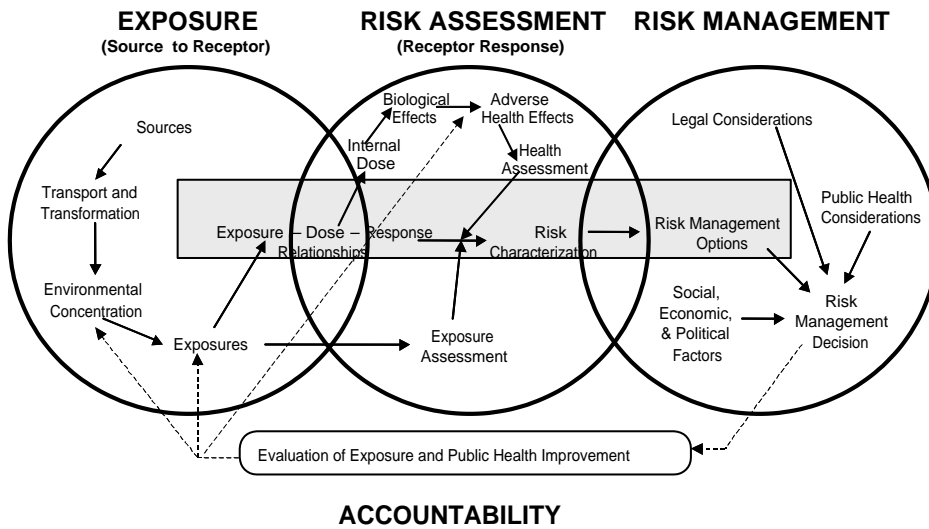
**Table 2.1 Relation of atmospheric environment science questions, research topics, paradigm components and framework subjects**

<b>Science Questions</b>	<b>Research Topics (NRC Research Topics #)</b>	<b>Research Paradigm Component *</b>	<b>PM Management Framework Subject**</b>
What is the atmospheric characterization of PM (and co-pollutants); its mass, composition and variability?	Ambient Measurements Methods and Observations (RT#11)	Environmental concentrations	Atmospheric concentrations
What are the sources of PM (and co-pollutants) and precursors?	Emissions Characterization (RT#3) Emission Controls (RT#11)	Sources Risk Management Options	Emissions Reduction Options
What are the processes that govern PM (and co-pollutants)?	Atmospheric Chemistry and Processes (RT#4) Air Quality Modeling: source and receptor (RT#4)	Transport and transformation	Atmospheric processing and meteorology

\* See Figure 2.1 \*\* See Figure 2.2.

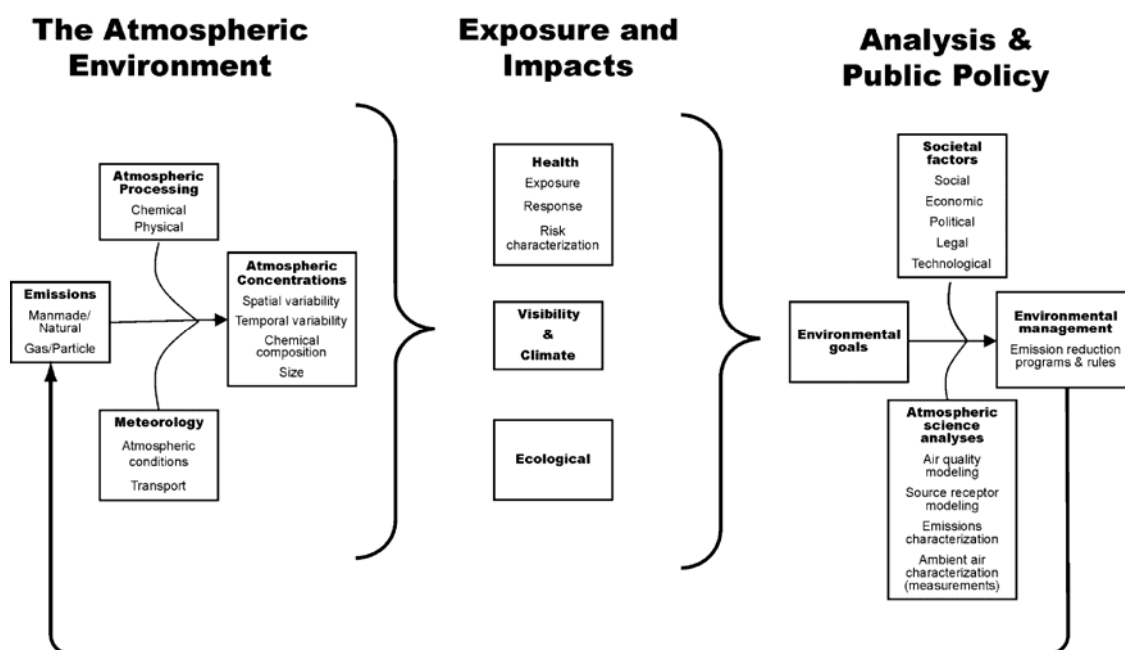
**Figure 2.1**

**Paradigm for Federal Research on Particulate Matter**



**Figure 2.2**

**Framework for informing PM management**



**Where we started - early state of science**

In 1998, there was a clear need for major science advances to characterize air pollution sources and atmospheric processes, both to inform exposure and health studies that underlay national standards review, and to support planning and implementation efforts for effective emission reductions to attain standards. There were inadequate methods to measure the many sizes and species of PM and its precursors and there was a limited understanding of atmospheric chemistry. Only slow and simplified complex computer models tying source emissions to ambient PM levels existed. Lastly, the methods to characterize emissions of PM from many major source categories were inaccurate.

### **Ambient Measurement Methods and Observations - Uncertainties**

The overriding uncertainty was an inability to fully characterize the PM polluted atmosphere due to the lack of ambient measurement methods to monitor PM's many size fractions, species, and precursors. The FRM PM<sub>2.5</sub> had been recently established, but yet to be arrayed in a national network or fully challenged. Built-in artifacts and biases of the FRM were known to exist. Neither routine, nor in some cases research grade, measurement methods were available for carbonaceous (OC and EC) PM, ultrafines (< 0.1 μm), and coarse PM (PM<sub>10-2.5</sub>). As a result, PM speciation (both spatial and temporal) was largely unknown, including for the large carbonaceous fraction and ultrafine fraction, except for insights from the IMPROVE network developed for haze monitoring.

### **Emissions Characterization - Uncertainties**

*NRC questions: "What are the size distributions, chemical composition, and mass-emission rates of particulate matter emitted from the collection of primary-particle sources in the United States, and What are the emissions of reactive gases that lead to secondary particle formation through atmospheric chemical reactions?"*

In order to address the challenges posed by the NRC's questions above, the Agency had to: 1) to produce better information on the composition of source emissions (e.g. source profiles) to enhance the accuracy of air quality and source-receptor models, and to improve the data available for health studies, 2) to develop models, measurement techniques, devices, and information applicable to source categories where existing emissions information was inadequate; and 3) to balance the research needed to support states develop more accurate mass emissions inventories for NAAQS implementation with the research to improve chemical speciation, size distributions, and source signatures and profiles across the board.

Specific uncertainties to be addressed by the Agency recognized that the existing emissions inventories and source characterizations were inadequate. Inventories were mostly for primary PM and based mostly on PM<sub>10</sub> methodologies. They contained little in the way of primary PM<sub>2.5</sub> information (e.g. size distribution and chemical composition). They included some gaseous species (SO<sub>2</sub> and NO<sub>x</sub>) for some source categories (utilities and autos), but poorly characterized other gaseous species (NH<sub>3</sub>, OC, EC) from all sources; and generally poorly characterized important open and fugitive sources (e.g. fires and animal feeding operations).

### **Air Quality Modeling - Uncertainties**

*NRC question: "What are the linkages between emission sources and ambient concentrations of the biologically important components of particulate matter?"*

Adopting the classifications used by the NRC, the Agency generally saw this question in terms of process understanding and modeling uncertainties. The Agency recognized that understanding the **atmospheric chemistry and processes** that models rely on was fundamentally important and needed to be strengthened. The chemical process involved in secondary PM and ozone formation (nitrate, sulfate, and secondary organic aerosols) was very uneven. NO<sub>x</sub>/NH<sub>3</sub> chemistry was fairly well known, as was NO<sub>x</sub>/VOC chemistry, except for that involving some aromatics. NO<sub>x</sub>/SVOC chemistry was somewhat characterized, but OC and secondary organic aerosol (SOA) chemistry were poorly characterized. The interaction among SO<sub>x</sub>, NO<sub>x</sub>, VOC, SVOC, and NH<sub>3</sub> were poorly understood. Continental transport (i.e. the relative regional and local contribution) was poorly understood as was intercontinental transport (i.e. the global contribution). Further, the modules representing the chemistry and process steps in models were too cumbersome and too slow.

**Source-oriented models** appeared to provide accurate estimates of some PM products (e.g. sulfates), but fell short for others, notably nitrogen compounds such as ammonia and nitrates and organic aerosols. For organic aerosols there was a need for a better understanding of the processes and precursors that affect SOA formation. Part of this problem resulted from the emissions inventory uncertainties described above. In addition, there was a lack of necessary field data to fully evaluate these models, though PM<sub>2.5</sub> data (including speciated data) was expected to be accumulated over the coming 2 to 3 year period through the national monitoring network and operation of the Supersites program. Specifically, source oriented modeling was: designed for episodic and not annual analysis; displayed in too large a scale (i.e. regional to urban scale on 12-36 km grids where neighborhood to global scales were needed); multi-pollutant in configuration but heavily biased for nitrates and OC, with SOA being uncertain; and evaluated for ozone, but not PM.

**Receptor-oriented models** were only able to approximate the complex physical reality of emission sources, and were limited where secondary products were involved. They were able to identify the presence of secondary contributions and estimate their magnitudes, but were much less able to determine the sources of their precursor emissions. Further, their uncertainty had to be evaluated by examining the degree of consistency among receptor-oriented models and by comparing results to source-oriented models rather than by means of an observable and independent benchmark. Specifically, receptor oriented modeling was: very useful for primary pollution (PM<sub>10</sub>), but severely limited for PM<sub>2.5</sub>; lacking many of the source profiles needed by most models (CMB), and an area of rapidly developing technology without an evaluation protocol.

## **What work has been done?**

Over the past six years, roughly halfway through the NRC portfolio, the Agency and its extramural research partners have made major scientific advances and significantly expanded knowledge of source emissions characteristics and atmospheric processes that can be used to support health studies and plan and implement effective emission reductions strategies. A complete array of PM monitoring and characterization methods has been developed and field

tested. Accurate methods have been developed to measure sizes and compositions of emissions from diverse and often widely dispersed sources. Data from field and laboratory studies have led to a better understanding of chemistry and processes of PM. Faster, more complex computer models that tie source emissions directly to ambient PM levels have been produced and evaluated.

### **Ambient Measurement Methods and Observations - Accomplishments**

Federal Reference (and Equivalent) Methods: The FRM for PM<sub>2.5</sub> has now been validated in the field and used in the National Monitoring Network to collect the three years of data necessary for use in compliance determinations. With the judicially directed need to monitor a separate coarse fraction, prototype samplers have been developed, deployed and are entering their final testing phases. Ongoing equivalency determinations for the PM<sub>2.5</sub> FRM have led to several alternative methods suitable for use in national compliance monitoring.

EPA Supersites: Seven sites distributed throughout the nation were competitively selected to intensively characterize PM and associated co-pollutants and to provide opportunities to test the latest technologies in aerometric analyses. Many new ambient monitoring technologies were tested and validated including approaches to make continuous measurements, single particle analyses, and others. The five eastern sites were organized into the cooperative Eastern Supersites Program that designed intensive, seasonal studies over a 13-month period from 2001 to 2002. The resulting data comprise the most extensive database collected to date on PM and its co-pollutants, and as a hall mark of this program are available on the web for public, scientific, and programmatic use. Analysis, synthesis and communication of results from this program are just now peaking, including an initial roll out at the AAAR Supersites Specialty Conference in Atlanta during February, 2005.

### **Emissions Characterization - Accomplishments**

ORD, in collaboration with OAR, has made substantial inroads in compiling data on conventional (industrial) and less conventional (agricultural and fire) sources of PM and its precursor emissions. Field and laboratory studies have significantly advanced our understanding of the chemical and physical characteristics of these source emissions, resulting in new and revised source profiles. Many of these profiles have been added to the OAQPS SPECIATE database where they are used directly by states as inputs for source receptor models. Researchers have developed specialized and complex measurement techniques to determine detailed particle sizes and compositions from diverse and often widely dispersed sources such as wildfires and concentrated animal feeding operations (CAFOs).

Recent major advances include having: 1) developed a dilution sampling system that collects emissions that mimic the behavior of an exhaust plume; 2) collected data to improve mass emission factors as well as PM composition and size information for residential wood combustion devices (including wood stoves operated under real-world conditions), a heavy-duty diesel truck tested during on-highway operation, and various industrial boilers and combustors, where the impacts of fuel type and composition, varied operating conditions, and performance data for pollution-control devices have been included; 3) addressed the open biomass burning problem using unique tracers and chemical fingerprints to estimate emission rates; 4) characterized fugitive road dust contributions; 5) developed a method using a Fourier transform

infrared (FTIR) laser system to measure ammonia emissions from hog barns and lagoons that can be used to measure other compounds, including methane and low molecular weight organic compounds from diffuse sources; and 6) partnered with industry to improve the capture of fine PM from coal-fired power plants by applying an electric field to conventional baghouses that can be retrofitted to plants currently using an electrostatic precipitator or fabric filter systems. The improved source emissions data and measurement techniques are now in use by states and others to improve their emissions inventories.

### **Atmospheric Chemistry and Processes - Accomplishments**

ORD continues development of a PM chemistry module to predict ambient compositions and concentrations of PM<sub>2.5</sub>. A first phase focused on SOA formation and its key chemical and physical processes that control its yield and composition from atmospheric transformations of aromatic compounds, biogenic hydrocarbons, and relevant mixtures of hydrocarbons. A series of smog chamber experiments have been conducted in which hydrocarbons were irradiated in the presence of NO<sub>x</sub> to assess the effect of environmental parameters such as relative humidity on the yield and chemical composition. Latter work has included irradiating  $\alpha$ -pinene, a representative biogenic compound, with a NO<sub>x</sub>/air mixture. This work has established unique biogenic SOA tracer compounds and the quantitative relationship between those compounds and total biogenic SOA.

### **Air Quality Modeling - Accomplishments**

Source-oriented modeling: The initial Community Multiscale Air Quality (CMAQ) model was released in 1998. New CMAQ model versions have since been released for public access roughly on an annual basis with ongoing development and inclusion of the latest aerosol model. The most recent regulatory version of CMAQ, released in June 2002, incorporates state of the science atmospheric processes, emissions models, and greatly speeded up multi-processing that cuts run times to a fraction of earlier speeds. CMAQ has been partially evaluated using data from the IMPORVE network and is now being further evaluated with the PM<sub>2.5</sub> data from the Speciation Trends Network (STN) and recently conducted large field studies. In particular, the model is being improved through the incorporation of newly developed chemical modules that describe PM's complex chemistry largely focused on nitrates and secondary organic aerosols. Significant improvements in the predictive capability of CMAQ are expected by the next major release in 2005.

A new major application of EPA's CMAQ model to real-time air quality forecasting for ozone and PM has been undertaken. The current coupled (NOAA – EPA) Eta-CMAQ system now produces hourly forecasts of ozone and other photooxidants on a three-dimensional model grid covering the eastern U.S. with a grid resolution of 12 km. CMAQ is now routinely used in many States.

Receptor-oriented modeling: ORD is providing user-friendly versions of receptor-based models that state and local regulators can use. Two PC-based models have been developed by EPA; the Chemical Mass Balance (EPA CMB8.2) and UNMIX models. Another, the Positive Matrix Factorization (PMF) method has been developed under STAR grants and is being brought in-house (as PMF 1.0) and evaluated along with a beta version of UNMIX. The CMB model has been released with full documentation and user guides that include application examples and is

currently in-use by many state agencies. Initial versions of a Quantitative Transport Bias Analysis (QTBA) are being developed that utilize air mass trajectory data and source contributions from receptor models to identify source areas and quantify relative source contributions to air pollutant levels at a receptor location such as an ambient monitor, or region. Recent EPA research using radiocarbon ( $^{14}\text{C}$ ) measurements has made possible a direct estimation of the fraction of  $\text{PM}_{2.5}$  carbon that is biogenic. The measurements are technologically complex, but can now be performed in an essentially routine manner at several specialized laboratories in the U.S.

## **What we now know**

### **Ambient Measurement Methods and Observations - Insights**

Federal Reference (and Equivalent) Methods: As a result of several years of field operation and scrutiny under the Supersites program, the FRM for  $\text{PM}_{2.5}$  is now fully evaluated and its artifacts and biases are known. Its operating requirements, limitations in collection and reporting periods, and costs are also known leading to the commonly supported goal of producing a continuous, real-time measurement that can reveal rapid cycles and peaks not previously apparent. As a result of legal action associated with the 1997 PM NAAQS, there is a mandate for a  $\text{PM}_{10-2.5}$  (Coarse) FRM. In 2003-2004 ORD conducted several field studies of the performance of possible  $\text{PM}_{\text{coarse}}$  methods. The results have been encouraging, and manufacturers are now producing second-generation instruments that will be tested by EPA during 2005.

Speciation: For the inorganic species of PM and its precursors, there are accurate, precise and comparable measurement methods available for sulfates, nitrates, ammonium, total carbon, most trace elements, and transition metals. Some  $\text{NO}_x/\text{NO}_y$  species retain biases that are undesirable. The measurement of the carbonaceous species of PM, elemental or black carbon (EC) and total Organic Carbon (OC), remain the subject of intense method development. Of the hundreds of compounds contained in the OC fraction, less than 20% can be routinely identified. Methods are now available to routinely measure ultrafine particles by mass and number, but their chemical speciation remains even more difficult than it is for the  $\text{PM}_{2.5}$  fraction.

Field Studies: Early field intensives and the follow-on work of the Supersites program, have revealed and continue to reveal important information about the many facets of PM. Eastern  $\text{PM}_{2.5}$  is dominated by sulfates and OC, and Western  $\text{PM}_{2.5}$  by nitrates and OC, though fractions change seasonally. Generally winter nitrate is higher than summer, and urban higher than rural. There are important regional contributions with 50-70% of locally observed PM coming from upwind sources. There are important urban to rural concentration gradients and gradients across urban areas. Most summertime OC in the East appears to be biogenic, and most of this appears to be secondary in formation.

### **Emissions Characterization - Insights**

Research has demonstrated that a dilution sampler system (DSS) can be effectively used to determine the phase distribution of semi-volatile compounds under conditions similar to those

that occur in the diluted plume immediately downwind of a source. Using this method emissions from a dozen important source categories have been characterized for PM mass, PM size distribution, speciated organics, elements, ions, and elemental vs. organic carbon. The detailed chemical composition of emissions from a residential oil-fired furnace, a commercial jet aircraft engine, a large residual oil-fired utility boiler, and a large coal-fired utility boiler are now known. There are now also new and improved source sampling and chemical analysis methods for fine PM, particularly the organic fraction. In addition, a new on-road laboratory (the Diesel Emissions Aerosol Laboratory or DEAL) has shown the effects of natural cooling and dilution on the formation of volatile PM. The technique was tested on jet aircraft engine exhaust in 2004. These data will assist states understand the contributions of aircraft to ambient PM around large airports.

A novel measurement method called Vertical Radial Plume Mapping (VRPM) which utilizes multipath optical remote sensing instruments coupled with real-time processing algorithms has been developed and is now capable of producing spatially-resolved  $\text{NH}_3$  emission measurements from animal feeding operation (AFO) sources. As a result, there is a significantly better understanding of how emissions from the largest  $\text{NH}_3$  category varies with the different types of feeding operations and with different possible emission control approaches. Further ammonia air/surface exchange rates have been measured for corn and soybean both near and downwind of animal production facilities. This information on exchange rates combined with improvements in emissions data from the open path measurement method, has led to a better understanding of how the scavenging of  $\text{NH}_3$  by vegetation impacts the actual  $\text{NH}_3$  that is available to react with other PM precursors.

Field testing and collaborations with other federal agencies, including NASA and NOAA has led to improved models of emissions from wildfires and prescribed burning. Field tests of biogenic emissions has improved the Biogenic Emission Inventory System (BEIS) model, which has been a key factor in better understanding secondary organic aerosol formation. Finally, early prototypes of an operating mode-based (e.g. modal) mobile sources emission model have been successfully tested. The MEASURE model incorporates data on emissions during specific driving conditions, such as cold starts, acceleration, and cruise, and allocates those emissions to specific locations where such operating modes occur (neighborhoods, freeway on-ramps, etc.) These data are helping guide the efforts of OTAQ in the development of their next-generation mobile model, MOVES and providing highly spatially and temporally allocated emissions for inventory development.

### **Atmospheric Chemistry and Processes - Insights**

Smog chamber results clearly demonstrate that aromatic compounds emitted into the atmosphere contribute to SOA formation through atmospheric transformations that form oxidation products which are partially absorbed into the organic films on pre-existing  $\text{PM}_{2.5}$ . SOA yields have been found to be strongly influenced by the total mass of organic compounds present, but were not affected significantly by typical daytime relative humidity. Laboratory results also demonstrate that SOA compounds from aromatic compounds are far less effective in taking up liquid water—which contributes to regional haze—than sulfate and nitrate compounds. SOA chemical composition studies are consistent with the formation of multi-functional oxygenated compounds, thus providing important tracer compounds for use in source-receptor relationships.



Finally, it was demonstrated that as much as 75% of the SOA from synthetic automobile exhaust could be explained by its aromatic content.

Biogenic hydrocarbon isoprene, long thought not to contribute to SOA formation, was irradiated in the presence of NO<sub>x</sub> in both the presence and absence of SO<sub>2</sub>. In the absence of SO<sub>2</sub>, as expected, there was little evidence of SOA forming, however, in its presence, the SOA yield of isoprene contributed significantly. Although these laboratory data were insufficient to extrapolate the results to ambient conditions, the results do suggest acid catalyzed reactions of isoprene or some other form of SO<sub>2</sub>-assisted reactions may be contributing to ambient SOA concentrations.

Studies by the Southern California Particle Center and Supersite, one of EPA's five PM Centers, are fully characterizing PM fine and UF, including seasonal and diurnal patterns, and source apportionment markers like hopanes for mobile sources, levoglucosan for wood combustion, and an indicator of photochemical secondary organic aerosol formation, 1,2 benzenedicarboxylic acid. Measurement and modeling of naphthalene (half of which comes from the use of gasoline and diesel vehicles) is demonstrating the ability of human exposure models to give more real time and finer resolution exposure data for health studies.

### **Air Quality Modeling - Insights**

Source-oriented modeling: Perhaps the greatest development in source-based modeling is the speed up in processing time over the last few years. The model can now be run in real time for ozone episodes and is now routinely used for ozone air quality forecasting in the eastern U.S. In regard to CMAQ's ability to forecast ozone episodes it has been evaluated in forecast mode over the eastern U.S. during the past two summers (2003 and 2004) and shown to be performing well and providing value over a persistence forecasting for both 1-hr and 8-hr maximum daily ozone predictions. The model was thoroughly evaluated against monitoring data several years back and is now being routinely used as an air quality management tool for national rule development and state implementation planning.

CMAQ is now able to predict PM on daily and annual basis. With improved processing times, annual runs for PM can be done now in a week to ten days. Based on initial evaluations to date using IMPROVE, STN, CASTNet, and Supersite data, the model handles sulfates and PM<sub>2.5</sub> mass reasonably well and there have been substantial improvements in prediction of total and aerosol nitrates. Carbonaceous PM species predictions remain uncertain.

Receptor-oriented modeling: CMB fully apportions exposure to the spectrum of sources and is highly dependent on the quality of the constituent-linked source-profile database. UNMIX and PMF internally generate source profiles from the ambient data and will probably be a useful tool for handling the vast amount of data being gathered by the national Speciation Trends Network. Both UNMIX and PMF are in the early stages of development and testing, with developmental work focused on establishing a set of key constituent species used to tag, identify, and separate major source categories. Model evaluation continues to use alternative approaches to validation against observations. Current protocols rely on method inter-comparison, though newly emerging techniques such as comparison to synthetic data sets is being researched.

Through  $^{14}\text{C}$  work, we now are learning that during the summer in the Southeast U.S. a large fraction of OC is biogenic. Further when  $^{14}\text{C}$  results are combined with other types of measurements (e.g. OC/EC ratio and molecular organic tracers of SOA) there is an indication that a large part of the biogenic aerosol is of secondary origin.

## **Implications for future research**

### **Ambient Measurement Methods and Observations - Implications**

There is a need for continued development and improvement of measurement methods for a wide variety of atmospheric constituents, improved understanding of the uncertainties associated with the methods, and improved sensitivity, selectivity, and time-resolution. Methods are needed for ozone precursor species that include the measurement of nitrogen oxides ( $\text{NO}$ ,  $\text{NO}_2$ ), formaldehyde, and volatile organic compounds (VOC). FRM and FEM methods that include continuous and semi-continuous methods for PM mass (fine, coarse, and  $\text{PM}_{10}$ ) need to be fully evaluated and inter-compared.

Results from current work under eight STAR grants to improve carbonaceous PM characterization will need to be converted for routine application. Included are efforts: to develop, improve, and evaluate advanced measurement techniques for source apportionment of organic PM (ATOFMS, TD-GC/MS, AMS, on-line LC/MS, PIAMS) – 5 grants; to integrate the thermal behavior and optical properties of carbonaceous PM to resolve differences in analysis methods (Improve vs. STN) – 2 grants; and to evaluate and minimize organic aerosol sampling artifacts – 1 grant.

Final results from the Supersites program with its insights on PM measurement approaches, processes and source contributions needs to be written up and disseminated. This includes the development of an integrated synthesis of key policy relevant findings based on 17 science/policy relevant questions developed by EPA/ORD in conjunction with other key personnel at EPA, in state and regional planning organizations, and the private sector.

### **Emission Characterization - Implications**

The key areas of concern for ORD's future PM emissions characterization research program lie in two areas, carbonaceous particles and emissions from dispersed sources (area and mobile). In both areas, information is needed to quantify the rates and characteristics of emissions and the variability in those measures.

Mobile Source Emissions: Research is needed to fully characterize real-world emissions from on-road and off-road mobile sources including the development of mobile source emission profiles and markers for use in human exposure and air quality receptor models. In this regard evaluation and application of portable emission measurement systems (PEMS) and open-path methods (e.g. OP-FTIR and TDLs) would be most useful. Emissions for one major subcategory, heavy duty diesels, need to be characterized over the range of engine and fuel types, operating levels, and road conditions likely to be encountered in coming years. School buses are of significant concern here. Similarly, jet aircraft emissions need to be characterized over varying operating conditions and while burning different fuels. Ultimately a more flexible and accurate

approach to model mobile source emissions, incorporating differences in vehicle operating mode and emission characteristics and transportation network details is needed. Such improved methodologies are needed for incorporation into EPA's future mobile source emission models (e.g. MOVES) that will be the successor to OTAQ's current mobile source model, MOBILE.

Area Source Emissions: Research is needed to further improve models of biogenic pollutant precursors taking advantage of the potential presented by satellite imagery. This is especially true for emissions from biomass burning and their contribution to PM and ozone. Developing model capabilities that account for constituents such as CO and VOCs in relation to fuel consumption and fraction of biomass burned are most desirable. Continued investigation of agricultural NH<sub>3</sub> emissions and the air/surface exchange of NH<sub>3</sub> over fertilized crops is also needed.

Control Technology: The use of wet scrubbers at power plants is expected to increase in the near future and technologies capable of providing simultaneous multi-pollutant control are needed. Bench-scale facilities that have confirmed the ability to achieve nearly complete NO oxidation and coincident mercury removal need to be tested to optimize use of ozone and investigate other cost-effective oxidants in addition to examining the removal/fixation of nitrates in dissolved scrubber liquids. Further, bench-scale studies are needed to characterize the effect of SO<sub>3</sub> on mercury capture using conventional sorbents and to identify flue gas conditions and sorbents that favor the combined removal of SO<sub>3</sub> and mercury. Lastly, the causes of excessive SO<sub>3</sub> formation from FGD and SCR controls, and the potential incidence of acid aerosol plume problems, and approaches to mitigating these adverse impacts needs to be examined with the goal of identifying ranges of most susceptible operating parameters.

### **Atmospheric Chemistry and Processes - Implications**

The further examination of the processes of SOA formation and the development of new computational techniques for this and other chemistry studies are needed. Computational techniques that use quantum mechanical calculations to predict properties influencing chemical and physical reactions that supplement chamber studies are needed to produce a less resource-intensive means for filling current gaps in atmospheric chemistry and process research. Further research is needed to determine whether traditional gas-aerosol phase partitioning, until recently the sole mechanism for SOA formation, is sufficient to explain laboratory and ambient field data. Field research is needed to assess the extent to which biogenic SOA is an important PM<sub>2.5</sub> constituent on national and annual scales, adding to recent evidence coming out of Supersite and STAR grant studies. Seven STAR grants are examining the carbonaceous PM phenomena; three improving emission source estimates of primary organic aerosol (POA) and secondary organic aerosol (SOA) precursors, and four studying SOA formation mechanisms, including cloud processing, SOA from aromatics, and biogenic VOC precursors.

### **Air Quality Modeling - Implications**

Source oriented models: Current and future work on the Community Multiscale Air Quality (CMAQ) model is needed to improve its prediction of nitrate and organic particulates and its processing speed, and to complete its evaluation. Specific needs include: adding the nucleation mode for PM to the current version, enhancing CMAQ's ability to predict coarse PM by adding sea salt and road salt, incorporating aerosol processes in fog conditions, developing the ability of

the CMAQ to predict ambient concentrations at smaller scales (e.g., at the neighborhood scale), continuing inverse modeling approaches to improve emission inventories, enhancing the model to address international transport of PM and provide air quality forecasts of PM, and in the longer term, including mechanisms that treat meteorological and chemical processes simultaneously (as opposed to using separate mechanisms as in current models), allowing more accurate treatment of the real-world interactions between meteorological and chemical processes.

Receptor-oriented models: Model development, testing, and application is an ongoing need. Two advanced receptor modeling tools are subject of current focus, UNMIX (EPA version 3.0), and the Positive Matrix Factorization - PMF (EPA version 1.0). In addition, methods such as EPA's Quantitative Transport Bias Analysis (QTBA) are being developed to identify source areas and quantify relative source contributions to air pollutant levels at a receptor locations in the form of hybrid receptor models. This development work needs to continue. Ultimately an independent evaluation protocol, comparable to that used for source-based model evaluation, needs to be developed and applied to these models. EPA has invested heavily in these models through its STAR program and results from this work will need to be incorporated into the Agency's regulatory models. Three grants go to evaluating and improving receptor models for PM source apportionment. Four grants go to integrating receptor, source-based, and inverse modeling for PM source apportionment. Four grants go to improving measurement methods for molecular tracer species and identifying new molecular tracers for source apportionment. One goes to developing a next generation receptor model (combining UNMIX and PMF).