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Regional-Urban Scale Modeling of Fine Particulates Using the U.S.EPA Models-3 Community Multiscale Air Quality Modeling System

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ABSTRACT

Recent evidence indicates that fine particles, those 2.5 μm and smaller, adversely impact human health causing increased mortality and morbidity; further, they diminish ambient air quality with decreased visibility. Typically, particles in this size range arise as either by-products of atmospheric reactions of sulfur, nitrogen, and organic pollutants or as primary pollutants emitted naturally or from anthropogenic sources. In this presentation, we describe the U.S. Environmental Protection Agency's new modeling framework, Models-3, and its first version for air quality called the Community Multiscale Air Quality (CMAQ) model. Models-3/CMAQ is a new generation, state-of-science, comprehensive air quality modeling framework. With a "one atmosphere" paradigm, it is designed to be capable of addressing holistically and inclusively, the major air quality issues such as photochemical smog, particulate matter, airborne toxics, and Air Quality Related Values (AQRVs) including acidic, nutrient and toxic deposition, as well as visibility. For particulate matter (PM), number and size distributed sulfate, nitrate, organic and aerosol-bound water are predicted on three dimensional grid cells for domains encompassing regional and urban scales. Models-3/CMAQ is scheduled to be publicly released in 1998, and will be a community-based tool for predicting PM concentration fields from current emission distributions as well as for analyzing and assessing the viability of optional control strategies to achieve compliance with National Ambient Air Quality Standards (NAAQS). The PM components in this system are derived to a large extent from the prototype Regional Particulate Model (RPM) (Binkowski and Shankar, 1995). The fundamental features of the aerosol formulations include a bimodal size distribution of particles in the sub-micron range, and aerosols that are internally well mixed. Size dependent dry deposition parameterization, aqueous phase aerosol dynamics, and nucleations are included among the various major atmospheric processes modeled. Considerations for extensions and applications of Models-3/CMAQ are discussed.

I. INTRODUCTION

This paper briefly discusses the background, rationale, and context for the design of the air quality modeling framework, Models-3/CMAQ. The basic features of the Models-3 framework, the science components of CMAQ, and a description of the aerosol modeling components follow. Finally, some operational issues and application opportunities for PM modeling will be discussed.

A. Background: Evidence for adverse impacts to human health and to air quality due to particulate matter (PM) loadings in the atmosphere is increasing (U.S.EPA, 1996a,b). Evidence for both acute (mortality) and chronic (morbidity and reduced lung functions) effects suggests a need for investigating options for reducing the atmospheric particulate burden. Other issues impacted by airborne PM include visibility, and deposition of acidic, nutrients and toxic substances to sensitive ecosystems. Advanced air quality simulation models are needed as tools for scientific analyses of current PM loadings and their distributions as well as to provide a framework for determining the efficacy of various control scenarios. The concentration, chemical composition, and size distribution of airborne PM are controlled by numerous atmospheric processes that operate over large ranges of temporal and spatial scales. The source contributions include primary particulates as well as the sulfur, nitrogen and organic air pollutant precursors for secondary particulates that are produced out of complex gas, aqueous and heterogeneous phase chemistry and dynamic processes. Particles generally are distributed bimodally by size in the atmosphere, with the minimum of the distribution between 1 and 3 μm aerodynamic particle diameter separating the fine-mode from the coarse- mode particles. Due to their adverse impacts, the U.S. Environmental Protection Agency has a pending new regulation, a statutory requirement to establish NAAQS for fine particles, PM2.5, to protect human health, and to perform AQRV assessments of their impacts on the environment. A brief discussion follows:

National Ambient Air Quality Standards (NAAQS).

The Clean Air Act establishes regulatory requirements for six criteria air pollutants, one of which is PM, all of which adversely affect human health. Criteria review of each NAAQS pollutant is conducted periodically as new evidence and information emerge that may require refinement and/or modification as necessary. Subsequent to its latest review, the U.S. Environmental Protection Agency (U.S.EPA, 1996a) has proposed the establishment of an additional PM standard for fine particles, PM2.5. Currently under consideration are two new forms of the primary standards, one for an annual (long-term) and another for a daily average (short-term) for fine particles set with a 2.5μm upper limit in size. This action is in addition to revision of the form and value of the current standard based on PM-10 (all particles less than or equal to 10 μm). Cities and areas found to be in non-compliance will require some plan of controls which will allow such areas to achieve the NAAQS targets.

Air Quality Related Values (AQRVs) assessments.

Visibility is an AQRV; Federal land managers such as the U.S. Parks Service and the U.S. Forest Service must apply models in their strategy for permitting new sources for the prevention of significant deterioration (PSD) requirements in Class I areas. Visibility reduction is of course, directly attributable to the particulate matter burden in the atmosphere. Another AQRV concerns the adverse impacts of atmospheric deposition of some pollutant species to sensitive receptor environments. These species include acidic, nutrients, and toxic compounds; each class of such species is associated with aerosol particles. The association with acidic/nutrients deposition of sulfates and nitrates are relatively well known. Less is known about the role of particles on the deposition of semi-volatile organic compounds (SVOCs). Many SVOCs are particle-bound, and can be deposited in wet or dry form to sensitive water bodies and their contributing watersheds. Subsequently, great magnification of minute quantities of these toxins by bioaccumulation through the aquatic food chain can lead to damage to higher life forms and eventually to man through indirect exposure. SVOCs can exist under normal atmospheric conditions in both gaseous and aerosol forms simultaneously. Thus, semi-volatile toxic pollutants such as dioxins and polycyclic aromatic hydrocarbons (PAHs) require complicated modeling of both gas or particle phases. Modeling SVOC is especially challenging since many factors may affect their transport and deposition. These classes of compounds are typically complex distributions of congeners with varying volatility and toxicity properties. Variations in meteorological conditions affect the volatility of gases that have attached themselves to particles and must be considered. The transport scales of SVOCs vary from urban to regional and larger spatial scales, thus, they require multi-day simulation to characterize an episode. All processes active on such scales including cloud process, turbulent mixing, chemistry must be incorporated into scientifically credible models.

B. Rationale, State-of-Air Quality Simulation Modeling: Air quality models are tools used to study and develop strategic control strategies for implementing the requirements of the NAAQS, once set. Models, together with monitoring programs provide information regarding areas in non compliance, and information on the contributing sources. The scope of control strategies may be national or regional such as in the case of acid deposition or at state and local levels as regards photochemical oxidants (ozone). Information from models is used as input to economic models for cost analyses and to perform regulatory impact analyses (RIA). The modeling objective is to provide the basis for investigating control options for achieving the NAAQS and when used in conjunction with economic models, provide the most cost effective control strategies. Since atmospheric PM contain both local as well as regional sources of both primary emissions and precursors of secondary pollutants, models provide critical support toward developing policy delineating federal vs. state jurisdictions in the overall plans. It is becoming increasingly understood by both the scientific and policy communities that the chemistry and transport of photochemical oxidants and particulate matter in the atmosphere are closely, and intricately linked. Thus, models of air quality are required to treat the atmosphere more comprehensively and holistically in order to study and develop the most effective control strategies to handle both the NAAQS for criteria pollutants as the related AQRV issues including deposition and visibility. Additionally, such models can serve a benchmark against which reduced form models developed specifically for screening purposes or for exploring wide range of control options can be checked.

The development of comprehensive air quality models that has explicit treatments for particulate matter is a penultimate challenge to the modeling community. It requires the development and implementing of additional processes and improved science description into such models without significantly sacrificing operational performance for conducting practical applications. In addition to the complexities of modeling ozone and acid deposition, PM modeling must also handle the complication of gas-to-particle conversion, particle formation, particle chemistry and the highly temporal and spatial distribution of particle size and composition due to dynamics of particle growth and deposition. Particle lifetimes and their transport distances depend on both size and composition. Transport distances for larger particles is less than for smaller ones due simply to greater gravitational settling. These added and improved science descriptions will add significantly to the computational burden. The Models-3/CMAQ modeling framework described below is an attempt to address these challenges.

II. MODELS-3/CMAQ

The U.S. Clean Air Act of 1990 mandates controls for various pollutant categories and issues, including photochemical oxidants, acid deposition, and toxics, to meet pollutant targets for National Ambient Air Quality Standards (NAAQS). The recent health and environmental effects data are leading to revised NAAQS requirements which include: (a) new forms of the ozone standard from a peak one hour standard to an eight hour standard, and an integrated standard (such as SUM06 in which the sum of all hourly ozone values that exceed some reference level such as 60 ppb applicable for to the spring to fall growing season); and (b) a new standard designed to protect health by establishing criteria for daily and annual averages for fine particles (PM2.5). Such changes will require additional or more robust science description of processes in the current air quality models. Increasingly, it is recognized that control strategies addressing each air pollutant issues separately is either inadequate, or wrong. Conversely, models that are able to treat the atmosphere, holistically, as a complex mixture of pollutants, that can provide predictions of pollutant distribution over enormous time scales from sub seconds for chemical systems to annual for standards and objectives, and from scales that vary from local scale for human exposure to regional for handling the contributing sources will be necessary. With such requirements, there is the need to address and to improve the state of science in the description of the important contributing processes to perform the anticipated and requisite air quality predictions. Experience has amply shown that it is highly impractical, costly, and cumbersome to retool air quality simulation models for each new requirement; thus, we envision the need for a fresh new approach that minimizes past modeling problems, and yet powerful enough to absorb new requirements in a timely and cost-effective way. One approach is to design, develop, and assemble a community-based modeling system that is user friendly for both the science and policy communities. Such a system should be robust enough to enter and evaluate new science descriptions without requiring major retooling of the computational framework for each science realization, and for a revised or new policy or regulatory requirements. Tools should be provided to perform model predictions and model quality analyses, which permit ease of assessments from its outputs, be it science evaluation to policy applications. In response, the U.S.EPA has been developing a major new, advanced operational modeling framework that addresses these pollution issues, comprehensively. The Models-3/CMAQ modeling framework is nearing the completion for public release. Models-3/CMAQ is a flexible and general modeling framework that addresses NAAQS and AQRV issues in a comprehensive manner. Models-3 is designed to support computational scalability for multi-pollutant and multiscale air quality simulation while taking advantage of the enhanced computational capabilities provided by high performance computing and communication (HPCC) architectures. CMAQ is an emissions-based, Eulerian air quality modeling framework which integrates state-of-science physical and chemical science process algorithms with efficient numerical solvers and data linkages. The inclusion of particulates in air quality simulation models will allow the capability for modeling heterogeneous processes. The various processes inclusive of transport and deposition as well as the chemistry is therefore much more adequately and credibly simulated. Models-3/CMAQ will provide a basis for understanding the complex temporal and spatial distribution of air pollution on scales ranging from land-use to regional (sub-continental) scales. The following discussion is a brief summary of its major features. For a more detailed description of the system see Dennis et al. (1996) and Byun et al. (1995 and 1997).

The Models-3 framework is structured so as to fulfill functionalities needed to support a wide range of users from scientists and modelers to policy makers. Models-3's Graphical User Interfaces (GUIs) allow the users to design, customize, and refine modeling studies. The Study Planner sets up studies ranging from simple analyses of modeled or observed databases, to highly complex multiple runs of comprehensive nested model simulations of CMAQ. Implementation and execution of studies invoke key framework subsystems including: (1) the Dataset Manager performs manipulations (registers, search, updates, archives) of observations and model output datasets; (2) the Source Code Manager allows the retrieval and archival of source code files and the Model Builder constructs models from optional process modules and processors; (3) the Program Manager allows the user to enter and register and manage executable programs (codes and scripts); (4) the Science Manager registers and sets up persistent science objects such as grid, domain, spatial resolution, and episode definition; it also sets up chemical mechanism and science processes (Persistent objects, once registered eliminates the need for reentry of such prescription); and (5) a Toolkit for analysis and visualization of modeled and observed data. The air quality concentration and deposition fields are solutions to science formulations of the fundamental conservation laws and the outputs are hourly gridded fields of concentration and deposition for multiple day episodes. Aggregation techniques (Eder and LeDuc, 1996) are being developed and refined for inclusion in the Models-3 toolkit for computing longer than episode (seasonal to annual) average model outputs.

III. PARTICLE MODELING

This section describes the development of an initial prototype and the migration of the PM modeling to the Models-3/CMAQ version. At the outset, two methods for modeling aerosol size distribution were reviewed. Initial efforts to model particulates on regional scales with a sectional representation for the particle size distribution proved to be unsuitable for our purposes in two ways. First, computer time was excessive with simulations taking as much as 23 hours for a 24 hour simulation. Second, the size distribution using a recommendation of nine sections for PM2.5 and PM10 was highly inaccurate. We subsequently adopted the modal approach of Whitby et al. (1991), based on findings of Whitby (1978), in which the size distribution of sub-micron particles are represented by a nuclei or Aiken mode and an accumulation mode. This paradigm provided the basis for practical computations, and lead to the development of the EPA's Regional Particulate Model (RPM) prototype (Binkowski and Shankar, 1995). The following sections describe the initial prototype, followed by a discussion of the Models-3/CMAQ version.

EPA's Regional Particulate Model (RPM): RPM is based upon the EPA's Regional Acid Deposition Model (RADM), an Eulerian Framework model. In the RADM (described in Chang et al., 1987 and 1990), input data from meteorology and emissions processors is used to drive the Chemical-Transport Model (CTM). The meteorological fields are computed using the Penn State/NCAR Mesoscale Meteorological model, Version 4, with Four-Dimensional Data-Assimilation incorporated to constrain its computational errors (MM4-FDDA). The Flexible Regional Emissions Data System (FREDS) prepares gridded emissions fields from anthropogenic sources (area, point and mobile sources) as well as those from biogenic sources. These data are processed by the CTM which generates gridded concentrations of secondary pollutant species, including sulfates and nitrates and of surface deposition. The RPM utilizes RADM outputs and produces bimodally distributed particulates. The size distribution is the superposition of two interacting lognormal sub-distributions. The current version of RPM has been formulated to predict gridded fields of sulfate, nitrate and organic aerosols species. The chemistry is handled as follows: Hydroxyl radicals oxidize SO_2 in the presence of water vapor to produce sulfuric acid, which then either condenses onto existing particles or forms new particles. New particles are formed as proposed by Kerminen and Wexler (1994) when a critical concentration of sulfuric acid is exceeded. The acidity and composition of the sulfate aerosols depend upon ambient levels of ammonia. Modeled particles are internally mixed uniformly, and can grow or shrink with respect to its water content when the relative humidity exceeds the aerosol's deliquescence point. The water-aerosol mix is assumed to be proportional to the sulfur content for acidic particles, is unaffected by the presence of organics, and responds to a nitrate content only if the system is neutralized sufficiently by ammonium. The aerosol swelling or shrinking affects their size distribution. Secondary aerosol nitrates are produced as a reaction between nitric acid and gas phase ammonia that remains after neutralizing H_2SO_4 (Saxena et al., 1986). Secondary Organic Aerosols (SOA) are produced in the atmosphere from gas-phase precursors by yields for oxidation of various reactive organic gases (ROG) by hydroxyl radicals to the lumped gas-phase species of the RADM-2 mechanism (Stockwell et al., 1990), i.e.,

$$\text{Production rate} = [OH]^* \text{ sum } \{C_n k_n \, [ROG]_n\}$$

where C_n and k_n are empirical constants and reactivities specific to n classes. Currently, RPM model five (n=5) ROGs, HC-8 (alkanes), OLI (internal alkenes, including monoterpenes), and three aromatics (TOL (toluene and less reactive aromatics), CSL (cresol and other hydroxy substituted aromatics) and XYL (xylene and more reactive aromatics)). In RPM, the rate of production of SOA was computed from the hydroxyl-ROG reactions using archived values of hydroxyl radicals and organic precursors from RADM simulations. This procedure causes no feedback to photochemical oxidant formation in the RADM simulations. RPM incorporates all important contributing atmospheric processes that affect the transport and changes in the aerosol composition, distribution and concentration. For example, cloud processes in RPM shifts the sulfate produced in cloud water to the larger (accumulation) mode upon evaporation of the cloud water. Also, it is assumed that the larger (accumulation) mode contains the cloud condensation nuclei; however, the smaller mode containing the Aitken nuclei is not activated in clouds, but is scavenged by cloud droplets. Aerosols are dry deposited according to a size distributed deposition velocity parameterization. Preliminary results have been presented in Ching et al. (1995) and Binkowski and Ching (1996).

Models-3/CMAQ Version for PM2.5: The CMAQ modeling version for PM2.5 is much more complete and efficient than the RPM version. In the current implementation, the various contributing processes to PM2.5 are coupled and integrated directly into the chemistry-transport model, in contrast to the RPM prototype. This version has the same secondary components as RPM (sulfate, nitrate, ammonium, and organics) along with primary emissions. The fully interactive approach of Pandis et al. (1992), in which the gas-phase chemistry operates interactively with the aerosol production, ie., the aerosol yields will be accounted for as additional gas-phase sinks, thus depleting the ROG concentrations in proportion to SOA production. Models-3/CMAQ model will handle anthropogenic and biogenic organic contributions to particles separately. The emission of fine primary particles and coarse primary particles are handled as follows. PM2.5 is apportioned to the two lognormal modes which were used in RPM. A coarse mode distribution will be added to model PM10. In addition to anthropogenic PM10 emissions, emissions of wind-blown dust and marine aerosols can be incorporated. The numerical solvers have already been improved for accuracy and robustness. The code structure to be implemented follows that of the photochemical module and thus, can be used in an Eulerian model, a Lagrangian model, or as a stand-alone box model. Unlike the original RPM, the Models-3/CMAQ will interact with the photochemistry at the synchronization time step which is set by a Courant condition determined by the horizontal wind speed and the grid cell size. This means that the Models-3/CMAQ is run using only meteorological and emissions information as input in contrast to RPM which requires a prior simulation using RADM to provide hourly values of photochemical outputs. This advance also provides a way of testing heterogeneous interactions between the gas and particle phases. This is a necessary feature for the study of reactive semivolatile species or for the quenching of radicals. Within the Models-3/CMAQ framework, model outputs of PM2.5 mass, chemical composition, and number and size distribution will be predicted for up to three nested domains with grid size resolution of 36-, 12- and 4-km.

IV. DISCUSSION

One of the major uses of PM models described here will be to investigate and provide regional particulate distributions for conducting assessments of current and future emissions projection scenarios in support of the NAAQS standard for PM10 and a potential one for fine particulate matter, PM2.5. A major limitation for implementation of CMAQ in regulatory applications is the modeling of seasonal and annual average concentration fields from CMAQ episodes consisting of up to five days of simulation time. To circumvent this problem, results from an aggregation method, initially developed for acid-deposition applications (Brook et al., 1995a,b) have been applied to a limited number (thirty) of RADM 5-day simulations in order to provide estimates of long-term (annual) ambient air concentrations of fine particulate matter. The aggregation method is based on the premise that at any given location, ambient air concentrations of fine particulate matter are governed by a finite number of different, though recurring meteorological regimes. The aggregation procedure estimates mean annual concentrations using a predetermined set of model simulations selected from the meteorological strata. Calculation of the mean annual concentrations makes use of weighting/scaling factors that are based on the frequency of occurrence and the expected concentration for each of the strata associated with the events selected for aggregation. Efforts will be needed to investigate the adequacy of the current capability developed for the acid deposition studies for the PM requirements. This is an issue of critical importance.

Several important applications and extensions to Models-3/CMAQ-PM2.5 are discussed below: With the composition, size distribution, and concentration levels known, optical parameters can be computed. A measure of visibility is the deciview ($= 10 \ln[B_{ext}/0.01]$) as discussed by Pitchford, and Malm (1994). Preliminary modeling results of spatial distribution of visibility in deciview units with values of zero (extremely good visibility) to 40 (very poor visibility) indicated, agrees with the typical range of median summer visibility in the eastern U.S. namely, 20-32 deciview units (Pitchford and Malm, 1994).

Another application of CMAQ is the extension to the modeling of SVOCs. The portion of the total atmospheric concentration of SVOCs that exist in gas and particulate forms are defined in terms of gas/particle (G/P) partition functions (Junge 1977, Pankow 1987). These G/P partition functions are typically functions of air temperature and the overall aerosol loading of the air. The results of ambient monitoring investigations have previously suggested that the surface area concentration of the total aerosol loading is a primary determining factor for the G/P partitioning of most SVOC compounds.

Consideration must also be given to the possibility that particle absorption may be more important than particle adsorption in drawing SVOCs into the aerosol form and that the volume concentration of total aerosol loading may be a more accurate indicator of G/P partitioning, at least for some SVOCs. Studies to incorporate both the adsorptive and absorptive theories in modeling the G/P partition functions will need to be conducted. CMAQ model simulations will provide the particle mass loading and particle size distribution information required to estimate G/P partitioning of SVOCs. A demonstration analysis was performed (Ching et al., 1996) for relatively high volatility organochlorines and relatively low volatility persistent aromatic hydrocarbon pollutants. They show that using gas to particle partition functions based on formulations of Pankow (1987) in conjunction with predicted aerosol surface area indicate that PM modeling approach can handle the full range of volatility of various pollutants.

Finally, model evaluation is an essential component of science-based PM models. Initial efforts will compare model results against available field observations from special field studies including the Eulerian Model Evaluation Field Study (EMEFS), (which provided a basis for evaluating RADM) and the more recent Southern Oxidant Study (SOS) in the Nashville area. The SOS, while primarily an oxidant research study, contained some limited data on PM that will be useful for the initial evaluation. In both studies, special intensive sampling periods using aircraft platforms collected Active Scattering Aerosol Spectrometer Probe (ASASP) and Forward Scattering Spectrometer Probe (FSSP) data and filter data for mass and composition information. The EMEFS Intensive study was performed during August-September 1988 and May 1990 in the eastern U.S. and the SOS, July 1995. The EMEFS flights were generally designed to characterize regional distributions while the SOS-Nashville study focus was on urban scale characterizations. The analyses of the data will be conducted using Pointer-Flyer methods on model results to facilitate the comparison with observed fields from aircraft sampling. Additionally, it is intended to utilize measurements from other sampling programs, including special aerosol measurements including TEOMs and special research grade aerosol samplers at EPA sites currently being set up in Baltimore and Phoenix. These ground-based samples provide a means to check the model predictions for longer term ground level exposures on time scales extending from hourly to daily samples, which when aggregated, provide longer term samples. Other candidate databases include the Interagency Monitoring of PROtected Visual Environments (IMPROVE) database, the database from the Measurement of Haze and Visual Effects (MOHAVE) study, and the Southeastern Aerosol and Visibility Study. Evaluation studies are intended to provide the basis for continued refinements of the PM modeling; such studies are part of an overall evaluation, the first phase is targeted to support the recommendation for the initial Models-3/CMAQ prototype which is scheduled for public release in mid-1998.

DISCLAIMER

This paper has been reviewed in accordance with the U.S. Environmental Protection Agency's peer and administrative review policies and is approved for presentation and publication. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

REFERENCES

1. Binkowski, F.S.; Shankar, U. The Regional Particulate Model: Part I. Model Description and Preliminary Results. J. Geophys. Res., 1995 100(D12),1995 26,191-26,209.
2. Binkowski, F.S., Ching, J.K.S. "Regional scale distribution of fine particulate mass and visibility from the EPA Regional Particulate Model," *Preprint Volume of the Ninth Joint AMS-A&WMA Conference on Applications of Air Pollution Meteorology*, Atlanta, January 28-February 2, 1996, Air & Waste Management Association: Pittsburgh, 1996, pp.565-569.
3. Brook, J.R.; Samson, P.J.; Sillman, S. Aggregation of selected three-day periods to estimate annual and seasonal wet deposition totals for sulfate, nitrate and acidity. Part I: A synoptic and chemical climatology for Eastern North America, J. Appl. Meteor. 1995a 34, 297-325.

4. Brook, J.R.; Samson, P.J.; Sillman, S. Aggregation of selected three-day periods to estimate annual and seasonal wet deposition totals for sulfate, nitrate and acidity. Part II: Selection of events, deposition totals and source-receptor relationships, J. Appl. Meteor. 1995b 34, 326-339.
5. Byun, D.W., Hanna, A., Coats, C., Hwang, D., "Models-3 Air Quality Model Prototype Science and Computational Concept Development," *Transaction of A&WMA Specialty Conference on Regional Photochemical Measurements and Modeling Studies*. Nov 8-12, 1993, San Diego, CA, 1995; pp 197-212.
6. Byun, D.W.,Ching, J.K.S., Novak, J., Young, J. "Development and Implementation of the EPA's Models-3 Initial Operating Version: Community Multiscale Air Quality (CMAQ) Model", *Conference Proceedings, Air Pollution Modelling and its Applications XII*, Ed S.E. Gryning and N. Chaumerliac. Plenum Publishing Corp, 1997.
7. Chang, J.S.;Brost, R.A.; Isaksen, I.S.A.; et al., A three-dimensional Eulerian acid deposition model: physical concepts and formulation, J. Geophys. Res. 1987 92, 14,681-14,700.
8. Chang, J.S., Binkowski, F.S., Seaman, N.L., Byun, D., et al.,The Regional Acid Deposition Model and Engineering Model, NAPAP SOS/T Report 4. In National Acid Precipitation Assessment Program, Acidic Deposition: State of Science and Technology, Volume 1, Washington, D.C., 1990.
9. Ching, J. K. S.; Binkowski, F.S.; Bullock, Jr.,O. R. Deposition of semi-volatile air toxic pollutants to the Great Lakes: A regional modeling approach. Environ. Toxicol. Chem.1996 (in press).
10. Ching, J.K.S., Binkowski, F.S., Pleim, J.E. "Preliminary results: Modeling fine particulate mass for the eastern United States using the EPA Regional Particulate Model," *Preprint, 21st NATO/CCMS International Meeting on Air Pollution Modeling and Its Application*, November 6-10, 1995, Baltimore, MD, 1995; pp 135-144.
11. Dennis, R.L.; Byun, D.; Novak, J.H., et al., The next generation of integrated air quality modeling: EPA's Models-3, Atmos. Environ. 1996 30, No. 12, 1925-1938.
12. Eder, B.K., and LeDuc, S.K.,"Can selected RADM simulations be aggregated to estimate annual concentrations of fine particulate matter?" Reprints of the *11th Annual International Symposium on the Measurement of Toxics and Related Air Pollutants*, Research Triangle Park, NC, 1996 732-739.
13. Hanna, A.F., Binkowski, F.S., and Shankar, U. "Analyses of regional visibility in the United States using Aerosol Models," *Proceedings of the A&WMA conference on Regional Photochemical Measurement and Modeling Studies*, November 8-12, 1993, La Jolla, CA, 1993 p742-757.
14. Kerminin, V.-M., and Wexler, A.S. Post-fog nucleation of H_2SO_4-H_2O particles in smog. Atmos. Environ., 1994 (28) 2399-2406.
15. Junge, C. E. Basic considerations about trace constituents in the atmosphere as related to the fate of global pollutants. In Fate of Pollutants in the Air and Water Environments (edited by I. H. Suffet), Part I, 1977 pp. 7-26. J. Wiley, New York.
16. Pandis, S.N.; Harley, R.A.; Cass, G.R.; Seinfeld, J.H. Secondary organic aerosol formation and transport, Atmos. Environ.1992 (26a) 2269-2282.
17. Pankow, J. F. Review and comparative analysis of the theories on partitioning between the gas and aerosol particulate phases in the atmosphere. Atmos. Env.,1987 21, 2275-2283.
18. Pitchford, M.L.; Malm, W.C. Development and applications of a standard visual index. Atmos. Environ.1994 (28) 1049-1054.
19. Saxena, P.; Hudischewskyj, A.B.; Seigneur, C.; and Seinfeld, J. H. A comparative study of equilibrium approaches to the chemical characterization of secondary aerosols, Atmos. Environ. 1986 (20) 1471-1483.
20. Stockwell, W.R.;Middleton, P.; Chang, J.S. The second generation regional acid deposition

model chemical mechanism for regional air quality modeling. J. Geophys. Res., 1990 95, 16,343-16,367.

21. U.S. Environmental Protection Agency; Air quality criteria for particulate matter. Washington, DC: Office of Research and Development. EPA/600/P-95/001aF-001cF; April 1996a.

22. U.S. Environmental Protection Agency; Strategic Plan for the Office of Research and Development. Washington, DC: Office of Research and Development. EPA/600/R-96/059; May 1996b.

23. Whitby, E.R., P.H. McMurry, U. Shankar, and F.S. Binkowski; Modal Aerosol Dynamics Modeling, EPA/A600/3-91/020, U.S. EPA, Research Triangle Park, NC 1991.

24. Whitby, K.T. The physical characteristics of sulfur aserosols, Atmos.Environ., 1978 (12)135-159.

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15. SUPPLEMENTARY NOTES

16. ABSTRACT

Recent evidence indicates that fine particles, those 2.5 μm and smaller adversely impacts human health causing increased mortality and morbidity; further, it diminishes ambient air quality with decreased visibility. Typically, particles in this size range arise as either by-products of atmospheric reactions of sulfur, nitrogen, and organic pollutants or as primary pollutants emitted naturally or from anthropogenic sources. In this presentation, we describe the U.S. Environmental Protection Agency's new modeling system, Models-3, and its first version for air quality called the Community Multiscale Air Quality (CMAQ) model. Models-3/CMAQ is a new generation, state-of-science, comprehensive air quality modeling system. With a "one atmosphere" paradigm, it is designed to be capable of addressing holistically and inclusively, the major air quality issues such as photochemical smog, particulate matter, airborne toxics, and Air Quality Related Values (AQRVs) including acidic, nutrient and toxic deposition, as well as visibility. For particulate matter (PM), number and size distributed sulfate, nitrate, organic and aerosol-bound water are predicted on three dimensional grid cells for domains encompassing regional and urban scales. Models-3/CMAQ is scheduled to be publicly released in 1998, and will be a community-based tool for predicting PM concentration fields from current emission distributions as well as for analyzing and assessing the viability of optional control strategies to achieve compliance with National Ambient Air Quality Standards (NAAQS). The PM components in this system are derived to a large extent from the prototype Regional Particulate Model (RPM) (Binkowski and Shankar, 1995). The fundamental features of the aerosol formulations include a bimodal size distribution of particles in the sub-micron range, and aerosols that are internally well mixed. Size dependent dry deposition parameterization, aqueous phase aerosol dynamics, and nucleations are included among the various major atmospheric processes modeled. Considerations for extensions and applications of Models-3/CMAQ are discussed.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/ OPEN ENDED TERMS	c. COSATI

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