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AIR QUALITY MODELING OF PM2.5 SPECIES

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1. INTRODUCTION

The United States Environmental Protection Agency (EPA) recently passed the regional haze rule which seeks to improve visibility in all Class I designated areas. Additional regulations including the 8-hour ozone and PM2.5 National Ambient Air Quality Standards (NAAQS) are planned for implementation in the near future. Existing scientific evidence shows that regional haze, fine particles, and ozone have common precursor pollutants, emission sources, atmospheric processes, spatial scales of transport, and geographic areas of concern. It is, therefore, desirable to integrate visibility control strategies with those for fine particles and ozone.

In the past, three-dimensional atmospheric chemistry and transport models, or photochemical models, were applied to assist in the development of regional pollution control plans. Given the needs to develop strategies to improve visibility and further reduce regional ozone, a one-atmosphere photochemical model should be applied that will accurately predict both and take their chemically coupled nature into consideration (Meng et al, 1997).

This document outlines the efforts by Lake Michigan Air Directors Consortium to apply multiple one-atmosphere photochemical models to the Eastern United States and compare the model results against each other and to observed values from a variety of monitoring networks. The same domain and domain projection scheme will be used for all models to facilitate comparison between models. All models will be driven by the exact same set of meteorological and emissions data. The emissions will be as similar as possible given the different PM speciation schemes utilized by each photochemical model.

1.1 Goals and Objectives

The goal of this study is to apply photochemical models as consistently as possible to support the selection of a best modeling approach for the development of future State Implementation Plans. The objectives necessary to achieve this goal are outlined below:

1) Compare relative differences in estimates by each of the photochemical models
2) Compare photochemical model estimates to observed estimates
3) Determine relative costs for running each model in terms of file storage size, execution speed, and staff time required for implementation

2. METHODOLOGY

Several one-atmosphere photochemical models, including the Community Multiscale Air Quality modeling system (CMAQ) and the Regulatory Modeling System for Aerosols and Deposition (REMSAD), were applied using a common set of raw meteorological and emissions data to a summer and winter episode. The Particulate Matter Comprehensive Air Quality Model with Extensions (PMCAMx) and the Comprehensive Air Quality Model with Extensions (CAMx) version 3.1 with aerosol chemistry mechanism 4 will be applied in the near future as an extension of this project.

Episodes that coincide with increased PM2.5 speciation measurements in the Upper Midwest were selected for this study. Daily measurements of PM2.5 species were taken as part of the March Midwest study from August 3, 1999 to September 11, 1999 and again from January 10, 2000 to February 18, 2000.

Each photochemical model will be applied to the exact same grid domain and Lambert projection centered at (-97,40) with true latitudes at 33 and 45. The domain consists of 87 cells in the X direction and 95 cells in the Y direction covering the Eastern United States with 36 km size grid cells. The vertical atmosphere up to 100 millibars is resolved with 16 layers, most of which are in the boundary layer.

2.1 Meteorological Inputs

Meteorological input data for the photochemical modeling runs were processed using NCAR's 5th generation Mesoscale Model (MM5) version 3.5 (Dudhia, 1993). Each episode was initialized with ETA model output data as a first guess analyses

field. The terrain input file was interpolated from the 24 category United States Geological Survey (USGS) 10 minute (~19 km) data for the 36 km domain.

Other important MM5 parameterizations and physics options applied to each episode include the simple ice microphysics, Kain-Fritsch cumulus scheme, Rapid Radiative Transfer Model, Pleim-Chang planetary boundary layer, and the Pleim-Xu land surface module (Grell et al, 1994).

2.2 Emissions Inputs

Emissions data will be processed using EMS-2001. The EMS-2001 model is selected for its ability to efficiently process the large requirements of regional and seasonal or daily emissions processing. In addition to extensive quality assurance and control capabilities, EMS-2001 also performs basic emissions processes such as chemical speciation, spatial allocation, temporal allocation, and control of area, point, and motor vehicle emissions (Janssen, 1998).

Outputs from EMS-2001 include a coordinate-based elevated point source file and gridded emissions estimates for low-point, area, motor vehicle, and biogenics sources. The anthropogenic emissions were based on the 1999 National Emission Inventory.

The biogenic emissions were estimated with EMS-2001 using BIOME3/BEIS3 and the BELD3 landuse dataset. Other inputs to the biogenic emissions model include photosynthetically activated radiation (PAR) and 15 m temperature data output from MM5. The 15 m temperature data was selected for its spatial representation of the tree canopy layer. MM5 output was used to approximate PAR from short-wave downward radiation by application of a conversion factor to estimate the visible light fraction of the spectrum (Baker, 2001).

2.3 Landuse Inputs

Each photochemical model applied for this exercise uses the same 11 landuse categories to describe the surface. The landuse data is based on the USGS Global 30 second vegetation database. The 30 second data was aggregated to the appropriate grid resolution for photochemical modeling.

2.4 Photolysis Rate Inputs

A number of chemical reactions in the atmosphere are started by photodissociation of certain trace gases. Photochemical models require these photodissociation rates be input to accurately estimate these types of reactions. Each of the photochemical models applied for this study utilize a slightly different approach to photolysis rate estimation. CMAQ was applied with day specific photolysis rate look-up tables. REMSAD can only be applied with a single look-up table that represents an entire calendar year.

CMAQ utilizes a pre-processor, JPROC, to provide photolysis rates as a function of altitude, latitude, and time. Photolysis rates are estimated by JRPOC for six latitudes (10 to 60 degrees North), seven altitudes (0 km, 1 km, 2 km, 3 km, 4 km, 5 km, and 10 km) and ∀8 hours of deviation from local noon (US EPA, 1999). These rates are calculated for each day of the episode and take ozone column attenuation into account with observations from the TOMS satellite program.

REMSAD is currently released with photolysis rates based on height and solar zenith angle under constant albedo, ozone column, and haze. There are 15 heights represented in the table ranging from 0 to 14,000 meters above sea level and 10 zenith angles ranging from 0 to 86 degrees. The constant for albedo is 0.08. This albedo value represents a very reflective surface condition, usually associated with urban and barren areas.

The haze constant is 0.2 and the ozone column constant is 0.318 (SAI, 2002). Ozone column values typically range from .285 to .360, so the constant used in REMSAD appears to approximate an average value. The REMSAD photolysis rate table is used for the entire year and does not incorporate daily ozone column data for rate attenuation.

2.5 Initial and Boundary Concentrations

Boundary conditions represent pollution inflow into the model and initial conditions provide an estimation of pollution that already exists. The initial conditions are usually considered to be background concentrations of pollutants. Both initial and boundary conditions may vary in time and in vertical space. The impact of initial concentrations within the boundary layer is small over month-long episodes, but a larger impact

may occur in the upper troposphere (Tonneson et al, 2001).

The initial and boundary conditions used in each model will be consistent in the horizontal and vertical direction and based on profiles released by EPA with the June 2002 release of the CMAQ model. Where an initial or boundary concentration is not specified for a pollutant the model will default to a near-zero concentration.

2.6 Model Configuration

Each of the photochemical models will be initiated at midnight Eastern Standard time and run hourly for 24 hours. Table 1 outlines the more important parameterization and module selection for each model (SAI, 2002; US EPA 1999).

Model	**CMAQ**	**REMSAD**
Version	June 2002	7.03
Gas-Phase Chemistry	cb4_ae2_aq	Micro-CB4
SOA estimation	Yields	
Plume in grid (NOx)	No	No
Horizontal transport	PPM	Smolar-kiewicz
Vertical transport	Bott	Bott
Particle Size	Modal	Fine & coarse
Chemistry solver	Hertel/ MEBI	Hybrid Fast
Aqueous Phase Chemistry	Explicit 1-section	Empirical
Wet & Dry Deposition	Yes	Yes

Table 1 Applied Parameters and Modules

3.0 RESULTS

Model results from CMAQ and REMSAD were compared to measured concentrations for a period in January 2000 (10^{th} to 20^{th}) and August 1999 (8^{th} to 28^{th}). Each modeling period was allowed to spin up for 9 and 7 days respectively to reduce the influence of initial concentrations.

Model estimates are compared to 16 Improve sites, 8 CASTnet sites, and 3 sites from the March Midwest study for the January episode. August modeling results were compared to 17 IMPROVE stations, 8 CASTnet stations, and 6 March Midwest monitors. CASTnet and IMPROVE monitors sample every 3 days and March Midwest stations collect daily measurements. All monitors collected 24 hr average samples. Most monitors are located in rural areas. The March Midwest study includes 2 urban sites in the winter episode and 5 urban sites in the summer episode.

All applied models show similar trends compared to monitored PM2.5 specie measurements. Nitrate and “other fine mass” are over-predicted while elemental carbon and organic carbon are under-predicted. Even species that are not grossly over or under predicted, such as sulfate, show little correlation between measured and predicted concentrations.

The systematic biases seen between model prediction and monitor concentrations over the entire Eastern United States indicate multiple components of the emission inventory need further examination.

The magnitude of predicted and measured PM2.5 mass shows general agreement. The composition of the predicted and measured fine mass is quite different, as illustrated at the Athens, OH and Cincinnati, OH locations (Figures 1 and 2). This clearly shows that the modeled PM2.5 species do not show agreement with measured values and how misleading model performance statistics of total PM2.5 mass can be. This also illustrates how difficult it would be to formulate an effective control strategy since reductions in anthropogenic emissions would have little impact on PM2.5 mass dominated by “other” PM2.5.

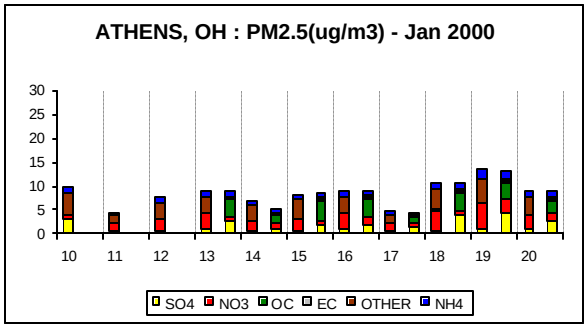

Fig. 1 Predicted (left) and observed (right) pairs of PM2.5 species with REMSAD

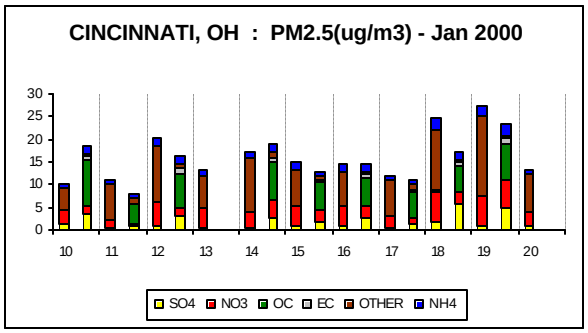

Fig. 2 Predicted (left) and observed (right) pairs of PM2.5 species with REMSAD

4.0 DISCUSSION

The relative cost of running each of these photochemical models in a full production mode should be considered in addition to model performance. Ultimately, annual modeling runs will need to be applied to a near-continental scale grid for regional haze. The cost associated with this type of modeling application is much higher using CMAQ as opposed to REMSAD. CMAQ takes approximately twice as long to simulate an episode day and requires a significantly greater amount of disk drive storage space for model inputs and outputs. For example, to model an entire year with CMAQ the base-case emissions inputs alone add up to a quarter of a terabyte for a continental United States scale grid (147x111x16 grid cells).

Staff resources required for CMAQ application are also higher than REMSAD. The number of meteorological input variables required by CMAQ is significant and demand more staff attention to adequately quality assure.

The systematic biases shown by multiple photochemical models for the PM2.5 species demonstrate that much more work needs to be done before a final decision can be made about the selection of a particular model or modeling approach for regulatory applications.

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