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## 1. INTRODUCTION

Coupled models of atmospheric chemistry, aerosol dynamics, and atmospheric dynamics are needed to fully evaluate measurements of aerosols and their precursors during intensive field campaigns. We recently modified gas-phase photochemistry models in zero and one dimensions (0-D and 1-D, respectively) to include modules describing the formation and removal of aerosols from the atmosphere. The aerosol module is based on the one used in the Community Multiscale Air Quality (CMAQ) regional-scale chemical-transport model.

## 2. THE CMAQ MODEL

The CMAQ aerosol module was coupled to the 0-D box model during the past year. The aerosol code represents aerosol size distributions as three different size modes (Aitken, accumulation, and coarse), with a log-normal function describing the size distribution in each mode. The SORGAM code represents the formation of semivolatile organic compounds and their gas-particle partitioning (Schell et al. 2001). A total of 28 different components are modeled in the three size modes. The model resolves the chemical compositions of aerosols derived from sulfur, nitrogen oxides, ten different hydrocarbons, sea salt, and dust. Explicit chemical composition of sea salt and soil dust are not presently available. These features will be added in collaboration with the University of North Carolina. The group there developed the aerosol module currently used in CMAQ and adopted for our box and 1-D models. The aerosol model included in the 0-D model calculates nucleation, condensation, evaporation, and coagulation rates of the aerosols in a given air parcel with specified precursor gas concentrations and water vapor content.

Box models are typically used to analyze data collected from aircraft platforms in either the equilibrium mode or the steady-state mode. In the equilibrium mode the model solves the equation

$$P_i = L_i n_i \quad (1)$$

Here  $P_i$ , ( $\text{cm}^{-3} \text{s}^{-1}$ ),  $L_i$  ( $\text{s}^{-1}$ ) denote the photochemical production and loss frequency for species  $i$ , whose concentration ( $\text{cm}^{-3}$ ) is  $n_i$ . This approximation is valid for species with photochemical time constants of less than an hour (Kotamarthi et al. 1997).

The calculation of  $P_i$  and  $L_i$  uses fixed values of  $\text{O}_3$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{CH}_4$ ,  $\text{SO}_2$ , and  $\text{NO}$ . For the applications of interest here the main use of this model is to derive the available sulfate in the air parcel and predict the instantaneous rates of sulfate particle production. Thus, this model will be of great use in evaluating aircraft-collected data on sulfate particle production rates and precursor gases as measured and predicted by the model. The nucleation rates modeled in many of the current-generation aerosol models were compared by Zhang et al. (1999). The results show wide variation (up to a factor of 10) in particle production rates. The CMAQ aerosol model uses parametric representation of nucleation rates based on laboratory-derived nucleation rates (Harrington and Kreidenweis 1998) as a function of relative humidity and temperature.

As data become available from near-plume and clean-air measurements from the aircraft platform of the U.S. Department of Energy's Atmospheric Science Program, these parameterizations and their representation in the model will be revisited and modified as needed. Another application of the 0-D model will be to evaluate the modeled and measured yields of secondary organic aerosols used in the SORGAM code. As the yield factors in the model are based primarily on limited smog chamber studies (Odum et al. 1997), evaluating these rates with measured formation rates of secondary organics in the polluted planetary boundary layer (PBL) is of interest. We will present some preliminary results from the model.

## 3. PROCESS-SCALE 1-D MODELS

We developed a 1-D PBL model with a 2.5-level turbulence closure model based on the  $\kappa$ - $\epsilon$  theory. Rodi (1985) discussed the fundamentals of this type of PBL model. This approach has been used for modeling nocturnal boundary layers (Uno et al. 1989) and neutral and stable boundary layers (Duynderke 1988; Kotamarthi and Carmichael 1993). See these references for the equations describing the dynamic evolution of the PBL.

More recently, as discussed below, we coupled this PBL dynamics model to (1) a photochemical model with

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72 species, 132 thermal reactions, and 52 photolysis rates to calculate the evolution of aerosol precursors and (2) the CMAQ aerosol module to calculate the evolution of aerosols within the PBL. The model now includes higher-order closure terms for chemical trace gases to account for the effects of turbulent mixing on the evolution of the trace gases and aerosols (Wesely and Kotamarthi 2002; Kotamarthi and Wesely, 2002). The aerosol precursor gas-phase chemistry and the aerosol module are similar to those described for the 0-D box model. In addition, the 1-D model calculates dry deposition losses for some gases and aerosols that are

prescribed at fixed values at the model surface for the course of the simulation. Emissions at the surface can be prescribed for a number of precursor gases and aerosols. This model is now being tested for evaluating the aerosol module.

In the immediate future we plan to replace the parameterized radiation calculations (Pielke 1984) with the Rapid Radiative Transfer Model (RRTM) for shortwave and longwave regions. RRTM can account for aerosol effects on radiation in the shortwave spectrum. Results of calculations with the 1-D model are in Figures 1 and 2. Additional results from these two models and comparison with existing field data sets will be presented.

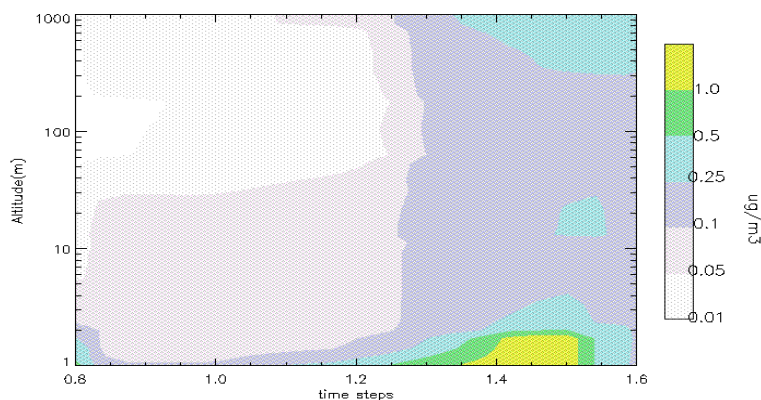


Figure 1: Distribution of organic aerosols generated from aromatic compounds in the 1-D model with the CMAQ aerosol module. The figure shows the evolution of aerosol profiles in the lower 1 km of the model, given a fixed boundary condition of precursor gases at the surface. The simulation started at 6 p.m. local time and ended 24 h later.

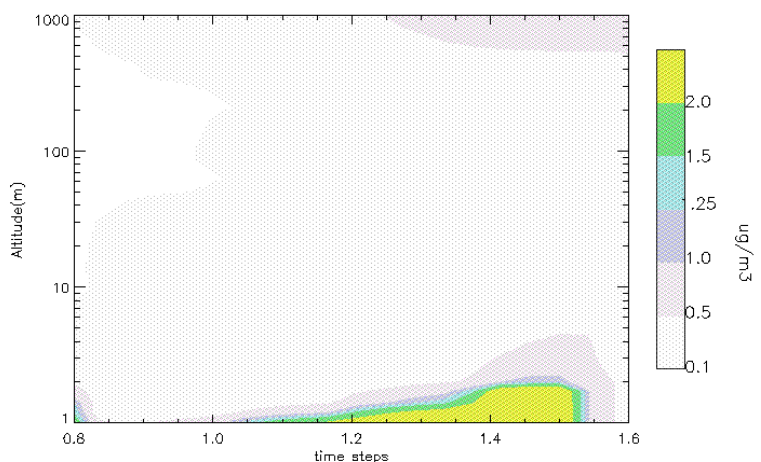


Figure 2: Distribution of organic aerosols generated from biogenic compounds in the 1-D model with the CMAQ aerosol module. The figure shows the evolution of aerosol profiles in the lower 1 km of the model, given a fixed boundary condition of precursor gases at the surface. The simulation started at 6 p.m. local time and ended 24 h later.

#### 4. ACKNOWLEDGEMENT

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