PARTICULATE MATTER MODELING IN CENTRAL AND NORTHERN CALIFORNIA

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1. INTRODUCTION

The southern part of the Central Valley of California, also known as the San Joaquin Valley (SJV), is one of the most polluted regions of the United States in terms of both particulate matter and ozone. In this region, these pollutants show distinct seasonal behavior with high ozone during the summer, high particulate matter with aerodynamic diameter less than 10 micrometers (PM_{10}) during the fall, and high particulate matter with aerodynamic diameter less than 2.5 micrometers ($PM_{2.5}$) during the winter (Chow et al., 1996; Chow et al., 1999). While the SJV is making significant progress towards attaining the National Ambient Air Quality Standards (NAAQS) for PM_{10}, attaining NAAQS for both $PM_{2.5}$ and ozone still remain a challenge.

To better understand the extent and formation mechanisms of particulate matter in central and northern California, a limited measurement campaign, known as the Integrated Monitoring Study of 1995 (IMS-95), was carried out in the SJV (Solomon and Magliano, 1999; Chow et al., 1999). Subsequent analysis (Kumar et al., 1998; Pun and Seigneur, 1999) and modeling (Held et al., 2004; Kleeman et al., 2005) of IMS-95 measurements revealed that the majority of $PM_{2.5}$ in the SJV during the winter is in the form of ammonium nitrate (NH_4NO_3) and that the formation of NH_4NO_3 is limited by nitric acid (HNO_3), not by ammonia (NH_3). It was also found that HNO_3 formation was limited by oxides of nitrogen (NO_x) rather than by volatile organic compounds (VOC) (Kleeman et al., 2005). Based on the experience gained during the IMS-95 study, a more comprehensive field monitoring study, known as the California Regional $PM_{10}/PM_{2.5}$ Air Quality Study (CRPAQS), was conducted from December 1999 to February 2000 (Magliano et al., 2001). This paper describes a collaboration among photochemical modelers at the California Air Resources Board (CARB) and the University of California at Davis now in progress to interpret the measurements made during CRPAQS. Some preliminary results of the photochemical modeling are also presented in this paper for the period of December 25, 2000 to January 07, 2001.

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2. METHODS

The modeling domain, shown in Figure 1, includes a part of the Pacific Ocean in the west, the Mojave Desert in the east, the northern Sacramento Valley in the North, and the Tehachapi Mountains in the south. The domain consists of 185x185 (4x4) km^2 grid cells; the number of vertical levels and the placement of the domain top differ based on the photochemical model used.

The CRPAQS meteorological network, consisting of a large number of surface and upper air sites, was used to generate meteorological fields for the modeling period using a diagnostic meteorological model (Goodin et al., 1979) as described by Held et al. (Held et al., 2004). Prognostic meteorological fields were also generated using the Fifth-Generation Penn State/NCAR Mesosclae Model (MM5) (Grell et al., 1994; Seaman et al., 1995) without observational nudging (Gürer, 2005).

Emissions inventories were prepared based on CARB emission estimates for both gaseous and particulate pollutants (Allen, 2005). A NO_x hot spot was observed in the emissions inventory for the Bakersfield area. This was also evident from

the comparison of modeled and observed NO_x concentrations where the modeled value was ~2 times larger than the observation. These excess NO_x emissions were found to suppress the modeled ozone (O_3) concentrations in that area compared to the observations. However, the modeled and observed values of carbon monoxide were in good agreement for this area. Thus, we used the observed CO/NO ratio to scale NO_x emissions relative to CO in that area. This resulted in a decrease of ~60% in NO_x emissions. The CMAQ results presented here are for this case. Investigations are already in progress to understand the causes of and remedies for this inventory NO_x hot spot in the Bakersfield area (Allen, 2005).

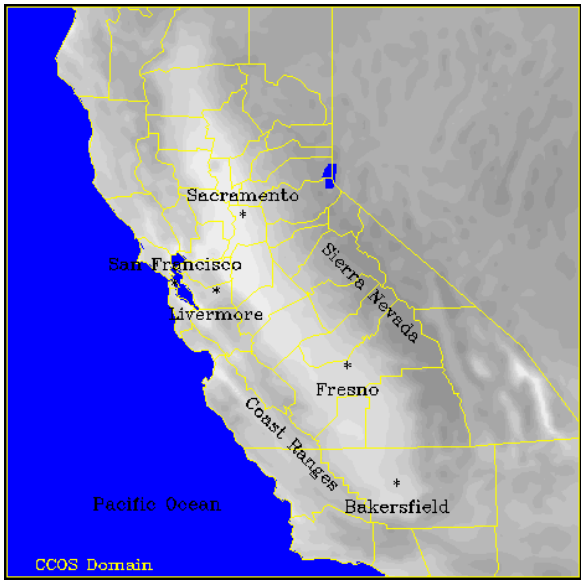

Figure 1. CMAQ horizontal domain for this study, same as the CCOS study.

The boundary and initial conditions for ozone were based on ozonesonde observations in northern California. Boundary and initial conditions for other species were set to be negligible, so that local emissions control the concentrations in the modeling domain.

Three different photochemical models are being used for modeling. The first is Version 4.4 of the Community Multiscale Air Quality (CMAQ) Modeling System (Byun and Ching, 1999) of the United States Environmental Protection Agency (US EPA) as distributed by the Community Modeling & Analysis System (CMAS) at the University of North Carolina, Chapel Hill, and modified for conditions in California by Liang and Kaduwela (2005). This model employs a modal approach to represent the size distribution of particulate matter.

The second model is the above version of CMAQ with a sectional representation of particle size distribution as described by Zhang and Wexler (2003). This version of CMAQ, known as CMAQ-UCD, contains a mechanistic, fully dynamic, internally-mixed, sectional aerosol module, which evolves from the Aerosol Inorganic Model and related work (Wexler and Seinfeld, 1990; Wexler et al., 1994; Potukuchi and Wexler, 1995ab; Sun and Wexler, 1998a,b; Wexler and Clegg, 2002). CMAQ-UCD employs three condensation/evaporation schemes: replacement, coupled, and uncoupled transport, as appropriate, avoiding substantial numerical stiffness due to rapid pH changes. It adopts a simplified aerosol thermodynamics scheme, able to predict particle phase states and water contents quickly and reasonably. The integration is accomplished using a computationally efficient asynchronous time-stepping (ATS) method, where particles in different sizes integrate with different time scales (Zhang and Wexler, 2005).

The third model is the UCD/CIT photochemical model. Details of this model have been published previously (Kleeman and Cass, 2001; Kleeman et al., 1997; Mysliwiec and Kleeman, 2002; Ying et al., submitted for publication). Unlike CMAQ, the UCD/CIT air quality model tracks particles emitted from different sources separately through the mathematical simulation of atmospheric processes. In addition to more accurately representing the heterogeneous nature of airborne particles, the source-oriented external mixture also predicts the contribution that each emissions category makes to airborne particulate matter concentrations at downwind receptor sites. This technique for the source apportionment of primary particulate matter shows excellent agreement with the Chemical Mass Balance source apportionment method (Held et al., 2005).

Modeling was conducted from December 17, 2000 to January 07, 2001. The first 8 days are considered to be spin up days and results are presented for December 25, 2000 through January 07, 2001

3. RESULTS AND DISCUSSION

We present results only for the US EPA Version 4.4 of CMAQ with modal representation and as modified by Liang and Kaduwela (2005). The meteorology input for this simulation was obtained using the MM5 meteorology model without observational nudging. The vertical extent of the domain was up to 100 mb with 15 layers with increasing thickness. The first layer had a thickness of ~30 m.

Figures 2-4 show the 24-hour $PM_{2.5}$ concentrations for the modeled period for Fresno, Angiola, and Bakersfield. Locations of both Fresno and Bakersfield, which are the major urban areas in the central and southern SJV, are shown in figure 1. Angiola is a rural area between Fresno and Bakersfield.

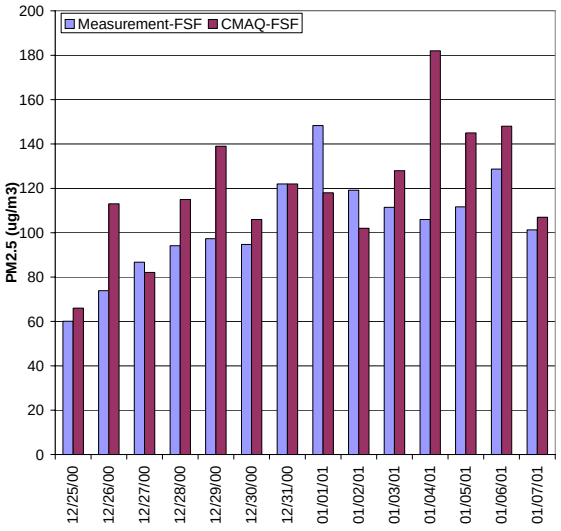

Figure 2: $PM_{2.5}$ concentration in Fresno.

As shown in figure 1, in Fresno the measured 24-hour $PM_{2.5}$ concentration varied between ~60 $\mu g/m^3$ and ~150 $\mu g/m^3$. For reference, the 24-hour $PM_{2.5}$ NAAQS is 65 $\mu g/m^3$. Measurements at Angiola (figure 2) were between ~25 $\mu g/m^3$ and ~125 $\mu g/m^3$, which were lower than the 24-hour $PM_{2.5}$ values at Fresno. Measurements at Bakersfield were comparable to those at Fresno. The modeled values are in good agreement with the measurements even though the model does not accurately reproduce trends in the measurements for each monitor. For example, at Bakersfield, the model over predicts the first half of the episode and under predicts the second half.

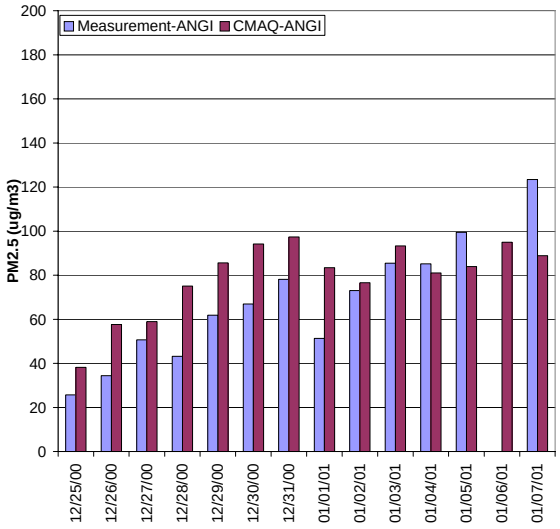

Figure 3: $PM_{2.5}$ concentration at Angiola.

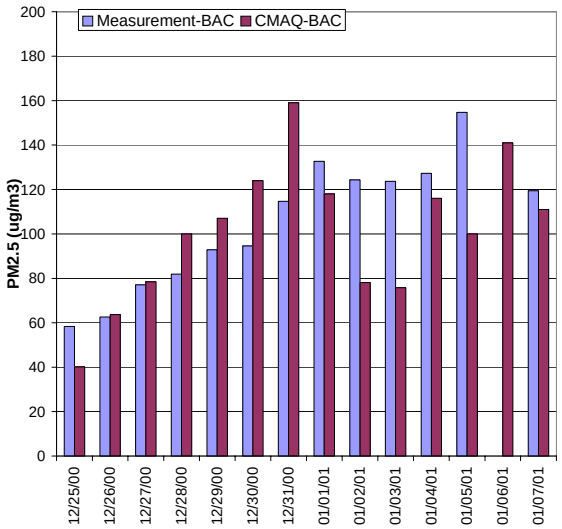

Figure 4: $PM_{2.5}$ concentration at Bakersfield.

However, the model is capable of simulating the relative trends observed at different monitors. For example, the measured $PM_{2.5}$ values remain low at Angiola until the end of the episode relative to those at Fresno and Bakersfield where they reach maxima in the middle of the episode. The model predicts this trend.

To understand the formation mechanisms and diurnal behavior of $PM_{2.5}$ in the SJV, we will continue this investigation. Future plans include comparison of model predictions and

measurements for short-term averaged PM and hourly averaged for gases. We will also investigate the models' ability to predict the observed vertical distributions of pollutants.

4. SUMMARY

We have simulated both gaseous and particulate matter measurements made during the CRPAQS using a modified Version 4.4 of the CMAQ Modeling System. We find satisfactory agreement between simulation and measurement for 24-hour averages of $PM_{2.5}$. Further comparisons of simulated and observed results are necessary to understand formation mechanisms and diurnal behavior of particulate matter in SJV.

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