LONG-TERM ONE-ATMOSPHERE CMAQ MODELING IN CENTRAL CALIFORNIA: MODEL PERFORMANCE EVALUATION AND PREDICTED TRENDS

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1. INTRODUCTION

As state regulatory bodies hasten to develop implementation plans to reach goals dictated by the US EPA Regional Haze Plan and $PM_{2.5}$ and ozone National Ambient Air Quality Standards (NAAQS), there is a clear need for extensive and rigorous chemical transport modeling to support and guide this work. In an effort to adequately address the effects of emissions controls on atmospheric particulate matter concentrations and ozone, there has been a move away from episodic modeling and towards longer term simulations that allow the consideration of important seasonal and regional differences in pollutant concentrations. While the environmental and temporal conditions that characterize high concentration "episodes" vary between species, pollutants such as ozone and PM are inextricably linked. Long-term modeling is required, therefore, in order to construct consistent control strategies where the control of one pollutant is not at the detriment of another. In central California the annual $PM_{2.5}$ NAAQS is considerably more restrictive than the 24-hour standard; so much so that meeting the 24-hour standard would not ensure the attainment of the annual standard, though the reverse may be true. This thus makes annual modeling an imperative for this region.

The California Regional PM_{10}/$PM_{2.5}$ Air Quality Study (CRPAQS) was a rigorous measurement campaign designed to study the important chemical and physical processes involved in the formation and evolution of particulate matter in Central California (Chow et al. 2006). The 14-month campaign extended from December 1999 through January 2001 and provided a wealth of data for model evaluation. In this presentation, CMAQ model results for a 14-month simulation are compared to speciated and total PM mass data collected during CRPAQS. Performance statistics and time-series plots indicate adequate model performance. Potential improvements that may lead to enhanced model performance are also outlined.

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2. MODEL APPLICATION

2.1 Modeling Domain and Setup

The geographically heterogeneous modeling domain used here covers Central California and part of the Pacific Ocean with 63 x 63 horizontal grid cells at 12-kilometer resolution (Figure 1). The vertical structure is composed of 15 layers of varying thickness and extends to approximately 15 kilometers above sea level. The finest resolution belongs to those layers close to the surface. These layers match the vertical structure of the preprocessed meteorological inputs.

In order to reduce the time required to run a continuous 14-month simulation over this domain of nearly 60000 cells, the December 1999-January 2001 simulation was split such that each month was simulated separately on a single processor. The monthly simulations were each run with an 8-day spin-up period.

2.2 Model Inputs

Meteorological inputs to CMAQ were preprocessed with MCIP using results from a non-FDDA mesoscale meteorological model (MM5) simulation (Grell et al. 1994). Gaseous and particulate emissions were prepared internally at the California Air Resources Board and represent winter weekday and weekend emissions typical of the region. The SAPRC99 chemical mechanism was employed to treat gas phase chemistry and AE4 and AQ aerosol and aqueous phase chemistry modules were activated to account for the physical and chemical transformations in the aqueous and aerosol phases. Initial and boundary conditions were based on wintertime surface observations and ozonesonde profiles (Newchurch et al. 2003).

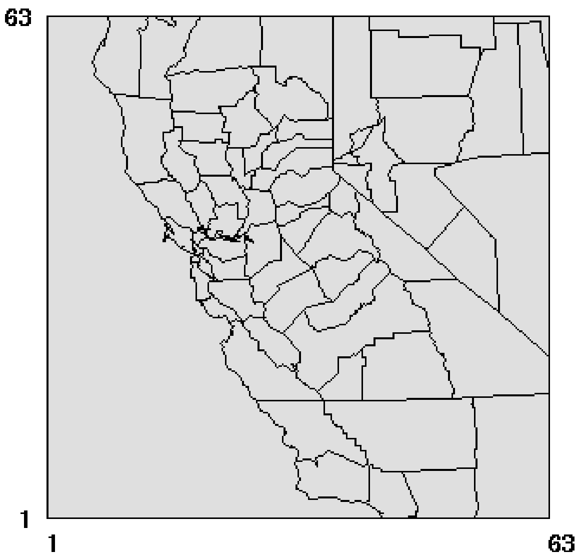

Fig 1. 63 x 63 cell modeling domain

2.3 Observations

The California Regional $PM_{10}/PM_{2.5}$ Air Quality Study led to a spatially and temporally extensive set of speciated and total particulate mass measurements in rural and urban environments throughout the San Joaquin Valley and its surroundings (Chow et al. 2006). Measurements included every-sixth-day 24-hour samples throughout the campaign and more frequent sampling during the winter intensive operating periods.

3. RESULTS

One gauge of model performance is to quantify and qualify the ability of the model to simulate observations. Here model results of total and speciated particulate mass concentrations from the 14-month CMAQ simulation are comparable to the general trends and average values of observed concentrations during the simulated period. Scatterplots for monthly averaged species concentrations for PM_{10} and $PM_{2.5}$ are shown in Figure 2 with mean fractional error (eq. 1) and mean fractional bias (eq. 2) given in the figure inset.

$$MFE = \frac{100}{N}\sum_{i=1}^{N}\frac{|M-O|}{(M+O)/2} \qquad (1)$$

$$MFB = \frac{100}{N}\sum_{i=1}^{N}\frac{(M-O)}{(M+O)/2} \qquad (2)$$

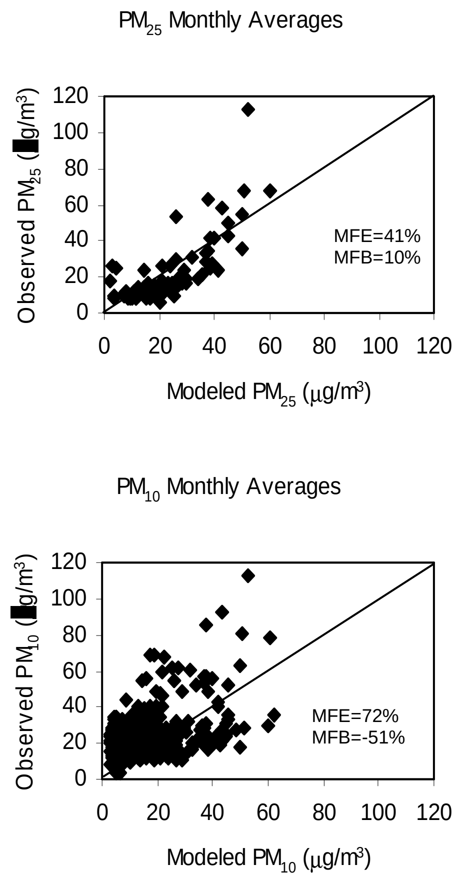

Fig. 1. Scatterplots of monthly average $PM_{2.5}$ (top) and PM_{10} (bottom) for all sites in the domain with sufficient measurements of PM_{10} and $PM_{2.5}$.

Boylan and Russell (2006) have proposed model evaluation metrics and goals for PM modeling where, generally-speaking, a model performance goal is said to have been met when the mean fractional error (MFE) ≤ 50% and the mean fractional bias (MFB) ≤ +/-30%. Similarly, model criteria is met when MFE ≤ 75% and the MFB ≤ +/-60%. If these same guidelines were applied here, PM_{10} concentrations would meet model performance criteria and the modeled $PM_{2.5}$ results would meet the model performance goal.

Time-series plots for individual species at the Fresno Supersite are given in Figures 3-6. These are meant to serve as an example of how the model tracks concentrations of the major components of PM. The model qualitatively and, to a slightly lesser extent, quantitatively tracks the behavior of individual species. The plots show that the elevated winter PM concentrations typical in Central California are reflected in both the observations and the model values. In general, the modeled and observed concentrations are similar with an exception late in the simulation (late December 2000 – early January 2001) when the model underpredicts most species. Part of this underprediction may be due to a mismatch between simulated and observed rainfall. The effects of mismatched simulated and observed rain events have yet to be examined. While only time-series plots for Fresno are shown, the model tended to track $PM_{2.5}$ and its components fairly well throughout the year in many locations.

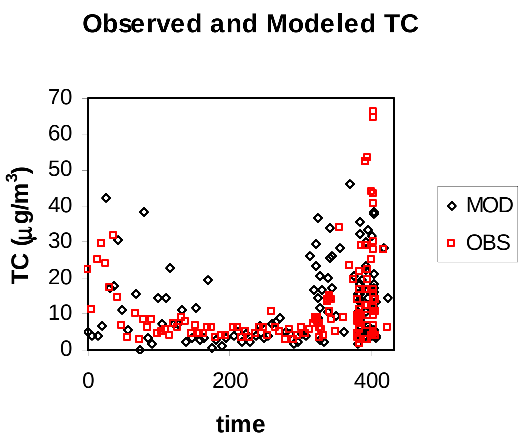

Fig. 3. Time-series of observed and predicted total carbon at Fresno over 14 months.

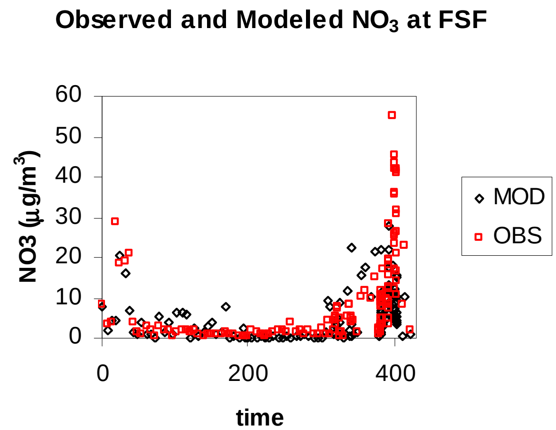

Fig. 4. Time-series of observed and predicted nitrate at Fresno over 14 months.

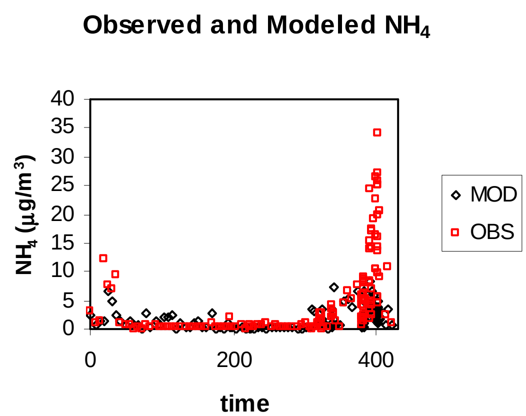

Fig. 5. Time-series of observed and predicted ammonium at Fresno over 14 months.

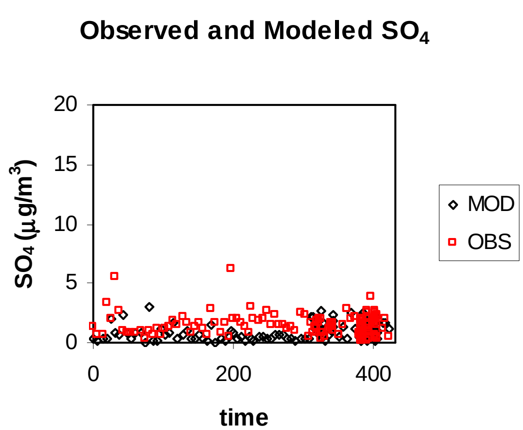

Fig. 6. Time-series of observed and predicted sulfate at Fresno over 14 months.

While the modeled concentrations were comparable with the observed trends and values, there were tendencies for the model to underpredict some species (sulfate and ammonium) and overpredict others (nitrate). Modeled organic carbon often matched observations fairly well. See Figure 7 for scatterplots of monthly averaged concentrations.

Potential reasons for lowered model performance include the relatively time-invariant emissions files (same weekday/weekend concentrations for all months) and time-invariant boundary conditions. A closer examination of the meteorology might also improve model performance (e.g., comparable observed and modeled rain events.)

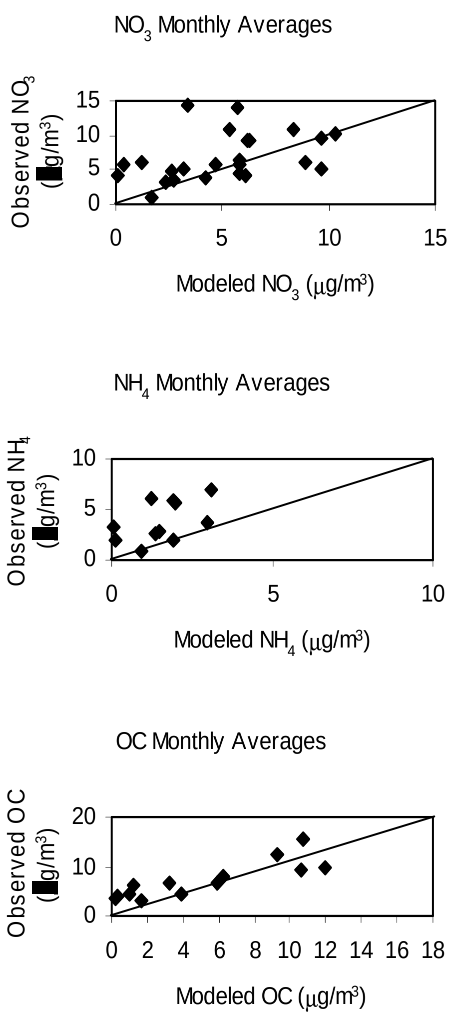

Fig.7. Scatterplots of monthly average concentrations of OC, NH_4, and NO_3

4. CONCLUSIONS

A 14-month CMAQ simulation spanning from December 1999 to January 2001 has been run for a 12-kilometer grid over central California, a region typically characterized by high PM concentrations and that includes areas designated as nonattainment for the national and state $PM_{2.5}$ and ozone standards. Comparisons with data collected during this time period give a first look at the model ability to guide the development of emission control strategies for diverse regions and seasons.

The model results are promising, in spite of the constant weekday/weekend emissions, as they adequately track the amount and temporal variation of observed PM_{10}, $PM_{2.5}$, and the individual component concentrations. Deviations from observed values will likely diminish if a greater degree of temporal variation is incorporated into the emissions and boundary conditions. In order to improve model performance, the next step will be to generate month-specific emissions and extract time-dependent boundary conditions from a global model.

5. REFERENCES

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