APPLICATION OF CMAQ-APT TO THE CENTRAL CALIFORNIA OZONE STUDY

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1. INTRODUCTION

Three-dimensional (3-D) models are frequently used to predict emission control impacts on concentrations of pollutants such as ozone and fine particulate matter ($PM_{2.5}$). Such models use a gridded representation of the atmosphere where atmospheric variables, such as chemical concentrations, are uniform within each grid cell. This approach averages emissions from elevated point sources within the volume of the grid cells in which they are released, and leads to significant errors for sources with spatial dimensions much smaller than that of the grid system. For example, stack plumes initially have dimensions of tens of meters, whereas the grid cell horizontal resolution is typically several kilometers in urban applications to about 100 km in regional applications. This artificial dilution of stack emissions leads to (1) unrealistic concentrations of emitted species near the stack, (2) incorrect chemical reaction rates due to the misrepresentation of the plume chemical concentrations and turbulent diffusion, and (3) incorrect representation of pollutant transport.

Over the past few years, EPRI has sponsored the development of a new state-of-the-science plume-in-grid (PiG) air quality model that can address the physical and chemical phenomena listed above explicitly, thereby providing a more realistic representation of the behavior of reactive plumes in the atmosphere. This PiG model consists of the reactive plume model, SCICHEM, imbedded into a three-dimensional grid-based model, the Community Multiscale Air Quality (CMAQ) modeling system. It is referred to as CMAQ with Advanced Plume Treatment (APT). An early version of CMAQ-APT was applied to explicitly simulate the plumes of two power plants for a five-day ozone episode in the Nashville/Tennessee valley area[1]. An improved version of the model was later used to explicitly simulate the plumes of the 30 largest NO_x point sources in the northeastern U.S. for a five-day episode[2]. This version of CMAQ-APT was based on the August 2000 release of CMAQ and SCICHEM Version 1302.

In this study, additional improvements and updates were made to CMAQ-APT. The updates were based on the latest release of CMAQ (Version 4.3, September 2003 release) and SCICHEM Version 1601. The model was applied in California for an episode during the Central California Ozone Study (CCOS) in July/August 2000. CCOS is one of the components of the Central California Air Quality Studies (CCAQS) program. It consists of a field program (conducted during the summer of 2000), data analysis, emission inventory development and modeling. CCOS was designed to characterize emissions, meteorology, and atmospheric processes affecting the production and fate of ozone in central California.

2. IMPROVEMENTS TO CMAQ-APT

CMAQ-APT consists of the host 3-D air quality model, CMAQ, and the embedded reactive plume model, the Second-order Closure Integrated puff model (SCIPUFF) with CHEMistry (SCICHEM). SCICHEM uses a second-order closure approach to solve the turbulent diffusion equations[3-5]. The plume is represented by a myriad of three-dimensional puffs that are advected and dispersed according to the local micrometeorological characteristics. Each puff has a Gaussian representation of the concentrations of emitted inert species. The overall plume, however, can have any spatial distribution of these concentrations, since it consists of a multitude of puffs that are independently affected by the transport and dispersion characteristics of the atmosphere. SCICHEM can simulate the effect of wind shear since individual puffs will evolve according to their respective locations in an inhomogeneous velocity field. The effects of buoyancy on plume rise and initial dispersion are simulated by solving the conservation equations for mass, heat, and momentum. The formulation of nonlinear chemical kinetics within the puff framework is described by Karamchandani et al. (2000)[6]. Chemical species concentrations in the puffs are treated as perturbations from the background concentrations. The chemical reactions within the puffs are simulated using a general framework that allows any chemical kinetic mechanism to be treated.

As part of the study described here, SCICHEM was modified to incorporate a state-of-the-science module for treating the effects of building downwash on plume rise and dispersion of stack emissions. The building downwash treatment is based on the Plume Rise Model Enhancements (PRIME) model[7]. PRIME incorporates the two fundamental features associated with building downwash: enhanced plume dispersion coefficients due to the turbulent wake, and reduced plume rise caused by a combination of the descending streamlines into the lee of the building and the increased entrainment in the wake. PRIME has been incorporated into the U.S. EPA regulatory model, ISC3. It has been tested against data from field studies and wind tunnels. The PRIME model was incorporated into SCICHEM by scientists at ARAP and the model was evaluated by AER scientists for the CCOS domain[8]. In SCICHEM-PRIME, the PRIME calculations are activated whenever building data are provided for a particular stack. PRIME is then used to describe the plume to a point beyond the building wakes and where the plume has achieved final rise. At this point, a SCICHEM source is then initialized with the appropriate size and emissions. SCICHEM-PRIME (Version 1601, January 2004 release), was embedded into the September 2003 version of CMAQ (Version 4.3).

3. MODEL APPLICATION TO THE CCOS DOMAIN

CMAQ and CMAQ-APT were applied for the July/August 2000 CCOS episode from 29 July to 2 August, 2000. A typical Great Basin high pressure system was observed during the course of this episode[9,10]. Prevailing winds were characterized by persistent inflow to the Central Valley from the central coast through the Carquinez Strait, passes and lower gaps in the coastal ranges. Peak inflow occurred in the afternoon and minimum inflow in the predawn hours.

Peak ozone values on July 30 occurred at Santa Clarita and in the San Joaquin Valley, where values near 130 ppb were recorded at Parlier and Edison. On 31 July, peak network ozone levels (120 ppb range) were measured at Livermore, Patterson Pass, and in the Sierra foothills east of Fresno. On August 1, peak ozone levels were experienced along the Sierra foothills from Sloughhouse to the San Andreas-Sonora area, and Kings Canyon. The only federal 1-hour exceedances on that day occurred in the Sacramento region, with the San Andreas station recording a peak value of 134 ppb.

Figure 1 shows the modeling domain for the simulations, which extends from Santa Barbara County in the south to Shasta County in the north, and from the Pacific Ocean into Nevada in the east. The domain is defined in a Lambert Conical Projection with reference latitudes at 30 and 60 N, the central meridian at 120.5 W, and the coordinate system origin at 120.5 W and 37 N. The southwest corner of the grid is 376 km west of and 292 km south of the coordinate system origin. The horizontal study domain is comprised of 185 x 185 grid cells with a resolution of 4 km, while the vertical grid structure consisted of 20 layers from the surface to the tropopause with finer resolution near the surface (e.g., the surface layer is 30 m deep).

The meteorological fields for the CMAQ and CMAQ-APT simulations were derived from a prognostic simulation conducted with the non-hydrostatic meteorological model, MM5, using four-dimensional data assimilation (FDDA). The emissions, initial conditions and boundary conditions were based on the corresponding inputs from another air quality model (CAMx). The MM5 meteorology and CAMx emissions, initial and boundary condition files for the CCOS modeling period were provided by the California Air Resources Board (ARB). These files were converted to CMAQ model-ready input. The modeling period for the CMAQ application was chosen to be from 12 GMT on July 29, 2000 to 12 GMT on August 2, 2000 based on the availability of input data.

Fifty-six (56) stacks from the ten plants that had the highest NO_x emission rates in the modeling domain were selected for explicit plume treatment in the CMAQ-APT simulation. The following air quality simulations were conducted with CMAQ and CMAQ-APT:

- A base case CMAQ simulation (i.e., all sources treated in the gridded framework)

- A CMAQ-APT simulation (i.e, the 56 selected point sources treated in the plume-in-grid framework and remaining sources treated in the gridded framework)
- A “background” CMAQ simulation (i.e,, emissions from 56 selected point sources not included in the simulation)

The purpose of the “background” simulation is to better understand the effect of using a plume-in-grid treatment. Relative to the results from this “background” simulation, the CMAQ-APT simulation and the CMAQ base simulation will show the effect of the NO_x emissions from these point sources with and without PiG treatment, respectively. In other words, we can get a measure of the ozone and nitric acid that can be produced (or titrated, in the case of O_3) in the plumes of these point sources with and without PiG treatment, particularly for isolated sources.

Model performance for both CMAQ and CMAQ-APT is currently being evaluated by comparing model results with hourly surface observations of O_3, NO_x, NO_y and CO at CCOS monitoring locations. In addition, the impacts of PiG treatment are being quantified by comparing the O_3 and HNO_3 results from the three sets of simulations.

4. SUMMARY

We have described improvements and updates to CMAQ-APT and described its application for a Central California Ozone Study episode in July/August 2000. The results from the study are currently being analyzed.

5. ACKNOWLEDGEMENTS

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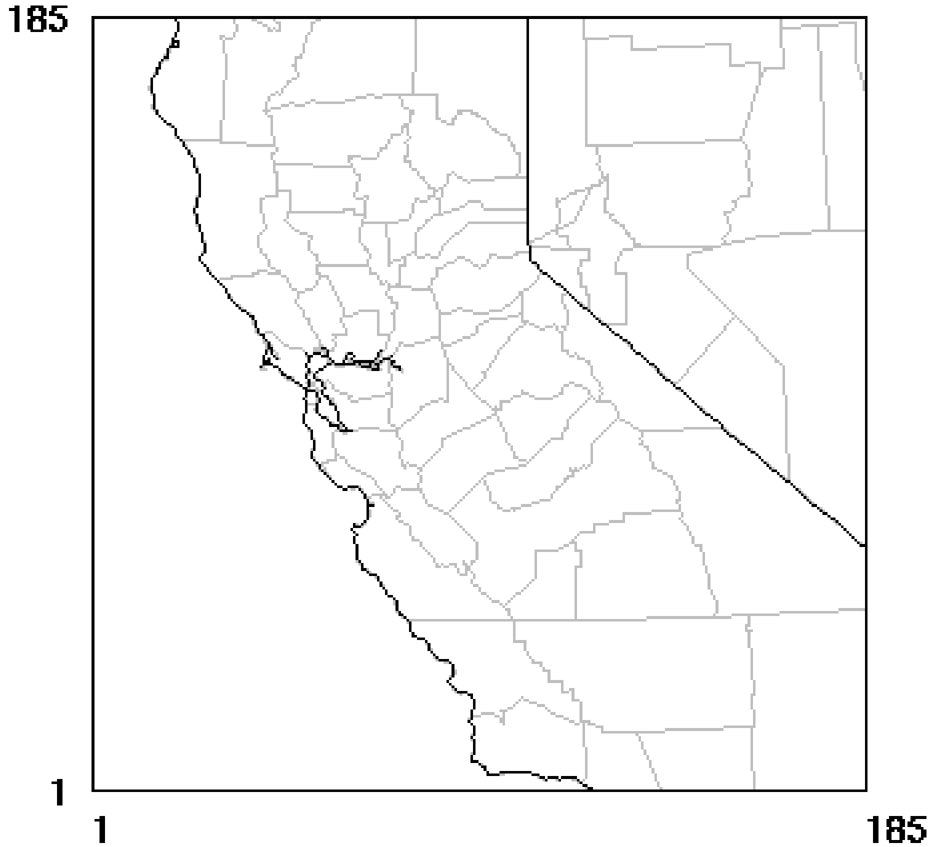

Figure 1. Modeling domain for the CCOS simulations