3.1 **SOME ISSUES RELATED TO THE SIMULATION OF POLLUTION DISTRIBUTION IN COMPLEX-TERRAIN AREAS**

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1. INTRODUCTION

The world is in the middle of a surge of urbanization, with some twenty megacities having arrived by the end of twentieth century. The population influx to the cities has necessitated providing of clean air and water, food, housing, healthcare and infrastructure for communication, governance, transportation and security. Of these, the quality of air is a factor of paramount importance, given that it is the medium of living and the constituents of air are intimately related to human health. Burgeoning population in cities have led to deterioration of air quality, which can be ameliorated only by careful planning and implementation of sound policy.

Through the National Ambient Air Quality Standards, the EPA impose limits on the amount of pollutants that can be present in the environment, and the most important of these pollutants are the CO, O_3, and PM (criteria pollutants). The State of Arizona currently is in non-attainment with respect to 1–hour O_3 and PM. In addition, the EPA has recently introduced a new 8-hour standard, and has requested the states to report their respective non-attainments areas by July 15th, 2003. Arizona State University researchers were contracted to perform the technical analysis for this boundary designation work, which involved extensive scientific and socio-economic analysis and modeling of present and projected future 8-hour ozone concentration of potential violation areas. The purpose of this communication is to discuss the ozone modeling results as well some of the modeling problems we faced during the project.

2. MODEL CONFIGURATION AND THE DESIGN DAYS OF SIMULATION

Standard community models, CMAQ (Community Multiscale Air Quality), MM5 (Penn State/NCAR Mesoscale Model) and SMOKE (Sparse Matrix Operator Kernel Emissions) were used, respectively, for the air quality, meteorology, and emission modeling. We employed two domains, with the outer domain covering the central part of the Arizona and the inner domain encompassing the Phoenix valley and surrounding mountains (Fig. 1).

The MM5 simulation was performed with 4 nested domains, with respective grid resolutions of 54 km, 18 km, 6 km, and 2 km. Vertically 27 layers were used with approximately 10 m agl as the lowest computational layer. The NCEP *Eta* model output (Grid 212 with 40 km spacing) was used to provide the initial and boundary values for the MM5 simulations and the data assimilation was performed using NWS soundings and surface measurements. The emission inventory for CMAQ was prepared using SMOKE based on Western Region Air Partnership (WRAP) inventory and an extensive GIS analysis. The biogenic emissions were also modeled by using SMOKE, utilizing the Biogenic Emissions Inventory System 2 (BEIS2) that estimates volatile organic compound (VOC) emissions from vegetation and nitric oxide (NO) emissions from soils based on meteorological conditions.

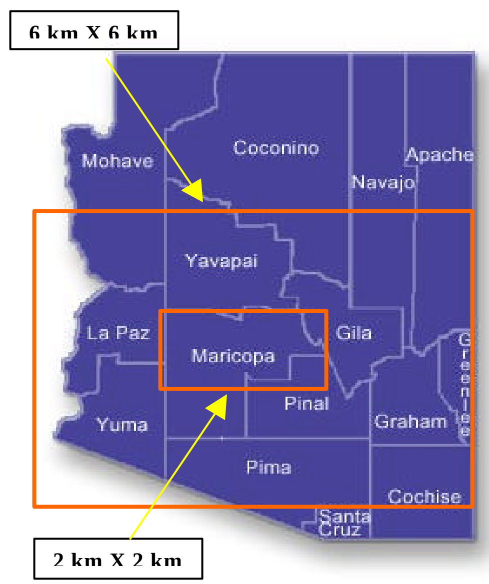

Fig. 1. The modeling domains and their relative locations with respect to the State of the Arizona. The name of each county is given as well.

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Two nested domains were used in CMAQ, which were identical to the innermost two domains of MM5, except that several lateral boundary cells were excluded. Observations from ADEQ routine monitoring stations and special measurements during the DOE's Phoenix '98 field experiment were used as initial and lateral boundary values for the outer domain. The selection of a sufficiently large outer domain allowed typical distances traveled by pollutants by thermal circulation to be smaller than the domain size, thus reducing uncertainties associated with lateral boundary values.

ADEQ recommended two design days for simulations based on the observations of elevated 8-hour ozone concentrations. The first is June 6, 2002 wherein high ozone concentrations were measured in the northeast part of the valley. The second day is July 12, 2002, where elevated 8-hour concentrations were recorded in the northwestern part of the Phoenix urban center as well as in the central valley area.

3. RESULTS

Local thermally driven wind circulation within the valley – up-slope (westerly) flow during day and down-slope (easterly) wind during night – was well simulated by the model. Available surface wind measurements from ADEQ routine monitoring stations and vertical wind profiles from a Radar Wind Profiler of ADEQ were used to evaluate the model results. Qualitatively, both near surface and upper-level winds showed reasonable agreement with the observations. The model performance was evaluated using standard statistical tools based on variables such as relative mean bias, mean difference, index of agreement, and RMS vector error. Generally, the values of the statistical variables were within the acceptable limits articulated in previous studies: e.g. Pielke and Pearce (1994), Sivacoumar and Thanasekaran (2001), Hanna and Yang (2001).

With regard to the ozone prediction, daytime maximum 1-hour ozone concentrations showed fairly good agreement with the observations, while nocturnal ozone concentration showed a deviation from the observations for both June 6th and July 12th cases. However, interestingly, CMAQ over-predicted ozone in the west and slightly, yet critically, under-predicted in the northeast station. The predictions agreed reasonably well with the observations at the central stations (Fig. 2). CMAQ produced significant diurnal variation of ozone at the west, while the observation did not show such a trend. Considering that the west station is located at a mountain summit, ozone precursors must be transported from a nearby source area. A modeling error was suspected for this anomalous prediction, as we describe below in Section 4.

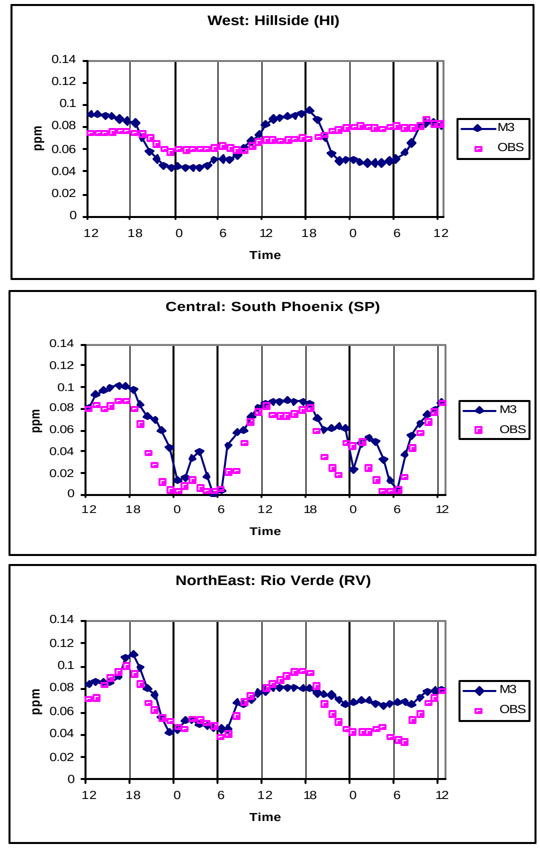


Fig. 2. Time series of observed and simulated 1-hour ozone concentration at a monitoring station located in (a) the West, (b) the central, and (c) the northeast of the valley for the June 6th case.

When averaged over the 8-hour period (Fig. 3), the central part of Maricopa County was simulated to be higher than 90 ppb, and its adjacent areas also were found to have elevated ozone > 85 ppb, national ambient air quality standard for 8-hour ozone. The elevated ozone concentration over most of the domain was possibly contributed by the meteorological conditions that were characterized by light wind, clear sky, and deep thermal convection.

Conversely, for the July 12th case, the elevated 8-hour ozone was mainly predicted in the vicinity of the Phoenix valley, which was due to limited transport resulting from moist convective cells and thunderstorm activities that were prevalent during that day (not shown).

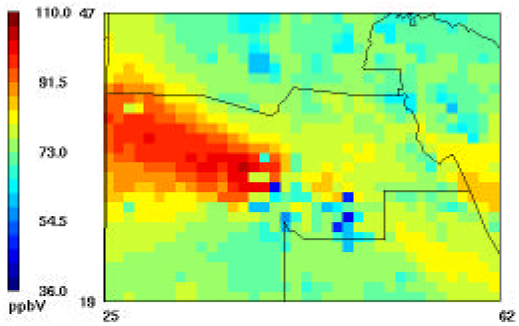
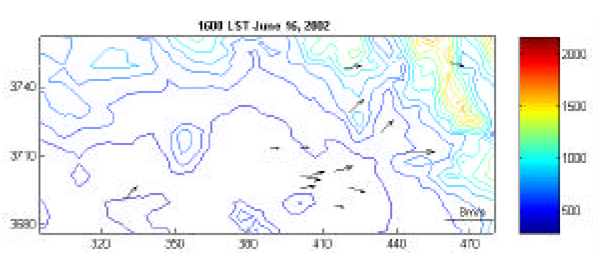


Fig. 3. Maximum 8-hour averaged ozone concentration on June 6th, 2002. County boundaries are marked by solid line.

4. DISCUSSIONS

Certain problems associated with transition periods were well evident from the CMAQ simulations, which indicate the formation of an ozone "blob" in the northwestern part of the domain. Note the maximum 8-hour ozone concentration oriented to the west of the modeling domain, the upstream of the urban center during the daytime up-slope winds (Fig. 3). These elevated levels are absent in the measurements, however, and scrutiny of MM5 and CMAQ simulations clearly indicated that the delayed transition in the simulations has led to high ozone in the northwest.

MM5 simulated persistent southeasterly winds whilst observations showed a shift from southeasterly to southerly during 1000 – 1200 LST. As an remnant effect of (erroneous) delayed transition, MM5 predicted fairly weak westerly winds into the afternoon, despite the observations indicated otherwise (Figs. 4 a,b). The ozone formed within in the urban core was supposed to be advected to the east by the up-slope flow that follow morning transition, but the delayed transition in the model caused the ozone movement to be biased toward northwest. This prolonged easterly winds transported more ozone and its precursors to the west than in reality. The difficulty of predicting transition is a bane of meteorological models, and the above anomaly points to the usual problem of inadequacy of transition parameterization in models.



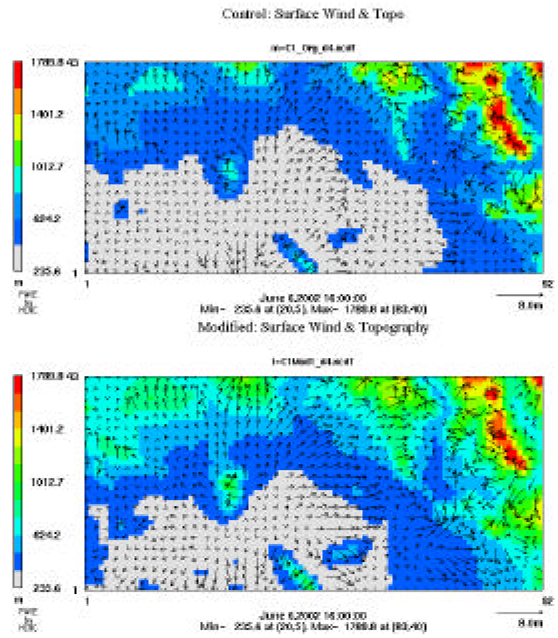


Fig. 4. Near surface wind field and terrain height in the inner modeling domain at 1600 LST June 6th 2002. (a) observations, (b) MM5 control run, and (c) MM5 modified run.

We therefore employed a new parameterization of eddy diffusivity in MM5 as an attempt to improve the prediction of transition. To this end, an eddy diffusivity suggested by Monti *et al.* (2002) was implemented, viz.

$$\frac{K_m}{s_w^2/\left|d\tilde{V}/dz\right|} = (0.34)\overline{Ri_g}^{-0.02} \approx 0.34$$

$$\frac{K_h}{s_w^2/\left|d\tilde{V}/dz\right|} = (0.08)\overline{Ri_g}^{-0.49} \approx (0.08)\overline{Ri_g}^{-0.5}$$

where, K_m and K_h are eddy diffusivity for momentum and heat, respectively, Ri_g is a gradient Richardson number, and s_w^2 is variance of vertical velocity.

The performance of the new parameterization was compared with that of the MRF scheme (Hong and Pan, 1996), which is known to perform better than or comparable to other default PBL schemes in MM5 (Bright and Mullen 2002). In addition, based on extensive VTMX field measurements (Doran *et al.* 2002), Monti et al. parameterization turned out to be in better agreement with observations than the MRF scheme (Lee *et al*. 2003). Hereafter, a simulation with the MRF schemes is referred as the control and that with the new parameterization as the modified run. In MM5 modified run, the easterly momentum during the morning transition appeared to be weaker than in the control run, and hence the westerly component was intense in the afternoon, which turns out to be closer to the observation (Fig. 4c). Fig. 5 shows the maximum 8-hour ozone on June 6th, 2002 predicted using the modified parameterization. Note that the elevated ozone concentration in the west is reduced significantly in comparison to the control run (Fig. 3).

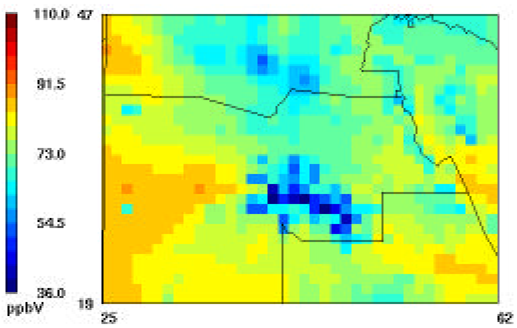


Fig. 5. Same as Fig. 3 except that eddy diffusivity parameterization from Monti *et al*. (2002) was used instead of the MRF scheme, one of the default PBL schemes in MM5.

5. CONCLUSION

The MM5-SMOKE-CMAQ modeling system performed reasonably well for the Phoenix basin, and it proved to be a useful tool for regulatory as well as research purpose. Even though both meteorology and air quality modeling results were in good agreement with the observations, both qualitatively and quantitatively, a closer analysis of results revealed a problem related to the morning (delayed) transition. The transition predictions were significantly improved by implementing a new simple semi-empirical eddy diffusivity parameterization scheme. This study indicates that sound physics and dynamics based parameterizations for morning (and evening) transition ought to be a priority in future model refinements.

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