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APPLICATIONS OF MODELS-3/CMAQ IN CALIFORNIA

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1. INTRODUCTION

For regulatory applications in the past, California used two major grid-based photochemical air quality models. They are the SARMAP Air Quality Model (SAQM) (DaMassa *et al.* 1996) and the Urban Airshed Model (UAM) (USEPA 1990). But the science of either model was not updated significantly, except for chemistry, during the past several years. With the availability of comprehensive data from several extensive field studies in California (Fujita *et al.* 1996, Watson *et al.* 1998, Fujita *et al.* 1999), we are now in a position to rigorously test air quality models for future regulatory applications. The leading models currently being tested are the Models-3/CMAQ modeling system (USEPA 1999), CAMx (ENVIRON 2002), SAQM, and CALGRID (Yamartino et al. 1989). The first three models accept meteorology inputs from prognostic meteorology models such as Mesoscale Model 5 (MM5) (Grell *et al.* 1994) and include both Carbon Bond IV (CBIV) (Gery 1989) and a fixed parameter version (SAPRC99f) of the1999 chemical mechanism of the State-wide Atmospheric Processes Research Center (Carter 2000). We have updated CALGRID to accept prognostic meteorological inputs and developed a flexible chemical mechanism interface to implement the SAPRC99f chemical mechanism.

The two applications presented in this paper are assessments of the CMAQ model in Southern California. The first application is an intercomparison of CMAQ results with those of CAMx and CALGRID for the 1997 August SCOS ozone episode. The second is the use of CMAQ in simulating air toxics concentrations in Southern California and intercomparison of CMAQ results with those of CALGRID. Both of these projects are still in progress and the results presented here are preliminary.

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2. MODELING THE SCOS-97 AUGUST OZONE EPISODE

The primary objective of the 1997 Southern California Ozone Study (SCOS), as described by Fujita *et al.* (1996), was a field experiment designed to collect air quality and meteorological data to support air quality modeling in southern California. To meet this objective, an intensive, supplemental monitoring program was conducted from July to October 1997 that included 26 RWP/RASS sites, six ozonesonde sites, four aircraft, and additional surface monitoring for ROG and criteria pollutant species. In spite of an anomalous year for meteorology caused by a strong El Nino event, five periods of high ozone concentrations were investigated with the intensive monitoring program; of which, two were selected for study using photochemical air quality models. One of these periods was August 4-7, 1997.

In this paper, comparisons among simulation results from the CMAQ, CAMx, and CALGRID air quality models were summarized for August 5, 1997. August 5 was part of a 5-day simulation period from August 3-7, 1997 and was the day on which the episode-high ozone concentrations were observed and simulated. The simulations were run using CBIV and SAPRC99f chemical mechanism and all of the meteorological inputs required by the various models were derived from output of the MM5 meteorological model. The modeling domain was 120x84x16, 5x5-km grid cells. The SCOS domain contains ocean, mountains, and deserts and is very difficult to model with meteorological

Table 1: The comparison of model results for the SCOS-97 August ozone episode.

STATSTIC	CALGRID		CAMx		CMAQ	
	CBIV	SAPRC	CBIV	SAPRC	CBIV	SAPRC
Observed Peak (ppb)	187	187	187	187	187	187
Sim. Station Peak (ppb)	163	179	167	191	183	184
Unpaired Peak Ratio	0.87	0.96	0.89	1.02	0.98	0.98
Normalized Bias (%)	+07	+24	+08	+25	+11	+19
Gross Error (%)	+29	+38	+26	+31	+35	+38

and air quality models. Within this domain, the MM5 meteorological fields were greatly improved by the use of the extensive SCOS meteorological data ingested into MM5 using observational FDDA. However, in spite of these improvements, MM5 tended to overestimate mixing heights, especially in the coastal regions, and overestimate wind speeds in mountainous and remote areas were there were few observational data.

On August 5, 1997 the peak ozone concentration observed in the southern California region was 187 ppb. The spatial distribution of the high ozone concentrations was limited; there were only 3 hours at any site with ozone concentrations of 170 ppb or greater, and only 6 hours with concentrations of 150 ppb or greater.

Comparisons of simulation results among the models were based on statistical measures outlined in USEPA (1991) modeling guidelines. Simulated concentrations of ozone were calculated for each set of modeling results, for each monitoring site in the domain. For these comparisons, the SCOS modeling domain was divided into 9 zones and statistical measures of unpaired peak ratio, normalized bias, and gross error (USEPA, 1991) were calculated independently for each model, and for each zone.

In this publication, the results from only Zone 4 (where the peak ozone concentration was measured) were summarized. Within Zone 4, there were 16 sites that recorded ozone concentrations.

The CALGRID, CAMx, and CMAQ peak simulated ozone concentrations with the CBIV chemistry ranged between 163 and 183 ppb (Table 1). Using CBIV, the simulated peak concentration underestimated the observed peak of 187 ppb. However, the unparied peak ratios were within the USEPA guideline of 80-120% (e.g., ±20%). All three models also met the performance guidelines for normalized bias (±15%), and gross error (35%). For CALGRID and CAMx, the peak concentrations using the SAPRC99f chemistry were 10-15% higher than using CBIV. However, for all three models, the normalized bias statistics from the SAPRC99f results were higher and exceeded model performance guidelines.

For the August 1997 SCOS episode, agreement among the simulation results from the CALGRID, CAMx, and CMAQ models was very good. Using the CBIV chemistry mechanism, each of the models met USEPA model performance guidelines. Simulated peak ozone concentrations were generally higher using the SAPRC99f mechanism, and these results were reflected in higher peak concentrations and in higher normalized bias measures. Given uncertainties in the emissions inventories used for air quality simulations, these results do not imply one mechanism is “better” than the other.

3.0 MODELING THE CONCENTRATIONS OF TOXIC AIR CONTAMINANTS

One objective of California’s Neighborhood Assessment Program is to conduct long-term regional-scale photochemical modeling of toxics air contaminants (TACs). This is an integral part of a modeling effort that also includes dispersion modeling and micro-scale computational fluid dynamic simulations.

The photochemical models used were the Models-3/CMAQ and CALGRID (with diagnostic meteorology inputs in this case). Both models used the SAPRC99f chemical mechanism updated to include 30 TACs and a total of 106 chemical species.

The modeling domain contained 87x67 4 km^2 grid cells. The number of vertical layers for CMAQ was 17 with top of the domain at 14.6 km. For CALGRID, 10 vertical layers were used with the top of the domain at 3 km.

Meteorological parameters were obtained from exercising both MM5 (for CMAQ) and CALMET (for CALGRID) (Scire *et al.* 2000) for the entire year of 1998. MM5 used analysis nudging but no four-dimensional data assimilation. Emissions inventories were prepared for each quarter of the year and weekdays and weekends. Thus, a total of eight inventories were prepared.

We intend to exercise CALGRID for the entire year of 1998 and CMAQ for four months representing each quarter. As a part of this effort, both CMAQ and CALGRID were exercised for the entire month of January 1998 and August 1-7, 1998. Reported in this publication are the results for August 1-7, 1998.

Table 2 shows the comparison of the observed peak ozone concentration in the domain with two model predictions. For the entire period, except for August 5th and 6th, CMAQ significantly over predicts the peak ozone concentrations, and CALGRID predictions generally agree better with observations. For both models, location of the predicted peak was in the general area of the observation.

Table 2: Domain peak one-hour ozone concentration for each day in ppb during August 1-7, 1998

Day	Observed	CALGRID	CMAQ
Aug1	157	155	209
Aug2	188	173	285
Aug3	165	163	294
Aug4	170	205	279
Aug5	202	147	234
Aug6	197	178	220
Aug7	206	120	277

Presented in Figure 1 is the ratio of observed TAC concentrations to model predictions for both models. These ratios represent 24-hour averages for all days and all stations. For the TACs (the first seven compounds in figure 1), ambient measurements were available at only five monitoring stations for two days. But for the inorganic pollutants (the last four compounds), ambient measurements were available from over 40 stations for each hour of the entire period. CMAQ underestimates the average ratio for TACs while CALGRID overestimates the ratio. For formaldehyde the overestimation by CALGRID is significant. It is difficult to identify the source of this overestimation because it could be due to inefficient photolysis, overproduction, or a combination thereof. Another significant discrepancy is the overestimation of NO by CMAQ and underestimated by CALGRID, while NO_2 ratios are comparable and very close to unity. The ratios for ozone reveal a limitation of using the average ratios. For CMAQ, the ratio is nearly unity, but from Table 2 we know that CMAQ significantly overpredicts the peak. This reveals that CMAQ must underpredict the non-peak ozone values and the predicted ratio agrees with the observation for the wrong reason.

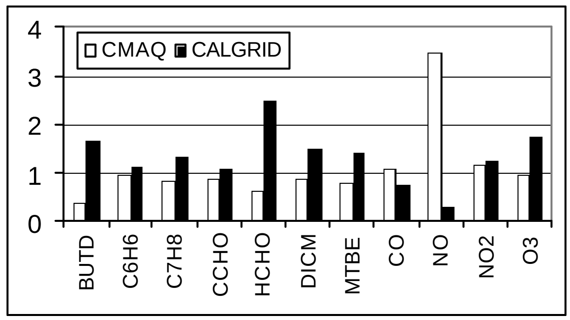

Figure 1: Ratio of Predicted-to-Observed 24-hr averages for toxic air contaminants. Graph represents average over all stations and August 1-7, 1998. The results are shown for 1,3-butadiene (BUTD), benzene (C6H6), toluene (C7H8), acetaldehyde (CCHO), formaldehyde (HCHO), dicholoromethane (DICM), methyl tertiary butyl ether (MTBE), carbon monoxide (CO), nitric oxide (NO), nitrogen dioxide (NO2), and ozone (O3).

We are currently conducting more detailed analyses of the model results to understand the sources of above discrepancies.

4. CONCLUSIONS

Based on the preliminary results of the two modeling efforts reported above, CMAQ, CAMx and CALGRID show similar model performances.

5. DISCLAIMER:

The management of the California Air Resources Board, the South Coast Air Quality Management District, or the San Diego County Air Pollution Control District did not review the results presented here. The opinions and conclusions stated here are entirely those of the authors and not necessarily those of the California Air Resources Board.

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