Appendix E2

Impacts of OGV Emission on South Coast Air Basin: An Air Quality Modeling Analysis

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Introduction

To investigate the impact of emissions from Ocean Going Vessels (OGVs) on onshore gaseous and fine particulate matter ($PM_{2.5}$) concentrations, a regional air quality model was used to simulate annual concentrations for Southern California. Two scenarios were simulated, one with emissions from OGVs and one without. The impact of OGVs on inland air quality was estimated from the difference between the two simulations.

Model Application

Model configuration

To simulate gaseous and PM2.5 concentrations, the Community Multi-scale Air Quality (CMAQ) model version 4.6 with sulfate tracking option was exercised for the year 2005 (http://www.cmaq-model.org/). The CMAQ model was developed by the U.S. EPA, and has been used by ARB in previous regional air quality modeling analyses. The year 2005 was selected because it was also used as the base year for the South Coast Air Quality Management District's $PM_{2.5}$ State Implementation Plan (SIP) development (SCAQMD, 2007).

For the analysis described herein, the emissions inventory and atmospheric chemistry were described using the Carbon Bond V (CB05) gas-phase chemical mechanism and the AERO4 aerosol modules. Within the CMAQ model, particulate matter were grouped into three log-normal modes that correspond to the ultrafine (aerodynamic diameter (D_p) < 0.1 μm), fine (0.1 μm $< D_p < 2.5$ μm), and coarse ($D_p > 2.5$ μm) particles sizes. Concentrations of $PM_{2.5}$ were the sum of the concentrations within the first two modes. The sulfate tracking option allowed the apportionment of PM sulfate from the chemical formation process, direct emissions, and initial and boundary conditions.

Domain setup

The modeling domain covers the South Coast Air Basin with 116 by 80 horizontal grid cells of 5 km (Figure 1). The vertical structure of the air quality modeling domain was determined by the layer structure of the meteorological model. In this analysis, there are nine layers extending to the top of the meteorological domain. The lowest eight layers extend to approximately 5 kilometers above surface.

The meteorological input fields required by the air quality model were generated using the MM5 prognostic meteorological model (Grell *et al.*, 1994). The MM5 model is recommended by the U.S. EPA (EPA, 2007) for air quality modeling applications and has been used for preparing ozone and PM SIP analyses in Central and Southern California. The MM5 model was used to generate hourly meteorological fields for the year 2005. The Meteorology-Chemistry Interface Processor (MCIP) version 3.2, which is part of the

CMAQ software package, was used to generate model-ready meteorological inputs for CMAQ model from the MM5 output files (http://www.cmascenter.org).

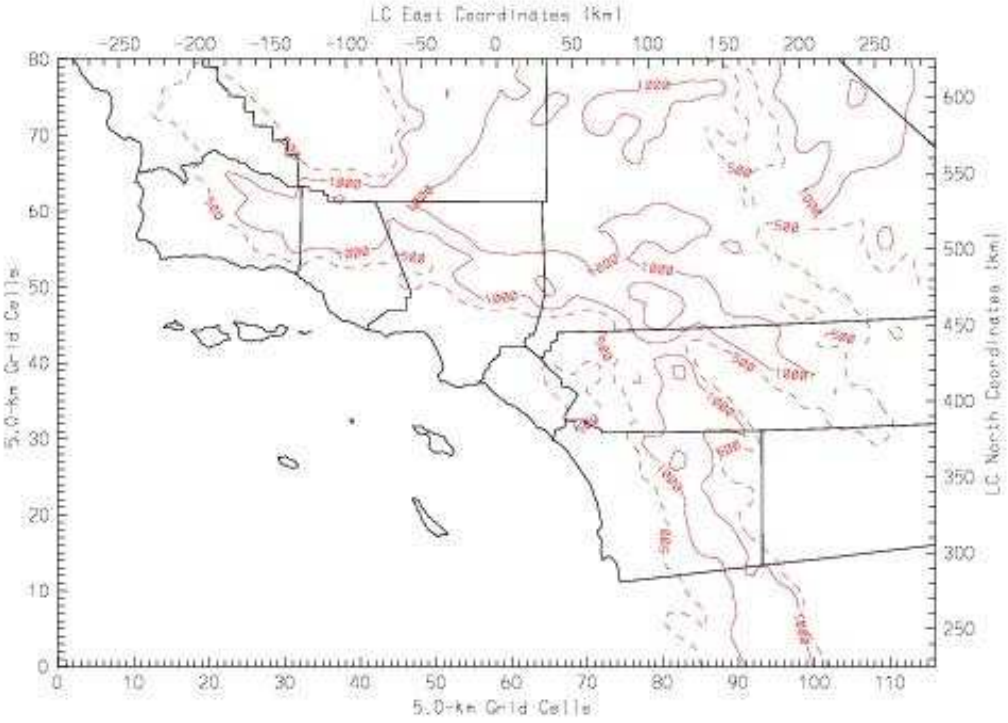


Figure 1. The Southern California Ozone Study (SCOS) modeling domain showing terrain contours.

Initial and boundary conditions

The boundary and initial gaseous and PM concentrations required for the air quality simulations were based on the U.S. EPA definition of "clean air" (EPA, 1991). Since the area of concern (Long Beach and Los Angeles) is near the center of the simulation domain, as shown in Figure 1, the impact of boundary condition (BC) would be minimal. Each simulation included a 10-day spin-up period to minimize the influence of the initial conditions.

Emission preparation

The year 2005 emission inventory used in the modeling analysis was generated using the ARB Emissions Inventory Forecast System (CEFS) and was consistent with that used by the SCAQMD in the preparation of their $PM_{2.5}$ SIP. The emissions inventory was gridded in the 4-km ARB statewide domain, and mapped into the 5-km modeling domain with mass conservation. The emissions inventory was defined in broad classes of

emissions including on-road mobile sources, biogenic emissions, elevated point sources, offshore shipping (e.g., OGVs), and other "area" sources. On-road mobile source and biogenic emissions were temperature-dependent. Hourly temperature fields were generated from observations to generate these emissions. The on-road mobile source emissions were also adjusted for the day of the week. For elevated point sources and other area sources, month-specific week-day and weekend-day emissions were generated. A single hourly inventory of OGV emissions was generated and assumed to be constant for the year. In CEFS, OGV was treated as an area emission source, thus all the OGV emissions were limited to the surface layer. The impact of OGV emission height on air quality model performance will be discussed in Appendix 2.

The OGV emissions inventory was mapped into existing shipping lanes and extended to 160 km (100 miles) offshore, well beyond the boundaries of the modeling domain. Only OGV emissions within the modeling domain were included in the modeling analyses. A comparison between OGV emissions and total emissions for the South Coast Air Basin is shown in Table 1. Gridded emissions for OGVs from selected gaseous and PM species are shown in Figure 2.

Table 1. The comparison between OGV emission and Total emission in the South Coast Air Basin.

Emission species	OGV emission (Tons/day)	Total emission (Tons/day)	%
NO_x	123.9	1662.8	7.45
SO_x	86.2	129.1	66.74
PM2.5 SO_4	1.6	15.9	10.07
PM2.5 EC	0.4	16.3	2.46
Other PM2.5	8.5	125.4	6.78

NO_x (= NO + NO_2 + HONO), SO_x (= SO_2 + SO_3), $PM_{2.5}$ sulfate (SO_4), EC, and unknown $PM_{2.5}$ account for 93.4% of total OGV emissions based on ARB's emission inventory. Table 1 shows the emission of main species emitted from OGVs compared with total emission in the South Coast Air Basin. Based on this comparison, 66.7% SO_x and 10% primary PM2.5 SO_4 were emitted from OGVs in the South Coast area. OGVs are also a significant NO_x emission source, and account for 7.4% of the total NO_x emission in the South Coast.

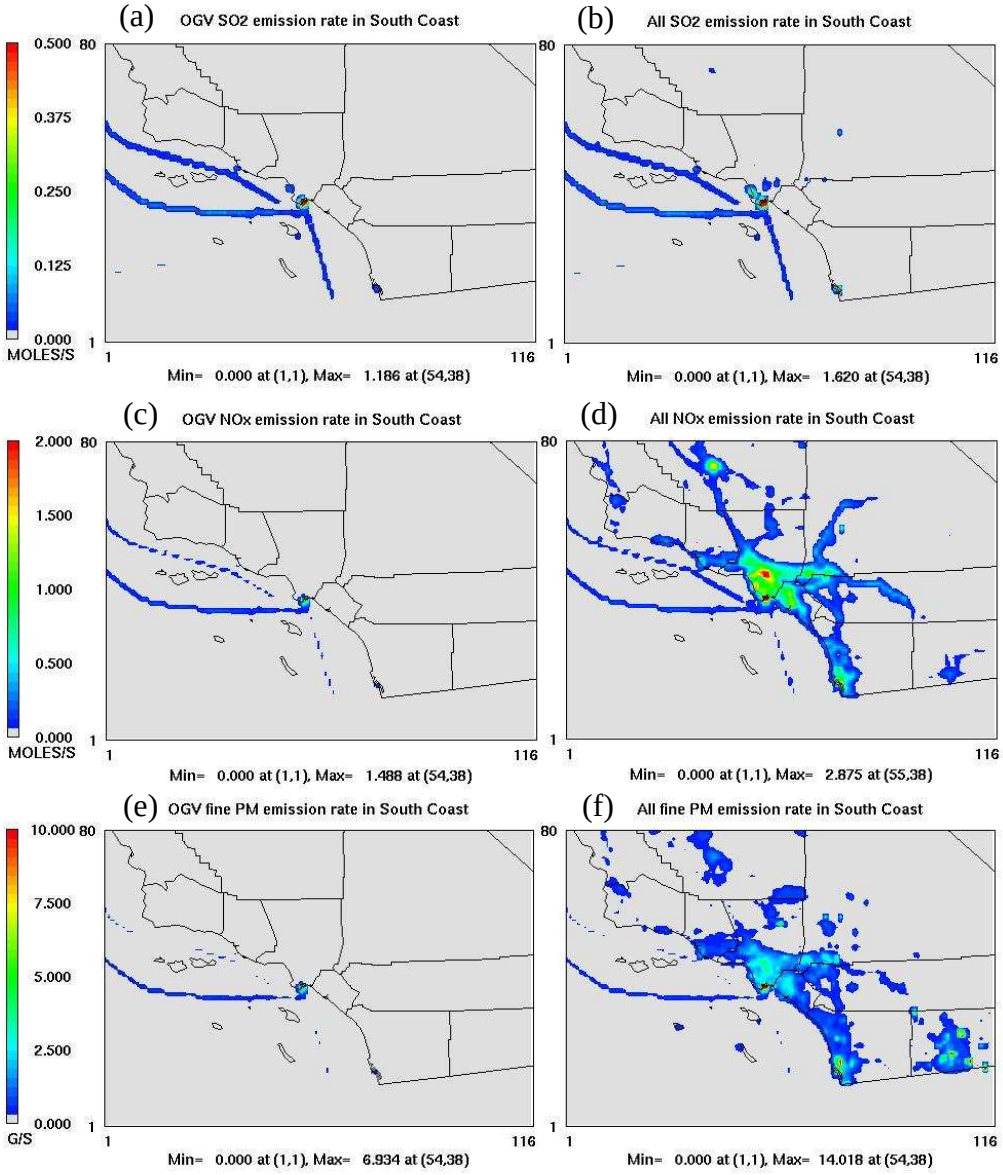


Figure 2. Plots of SO_2 and NOx emission rate from OGV and all emission sources. Panel (a) shows the emission rate (moles/sec) of SO_2 from OGVs, (b) the emission rate (moles/sec) of SO_2 from all emission sources in South Coast, (c) the emission rate (moles/sec) of NOx from OGVs, (d) the emission rate (moles/sec) of NOx from all emission sources in South Coast, (e) the emission rate (g/sec) of $PM_{2.5}$ (includes $PM_{2.5}$ SO_4, $PM_{2.5}$ EC, and other $PM_{2.5}$) from OGVs, and (f) shows the emission rate (g/sec) of $PM_{2.5}$ from all emission sources in the South Coast.

Simulation Results and Analyses

The CMAQ air quality model was run for the year 2005 using each of the two emissions inventory scenarios. Hourly gaseous and aerosol concentrations for each grid cell within the domain were calculated. In the first scenario, the emissions from all sources inside the modeling domain were included. In the second scenario, the emissions from OGVs were excluded. The results from each simulation were used to calculate, by grid cell, the annual maximum 8-hour ozone (O_3) concentration, and the annual average concentrations of $PM_{2.5}$, primary $PM_{2.5}$, $PM_{2.5}$ sulfate (SO_4), and $PM_{2.5}$ nitrate (NO_3). Since primary $PM_{2.5}$ is not explicitly defined in CMAQ model, it was arbitrarily defined as the sum of primary $PM_{2.5}$ sulfate and the non-reactive $PM_{2.5}$ species in the emissions inventory, including $PM_{2.5}$ elemental carbon (EC), primary organic carbon, and un-speciated $PM_{2.5}$. With the help of the sulfate tracking option, the contributions to modeled $PM_{2.5}$ sulfate from direct emission and from boundary and initial conditions could be identified, and they were then defined as primary $PM_{2.5}$ sulfate in this study. The primary $PM_{2.5}$ did not include concentrations of nitrate because from the modeling results it was not possible to distinguish between the primary and secondary components of this species. This is not a significant source of error since there are no significant amounts of primary nitrates in the emissions inventory.

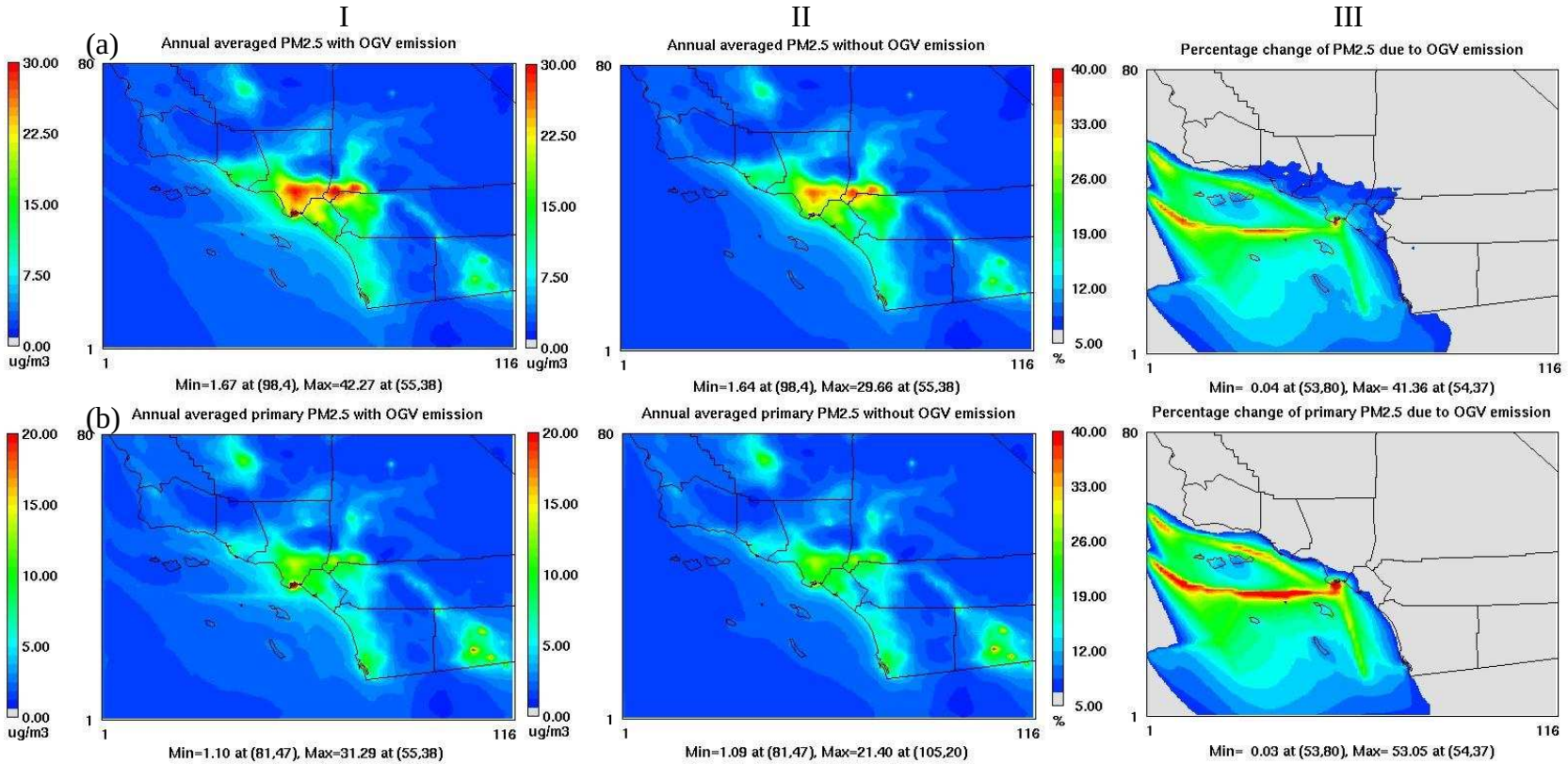
The differences in gaseous and particulate concentrations resulting from the two simulations were used to illustrate the impact of OGVs on air quality. In Figure 3, annual average concentrations of $PM_{2.5}$, primary $PM_{2.5}$, $PM_{2.5}$ SO_4, and $PM_{2.5}$ NO_3 are shown, along with the percentage change due to OGV emissions.

The greatest impact of OGVs on onshore $PM_{2.5}$ concentrations occurred in the vicinity of the Ports of Los Angeles and Long Beach, where emissions from OGVs accounted for approximately 25% of the $PM_{2.5}$ and 33% of the primary $PM_{2.5}$. More than 40% of the difference in $PM_{2.5}$ in the Port area was attributed to SO_4 concentrations. A broader spatial impact (>4% difference) of OGV emissions on SO_4 was predicted, covering most of the ocean area, coastline, and the Los Angeles Basin. However, concentrations of SO_4 and the proportion of $PM_{2.5}$ attributed to SO_4 decreased quickly inland from the coast. Compared to SO_4, less impact of OGVs on NO_3 was predicted, and most of the impact was onshore with a narrow range.

In Figure 4, the percent change in maximum 8-hour ozone concentrations that can be attributed to emissions from OGVs is shown. Along the coastline, the change in ozone concentrations was as much as 10%, and decreased inland. However, the maximum 8-hour ozone concentrations along the coast were generally less than 70 ppb (data not shown).

Conclusion

The results of this modeling analysis show that emissions from OGVs do impact onshore annual-average $PM_{2.5}$ concentrations within the South Coast Air Basin. Especially near the Ports of Los Angeles and Long Beach, emissions from OGVs contribute 25% or more to the total annual average concentrations. The impact of emissions from OGVs on $PM_{2.5}$ concentrations decreases quickly with distance from the coast inland, but contribute (>4% difference) impacts as much as 80 km (50 miles) inland.


I
II
III
(a)
Annual averaged PM2.5 with OGV emission
Annual averaged PM2.5 without OGV emission
Percentage change of PM2.5 due to OGV emission
30.00
22.50
15.00
7.50
0.00
ug/m3
40.00
33.00
26.00
19.00
12.00
5.00
%
80
1
116
Min=1.67 at (98,4), Max=42.27 at (55,38)
Min=1.64 at (98,4), Max=29.66 at (55,38)
Min= 0.04 at (53,80), Max= 41.36 at (54,37)
(b)
Annual averaged primary PM2.5 with OGV emission
Annual averaged primary PM2.5 without OGV emission
Percentage change of primary PM2.5 due to OGV emission
20.00
15.00
10.00
5.00
0.00
Min=1.10 at (81,47), Max=31.29 at (55,38)
Min=1.09 at (81,47), Max=21.40 at (105,20)
Min= 0.03 at (53,80), Max= 53.05 at (54,37)

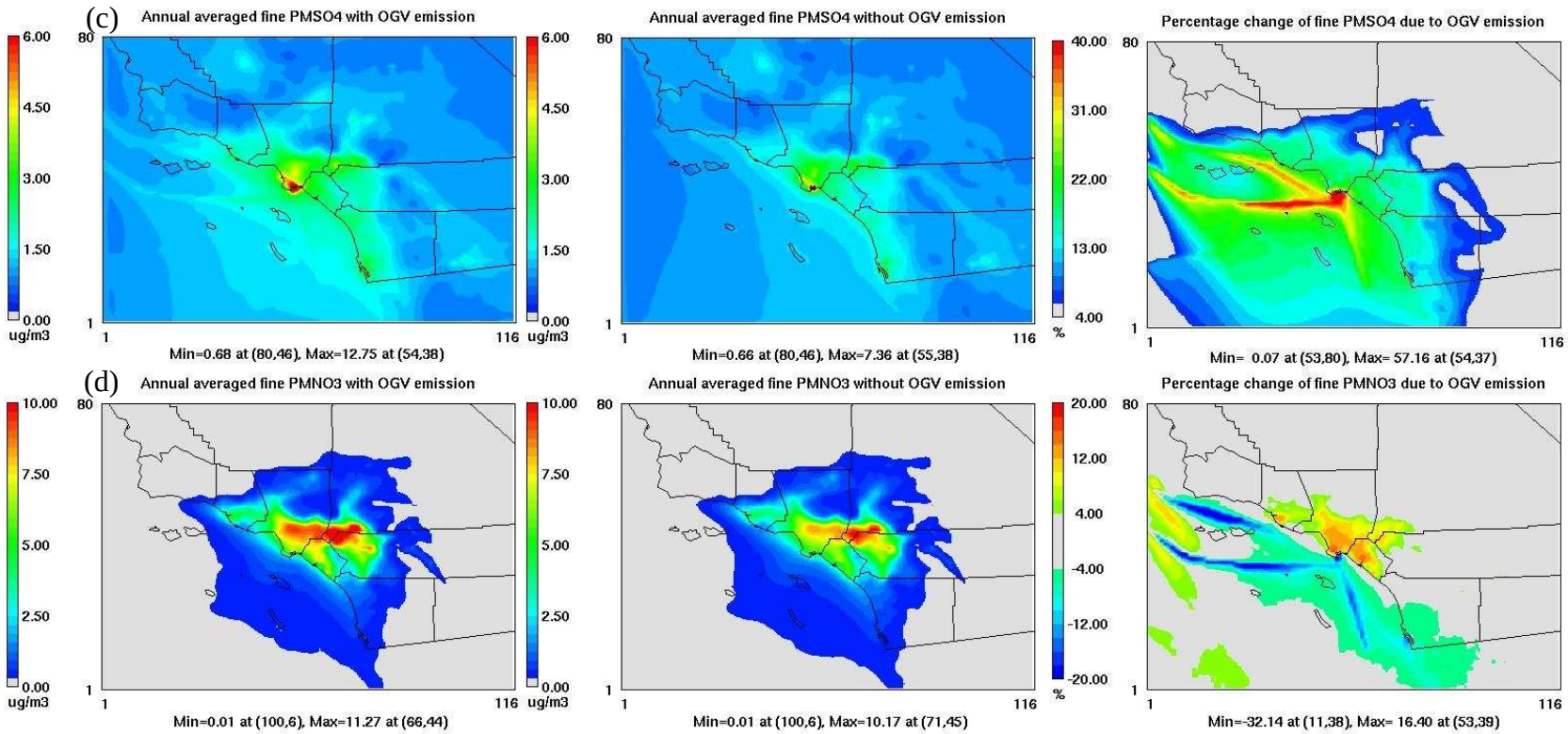


Figure 3. The comparison of annual averaged $PM_{2.5}$ (row (a)), primary $PM_{2.5}$ (row (b)), $PM_{2.5}$ sulfate (row (c)) and $PM_{2.5}$ nitrate (row (d)) predicted by CMAQ with OGV emission (column (I)) and without OGV emission (column (II)), and the estimated relative contribution from OGV emissions (column (III)).

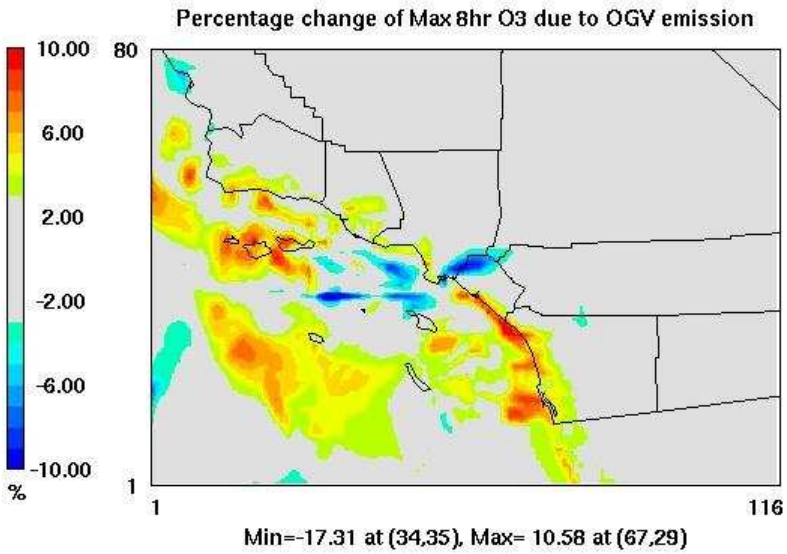


Figure 4. The relative change in annual maximum 8-hour O_3 concentration due to OGVs. Only the relative changes > 4% and < -4% are shown in the plot.

References:

(EPA, 1991) U.S. EPA, Guideline for regulatory application of the urban airshed model, U.S. EPA (1991). Research Triangle Park, North Carolina

(EPA, 2007) U.S. EPA, Guidance on the use of models and other analyses for demonstrating attainment of air quality goals for ozone, PM2.5, and regional haze, U.S. EPA (2007). Research Triangle Park, North Carolina http://www.epa.gov/scram001/guidance/guide/final-03-pm-rh-guidance.pdf

(Grell et al, 2007) Grell, A. G., J. Dubhia and D. R. Stauffer, A description of the fifth-generation penn state/ncar mesoscale model (mm5). NCAR Technical Note NCAR/TN 398+STR, National Center for Atmospheric Research, Boulder, CO (1994).

(SCAQMD, 2007) South Coast Air Quality Management District, 2007 air quality management plan, South Coast Air Quality Management District (2007). http://www.aqmd.gov/aqmp/07aqmp/index.html

Appendix 1: Model Performance Evaluation

To evaluate the performance of the regional air quality model for assessing the impact of emissions from OGVs, the CMAQ model simulation results for ozone (O_3) and $PM_{2.5}$ concentrations were compared with measurements within the South Coast Air Basin during 2005. The comparisons are summarized in this appendix.

Measurements

There were a number of sources of air quality data in the South Coast Air Basin during 2005. These include the State and Local Monitoring (SLAM) network, the STN network, and the MATES III network, which was a special purpose intensive monitoring study during 2005. Of these, the STN and MATES III networks emphasized speciated PM measurements and were the focus of the model performance analyses contained herein. There are two monitoring sites in the STN network and nine sites in the MATES III network, as shown in Table A1.

Most PM measurements are 24-hour averages. Therefore, for comparisons with measured concentrations, 24-hour averages were calculated from the hourly model simulation results.

Table A1. Monitoring sites

		Address	STN	MATES III
Los Angeles	LAS	1630 N. Main St.	×	×
Rubidoux	RUB	5888 Mission Blvd.	×	×
Anaheim	ANA	1010 S. Harbor Blvd.		×
Burbank	BUR	228 W. Palm Ave.		×
Compton	COM	720 N. Bullis Ave.		×
Fontana	FON	14360 Arrow Highway		×
Long Beach	NLB	3648 N. Long Beach Blvd.		×
Pico River	PIC	3713-B San Gabriel River Parkway		×
Wilmington	WIL	900 E. Lomita Blvd.		×

Comparison between model predictions and measurements

The comparisons of both gaseous and particulate species between CMAQ model predictions and STN network measurements are shown in Figures A1 – A4, and the comparison of PM species between model prediction and the MATES III network measurements are shown in Figures A5 – A7.

Figure A1 shows comparisons between simulated and measured concentrations of $PM_{2.5}$ SO_4, NO_3, and total $PM_{2.5}$ at the STN sites at RUB and LAS. Generally, CMAQ results agree better with measured concentrations at RUB than at LAS. At both sites, CMAQ slightly over-predicted $PM_{2.5}$ total mass, though the model under-predicted observed peak

concentrations. At LAS, high observed concentrations of $PM_{2.5}$ sulfate (SO_4) were obviously under-predicted. One possible reason may be that the monitoring site is close to the port, which is the major emission source of SO_2.

Figure A2 compares simulated and observed daily $PM_{2.5}$ total mass as a function of time at RUB and LAS. Generally, the CMAQ model showed better agreement with observations at RUB. However, extreme concentrations were under-predicted. At LAS, measured $PM_{2.5}$ concentrations were often over predicted.

Figure A3 provides comparisons between simulated and measured hourly averaged O_3 concentrations at RUB and LAS sites. While there is some scatter, simulated and observed concentrations were well correlated at these sites.

Figure A4 shows box-plots of hourly averaged O3 concentration predicted by CMAQ and observations at the STN sites RUB and LAS. The simulation results showed similar patterns compared with observation at both sites. However, some of the maximum observed concentrations were under predicted.

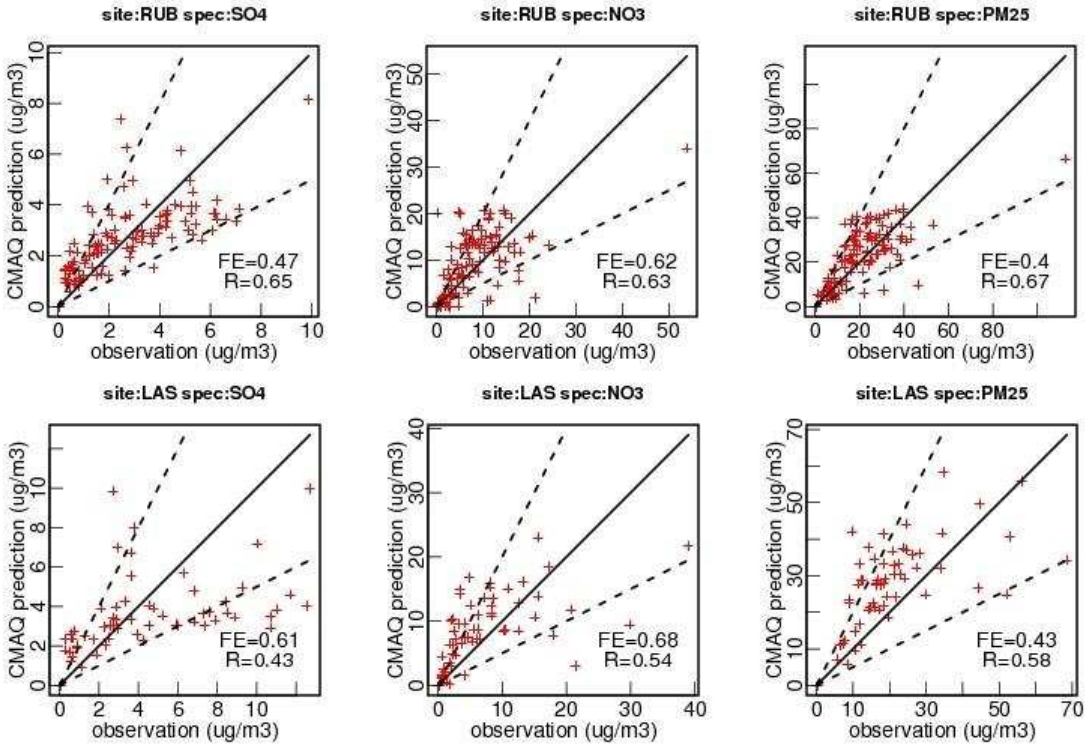


Figure A1. Scatter plots of model predictions and observations of $PM_{2.5}$ SO_4, $PM_{2.5}$ NO_3, and $PM_{2.5}$ at RUB and LAS. The observational data are from the STN network.

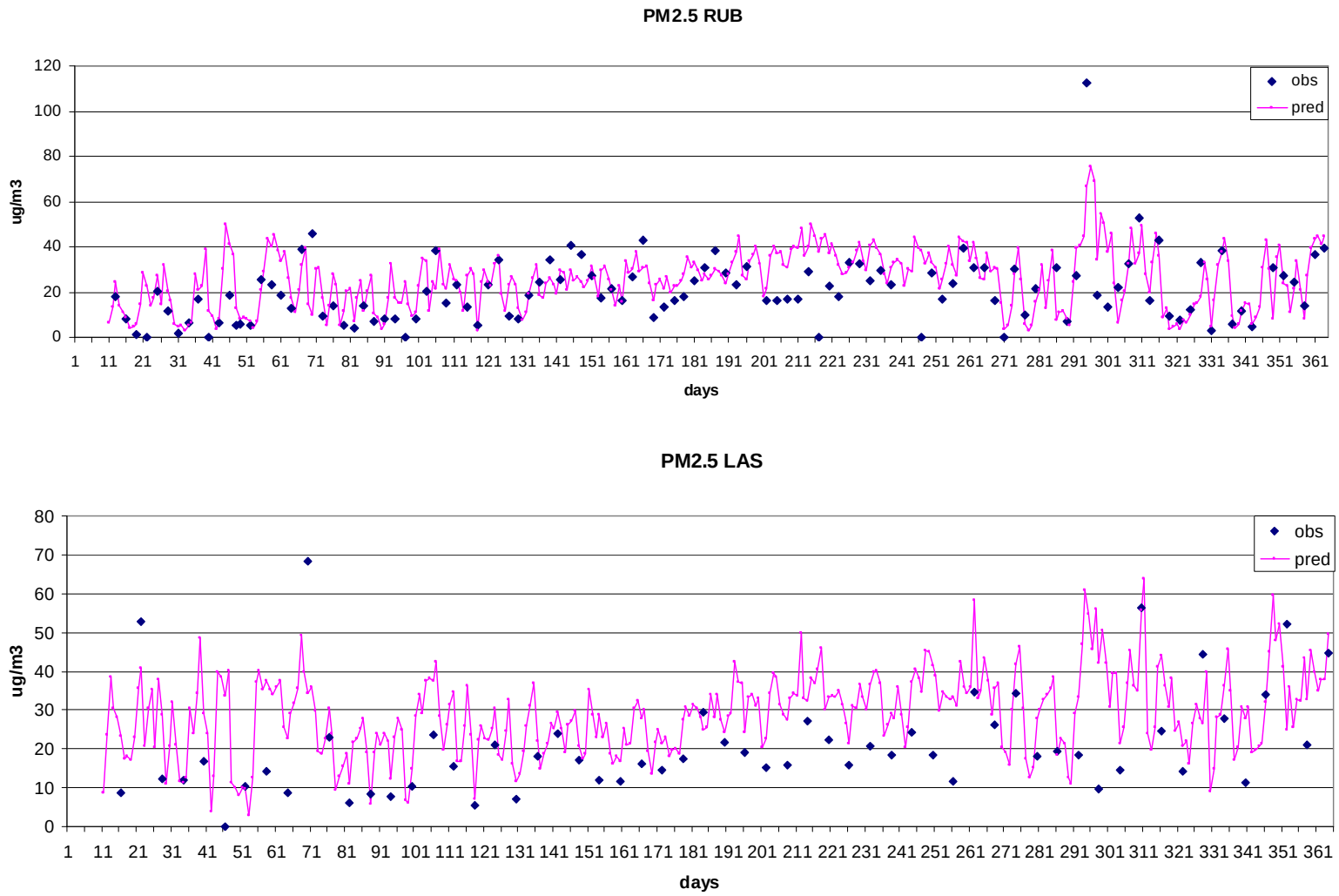


Figure A2. Time series plots of $PM_{2.5}$ model predictions and observations at RUB and LAS. The lines are model predictions, and the dots are measurement data. The observational data are from the STN network.

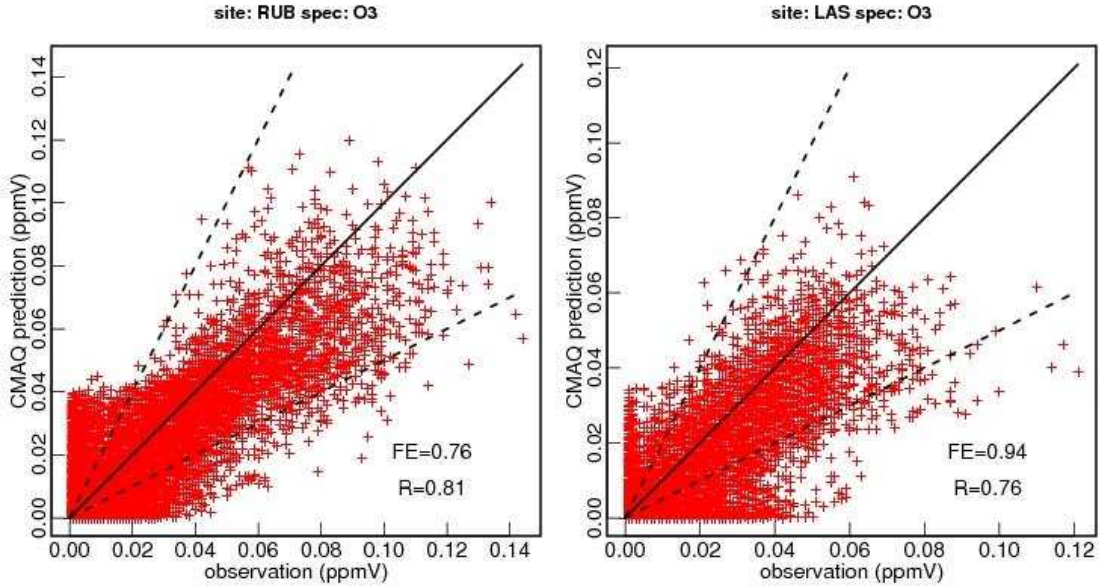


Figure A3. Scatter plots of model predictions and observations of hourly averaged O_3 at RUB and LAS. The observational data are from the STN network.

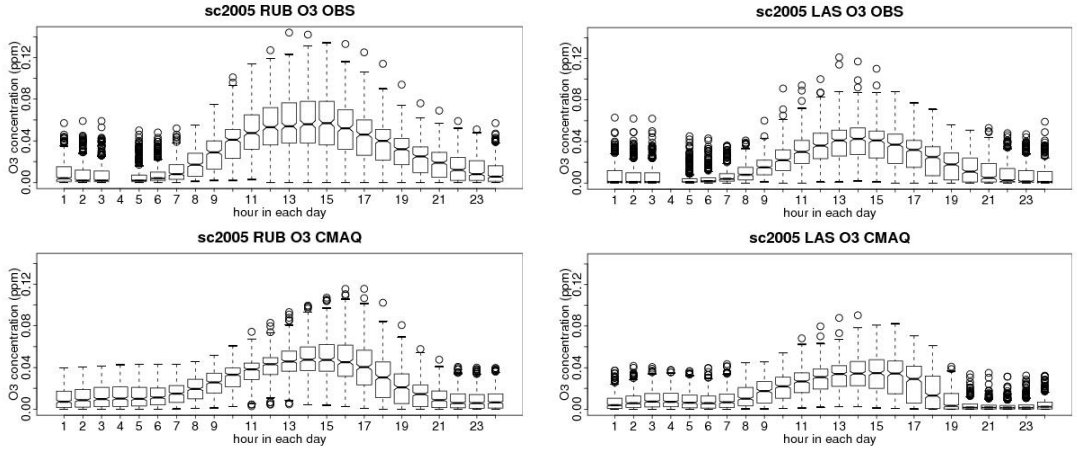


Figure A4. Comparisons of hourly averaged O_3 observations and model predictions at RUB and LAS. The top row shows observations, and the bottom row shows model predictions. The observational data are from the STN network.

Figures A5-A7 show scatter plots of $PM_{2.5}$ (A5), $PM_{2.5}$ nitrate (A6), and $PM_{2.5}$ sulfate (A7) at all nine MATES III network sites. The model could not predict some observed peak $PM_{2.5}$ values, but most data are evenly distributed along the 1:1 line, and between the 1:2 and 2:1 lines.

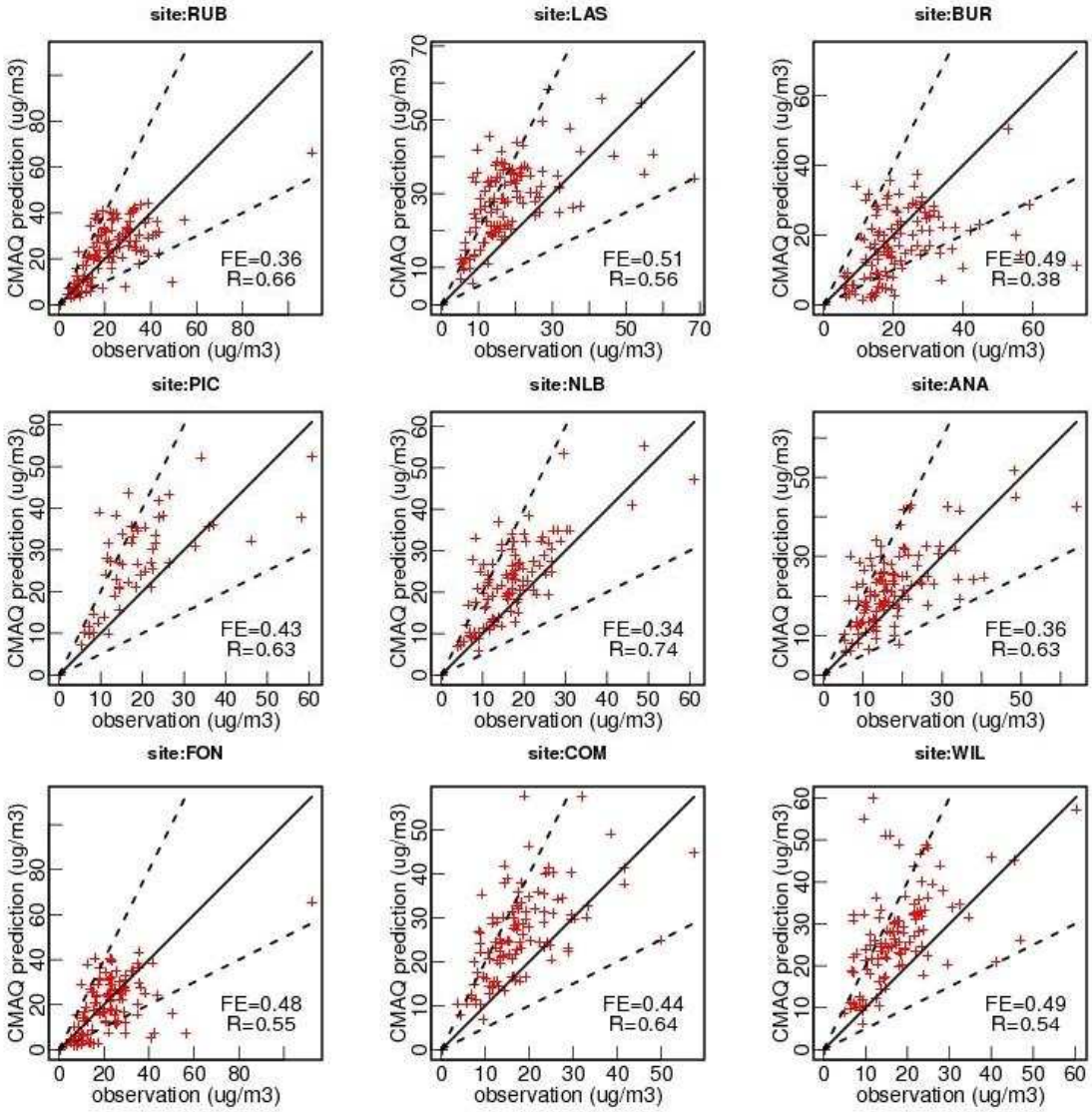


Figure A5. Scatter plots of model predictions and observations of $PM_{2.5}$ total mass at the MATES III network sites.

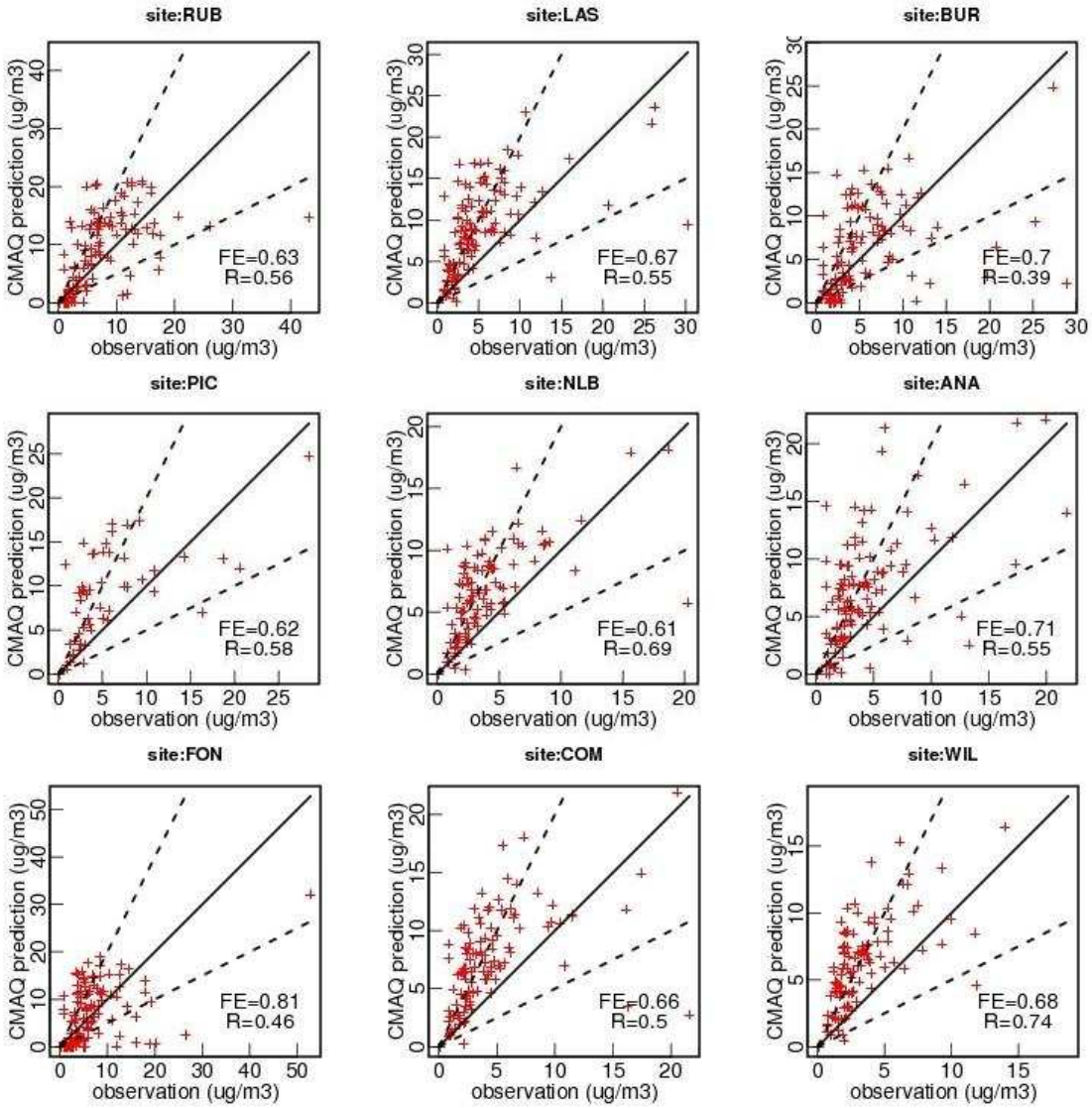


Figure A6. Scatter plots of model predictions and observations of $PM_{2.5}$ NO_3 at the MATES III network sites.

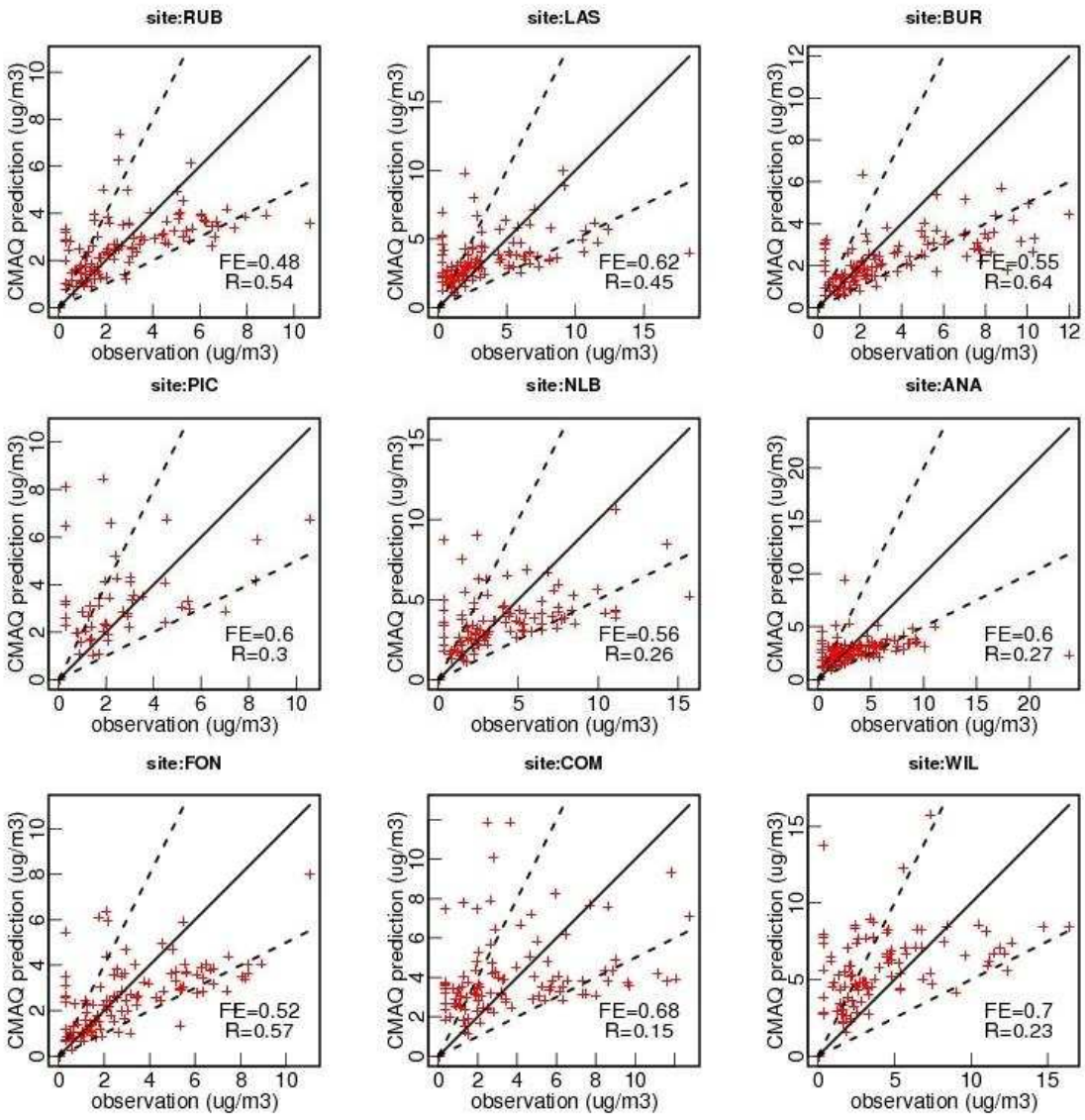


Figure A7. Scatter plots of model predictions and observations of $PM_{2.5}$ SO_4 at the MATE SIII network sites.

Statistical Analysis

There are currently no standard metrics for evaluating air quality model performance for long-term PM simulations, and no single statistical calculation can be effective in evaluating model performance for all species. A soccer plot is one typical and direct method for showing differences between model prediction and observations; these plots use Normalized Mean Bias (NMB) and Normalized Mean Error (NME), which are defined as below:

$$NMB = \frac{\sum_{1}^{N}(pred - obs)}{\sum_{1}^{N} obs} * 100\% \quad \text{(A1)}$$

$$NME = \frac{\sum_{1}^{N}|pred - obs|}{\sum_{1}^{N} obs} * 100\% \quad \text{(A2)}$$

Figure A8 is a soccer plot based on the calculated NMB and NME for O_3, total $PM_{2.5}$, NO_3, SO_4, NH_4, EC, and OC at the RUB and LAS sites The calculated NME values are less than 80%, and most NMB value are within the range of -40% and 40%. The tendency of the CMAQ model to under-predict $PM_{2.5}$ OC is the focus of current research by the U.S. EPA and others.

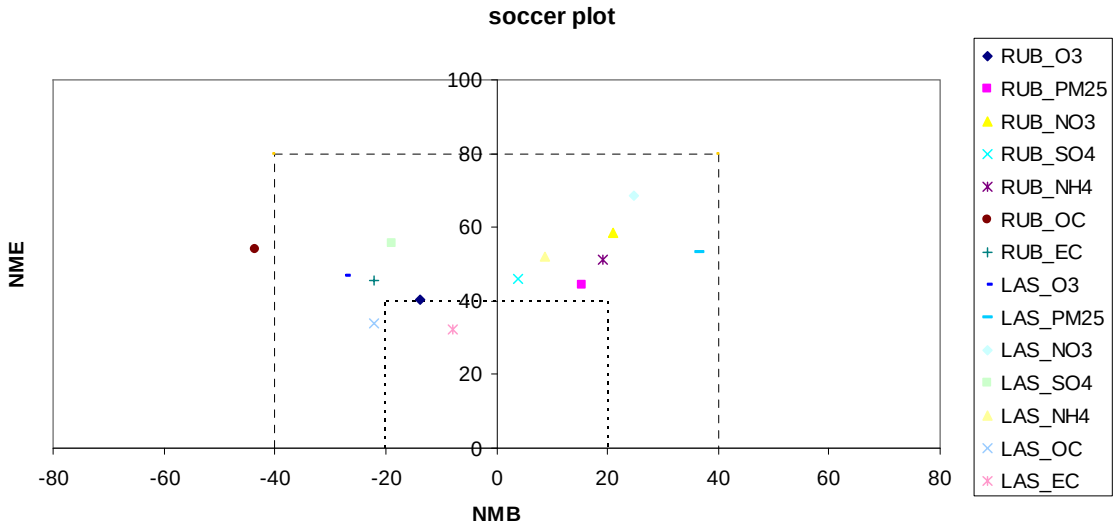


Figure A8. Soccer plot of model predictions at RUB and LAS. The observational data are from the STN network.

Conclusions

For total $PM_{2.5}$, the simulation results tended to over-predict observed concentrations at monitoring sites such as WIL and NLB near the coast. The agreement was better at sites such as RUB and FON located inland, and further away from the coastline. The simulation results tended to over-predict $PM_{2.5}$ NO_3 and under predict $PM_{2.5}$ SO_4. In general, simulated concentrations of $PM_{2.5}$ and $PM_{2.5}$ components agreed within a factor of two with observed concentrations.

Hourly simulated O_3 concentrations were well correlated with observations at the RUB and LAS sites. At most inland monitoring sites, for example RUB and FON, CMAQ predictions matched well with observations for $PM_{2.5}$ species, including total $PM_{2.5}$ mass concentration, $PM_{2.5}$ NO_3 and SO_4 concentration. Compared with measurements at other observation sites, which are closer to the coastline, the CMAQ model tended to over-predict observed $PM_{2.5}$ species concentrations.

Appendix 2: Difference of model prediction with OGV emissions from 1st and 2nd layers

In ARB's emission preparation system, OGV were treated as an area emission source. All the OGV emissions were assigned to the first layer of the CMAQ model, which covers the first 38 meters above the surface. In reality, some of the OGV emissions could have been released above 38 meters. In order to investigate the impact of OGV emission height on model performance, CMAQ model version 4.6 with Carbon Bond 05 (CB05) and AERO4 mechanism was used to predict the annual averaged $PM_{2.5}$ concentration in the South Coast under two emission scenarios: one with all OGV emissions assigned to the first layer (0 – 38 meters), and another with all OGV emission assigned to the second layer (38 – 154 meter). All other emissions were kept the same for both scenarios. The differences in model prediction on $PM_{2.5}$ are shown in Figure B1.

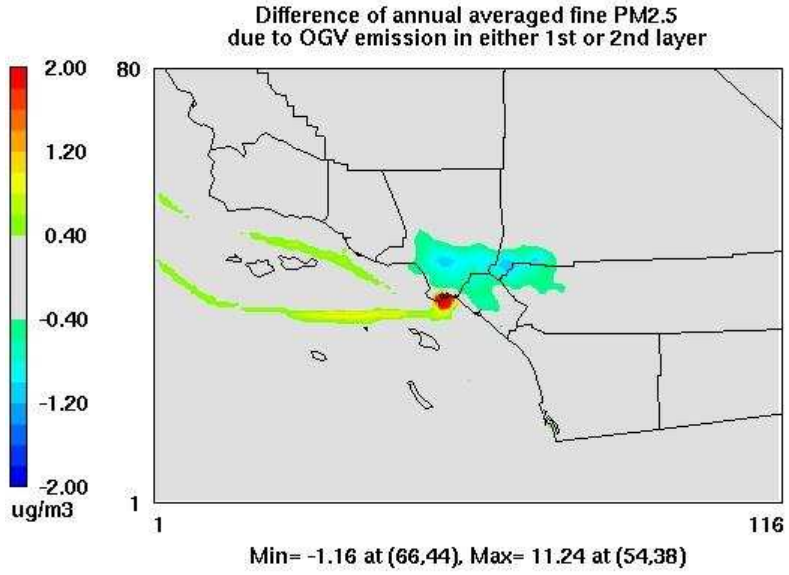


Figure B1. The difference in predicted annual-averaged surface $PM_{2.5}$ concentration with OGV emission in the first and second layers. Only changes > 0.4 and < -0.4 $\mu g/m^3$ are shown in the plot.

As shown in Figure B1, when the emissions were limited to the first layer, the concentrations were higher in the source areas. When the emissions were limited to the second layer, higher downwind concentrations were predicted. In reality, we believe that the emissions would be distributed in both the first and second layers. Thus, the actual in-land effects of OGV emissions could have a larger spatial distribution than predicted by the simulations reported in this study.