Ozone Episodes in US-Mexico Boarder Cities: Inferences based on Simulations and Satellite/Surface Data

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1. INTRODUCTION

Chemical transport models (CTM) are usually evaluated using surface measurements, but increasing availability of space-borne remote sensing products offers a new and powerful tool to conduct such evaluations. Extensive geographical coverage and frequent observations of satellite measurements are particularly attractive in this context as they minimize the necessity of interpolations among point surface measurements. The study reported herein assesses the usefulness of tropospheric satellite data, in combination with those of surface monitoring networks, in evaluating ozone predictions of an air quality model. The motivation was to investigate the feasibility of utilizing satellite data to improve the extent, severity and episodes of ozone pollution in the Southwestern US.

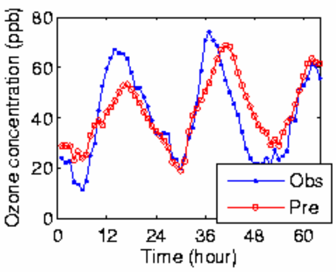

Figure 1 Time series of ozone concentration at San Diego

The design of the study was centered on an ozone episode over South California, including US-Mexico boarder in San Diego, on August 8-10, 2006, recorded by the EPA's Aerometric Information Retrieval System (AIRS). The maximum 1-hr/8hr ozone concentration exceeded 120ppb/80ppb at several sites in San Diego. The episode was particularly striking on the 9th August, and hourly variation of ozone concentration (averaged over all observational sites on San Diego) is given in Figure 1. The time begins at 00LT on August 8, 2006.

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2. DESCRIPTIONS OF THE MODELING SYSTEMS AND DATA

2.1 Model configuration and input data

The simulations were conducted for the design days August 8-10, 2006 using the regional air quality model system of Models-3 (MM5v3.7/SMOKEv2.3/CMAQv4.5.1). Two nested grids with horizontal resolutions of 36km and 12km and centers coinciding at (97ºW, 40ºN) were used for MM5/SMOKE/CMAQ. For CMAQ and SMOKE runs, the outer domain covered the Southwestern U.S. with 74×70 horizontal grid cells. The inner domain with 120×110 grid cells mainly included California, Arizona, Nevada and Utah. The coarse domain for MM5 covers the whole North American continent. The troposphere from ground to 100hPa was divided into 29 model sigma layers, with 16 unevenly distributed vertical layers within the lower 2000m. The lowest layer near the ground was 7m, and highest resolution was maintained near the ground to better capture boundary-layer processes. The data for initialization and side boundary conditions were from NCEP/ETA model, NCEP global surface observations and NCEP global upper air observations. The National Emissions Inventory (NEI) databases of 2001 (for the US) and 1999 (MEXICO) were used for air quality simulations. For runs with default initial/boundary conditions, the simulation began at 00GMT on August 4 and ended at 00GMT on August 11. The results of the first 4 days were discarded to account for the spin-up.

2.2 Data for Model Evaluation

The surface data used for CMAQ evaluation were from the AIRS; and for MM5 evaluation were from the California Air Resources Board (http://www.arb.ca.gov/aqmis2/paqdselect.php). The satellite data included: SCanning Imaging Absorption Spectrometer for Atmospheric Chartography (SCIAMACHY) (Bovensman et al. 1999), Ozone Monitoring Instrument (OMI)

(Pieternel et al. 2006) and Tropospheric Emission Spectrometer (TES) (Beer et al. 2001). SCIAMACHY provides tropospheric NO_2 vertical column densities (VCDs) with a resolution of 30km×60km at about 10:30LT; OMI provides tropospheric NO_2 VCDs with a resolution of 13km×24km at about 14:00LT; TES provides ozone profiles in troposphere with a higher resolution.

3. COMPARISON METHODS

3.1 Tropospheric NO_2 VCDs

For consistent comparisons both spatially and temporally, the simulated concentrations were integrated from the bottom to the model top and then integrated to the satellite pixel by the area-weighted method exactly at the time where SCIAMACHY/OMI data were collected. Some commonly used statistical parameters were calculated, which include: correlation coefficient (R), Mean Bias (MB) and Normalized Mean Bias (NMB). Considering that satellite data have gross retrieval errors (GRE), mean absolute bias (MAB) with CAMQ and mean gross retrieval error (MGRE) were calculated as:

$$MAB = \frac{1}{N}\sum_{i=1}^{N}(VCD_{CMAQ,i} - VCD_{SATT,i})$$

$$MGRE = \frac{1}{N}\sum_{i=1}^{N} GRE_i \ .$$

Here, $VCD_{CMAQ,i}$ and $VCD_{SATT,i}$ are the simulated and satellite-observed tropospheric NO_2 vertical column densities (VCDs) in the i^{th} pixel. GRE_i is the gross retrieval error for the i^{th} Pixel. N is the total pixel number.

3.2 Ground level O_3

The methods used to evaluate the model based on ground-level ozone include:

(1) Graphical procedure: Preparing scatter plot for all hourly prediction-observation pairs for all sites for each simulation, as recommended by the USEPA (1991) for model evaluations.

(2)Statistical Evaluations: The use of commonly used statistical parameters as discussed in section 3.1 for all model cells containing the observational sites

4. VALIDATION OF MODELING RESULTS

4.1 MM5

Bilinear interpolation was used to obtain simulated ground level parameters for each site in San Diego and Imperial Valley. In general, MM5 could capture the hourly variation of surface temperature very well. The average correlation coefficients for temperature in San Diego and Imperial Valley are 0.938 (range from 0.866 to 0.967, over 7 sites) and 0.885 (0.843 to 0.913, over 6 sites), respectively. However, the model generally overestimates the surface temperature all the time for San Diego and at night for Imperial Valley. The correlation for wind speed comparison is not as good as that for temperature; e.g., 0.457 for San Diego (ranging from 0.146 to 0.665; 8 stations) and lesser for Imperial Valley. The dominant surface wind direction generally changes twice a day, and modeled wind direction lags behind the data for San Diego whereas the model did not capture well the wind direction at Imperial well.

4.2 CMAQ

(i) Comparisons of surface O_3

The average statistical results for all model cells in the U.S. containing observational sites for the two domains are included in Table 1. For ozone in the coarse/finer domain, the correlation coefficient is larger than 0.6 for majority of cells. The NMB is between -25% and 25% at more than half of the cells. In the coarse domain, aside from two minuses, the positive correlation coefficient ranges from 0.13 to 0.95.

Table 1 Statistical results of ground Ozone between AIRS and CMAQ

Parameters	Coarse Domain	Finer Domain	TES-BC -Coarser
correlation	0.51	0.43	0.498
Slope	0.47	0.39	0.499
Intercept (ppb)	21.9	22.5	23.4
NMB(%)	6.5	-2.3	13.99
MB(ppb)	-6.8	-3.2	2.67
Sample(r>0)	194	237	192
No(r>0.6)	149	146	144
No(|nmb|<25%	133	147	135
No (r<0)	4	2	6

Here: the linear equation is Y=A×X + B, where X, Y, A and B refer to observed ozone, modeled ozone, slope and intercept.

As for Mexico, data from nine observational sites located in 6 different coarse model grids are available. The correlation of O_3 ranges from 0.29 to 0.76, with an average of 0.62. The model over-predicted the surface O_3 at most sites.

The performance (as quantified by the correlation coefficient) of coarse domain simulations is better than that of finer domain simulations. As for the twin cities with ozone episode, the temporal correlations in San Diego are quite good, but the simulated ozone maxima lagged the observations about 3 to 4 hours (Figure 1). Figure 2 shows a scatter plot for all (hourly) observations-simulations pairs in coarse domain.

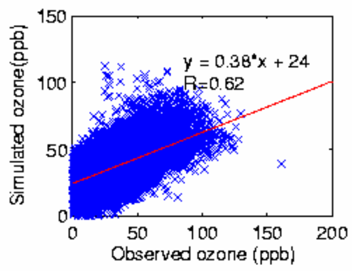

Figure 2 Scatter plot of hourly ozone

(ii) Comparison of NO_2 VCDs between SCIAMACHY and CMAQ

Composite distributions of NO_2 VCDs from SCIAMACHY and CMAQ for the coarse domain are shown in Figure 3, indicating that the model can reproduce the observed characteristics of NO_2 VCDs in the morning (around 10:30LT), especially for hot spots in areas such as Los Angeles and San Diego. Statistical results for the two domains are tabulated in Table 2. Table 2 indicate that the simulated NO_2 VCDs are highly correlated with SCIAMACHY observations, although the model under-predicted the tropospheric NO_2 columns approximately 57% of the time in coarse domain and 33% of the time in finer domain. However, MAB is somewhat smaller than MGRE in two domains.

(iii) Comparison of NO_2 VCDs between OMI and CMAQ

Composite distributions of NO_2 VCDs from OMI and CMAQ for the coarse domain are shown in Figure 4, which shows that the model can replicate the observed characteristics of NO_2 VCDs, especially those hot spots of high NO_2 columns. The statistics of comparisons are shown in Table 2, which shows that the simulated NO_2 VCDs correlates reasonably well with OMI. The model, however, under-predicts the tropospheric NO_2 column content in approximately 75% of the stations in the coarse domain and 68% in the finer domain. For OMI, the MAB is larger than MGRE.

The above comparisons show that the model predicts better the spatial distribution of tropospheric NO_2 VCDs in the finer domain, perhaps due to increased resolution of the pollution inventory. In addition, the model under-predicts NO_2 when compared with both SCIAMACHY in the morning and OMI at ~ 14.00LT, but the negative bias in the latter is larger. The anachronous pollution inventory is perceived to be a large source of uncertainty, and an updating of the available inventory is recommended for better results.

5. THE USE OF TES DATA FOR CMAQ/INITIAL/BOUNDARY CONDITIONS

To assess the usefulness of satellite data of the troposphere in CMAQ calculations, the TES -based ozone profiles (obtained at 06:00 UTC, August 4) were interpolated to the 3D model grids of 36km resolution to implement as the initial condition for CMAQ (in lieu of CMAQ default initial condition). Also, the TES data at 06:00 UTC on August 4 and 8 were interpolated to boundary grids to implement as boundary conditions. The data of August 4 were used for August 4-7 and of August 8 were used for August 8-10. The statistical results with surface ozone and satellite observations were compared with those obtained with default boundary/initial conditions of CMAQ.

5.1 Surface Ozone

Statistics of comparisons for surface ozone concentrations between observations and CAMQ simulations (with and without TES data ingestion) are tabulated in Table 1. Accordingly, the differences between the two simulations are negligible for most cases.

5.2 Comparison with Tropospheric NO_2 (OMI and SCIAMACHY)

Statistical comparisons between simulated (with TES initial and boundary conditions) and SCIAMACHY and OMI observations are tabulated in Table 2. There is either very little or no change of performance of CMAQ when TES data are ingested as initial/boundary conditions.

5.3 Comparison of tropospheric O_3

profiles

Simulations with default initial/boundary conditions under-predicted ozone in the upper troposphere in different land use divisions considered in this study. For heights above 8km, the simulated ozone concentration was ~ 70ppb, which is close to the default no-flux boundary conditions of CMAQ (70ppb) at the model top. In the lower troposphere, however, the predicted and TES-measured ozone showed better agreement. Also note that CMAQ employs zero-gradient (Neumann) boundary condition in the lateral direction, thus making the effects of side boundaries weaker.

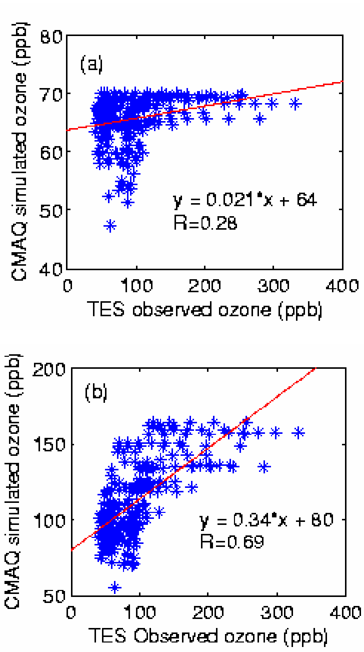

Figure 5 Comparisons of ozone concentration in the upper troposphere (over 500mb) between CMAQ and TES ((a): Simulations without TES input data; (b) Simulations with TES input for initialization)

For cases where TES data were used for initial/boundary conditions, a significant improvement was noted in CMAQ predictions for the upper troposphere when compared with subsequent TES observations, which can be seen from the plots shown in Figure 5. Here the correlation coefficient changed from 0.28 to 0.69. Similar plots were also made for the lower troposphere, but the correlation was low, for both default and TES based initializations.

6. CONCLUSIONS

Models-3 (MM5/SMOKE/CMAQ) with emissions from the National Emissions Inventory (NEI) database of 2001 for the US and 1999 for MEXICO was applied to simulate an ozone episode in San Diego area occurred on August 9, 2006. Ground level observations of ozone and satellite observations of tropospheric NO_2 column contents and ozone profiles were used to evaluate the model performance. The modeled NO_2 VCDs were correlated well with SCIAMACHY measurements. The correlation between OMI and CMAQ are not as good as that between SCIAMACHY and CMAQ. The model underpredicted the tropospheric NO_2 column in terms of comparing with both satellites measurements.

In general, in most observational sites, the diurnal patterns of ozone were reproduced satisfactorily by CMAQ. For coarser and larger domains, two thirds of model cells containing surface observations showed a correlation larger than 0.6 and a NMB between -25% and 25% when (AIRS) and CMAQ (lowest level) are compared. In the case of comparisons for finer and smaller domains, similar levels of correlation and NMB were also shown by more than two thirds of model cells containing surface observations. The correlation for all hourly prediction-observation pairs in the coarse domain is 0.62.

The sensitivity tests with TES data as initial/boundary conditions did not show, when viewed in terms of correlation coefficients, an appreciable improvement in the predictions of surface ozone concentrations (AIRS observations); tropospheric NO_2 columns (SCIAMACHY and OMI); and ozone concentration in the lower troposphere (TES). This modification, however, did show a significant improvement in the correlation coefficient between CMAQ predictions and TES observations of the upper-tropospheric ozone.

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Table 2 Statistics of comparison between Satellite (SCIAMACHY/OMI) measurements and CMAQ simulations for the tropospheric NO_2 column content

Parameters	SCIAMACHY			OMI		
	Coarse	Finer	TES-BC	Coarse	Finer	TES-BC
Correlation(r)	0.775	0.812	0.618	0.4761	0.561	0.442
Slope	0.4313	0.6251	0.4813	0.1607	0.2997	0.228
Intercept	0.0736	0.0682	0.0657	0.1753	0.0335	0.0918
MB	-0.63	-0.51	-0.59	-1.12	-1.35	-1.15
NMB(%)	-51	-33	-46.7	-73	-68	-71.4
MAB	0.79	0.95	0.859	1.19	1.447	1.22
MGRE	0.81	1.02	0.82	0.75	0.878	0.76
Total Pixels	1607	371	1622	29637	6196	32496

Here: the linear equation is Y=A×X + B, where X, Y, A and B refer to satellite measured NO_2 column, modeled NO_2 column, slope and intercept. The units of MB, MAB and MGRE are 10^{15}moleculaes/cm^2

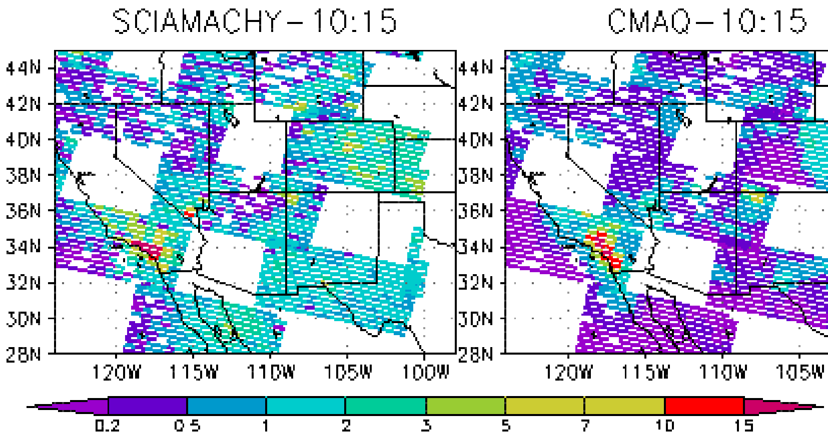

Figure 3 Distributions of tropospheric NO_2 columns from SCIAMACHY and CMAQ

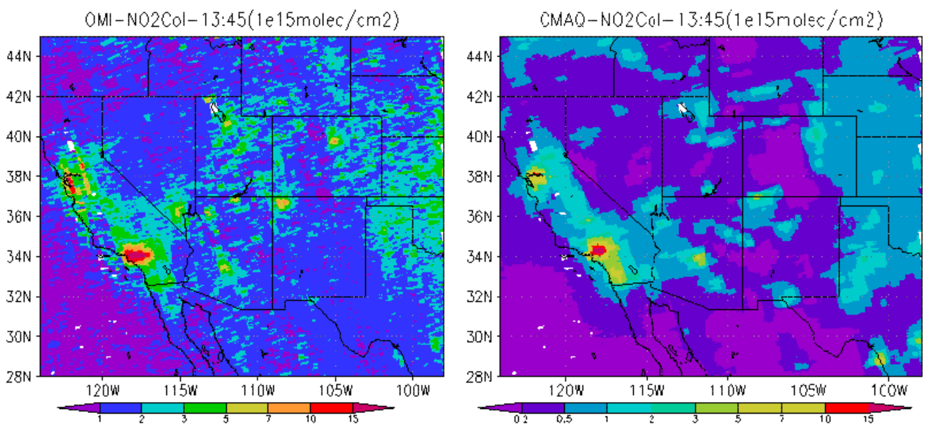

Figure 4 Distribution of tropospheric NO_2 columns from OMI and CMAQ