5.5 Apportionment of Contributors to Ozone in three U.S./Mexico Border Twin-cities

by

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1. Introduction

During the past decade, several sister cities along the U.S.-Mexican border, for example, San Diego/Tijuana**,** El Paso/Ciudad Juárez/Sunland Park and Calexico (Imperial Valley)/Mexicali have experienced air quality problems associated with ozone. While sometimes these problems are associated with local generation of ozone, in other times the transport of ozone and its precursors by flow cause these cities to bear the brunt of pollution generated elsewhere. Insights on geographical patterns, movements and photochemistry of ozone in the U.S.-Mexico border can provide valuable tools for policymakers in instituting ozone mitigating strategies. In this study, the integrated process analysis (IPA) technique of the Models-3 (MM5/SMOKE/CMAQ) air quality modeling system and the Hybrid Single Particle Lagrangian Integrated Trajectory model (HYSPLIT4) (Draxler, R. R., 1997) was used to apportion contributors to high ozone in the three twin cities listed above.

According to EPA's Aerometric Information Retrieval System (AIRS), high ground level ozone concentrations were observed at the three twin cities of the U.S./Mexico border during June 1-4, 2006, and thus this period was selected as the design days. In particular, San Diego recorded daily ozone episodes during June 2-4, Imperial Valley during June 1-3 and El Paso on the June 3 (see Figure 1a).

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2. Modeling System and Data

The simulations were conducted using the following codes: PSU/NCAR meso-scale meteorology model (MM5) v3.7; Meteorology-Chemistry Interface Processor (MCIP) v2.3; Sparse Matrix Operator Kernel Emissions Processor (SMOKE) v2.2; and Chemical Transport Model (CMAQ) v4.5.1.The simulation used a Lambert projection, centered at 40°N latitude and 97°W longitude, with 29 vertical layers from the surface to 100hPa (about 11-15km) and 13 unevenly distributed vertical layers within the lower 1000m, the layer closest to the ground being 7m to better capture boundary-layer processes. For MM5, four-dimensional data assimilation (FDDA) (3D and SFC) was used, with a horizontal resolution of 36km spanning the North American continent. For CMAQ and SMOKE, the domain covered the Southwestern US with 74×70 horizontal grids.

The data for initialization and lateral boundary conditions were from NCEP/ETA model, NCEP global surface observations and NCEP global upper air observations. The National Emissions Inventory (NEI) databases (2001 for the US and 1999 for Mexico) were used. CMAQ predictions were evaluated using AIRS data and MM5 using the California Air Resources Board (http://www.arb.ca.gov/aqmis2/paqdselect.php) data. The simulation began at 00UTC on May 28 and ended at 00UTC on June 5. The results of the first 4 days of spin up were discarded.

3. Validation of Model Results

3.1 MM5

In evaluating MM5, the simulated distributions of surface winds and pressure were compared with 3-hourly surface analysis charts from NOAA web (http://nomads.ncdc.noaa.gov:9091/ncep/NCEP.). Overall, the model replicates the observed flow and pressure patterns well. Then the bilinear interpolation was used to obtain ground level parameters (temperature at 2m, wind speed and wind direction at 10m) for each available station in San Diego, Imperial Valley and El Paso area.

The performance statistics for temperature are tabulated in Table 1. In term of the values of mean bias (MB), the temperature is somewhat overestimated in San Diego and El Paso and underestimated in Imperial; and the wind speed is overestimated in San Diego and Imperial and underestimated in El Paso. The index of agreement (I) reveals excellent performance for temperature, medium performance for wind direction and poor performance for wind speed. According to the rules postulated by Lu et al (1997) based comparing RMSDs of predictions and STD of observations, the MM5 performance is acceptable, except for the wind speed in San Diego and Imperial valley.

3.2 CMAQ

The distributions of maximum 1-hr ozone in the domain for June 3 are shown in Figure 1b, and only the grids containing observational sites are shown. Figures 1a and 1b show that the model in general reproduces the maximum 1-hr ozone distribution, although a tendency for under prediction can be seen.

There are 9 ozone monitor stations in San Diego, 6 in Imperial Valley and 11 in El Paso, TX and nearby Dona Ana, NM, based on which the performance evaluation is tabulated in Table 2. The model over-predicted the average ozone in San Diego and Imperial Valley and under-predicted in El Paso. The indices of agreement is medium, in San Diego (0.58~0.78), Imperial Valley (0.63~0.76) and El Paso (0.54~0.82). All RMSDs are within STDs of observations, but STDs of predictions are about one half of the observations, which may be a result of the over-prediction of ozone at night. Some exceptions could be seen, however, as far as the individual stations are concerned: e.g. RMSDs at the site SD-D (with highest elevation) and sites SD-E, I, F, H (lowest elevations and close to water) are larger than the corresponding STD of observations, but they have comparable values of simulated and observed STDs.

4. Process analysis for ozone formation

The IPA includes the integrated process rate (IPR) analysis and integrated reaction rate analysis (IRR). Using IPR, it was possible to estimate contributions of different processes to the ozone level at a given location. The model cells chosen for the three regions are defined as A, B and C in Figure 1a, and hourly IPR for five salient contributory processes are presented in Figure 2. These are: gas-phase chemical production (chem), horizontal transport (hadv), vertical advection (zadv), vertical diffusion (dif) and dry deposition (dep).

Note that all processes have diurnal variations. hadv and zadv are almost out of phase, with hadv transporting ozone into San Diego in late morning and early afternoon while transporting out at night. The opposite occurs in the Imperial Valley and El Paso. As expected, chem produces ozone during day and consumes at night with a positive maximum at around noon and negative maxima at sunset (18:00LT) and sunrise (06:00LT). Vdif roughly balances the deposition, but the former can be somewhat higher mostly at night; i.e. vdif +ddep >0 has two positive maxima (early morning and evening) and a minimum (noon), with the morning maximum corresponding to the rapid increase of ozone concentration in the morning. This shows that fumigation of ozone is very important to the rapid rise of ground level ozone in the morning. During the period of ozone increase in San Diego (~ 6:00 to 15:00), the main contributors are the vertical diffusion (dif), horizontal advection (hadv) and chemistry (chem); and for Imperial Valley and El Paso, the vertical diffusion (dif), vertical advection (zadv) and chemistry (chem). After peaking, the ozone in San Diego is removed by horizontal advection and titration and in Imperial Valley and El Paso by the vertical advection and titration at night.

It was also found that ozone is transported out of San Diego within the lower boundary layer at night, and there is an influx of ozone into the area during the day. Therein, the maximum influx usually occurs at the height of ~ 100 m at about 18 UTC (10 LT). On the other hand, in the lower boundary layer, ozone is transported into Imperial and El Paso during the night to early morning and out of it during the day. The maximum inflow of occurs at ~ 100m at about 06UTC in Imperial Valley and at 11UTC in El Paso at the same height.

5. Back trajectories analysis for all high ozone days in warm season of 2006

To understand the origins of ozone, HYSPLIT4 was used to calculate 72-h back-trajectories on all high ozone days (1-hr maximum > 80ppb) in the warm season (May to September) of 2006. FNL archived data provided by NOAA was used in back-trajectory calculation. The site with highest ozone from each region was chosen for the analysis, considering that the hourly ozone measurements during the warm season of 2006 show a high correlation with the nearby stations and thus are representative.

The starting height (100m) and time (18:00UTC, 06:00UTC and 11:00UTC for San Diego, Imperial and El Paso, respectively) of back trajectories corresponded to those of maximum ozone influx by transport. The results are shown in Figure 3. By cluster analysis (Brankov et al., 1998), these trajectories can be further grouped to show their potential origins. The ozone-rich air masses were mainly transported from the coastal area by north-westerly winds in the lower boundary layer to San Diego during the day time, augmented by a few trajectories from north or south (Mexico). For Imperial Valley, the back trajectories are mainly from to three directions, North West (22 days, Los Angles and San Diego), Southeast (16 days, Mexico), and North (4 days). For El Paso, the back trajectories originate mainly in Texas (13 days) and Arizona (8 days) and in a few cases in Mexico (5 days).

6. Summary and conclusions

Models-3 (MM5/SMOKE/CMAQ), with emissions from the National Emissions Inventory (NEI) database of 2001 (for the US) and 1999 (MEXICO), was used to simulate ozone episodes that simultaneously occurred in San Diego, Imperial Valley and El Paso area during June 1-4, 2006. Process analysis, together with back trajectories, was used to apportion the sources of ozone for three U.S.-Mexico border cities. The model predictions were evaluated against ground level observational data by computing conventional statistical measures, and the performance measures were found to be in acceptable ranges.

The integrated process rate analysis (IPA) was used to understand the reasons for high ozone concentrations three U.S./Mexico border cities. The results indicated that ozone was transported within the lower boundary layer into San Diego during day time and out during night and into the Imperial Valley and El Paso during night or early morning and out during day. The occurrence of high ozone is mainly contributed by vertical diffusion, horizontal advection and chemistry in San Diego; and, vertical diffusion, vertical advection and chemistry in Imperial Valley and El Paso. Based on results of IPA, back-trajectory analyses were conducted to understand the origins of such ozone in the warm season of 2006. The results indicated that ozone was transported from the coastal area of the northwestern California for the case of San Diego; Mostly from the east or coastal area of northwestern California and about one third from Mexico for the Imperial Valley; and from the Texas and Arizona for El Paso.

References:

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Table 1: Summary of statistical measures, in comparing observations to model predictions of temperature, wind direction (WD) and wind speed (WS)

Regions	Variables	Observed		Modeled		RMSD	*I*	MB
		Mean	STD	Mean	STD			
San Diego	Temp(K)	294.44	4.88	295.83	5.35	3.35	0.89	1.39
	WS(m/s)	1.38	1.20	2.92	1.36	1.96	0.60	1.54
	WD(deg)	258.45	76.41	245.51	97.76	73.10	0.81	
Imperial	Temp(K)	307.08	7.17	305.19	5.71	2.99	0.95	-1.88
	WS(m/s)	1.82	1.13	2.68	1.16	1.79	0.40	0.86
	WD(deg)	162.34	102.56	221.17	60.34	90.90	0.72	
El Paso	Temp(K)	298.00	4.96	299.06	4.55	2.55	0.93	1.05
	WS(m/s)	3.71	2.49	3.38	1.20	2.33	0.53	-0.33
	WD(deg)	125.63	68.94	129.70	41.43	65.74	0.58	

Reference: STD (standard deviation); RMSD (Root Mean-square Difference); I (index of agreement) is between 0 and 1, and 1 for perfect agreement. MB (Mean Bias);

Table 2 Statistical measurements of model performance for surface ozone

StaNO	MeanObs	MeanPre	Index	rmsd	Sta_D_Obs	Sta_D_Pre	MB
SD	41.08	57.96	0.69	24.64	25.05	15.12	16.88
IMP	50.91	53.42	0.64	17.94	22.13	8.95	2.51
TEP	48.26	40.87	0.75	14.61	19.23	9.61	-7.39

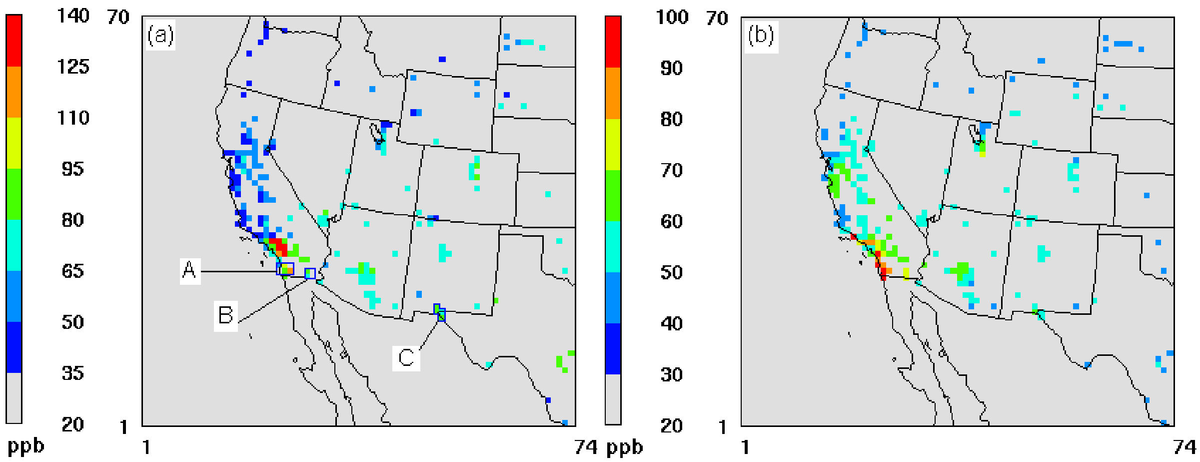


Figure 1 Distributions of maximum 1-hr ozone on June 3, 2006: (a) Observation, (b) Prediction. Here: blue open squares denoted by A, B, C refer to San Diego, Imperial and El Paso respectively, which was used for process analysis and Figures 3-5.

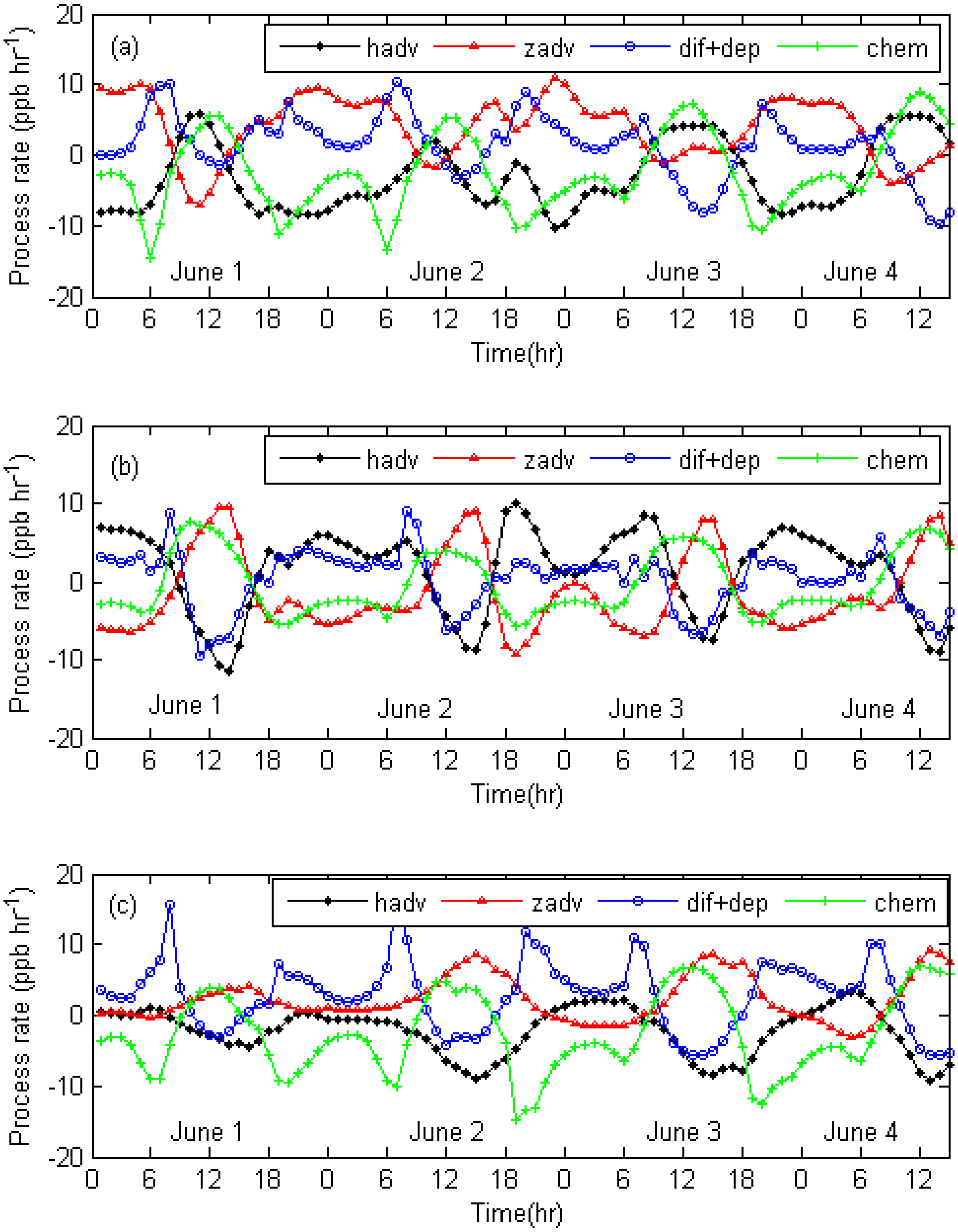
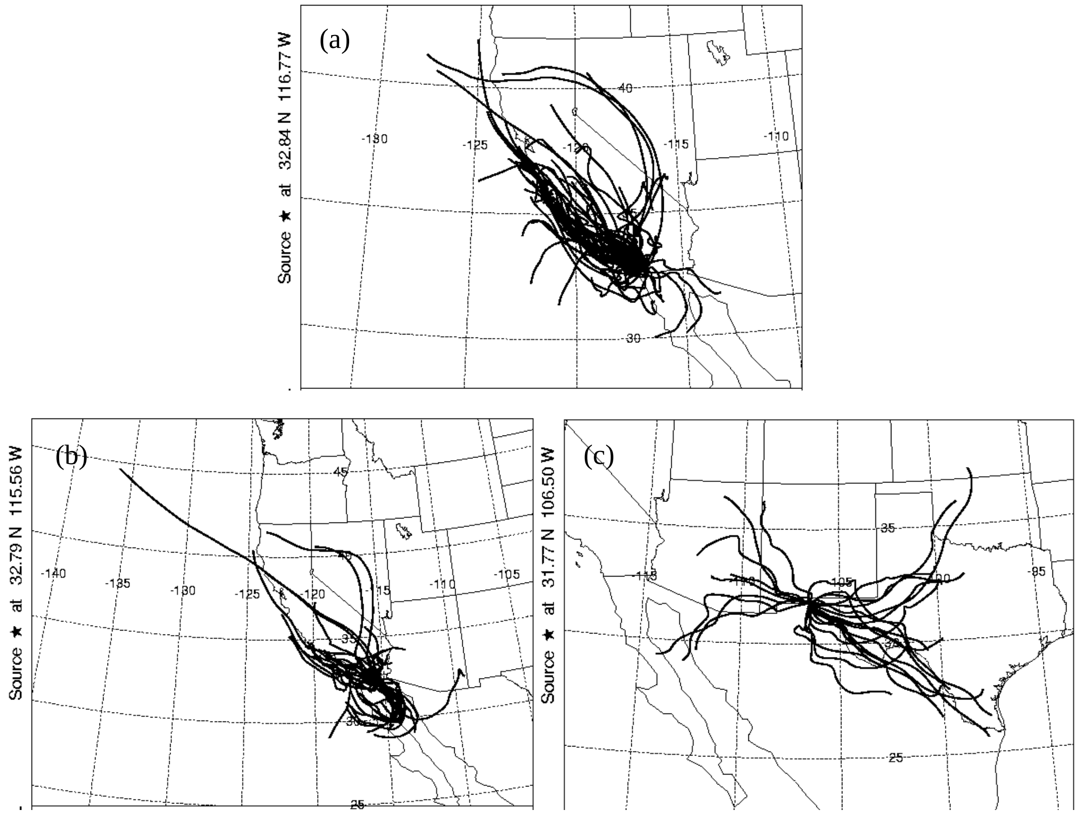


Figure 2 Relative contributions of individual rate processes to the predicted concentration at the surface (model) layer for San Diego (a), Imperial (b) and El Paso (c). (Local time)



(a) San Diego

Figure 3 Distribution of 72-hr back-trajectories on days that have maximum ozone (>80ppb) from May to September in (a) San Diego (63 days), (b) Imperial Valley (42 days) and (c) El Paso (26 days)