Mexico City air quality simulation

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ABSTRACT

The effect in ozone diurnal evolution due to changes in the hydrocarbons (HC) and nitrogen oxides (NOx) emissions temporal pattern under Mexico City Metropolitan Area (MCMA) conditions was simulated using the CIT (California/Carnegie Institute of Technology) airshed model. Changes involve the shift of one hour, backward and forward, in the emissions temporal pattern. The simulations include two scenarios, the former with a high hydrocarbon to nitrogen oxides (HC/NOx) ratio, closer to actual MCMA ratios, and the latter with a low ratio. The changes in the ozone peak are more important under this second case; i.e., increased ozone peak is observed when the emissions are shifted one hour earlier and decreased when the emissions are shifted forward.

No changes were observed in the solar time for the peak under either scenario. The results might be considered in good agreement with monitored data; the discrepancies, nevertheless, point those areas where the emission inventories are more uncertain.

INTRODUCTION

Air quality models have been emerged as a useful tool to assess the response of ozone to the adoption of given control strategies, as well as to determine those areas with larger impact.

An air quality model is a mathematical description of atmospheric reaction, transport, diffusion and fate of pollutants in a given region. The most important application of air quality modeling is the prediction of ozone evolution and other secondary atmospheric oxidants.

The CIT (California/Carnegie Institute of Technology) [1,2] airshed model has been selected to get insight of the effect in ozone formation due to changes in the time of the emissions of hydrocarbons and nitrogen oxides under Mexico City Metropolitan Area conditions. This model has been applied successfully to areas with similar ozone problems as the US California's South Coast Air Basin [3,4,5]. Due to the lack of reliable wind patterns for MCMA, the CIT photochemical code has been coupled to a wind field generated with the prognostic model HOTMAC [6].

Three cases under two different scenarios were simulated: the base case and the shift, one hour backward and forward, of the temporal pattern for total hydrocarbons (HC) and nitrogen oxides (NOx) emissions. The two scenarios involve high hydrocarbons to nitrogen oxides (HC/NOX) ratios (I), and low HC/NOx ratios (II).

METHODOLOGY

The CIT photochemical code has been adapted to be used under MCMA conditions. Within the model the LCC chemical mechanism [7] has been incorporated; under examination of the reactions involved in this mechanism it emerged as the appropriate to simulate the MCMA basin [8]. February 22, 1991, was selected for simulations as base case since enough information from intensive monitoring campaigns was available [9].

The emission temporal pattern for stationary sources was assumed as the difference in electric demand between weekend and week days [10]. For mobile sources emission pattern, the study of traffic in a pilot area was considered [11]; both temporal patterns are shown in Figure 1. The met and chemical fields were constructed from data provided by the Sedesol monitoring network [12].

For the airshed modeling a tridimensional grid in seven vertical layers, with 2400 meters as maximum height was used. The horizontal grid contains 14 x 16 cells, with 5 x 5 km2 each. The emission inventory comes from *Programa Integral de Lucha contra la Contaminación Atmosférica* (Comprehensive Program Against Air Pollution), and pollutant emission spatial distribution is reported in reference 13.

Airshed simulations were done for two scenarios: In Scenario I a high HC/NOx ratio (average from 600 to 900 hours) was considered. Recent hydrocarbon measurements show an averaged HC/NOx ratio of 35 [14]. For comparison simulations with low HC/NOx ratios were also performed, using the same simulation conditions.

The results for the diurnal ozone variation are compared with ozone data from several monitoring stations in different geographic zones of the MCMA:

these are, La Merced (located downtown), Acatlán and Tlalnepantla (at northwest), Pedregal (southwest) and Iztapalapa (southeast).

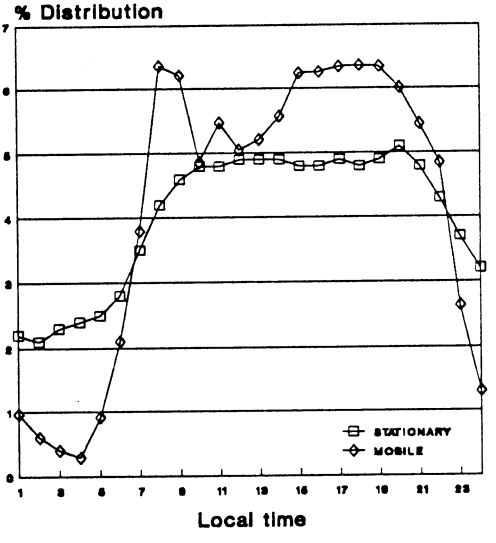


FIGURE 1. Temporal emission distribution

RESULTS AND DISCUSSION

The simulated diurnal ozone variation for base case under conditions of Scenario I is shown in figures 2 and 3; in such figures along with the simulated values for the cells corresponding to the sites where some monitoring stations are located, the one hour average monitored ozone values are also displayed.

The agreement between the monitored and simulated data is fairly good all over the city. The best agreement was obtained for the Pedregal station (Figure 2a) in the SW area. However, discrepancies between simulated and monitored data appear going from west to east and from south to north. The discrepancies at some stations, in particular at Merced and Tlalnepantla, advise of uncertainties in the emission inventories.

Within the same figures the effects in ozone levels due to changes in emissions, one hour in advance and delay, are also shown. Very little effect is appreciated in most of the cases; in fact the changes in ozone peak for the stations used for data comparison are within the range 0-15%. This last value is observed only at one site, Tlalnepantla, for the case of shifting the emissions one hour in advance. It is worth noting that at this station the worse agreement between simulated and monitored data was obtained.

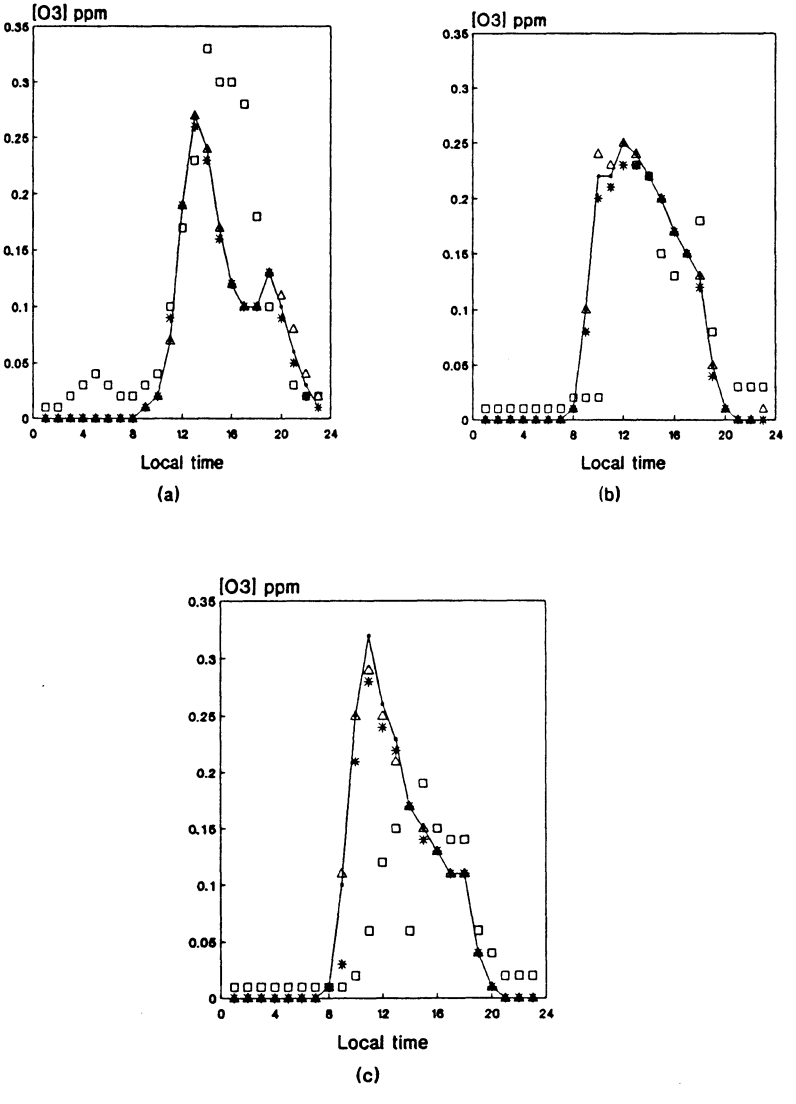
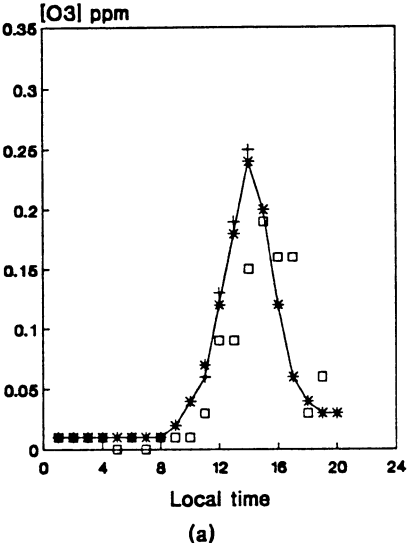


Figure 2. Scenario I ozone diurnal variation and effect of temporal emission pattern. Simulation for Base Case (—), Advance 1 hour (Δ), Delay 1 hour (✱), Monitored Data (□). (a) Pedregal Station (SW), (b) Iztapalapa Station (SE), (c) Merced Station (DT).



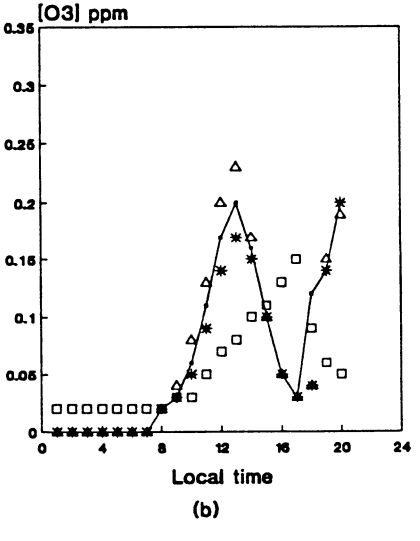


Figure 3. Scenario I ozone diurnal variation and effect of temporal emission pattern. Simulation for Base Case (—), Advance 1 hour (Δ), Delay 1 hour (✱), Monitored Data (□). (a) Acatlán Station (NW), (b) Tlalnepantla Station (N)

The shape of the ozone diurnal variation for the most stations, reflects a fast ozone peak formation and a very quick decrease in the afternoon. This behavior may be explained on the basis of the high hydrocarbon to nitrogen oxides regime in the afternoon, where the nitric oxide becomes the limiting species for the ozone-forming reaction

$$RO_2 + NO \text{ --> } RO + NO_2$$

and it becomes not kinetically important; instead, the reaction

$$RO_2 + O_3 \text{ --> } RO + 2O_2$$

becomes the driving reaction leading to a fast ozone elimination at this time of the day.

Ozone evolution depends both on the concentration and composition of the hydrocarbon mixture and on its ratio to NOx; a drastic increase of NOx emissions (ten times the corresponding values of each cell) was performed to produce Scenario II. The simulated HC/NOx average ratios (600 to 900) for both scenarios are shown in Table I.

Table I. HC/NOx ratios. Average 600 to 900 hours.

Station	Merced	Acatlán	Tlalne pantla	Iztapa lapa	Pedregal
Scenario I (High HC/NOx)	19.69	1.52	4.67	11.86	14.90
Scenario II (Low HC/NOx)	2.00	0.78	1.66	1.69	2.52

In the Table, it can be seen that the HC/NOx ratios for Scenario I simulations are closer to measured values than those with Scenario II. Nevertheless, the diurnal ozone evolution for Merced and Tlalnepantla base cases show much better agreement under this new scenario, as it may be seen in Figures 4c and 5b. These results confirm the assumption that for the cells containing such stations the NOx emissions were underestimated within Scenario I.

It is worth to note two additional features of this last simulation set. First, the discrepancy between the ozone values obtained for the Pedregal cell and the values reported by the monitoring station (Figure 4a) confirm that in this site the HC/NOx ratio should be high, as in Scenario I; probably the HC local emissions are related with mobile sources as stated in the MCMA emission inventory spatial distribution document [13]. Second, for the southeast part of the city

(Iztapalapa) the agreement of both simulated scenarios with monitored ozone concentration may be considered in reasonable good agreement; however, in both cases the maxima are slightly overestimated in the simulations and the time for the peak is either in advance or delay. Probably the ozone behavior in this station depends on the structure of the wind field, as if the gaseous mass is deviated to the southeast instead of the southwest direction.

Figures 4 and 5 also show the changes in ozone formation when the emissions temporal pattern is shifted by one hour respecting to the base case. Under this new scenario (II) a general trend is present, the ozone peak increases when pollutants are emitted in advance and decreases when the emissions are delayed.

TABLE II. Ozone peak concentration (ppm), time (h) and change (%) due to emission pattern

Station	Merced	Acatlán	Tlalne pantla	Iztapa lapa	Pedre gal
	Scenario I		High HC/NOx		
Base case	.32	.24	.20	.25	.27
Time	1100	1400	1300	1200	1300
1h advance	.29	.25	.23	.25	.27
Time	1100	1400	1300	1200	1300
Change	-9.4	+4.2	+15.0	0.0	0.0
1h delay	.28	.24	.17	.23	.26
Time	1100	1400	1300	1300	1300
Change	-12.5	0.0	-15.0	-8.0	-3.7
	Scenario II		Low HC/NOx		
Base case	.15	.20	.09	.27	.15
Time	1600	1600	1600	1600	1400
1h advance	.17	.23	.10	.32	.17
Time	1600	1600	1600	1600	1400
Change	+13.3	+15.0	+11.1	+18.5	+13.3
1h delay	.12	.18	.08	.22	.12
Time	1600	1600	1600	1600	1400
Change	-20.0	-10.0	-11.1	-18.5	-20.0

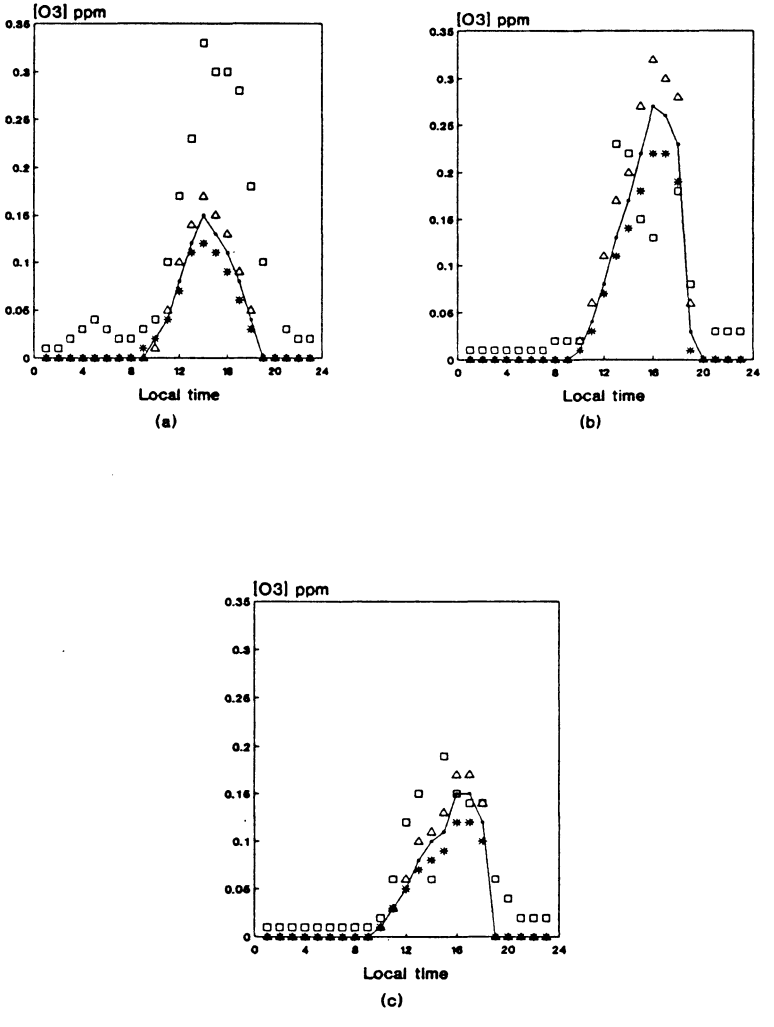
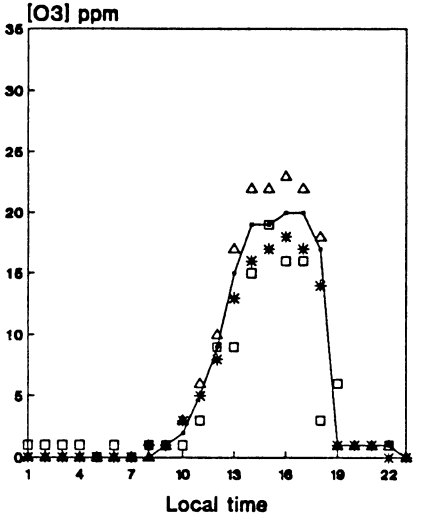


Figure 4. Scenario II ozone diurnal variation and effect of temporal emission pattern. Simulation for Base Case (—), Advance 1 hour (Δ), Delay 1 hour (✱), Monitored Data (□). (a) Pedregal Station (SW), (b) Iztapalapa Station (SE), (c) Merced Station (Downtown).



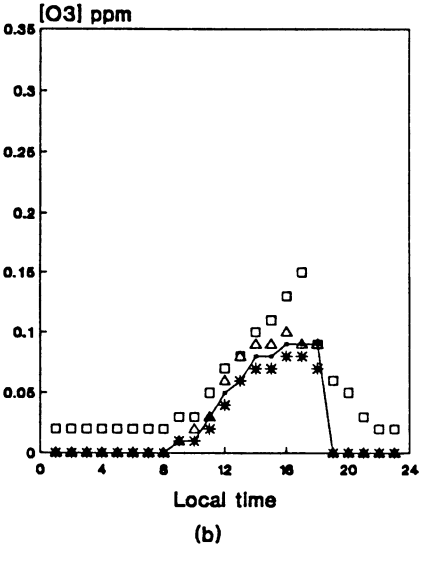


Figure 5. Scenario II ozone diurnal variation and effect of temporal emission pattern. Simulation for Base Case (—), Advance 1 hour (Δ), Delay 1 hour (✱), Monitored Data (□). (a) Acatlán Station (NW), (b) Tlalnepantla Station (N)

The time and values of the simulated ozone maxima are shown in Table II. A comparison between Tables I and II show that the ozone behavior is less sensible to change in emission time than to the prevailing HC/NOx ratio.

The increase in the ozone peak due to the advance of the HC and NOx emissions under scenario II may be explained on the basis that there are more ozone precursors available at sunrise, leading to earlier photochemical formation of free radicals. The contribution of meteorological effects may also be influencing the ozone formation since the reaction volume is small longer, i.e., the concentrations of the ozone precursors are higher and the reaction rates increase.

CONCLUSIONS

Ozone airshed simulation with the CIT air quality model under MCMA conditions show for Scenario I, characterized by a high HC/NOx ratio, following the regime detected in Mexico City, that shifts in emission pattern do not produce important changes in ozone formation and maxima values. The effect both in the time and the magnitude of ozone peaks are, in general, meaningless and represent an insignificant decrease in ozone production for the delay of emissions one hour.

Simulations under scenario II, characterized by low HC/NOx ratio, reveal some changes in ozone peak; nevertheless, the solar time when the peak occurs remains the same. The changes, in a range of 0-20%, show a trend to increase the ozone peak when the emissions time is shifted one hour in advance and to decrease it when the time of the emissions is delayed one hour. It is to be noted that the HC/NOx ratio has more influence in ozone formation than the shift in the emission patterns.

This work has shown that high HC/NOx ratio is predominant over the MCMA; however, sites as Merced and Tlalnepantla have also important NOx emissions.

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