Preliminary comparison of ozone concentrations provided by the emission inventory/WRF-Chem model and the air quality monitoring network from the *Distrito Metropolitano de Quito (Ecuador)*

R. Parra, V. Díaz
Corpaire: Corporación para el mejoramiento del aire de Quito
Corresponding author address: rparra@corpaire.org

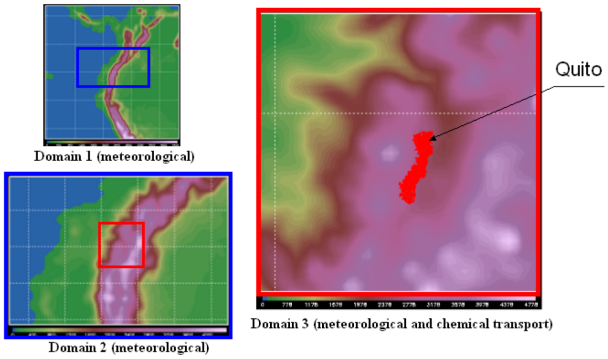
Abstract
The first emission inventory from the *Distrito Metropolitano de Quito (DMQ) (Ecuador)* and WRF-Chem were used to obtain O3 concentrations during the period 11th – 28th Sep/2006. A preliminary comparison with records of the automatic air quality monitoring network shows that during daytime hours, O3 concentrations are well captured by the model. During nighttime the model provides higher concentrations in both urban and suburban areas. It seems that background concentrations in the DMQ are lower than background values reported in the literature. The complex topography of the region, its allocation (next to the Equator), altitude (around 2800 masl) and the uncertainty of the emission inventory; are factors that could affect the performance of the model during nighttime. Results actually provided by the model are useful to track the behavior of O3 during daytime, when it is important to follow its increase owing to photochemical reactions. Average concentrations for the simulation period show correlation with altitude. Although model averages are higher than concentrations of the passive monitoring network, this tendency was ratified. Modeling helps to understand the link between emission sources and air quality in the DMQ. WRF-Chem needs to be tuned for the DMQ's conditions to capture well O3 concentrations during the whole day.

1 Introduction

The first version of the emission inventory from the DMQ was built by CORPAIRE [1], taking the year 2003 as baseline. Different emission models are being coded into a unique GIS tool called the *Sistema de Gestión de las Emisiones del DMQ (SIGIEQ)*. At present, emissions from on-road traffic, power facilities and other industries, vegetation, service stations and by use of solvents; are included within the SIGIEQ.
Hourly gas-phase emissions are speciated according to the Regional Acid Deposition Model (RADM) chemical mechanism [2]. They are used with WRF-Chem to simulate air quality in the DMQ.
The SIGIEQ/WRF-Chem model is considered the core of the future air quality forecasting model for the DMQ [3].
During 2006, the automatic stations recorded five times, hourly O3 concentrations higher than 120 µg m^{-3} [4]. Neither during 2005 nor 2006, no 8-hour O3 concentrations were higher than the updated WHO air quality guideline (100 µg m^{-3})[5].
In the DMQ the most important issues are both short-term and long-term exposures to PM2.5[4]. Average 2005/2006 PM2.5 concentration was 20.4 µg m^{-3}; twice the updated WHO air quality guideline (10 µg m^{-3})[5].
At present, diagnostic simulations of gas-phase are developed. In the future, aerosols will be included.
Incoming solar radiation is higher during summer season in the DMQ. Hence, in September an increase of O3 concentrations is recorded.
Modeling exercises of O3 provide first insights about the performance of the SIGIEQ/WRF-Chem model.
O3 mixing ratios obtained by modeling during the period 11th – 28th Sep/2006, were compared with data of the air quality monitoring network.

2 Domains for modeling

Figure 1 depicts the master and two nested domains used for simulation. The two first (d01: 27x27 km, d02: 9x9km) are used only for meteorological simulations. For the second subdomain (d03: 3x3 km), the chemical transport option is activated. Initial and boundary conditions were derived from one-way nesting using Final Analysis datasets from NCAR.



(Fig. 1: location of Quito and domains for modeling)

Table 1 summarizes the most important parameters. Simulations were made using WRFChem_v2.12_30may06. Boundary conditions were adjusted to 75% of default values.

Table. 1: Parameters for numerical simulation in the DMQ

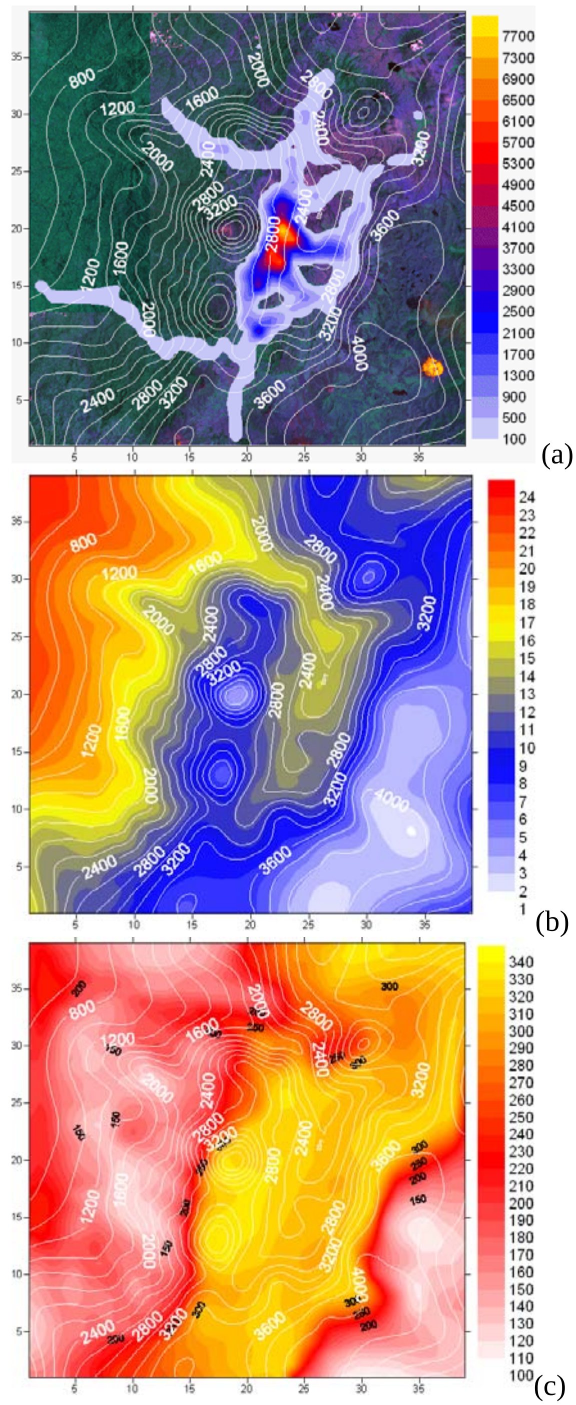
Parameters	**Values**	**Observations**
Domains		
e_we	100, 76, 40	
e_sn	100, 52, 40	
e_vert	26, 26, 26	
dx	27000, 9000, 3000	
dy	27000, 9000, 3000	
Physical parameters		
mp_physics	2	Lin et al.
sf_surface_physics	1	Monin-Obuknov
bl_pbl_physics	2	Mellor-Yamada-Janjic

3 The zone of study

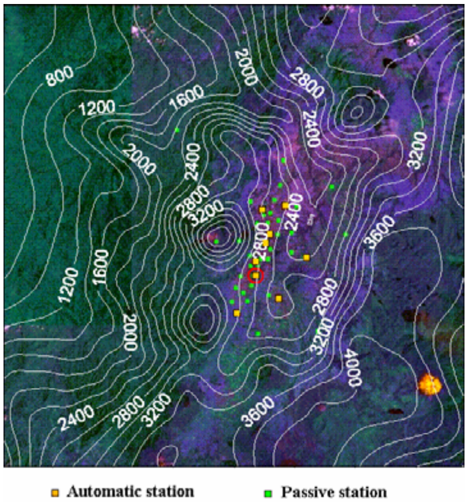
The DMQ is allocated near the Equator. It has a complex topography (Fig. 2) and its altitude is around 2800 masl. So, combustion processes are less effective due to less O2 than at sea level. Subdomain d03 has zones with height lower than 800 masl and higher than 4000 masl.
Meteorological WRF-Chem results show the expected reverse variation of the surface temperature with altitude. Figure 2 also shows the average incoming solar radiation during the simulation period.

4 Results

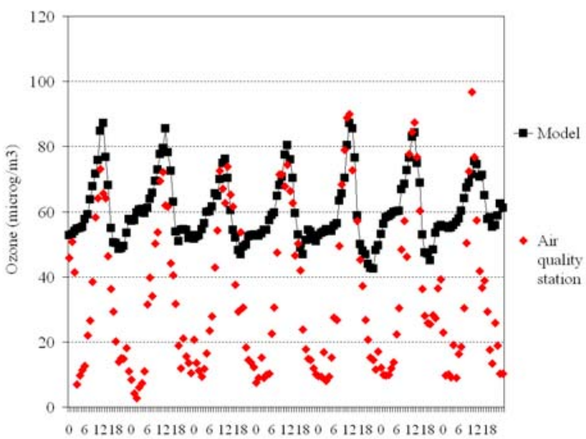
Figure 3 depicts the allocation of automatic (yellow dots, 9 stations) and passive (green dots, 43 stations) air quality stations, and the comparison between the model results and data recorded by El Camal air quality station.



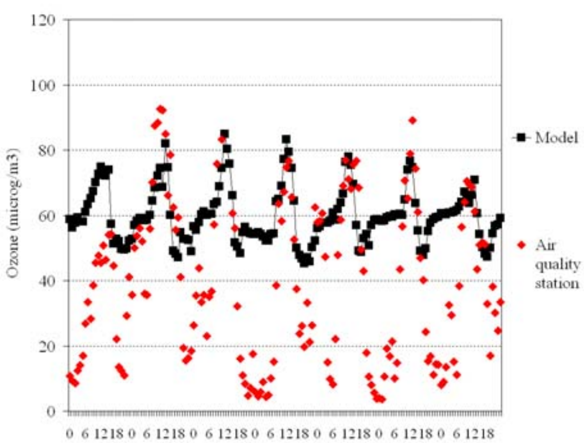
(Fig. 2: (a) topography (masl) and emission of CO (mol km^{-2} h^{-1}) between 07h00 – 08h00 for weekdays); (b) and (c), average surface temperature (ºC) and incoming solar radiation (W m^{-2}) during Sep/2006



El Camal air quality station (red circle)



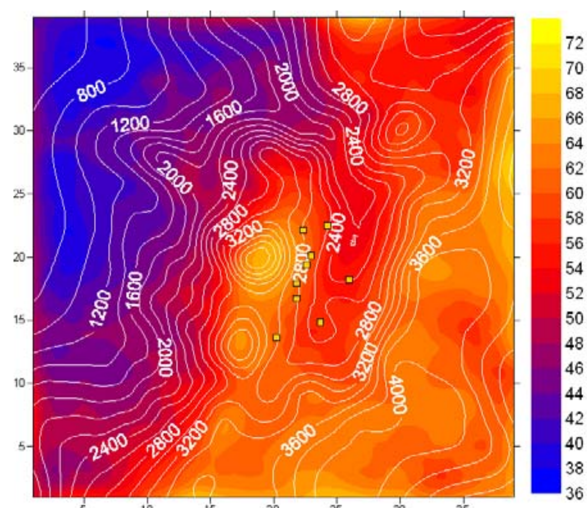
11th – 17th Sep/2006



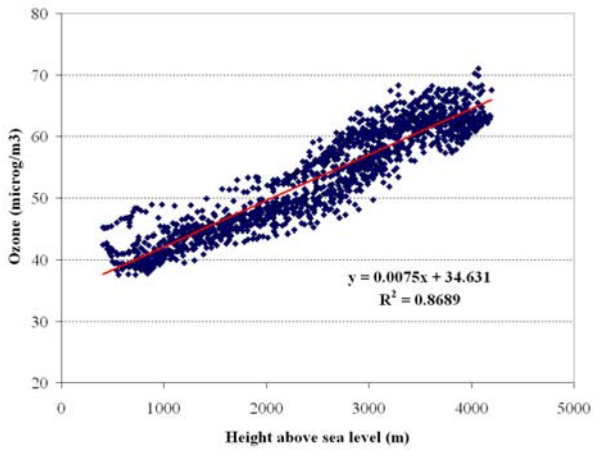
18th – 24th Sep/2006

(Fig. 3: hourly O3 concentration. Model results versus air quality records for the period 11th – 24th Sep/2006. El Camal station)

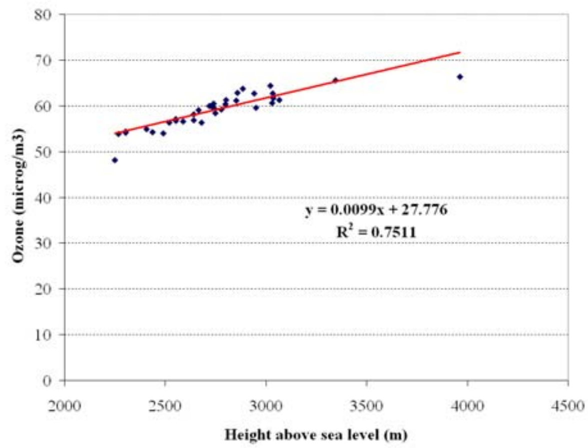
During daytime hours O3 concentrations are well captured by the model for most of the days (peak values until 90 µg m^{-3}). But, during nighttime the model provides concentrations between 50 – 60 µg m^{-3}, as long as records reach values until 5 µg m^{-3} in both urban and suburban areas.This behavior is similar to others air quality stations.
According to the information provided by the air quality network, it seems that O3 background concentrations in the DMQ are lower than background values reported in the literature. In remote locations, O3 concentrations typically range from 39 – 79 µg m^{-3} [6].
Results actually provided by the model are useful to track the behavior of O3 during daytime, when it is important to follow its increase owing to photochemical reactions.
Average concentrations for the simulation period are directly related with altitude (Fig. 4 and 5). This tendency was verified by records of the passive network. There is a significant increase in average O3 concentrations with altitude ($y = 0.0233x - 34.308$; $F_{1,41}=29.8$; $p<0.01$).
Model averages are higher than records due to its higher values during nighttime (Fig. 5)
Similar behavior of surface O3 mixing ratio with altitude is found in other regions [7]



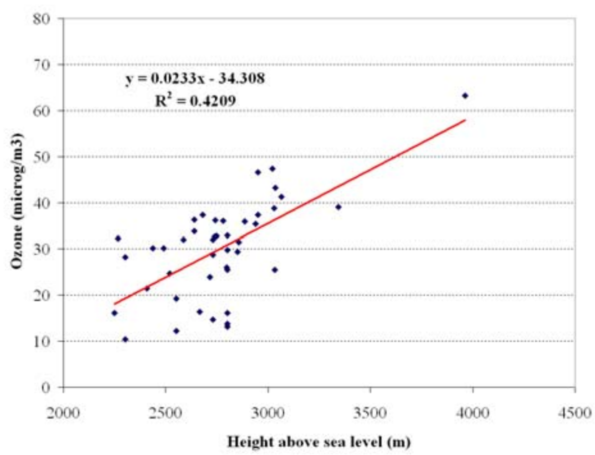
(Fig. 4: O3 average concentration (µg m^{-3}) for the period 11th – 28th Sep/2006)



SIGIEQ/WRF-Chem over all d03



SIGIEQ/WRF-Chem over the passive network points



Passive network

(Fig. 5: Variation of O3 average concentrations (µg m^{-3}) with altitude (masl) for the period 11th – 28th Sep/2006)

5 Conclusions

The particular features of the region and the uncertainty of the emission inventory, are factors that could affect the performance of the model during nighttime.

Owing to the high altitude, DMQ air contains less oxygen than at sea level. Determination of own emission factors, specially from on-road traffic, is a priority field of investigation. Updating the emission inventory is believed will improve the performance of the model.

In addition, WRF-Chem needs to be tuned for the DMQ's conditions in order to capture well O3 mixing ratios during the whole day.

In the future, aerosols emissions should be included to simulate PM2.5 pollution, the critical air quality issue in the DMQ.

The SIGIEQ/WRF-Chem model helps to understand the link between emission sources and air quality. At present it shows promising performance in the DMQ.

6 References

[1] CORPAIRE. *Inventario de Emisiones del Distrito Metropolitano de Quito 2003*. Quito-Ecuador, 65 p., 2006

[2] Stockwell, W.; Middleton, P., Chang, J. and Tang, X. *The Second Generation Regional Acid Deposition Model Chemical Mechanism for Regional Air Quality Modeling*. Journal of Geophisycal Research, 95 (D10), 16343 – 16367, 1990

[3] Parra, R.; Páez, C. Estrategia para el desarrollo de un modelo de predicción de la calidad del aire de Quito y resultados preliminares de la fase de diagnóstico. 1er Congreso Boliviano sobre Gestión de la Calidad del Aire Urbano. Cochabamba – Bolivia, 2006

[4] CORPAIRE. *Informe Anual 2006 de la calidad del Aire en Quito*. Quito-Ecuador, 2007

[5] WHO. *Air quality guidelines. Global update 2005*. (http://www.who.int/en/, May/2006)

[6] Seinfeld, J.; Pandis, S. *Atmospheric chemistry and physics. From Air Pollution to Climate Change*. John Wiley & Sons, Inc. New York (United States), 1326 p., 1998

[7] Ribas, A.; Peñuelas, J. *Surface ozone mixing ratios increase with altitude in a transect in the Catalan Pyrenees*. Atmospheric Environment, 40, 7308 – 7315, 2006