6.09 MODELING AN OZONE EPISODE IN THE GREATER ATHENS AREA, GREECE USING BOTH UAM-V AND A BOX MODEL

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INTRODUCTION

Atmospheric pollution in the Greater Athens Area (GAA) has been the subject of many studies (*Ziomas, I. et al.*, 1998; *Kalabokas, P.D.* et al., 2000; *Sotiropoulou, R.E.P. et al.*, 2004). All the researchers agree that the formation of high levels of photochemical pollutants in the GAA is due to a number of critical factors, namely the poor ventilation of the basin, the frequent appearance of sea breeze and intense solar irradiation combined with the high population density of the area and the intense anthropogenic activities. Numerical simulations with Air Quality Models demand a number of input data including emission rates, meteorological conditions, initial and boundary concentrations of chemical reactants. While such models are becoming increasingly sophisticated and capable of incorporating details physics and chemistry, a number of important issues and uncertainties still remain.

This study simulates an ozone episode in the GAA using the three-dimensional photochemical model UAM-V as well as a simple box model both of which are coupled with the meteorological Mesoscale Model (MM5). The case selected for the simulations is a severe pollution episode (14th and 15th September 1994) occurred during the MEDCAPHOT-TRACE experimental campaign. During these days a system of two sea breezes was developed in the area which favoured extremely high ozone concentrations in the northern and eastern periphery of the city.

METHODOLOGY

Spatial and temporal ozone concentrations patterns were derived from the UAM-V model while the mean hourly ozone concentrations at selected sites (operating stations of the routine monitoring network) were further reproduced with the box SAPRC Atmospheric Photochemical Mechanism model (*Carter, W.P.L*, 1988). A number of numerical experiments were performed for this episode where the most important factors were examined. It is revealed that most of the corrections/additions and modifications of the input data are necessary.

The different experiments confirmed the findings of the recent literature (*Hidy, G.M,* 2000) that ozone concentrations are clearly very sensitive to meteorological conditions, including the wind speed and direction and the intensity of mixing especially in the vertical direction. Especially, over a complex topography like the GAA, delicate balances are observed at the slopes of the mountains or between them where various sea breezes converge (*Svensson, G,* 1998). The photochemical model performed for various sets of meteorological fields that were produced from the MM5 model, which run with different initial nesting conditions. Moreover, in order to incorporate the effects of the urban sector on the wind speed and the diffusion coefficients, some corrections of the meteorological fields were also considered. In particular, the decrease of the wind speed inside the urban structure (*Masson, V*, 2000).

Concerning the emissions, another important area of uncertainty, some corrections/additions and assumptions have been considered. For the applications, the most up to date inventory has been used. The reference year is 1998 and it covers the transportation sector (*Symeonidis, P, et al.*, 2003) and the industry sources (Ministry of the Environment). The spatial resolution of the area sources is 2kmx2km on an hour basis. For the chemical speciation, the profile proposed by *Bossioli, E, et al*., (2002) for NMVOC emissions was applied. Apart from the industry and the transportation sector, the emissions from other critical sectors have also been encountered. Specifically, the role of the biogenic emissions was examined by incorporating the spatial and hourly distribution of the natural emissions (isoprene, a-pinene, other monoterpenes, unidentified). These were estimated based on literature emissions factors (*Roselle, S.J, et al.,* 1991; *Benjamin, M.T, et al.,* 1997) as a function of solar radiation and temperature. The calculations were based on a vegetation index, while the species composition of the biomass covered areas was roughly assumed. Finally, the NMVOC emissions of the suburban areas were dealt with special care. A different profile referred as 'city plume' profile (*Bossioli, E, et al*., 2002), was applied in the periphery of the basin in order to reflect the composition of the aged air masses. This brought additional NMVOC emissions, which is in accordance to *Klemm, O. and I.C. Ziomas* (1998).

Several numerical experiments have been performed examining the influence of the background ozone concentrations expressed in the eulerian models as boundary conditions. Information on the background ozone of the Athens' basin is mainly available from the MEDCAPHOT-TRACE experiment (*Suppan, P, et al*., 1998; *Kalabokas, P.D, and J.G. Bartzis*, 1998), but also from other recent studies (*Kalabokas, P.D*. et al., 2000). The critical contribution of the background ozone was confirmed by using both constant and daily varied O_3 concentration profiles.

Finally, all the important to ozone formation factors were also examined by the box model. The box model was applied either with CB-IV (*Gery, M.W, et al*., 1989), the approach considered by UAM-V or with SAPRC-99 (*Carter, W.P.L*, 2000) chemical mechanism.

RESULTS

The meteorological model performed several runs applying different initial conditions since the flow fields are sensitive to the magnitude and direction of the synoptic forcing (Svensson, 1998). Among these runs the one that reproduced more successfully the flow pattern in the GAA for both days was derived without nesting. In such case the synoptic conditions turned to be quite weak and permitted the system of both sea breezes from the SW and E to clearly develop in the basin. For the following photochemical simulations this set of meteorological data was considered.

In general, the spatial patterns of ozone concentrations were successfully reproduced by the simulations, for both days. An example is presented in figure 1, where all the additions and modifications discussed in the previous paragraph were considered. The model predicted successfully the low concentrations in the centre of the city as well as the transport of the city plume towards the axis of the sea breeze (SW-NE). However the UAM-V model didn't succeed to predict the high ozone concentrations observed at the suburban stations of Thrakomakedones (260μg/m^3) in the northern part of the basin (near the foothill of Parnitha) and Demokritos (340μg/m^3) in the eastern part (hill side of Hymittos), as other workers in the past (*Ziomas, I, et al*., 1998; *Svensson, G*, 1998; *Sotiropoulou, R, et al*., 2004). Although, the ozone concentration levels at these sites are mainly affected by the transport mechanism (they are on the way of the sea breeze), they are also very sensitive to local meteorological characteristics and to the reliable anthropogenic/biogenic emissions. Especially for the Thrakomakedones site, it was revealed that the concentration levels are also very sensitive to the emissions of the industrial area of Thriassion plane, as was also declared by *Flocas, E, et al.*, (2003). The results in the suburban stations (Demokritos, Zografou, Thrakomakedones, Marousi, Spata, Pendeli, Pireas and N.Smyrni) were improved, when the meteorological parameters modified in the urban sector.

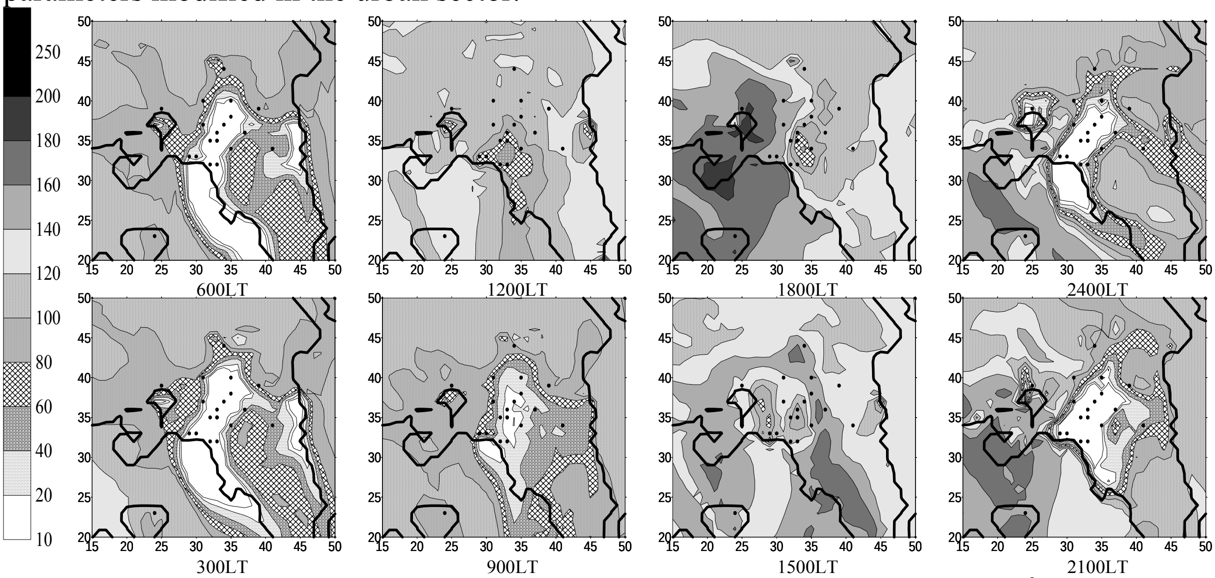

Figure 1: Spatial patterns of mean hourly ground O_3 concentrations in μg/m^3, for the 14th September 1994 for selected hours.

In figure 2, the comparison of the measured and calculated mean hourly ozone concentrations for the 14th September at selected sites are presented. The comparison reveals a good agreement for the background stations Aigina (SW), Spata (E) and Pendeli (N) as well as for the suburban stations (N. Smyrni and Geoponiki). A good agreement is also observed for the time when the maximum occur. The underestimation of the peak ozone concentration at the traffic station of Athinas was corrected when the emissions from the off road activities, which are very rich in NO_X, had been omitted. It is important to mention that the current emission inventory, is the first that registered the off road emissions which contain a high percentage of NO_X, responsible for ozone titration.

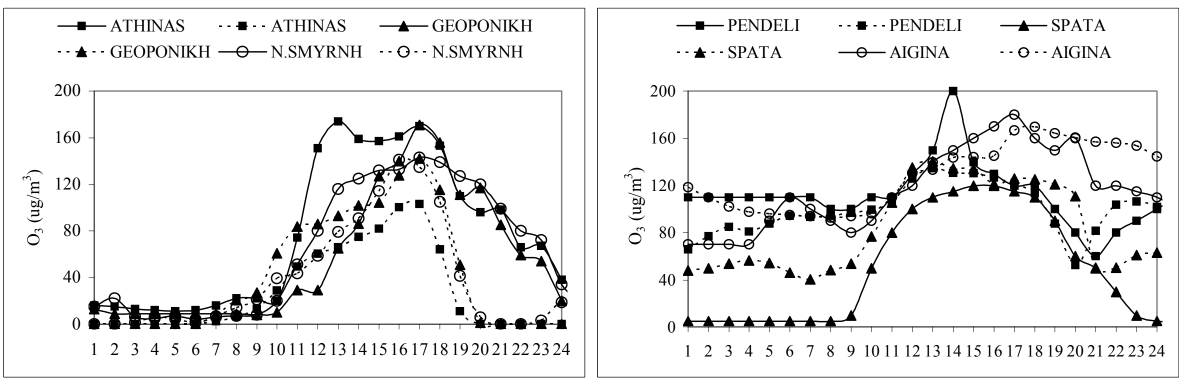

Figure 2: Calculated with UAM-V (dashed) and measured (solid) O_3 concentrations for the 14th September 1994 at selected sites.

Despite the limited physical conception of the box model, the high ozone concentrations at the suburban stations of Thrakomakedones and Demokritos have been reproduced. In figure 3 the maximum concentrations for the 14th September are presented for three suburban/background and one urban traffic station. The simulations were performed by considering two alternative scenarios for the anthropogenic emissions; a common speciation profile with city centre characteristics over the whole area, named ‘street’ and another one with increased VOC emissions, named ‘plume’ applied only over the suburban areas. There is an agreement between the observed and calculated values for the stations of Demokritos and Thrakomakedones. This is mainly attributed to the fact that in these areas the biogenic emissions have a major contribution, therefore, their high reactivity produces elevated concentrations. Moreover, the box model simulated more successfully than the UAM-V model, the limited values of ozone at the traffic station in the city centre (Patision). This result is quite reasonable since the box model resolves more accurately the street canyon than the eulerian model, which has a coarse resolution of $4km^2$. The suburban station at Liosia seems to be very sensitive to the different VOC emissions profiles. More specifically, the location of this station (on the sea breeze axis) is greatly favoured from the transportation of the city plume air masses and thus it feels the ‘plume’ speciation in the absence of biogenic emissions. Finally, comparing the results of the two chemical mechanisms, the SAPRC99 mechanism always gives higher concentrations.

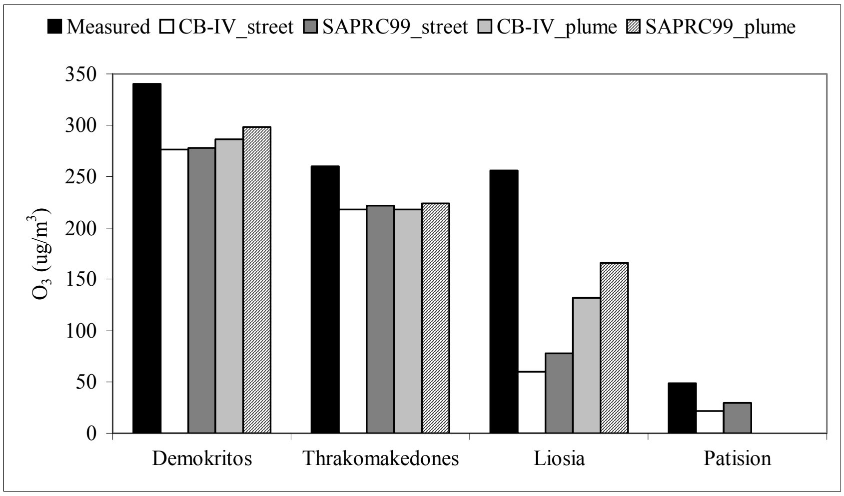

Figure 3: Calculated (box model) and measured maximum O_3 concentrations

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