The influence of the lateral boundaries and background concentrations on limited area photochemical model simulations

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Abstract: In this study an attempt was made to investigate the influence of the lateral boundaries and the background concentrations, on the predicted air pollutants' concentrations, as calculated by limited area, grid-based photochemical models. This influence is more pronounced in the case of mesoscale applications because of the limited domain. The lateral boundaries should be defined in such a way as to take into account the recirculation phenomena which occur as a result of the interaction of different scale atmospheric circulations. In addition, the influence of air pollutant sources located near the domain boundaries (inside or outside), on the concentrations of the photochemical pollutants inside the domain have to be considered. In this study the UAM-IV photochemical model has been implemented and simulations have been performed over the Athens Basin. It was found that the concentrations of the photochemical oxidants are mainly affected by the lateral boundary conditions, while the influence of the background is evident in the first hours of the simulation.

Keywords: model boundaries and initialization, model domain size, photochemical modelling.

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1 Introduction

Defining the boundary conditions is one of the most important issues in grid-based photochemical model simulations in that they influence the accuracy of the predicted oxidant levels (Sistla *et al.*, 1995). The propagation of the boundaries inside the modelling domain is associated with the domain size and the assimilated fields. Therefore, the influence of the imposed boundary values on the predicted oxidant levels has to be investigated in association with these two parameters. There is an obvious requirement of detailed meteorological inputs, especially in cases with strong regional scale circulations. Moreover, the existence of significant sources near the domain boundaries should be taken into account.

The background concentration of the air pollutants is also a significant parameter which is interdependent with the boundaries and the domain size. The influence of the background is expected to weaken quickly in areas with significant primary pollutant sources and to be more pronounced in remote areas.

In this study simulations with the UAM-IV photochemical model have been performed. The influence of the lateral boundaries is examined by calculating the spatial and temporal scales of transport from the boundaries to the interior of the model domain. The analysis is focused on investigating background and boundary effects while predicting air quality levels over the Attica Peninsula and the Saronic Gulf (Figure 1). Significant sources, including automobiles and central heating, are located in the Athens Basin. Major industrial installations including cement plants and refineries are located on the Thriassion plain. In addition, the two power plants at Lavrio (at the southeast part of the Attica Peninsula) and Aliveri (near the centre of Evoia island) are considered.

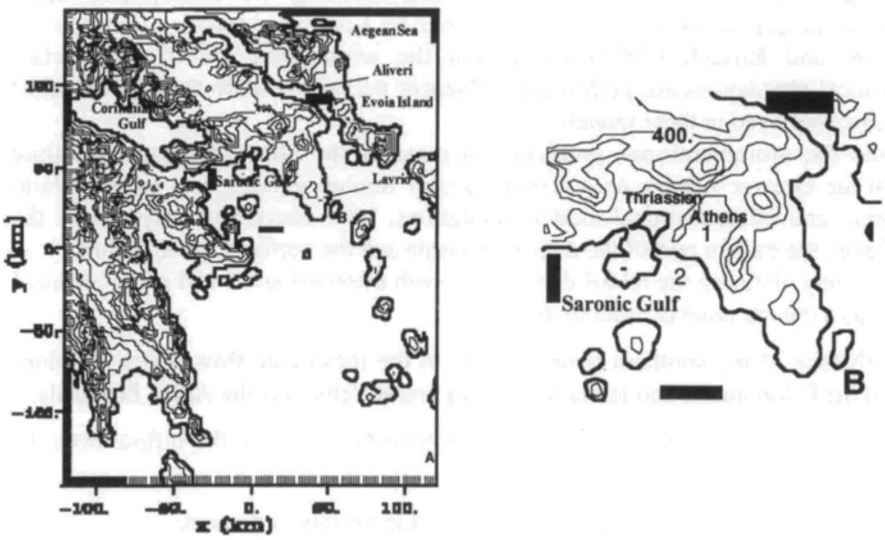

Figure 1 Topography inside the domains A and B used for UAM-IV simulations (contours are plotted every 200 m). The marked areas represent the areas of passive tracer releases.

The complexity of the physiographic characteristics of southern Greece, favours various scale circulations which control local-scale meteorological parameters. Observational, modelling and time-series analysis approaches have been implemented in the past in order to investigate the role of meteorology on the build-up of an air pollution episode, as well as the prediction of the next day concentration over the Athens Basin. Photochemical oxidant vertical profile, and primary and secondary transport mechanisms of pollutants were extensively investigated by field campaigns during extreme pollution episodes. In these experimental efforts, the role of sea breeze circulation over the Saronic Gulf and Athens Basin on the build-up of air pollution episodes were also studied by using synoptic analysis methods. The worst episodes over the Athens Basin were found to be associated with stationary anticyclonic conditions and/or warm air advection (Katsoulis *et al.*, 1988a, b; Kallos *et al.*, 1993; Kassomenos *et al.*, 1995; Varinou and

Kallos, 1996), or with situations where a counterbalance between sea breeze circulation and regional, or synoptic scale, circulations occurred (Kallos *et al.*, 1993).

Numerical model simulations have been performed in order to explore the role that various scale circulations play on the evolution of air quality episodes through trapping and recirculation processes. In such simulations, combined systems of atmospheric, dispersion and photochemical models have been used (Kassomenos, 1993; Pilinis *et al.*, 1993; Kallos *et al.*, 1995; Moussiopoulos, 1995; Lagouvardos *et al.*, 1996; Kotroni *et al.*, 1998). These methodologies are considered as integrated methods for air quality studies because they can provide a more realistic description of the dispersion characteristics and the spatial and temporal variations of pollutant concentrations. However, improper use of such systems may lead to unrealistic results. Selecting the model domain and initialization are two of the most crucial parameters for model simulations. As was pointed out in Kallos and Kassomenos (1994), Lagouvardos *et al.* (1996), Kotroni *et al.* (1998), these problems can be overcome by using models with two-way interactive nesting capabilities. The necessity of accurately defining the atmospheric fields introduced in air quality models was also mentioned by Kunz and Moussiopoulos (1995). Giovannoni and Russell (1995) stated that the wind field specification when photochemical simulations are performed, influences the results more than the chemical mechanisms employed in these models.

Despite the aforementioned problems, in most of the photochemical modelling studies in the Greater Athens Area (GAA), a very limited domain was used for both atmospheric and photochemical model simulations. This domain usually covers the Athens Basin, the eastern part of the Attica Peninsula and the northern Saronic Gulf.

In this study, defining the model domain (for both meteorological and photochemical models) was a crucial issue in order to discuss:

- the influence of the southern boundary due to the mesoscale flow which develops around the Peloponnese and interacts with sea breeze cells over the Attica Peninsula;
- the influence of the northeastern edge of the boundaries due to the inflow from the Aegean Sea;
- the influence of some major sources located outside the model domain;
- the influence of the western boundary because of the channelling effects along the Corinthian Gulf, where significant primary pollutant sources exist in the coastal area;
- the influence of the background concentrations on the simulated ozone levels.

The simulation period extends from 6–8 July 1994. During this period an important air pollution episode occurred in GAA (Peleg *et al.*, 1996). Hence, a large database of meteorological and air quality data was available from a measuring campaign in the framework of the T-TRAPEM project (Kallos *et al.*, 1997).

2 Meteorological conditions

During the simulation period stationary conditions prevailed over most of the Mediterranean. A high pressure system with weak pressure gradient was established over the region and weak synoptic flow was evident at the surface and aloft. Over the Aegean Sea this weak flow was from northern directions. Weak synoptic flow allows the development of thermal local-scale circulations in the area of interest. These local circulations lead to the formation of the most favourable conditions for air pollution episodes in the Attica Peninsula and Saronic Gulf (Kallos *et al.*, 1993). For a more detailed description of the prevailing meteorological conditions during the period 6–8 July 1994, see Peleg *et al.* (1996) and Kotroni *et al.* (1998).

3 Description of the modelling system

3.1 The RAMS model

Pielke *et al.* (1992) summarize the most important features of the Regional Atmospheric Modelling System (RAMS) which Colorado State University and the ASTER Division of Mission Research Corporation have developed. RAMS uses the full set of primitive dynamical equations with optional parameterization schemes for turbulent diffusion, solar and terrestrial radiation, sensible and latent heat exchange between the atmosphere, multiple soil layers, the kinematic effects of terrain and a vegetation canopy. An important feature of RAMS is its capacity of performing two-way interactive grid nesting which allows local fine mesh grids to resolve small atmospheric systems, while simultaneously modelling the large-scale environment of the systems on a coarser grid.

3.2 The UAM-IV model

The UAM-IV is a three-dimensional photochemical grid model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the physical and chemical processes in the atmosphere that affect pollutant concentrations (Morris *et al.*, 1990). The UAM-IV is based on the atmospheric diffusion or species continuity equation which represents a mass balance including all relevant emissions, transport, diffusion, chemical reactions and removal processes. In detail, the spatial distribution and composition of biogenic and anthropogenic NO_x and VOC emissions, the spatial and temporal variations in the wind field, the dynamics of the boundary-layer, the chemical reactions involving VOC, NO_x and other important species, the diurnal variation of solar insolation and temperature, the loss of ozone and ozone precursors by dry deposition and the ambient background of VOC, NO_x and other species are considered in the simulation of the photochemical processes. The UAM-IV implements version IV of the Carbon Bond Mechanism (CB-IV) for solving chemical kinetics.

3.3 Model set up

3.3.1 Meteorological model set up

For the present study three nested grids have been defined (Figure 2):

(a) The outer model domain (1) had a horizontal grid increment of 32 km with 140 × 90 grid points centred at 37.500°N - 23.500°E.

(b) The second model domain (2) had a horizontal grid increment of 8 km with 130 × 118 grid points centred at 37.932°N - 23.500°E.

(b) The fine model domain (3) had a horizontal grid increment of 2 km with 122 × 146 grid points centred at 37.500°N - 23.500°E.

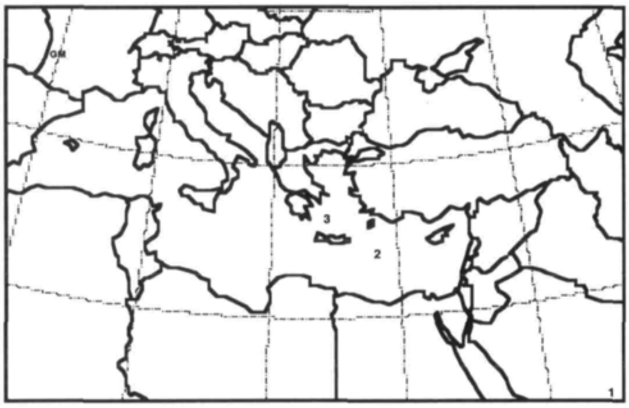

Figure 2 Domain of the three nested grids used for RAMS simulations.

Twenty-three vertical levels following the topography have been used in all grids, having 180 m vertical spacing near the ground, stretching to 1 km at an altitude of 6 km and remaining constant up to about 16 km. The inner grid has been defined so that it includes, in addition to the GAA, the island of Evoia on the east, the Corinthian Gulf on the west and the eastern Peloponnese. This extended fine grid was considered necessary for an accurate simulation of the atmospheric flow over such a complex terrain, in order to avoid any possible lateral boundary influence.

The simulation started at 00:00 UTC on 6 July 1994 and ended after 72 hours. The ECMWF 1° gridded analysis files were used in order to initialize the model and the ECMWF data are objectively analysed by the RAMS model on isentropic surfaces from which they are interpolated to the RAMS grids. These fields were used in order to nudge the lateral boundary region of the coarser grid every hour. The ECMWF fields of the climatological sea surface temperature (1° resolution) and topography derived from a 30 second (angle) terrain data retrieved from NCAR have been used for all grids. Moreover, vegetation type data with 10 minute (angle) horizontal resolution were used.

3.3.2 UAM-IV model set up

For the UAM-IV simulations two domains have been defined (Figure 1). For all UAM-IV simulations the meteorological fields of the inner grid of RAMS were used. Domain A coincides with the inner grid of RAMS. Both grids have a resolution of 2 × 2 km. The UAM-IV simulations in the present study started at 00:00 UTC on 6 July 1994 and ended after 72 hours. The emission inventory for the GAA was derived from the inventory proposed by Moussiopoulos *et al.* (1995) after appropriate adjustments.

In order to meet the scopes of this study two types of simulations have been performed. For the first type of simulations a passive tracer was released at specific locations at the grid boundaries (marked areas in Figure 1). Independent simulations have been performed for grids A and B. Releases of a high amount of the tracer were performed as given below:

- At the southwest corner of domain A (for the grid A simulation) and a part of the southern boundary of domain B (for the grid B simulation) to investigate the roles within the propagation of the boundary values of a) the mesoscale flow which develops around Peloponnese, and b) the sea breeze cell of the Saronic Gulf. Examining the propagation patterns of the southern boundaries is interesting because a) a regional scale transport of polluted air masses from Italy through the mesoscale flow around Peloponnese is evident (Kallos *et al.*, 1996), and b) recirculation phenomena in the Saronic Gulf due to the sea breeze cell might occur (Lallas *et al.*, 1983).
- At the northeast corner of domain A in order to trace the trajectory of the air masses advected inside the domain from the Aegean Sea. These air masses are possibly contaminated by the major sources located at the Dardanelles gap such as the urban area of Istanbul. Tracer releases were also made at the northern boundary of domain B in order to examine the influence of sources located outside this domain, such as the Aliveri power plant.
- At the western boundary across the Corinthian Gulf for domain A and at the western boundary across the exit of the Corinthian Gulf for domain B. The high mountains all around the Corinthian Gulf lead to an important channelling of the flow, with an exit over the Saronic Gulf. Thus, the definition of the model boundaries across the Corinthian Gulf has to take into account the significant pollutant sources at the coastal areas which are outside the model domain.

For the second type of simulations the photochemical processes were activated in order to examine the influence of the background concentrations on the build-up of the atmospheric oxidants. The implemented boundary and initial conditions were based on measurements with a research aircraft during the T-TRAPEM campaign. The resulting initial conditions consisted of the 'normal background', while a sensitivity test with reduced initial concentrations ('low background') has also been performed.

4 UAM-IV results

The effects of the western boundary vary when different domains are used. When domain B is used, this boundary is activated during late evening and night hours under the prevailing west-northwest flow. Owing to the selected domain size, the imposed boundary concentrations are advected to the southern part of the grid and need less than six hours to exit the domain (Figure 3a). Thus, any inaccuracy at the western boundary leaves domain B without affecting air quality inside the Athens Basin. When domain A is used, the tracer mass released at the western boundary needs more than 15 hours to reach the area of the Saronic Gulf. Inspection of the tracer concentration time series showed that the advected tracer mass remains inside the domain and later on, during the evening, affects the GAA (Figure 3b). These results support the suggestion that when a large domain is used the uncertainties at the boundaries remain inside the domain.

The effects of the southern boundary are more pronounced when domain B is used. In this case the southern boundary influences the GAA during the afternoon hours, due to the strengthening of the southerly flow associated with the development of the sea breeze cell over the Saronic Gulf. A tracer mass released at the southern boundary propagates fast towards the GAA with a time scale of three hours (Figure 4a). When domain A is used, there is no strong evidence of southern boundary effects over the GAA, under the prevailing meteorological conditions (Figure 3b). Nevertheless, under a stronger regional flow the propagation of this boundary towards the GAA is possible.

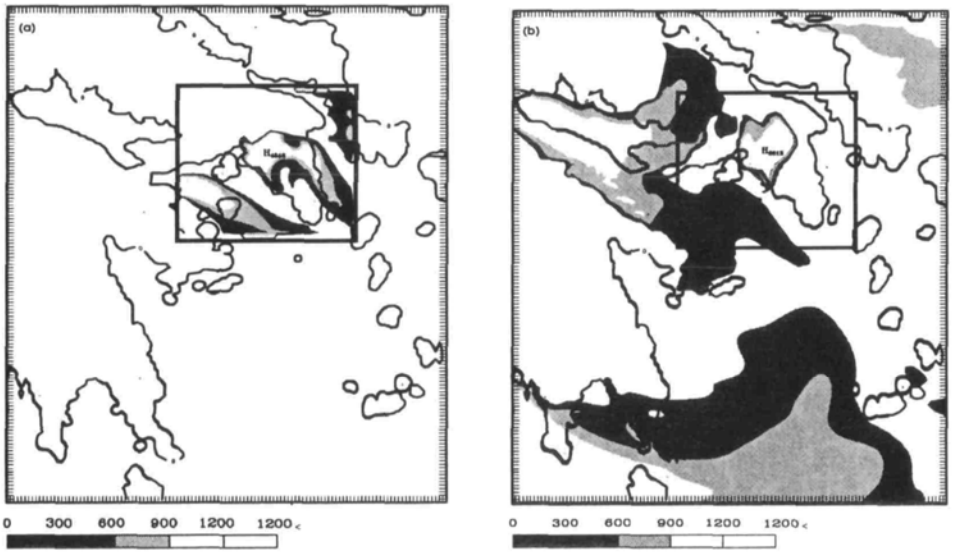

Figure 3 Tracer concentration field in the first layer of UAM-IV (300 ppm interval). a) Domain B, 06:00 UTC on 7 July 1994, b) Domain A, 20:00 UTC on 7 July 1994.

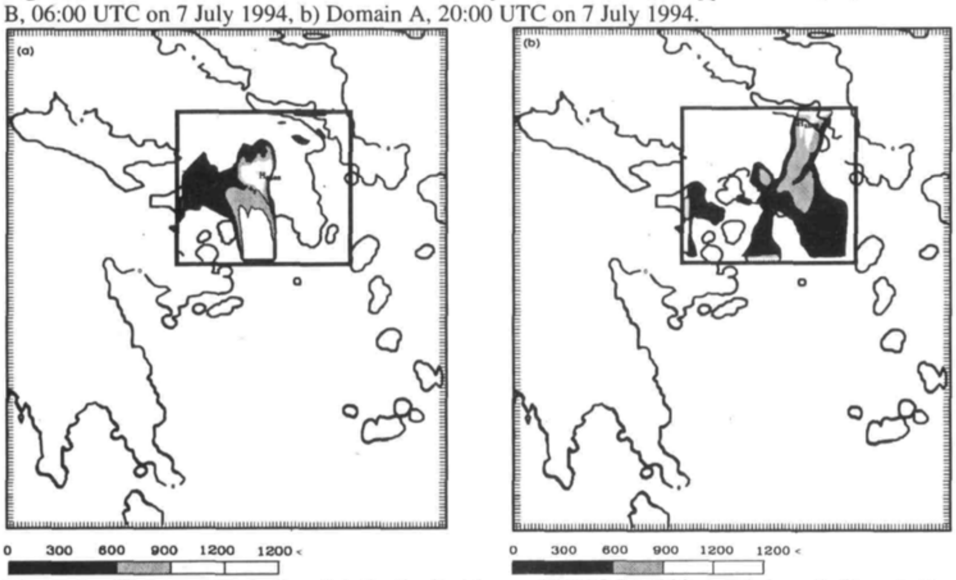

Figure 4 Tracer concentration field in the first layer of UAM-IV (300 ppm interval). Domain B, a) at 16:00 UTC on 7 July 1994, and b) at 11:00 UTC on 8 July 1994.

The northern boundary was found to affect the GAA when both domains A and B are used. The tracer mass released along this boundary is advected towards the GAA with a time scale of five hours, affecting the calculated fields over the Athens Basin and the eastern Attica peninsula (Figures 5a and 4b for domain A and B respectively).

The realistic representation of the GAA plume advection towards remote areas was also examined in association with the selected domain size. As is shown in Figure 5b, the implementation of domain A gives evidence that the plume from the GAA is advected to the south over the maritime area to the east of the Peloponnese. These results are supported by the high ozone concentrations measured in that area during the T-TRAPEM campaign (Peleg *et al.*, 1996). It was not possible to represent the GAA plume advection when domain B was used which is considered as a benefit of the large domain A.

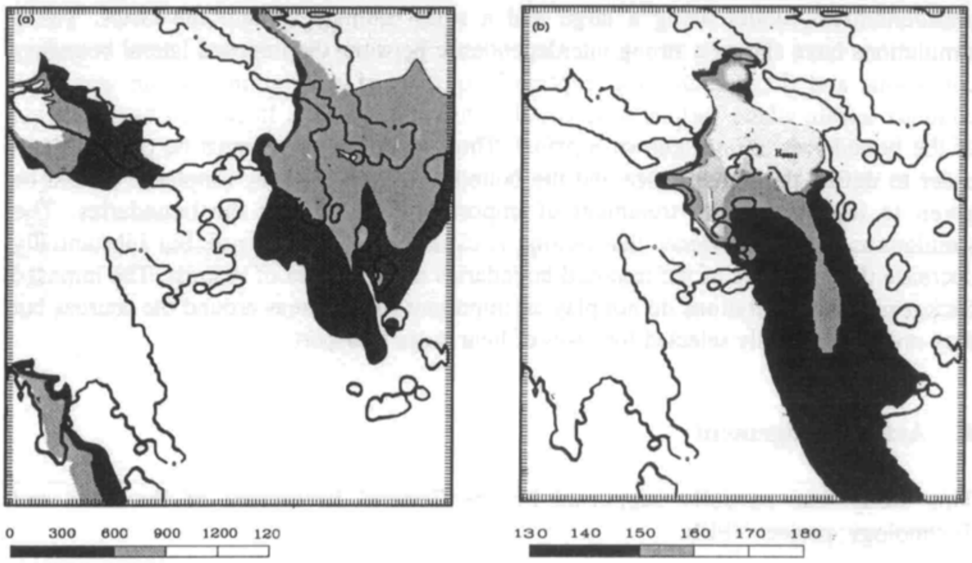

Figure 5 Tracer concentration field in the first layer of UAM-IV, Domain A, a) at 06:00 UTC on 6 July 1994 (300 ppm interval), and b) at 22:00 UTC on 8 July 1994 (10 ppm interval).

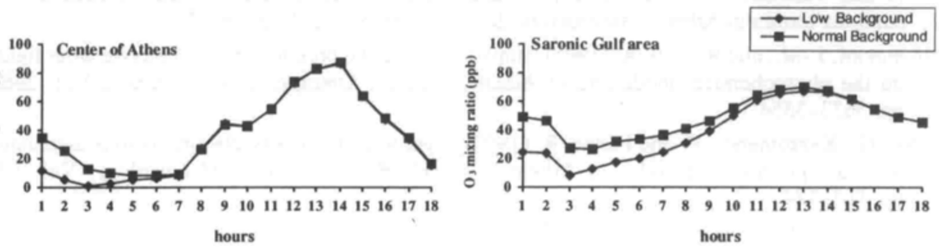

Figure 6 Simulated ozone concentrations at the centre of Athens and the Saronic Gulf for normal and low background.

The second type of simulation provided evidence that the influence of the background is more pronounced far away from areas with significant sources (Figure 6). Indeed, in the centre of Athens (location 1 in Figure 1) the calculated ozone concentrations for both low and normal background become equal seven hours after the simulation starts (07:00 UTC). This is due to the effects of local emissions, while over the Saronic Gulf (location 2 in Figure 1) ozone concentrations show a dependence on the background definition for a time scale of 14 hours.

5 Conclusion

In the frame of this study various simulations have been performed with a grid based photochemical model using a large and a small domain around the GAA. These simulations have shown a strong interdependence between the imposed lateral boundary conditions and the domain size, especially in case of simulation over an area with complex terrain where various scale circulations are developed. In such cases the effects of the boundaries are not known *a priori.* Thus, sensitivity tests must be performed in order to define the domain size and the boundary concentrations. Emphasis should be given to the appropriate treatment of important sources near the boundaries. The simulations provide evidence that nesting is expected not to eliminate but substantially decrease the influence of the imposed boundaries over the area of interest. The imposed background concentrations do not play an important role in areas around the sources but they must be carefully selected for cases of long range transport.

6 Acknowledgement

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