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An Investigation of the Factors Affecting the Ozone Concentrations in an Urban Environment

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ABSTRACT

Adjoint sensitivity analysis allows to assess the areas that have the largest impact on a given receptor site. The adjoint version of the Community Multiscale Air Quality (CMAQ v4.5) model was employed to perform a sensitivity analysis of ground level ozone for the episodic event of June 24, 2003, in the city of Athens assuming as a receptor site that of Agia Paraskevi Station. The 3-dimensional meteorology fields calculated using the Mesoscale Model 5 (MM5, Penn State University version 3.7.2) were used to produce high resolution daily air emissions inventories for the main anthropogenic and biogenic pollutants with 1-hour time step by an in-house built processor named EMISLAB. The meteorological prediction fields in combination with the emissions inventories were consequently fed as inputs to the CMAQ model. The ozone sensitivities were obtained with respect to pollutant concentrations and emissions. The distribution of the sensitivities in the computational domain for different times delineated the regions where perturbations in some concentrations would result in significant changes in the ozone concentrations in the area of interest (Agia Paraskevi, in this case) at the final time. The investigation yielded that the most significant influences were the transported O_3 and NO_x concentrations from the industrial area in the northern parts of the city and the road traffic from the city centre.

Keywords: Adjoint Model; Ozone Sensitivities; Emissions; Urban Area

1. Introduction

Three-dimensional atmospheric chemical transport models (CTMs) are tools used by the scientific community to predict the temporal and spatial distribution of air pollutants. Recent advancements in computational methods and resources have allowed the calculation of sensitivities of pollutant concentrations with respect to a large number of model parameters, improving our understanding of the changing chemical state of key atmospheric constituents in relation to their sources and sinks. The sensitivity analysis results in the calculation of the sensitivity coefficients (derivatives) of model outputs with respect to various inputs. Such sensitivity information can be used effectively in emission control strategies and air quality management.

There are two general techniques for computing sensitivity analysis, the forward and backward methods. In the forward approach, any perturbation in one or more input variables is propagated forward in time into various receptors [1,2]. In the backward (adjoint) mode, a perturbation in a receptor based metric is propagated backward in time through an auxiliary set of equations resulting in the calculation of its sensitivities with respect to a large number of perturbed input parameters [3].

The mathematical formulation of the adjoint sensitivity for nonlinear dynamical systems has been presented by [4-7]. The mathematical description of the adjoint sensitivity method applied to three-dimensional air transport and chemical models could be found in [8].

This paper presents an adjoint sensitivity analysis of ozone concentrations with respect to emissions performed for the city of Athens and the Greater Athens Area (GAA), at the receptor site of Agia Paraskevi, using the adjoint version of the Community Multiscale Air Quality (CMAQ v4.5) model [9].

2. Methodology

2.1. Input Data and Domain Description

CMAQ is a 3-D atmospheric chemical transport model [10] and is part of the operational meteorology and air quality forecasting system currently under development by the Environmental Research Laboratory (EREL) of NCSR “Demokritos” (Greece). The meteorology fields are produced by the Mesoscale Model 5 (MM5, Penn State University version 3.7.2), which has been parameterized for application to the particular geographical and climatic characteristics of the GAA. The MM5 output is used to produce high resolution daily air emissions inventories for the main anthropogenic and biogenic pollutants with 1-hour time step by an in-house built processor named EMISLAB. The meteorological prediction fields in combination with the emissions inventories are used as inputs to the CMAQ model.

The computational domain is designed to cover an area of 103 × 103 km^2 with 1 km × 1 km horizontal resolution (**Figure 1**). The case study considered was a pollution episode that occurred in the area during the period, June 23-24, 2003. Concentrations of air pollutants (O_3, NO and NO_2) were available from pollution monitoring stations, operating on a continuous basis under the supervision of the Greek National Air Pollution Monitoring Network (Ministry of Environment, MINENV). Ambient concentration values of O_3 and NO_2 were available from the Aliartos background station operated by MINENV.

2.2. Meteorology Simulation

The MM5 model was initialized at 00:00 UTC on June 23, 2003 using input meteorological data from the National Centres for Environmental Prediction (NCEP) Global Forecasting System (GFS) (6-hours resolution). **Figure 2** shows that the model results compared very well with the wind speed observational data (Hellenic National Meteorological Service) available from two stations, Elefsina and the El. Venizelos (Athens airport).

In general, the calculated meteorological fields showed that the both days were characterized by sea breeze conditions and rather low near surface winds that favoured the air pollution episode formation (**Figure 3**). Temperatures ranged from 30˚C - 35˚C between the two days, the highest temperature occurred on June 24, 2003 (**Figure 4**).

2.3. Air Quality

Firstly, the anthropogenic and biogenic emissions of NO, NO_2, NMVOC, SO_2 and PM were obtained using EMISLAB, on an hourly basis for the specific grid (1 × 1 km^2) (**Figure 4**). The calculated hourly emissions were used as input to the CMAQ model (**Figure 5**).

The chemistry-transport model CMAQ was started at 00:00 UTC on June 23, 2003 and performed a simulation of 48 hours. An example of the calculated O_3 concentration profile at Agia Paraskevi (suburban) station is shown in **Figure 6**. The near-surface concentration contours of NO_2, as predicted by CMAQ at 9:00 UTC on June 24, 2003, are shown in **Figure 7**.

3. Results

One suburban station Agia Paraskevi in the city of Athens has been selected for the adjoint sensitivity analysis which according to the annual report of the Ministry of

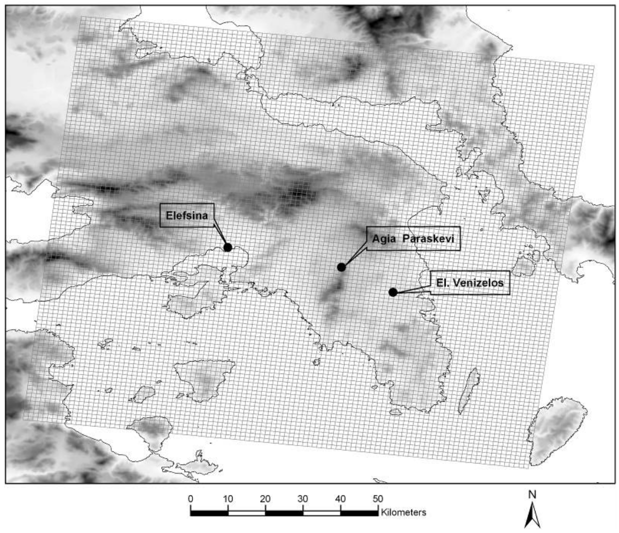

Figure 1. Modelling domain and location of the two meteorological station (Elefsina, El. Venizelos) and the receptor (Agia-Paraskevi) used in the adjoint analysis.

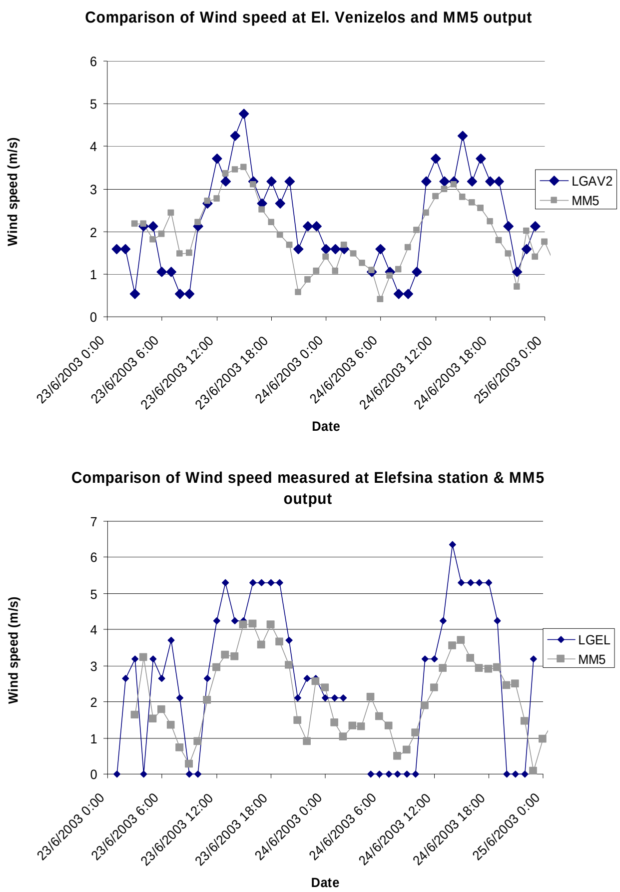

Figure 2. Comparison of the MM5 calculated wind speed (m/s) results and observations at the El. Venizelos airport (left) and Elefsina (right) stations.

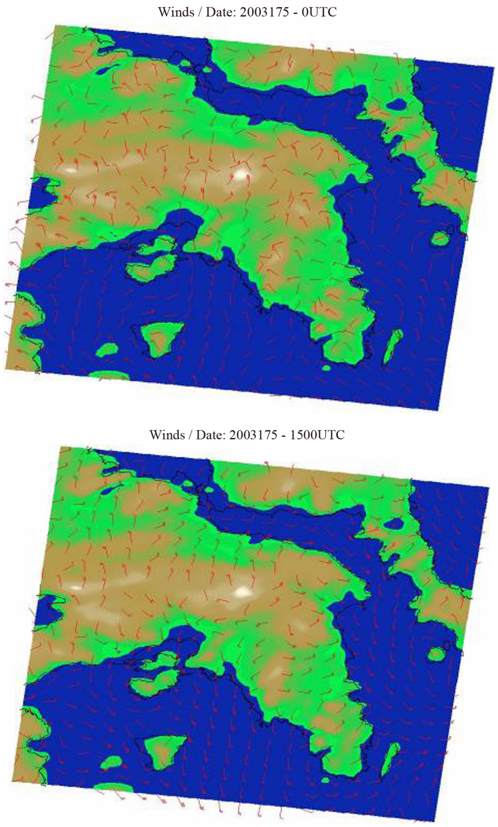

Figure 3. Wind fields (near surface) calculated by MM5 for June 24, 2003, at 00:00 UTC (left) and 15:00 UTC (right).

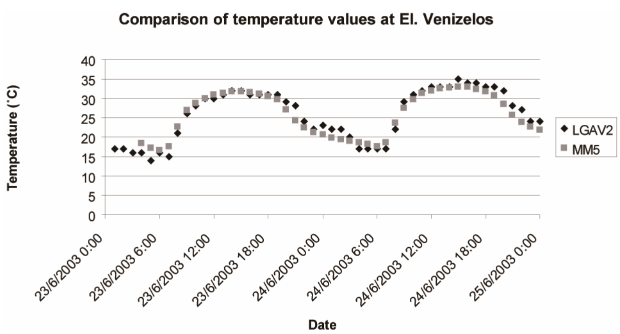

Figure 4. Surface Temperature temporal profiles as calculated by MM5 and observed at El. Venizelos (23-24, June, 2003).

the Environment exhibits the highest amount of episodic events (*i.e.* exceedances of maximum 8-h average value) on an annual basis. The adjoint model of CMAQ was run 12 hours backwards of the target time (output at 12:00, 09:00, 06:00, 03:00 UTC, June 24, 2003). The sensitivities of ground level ozone concentrations (model-calculated) with respect to concentrations and emissions of NO_x, CO, VOCs have been obtained. The distribution of the sensitivities in the computational domain for different times, (iso-surfaces) delineate the influence regions, *i.e.*, areas where perturbations in some concentrations will result in significant changes in the ozone concentrations in the area of interest (Agia Paraskevi) at the final time. The calculated sensitivities of ozone with respect to concentrations of gas pollutants (O_3, NO_2 and SO_2) are shown in **Figures 8-10**. The calculated sensitivities of O_3 with respect to emissions of pollutants (NO, NO_2) are shown in **Figure 11**.

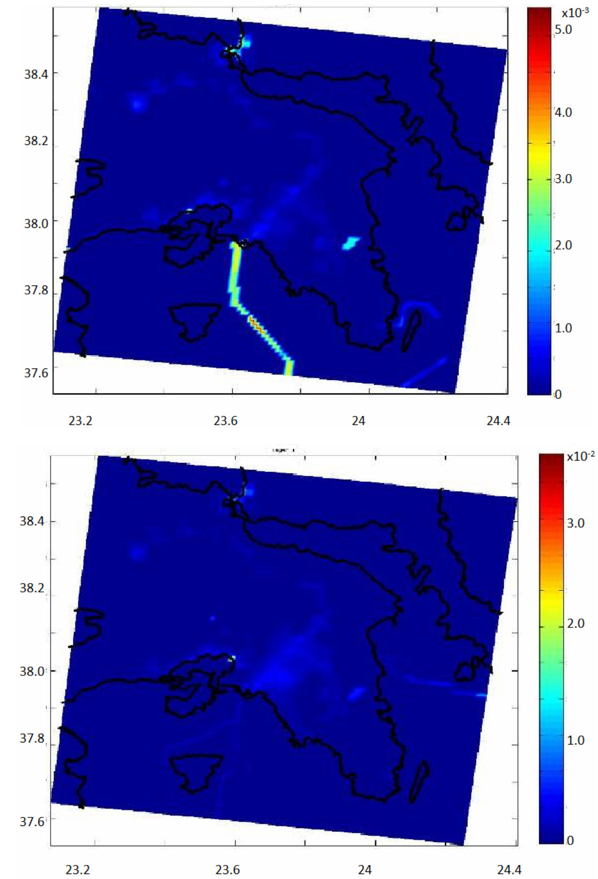

Figure 5. Emissions of NO_2 (Layer 1) calculated by EMIS-LAB for June 24, 2003, at 00:00 UTC (left) and 15:00 UTC (right).

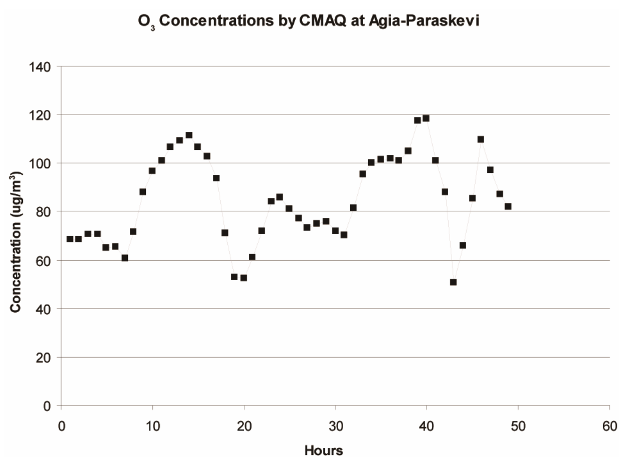

Figure 6. Temporal ozone profile from CMAQ at Agia Paraskevi station for 23-24 June, 2003.

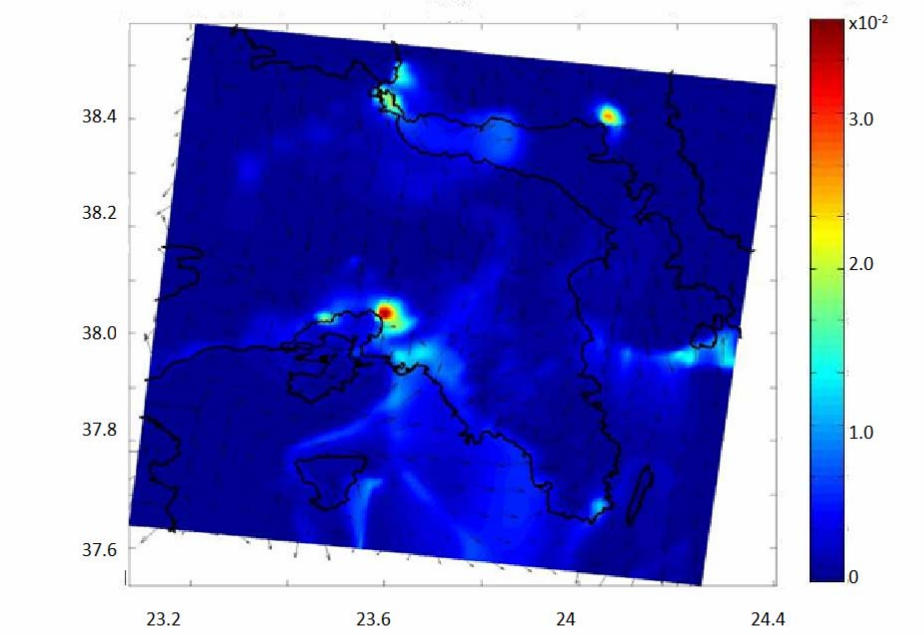

Figure 7. CMAQ calculated NO_2 concentrations on June 24, 2003, at 9:00 UTC.

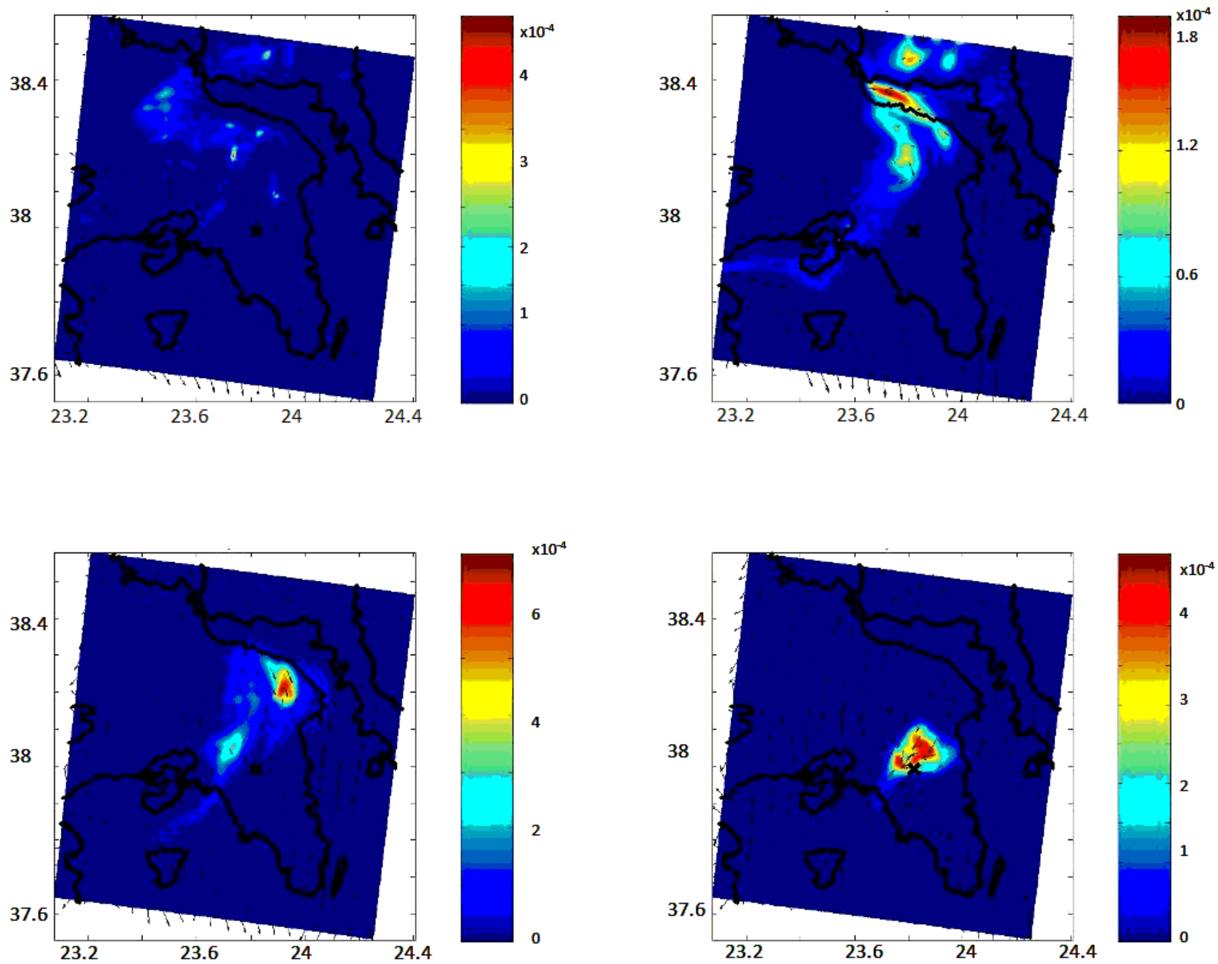

Figure 8. Calculated sensitivities (dO_3/dO_3) at the surface layer (at 3:00, 6:00, 9:00 and 12:00 UTC) (24 June, 2003).

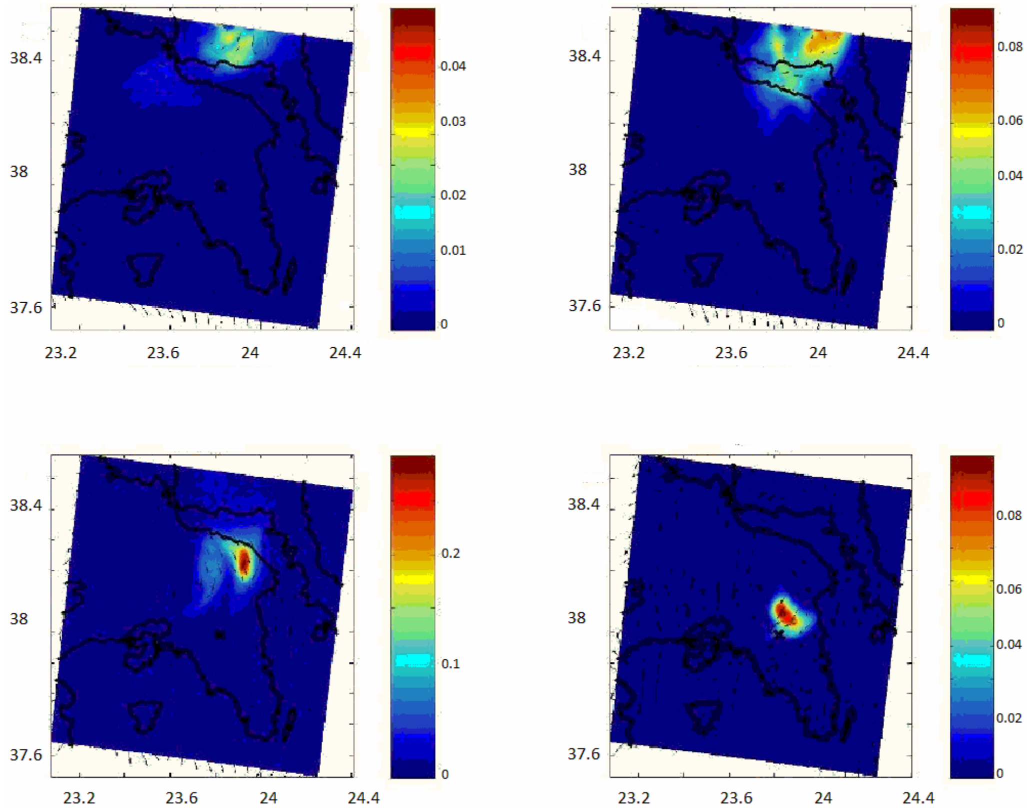

Figure 9. Calculated sensitivities (dO_3/dNO_2) at all model layers (at 3:00, 6:00, 9:00 and 12:00 UTC) (24 June, 2003).

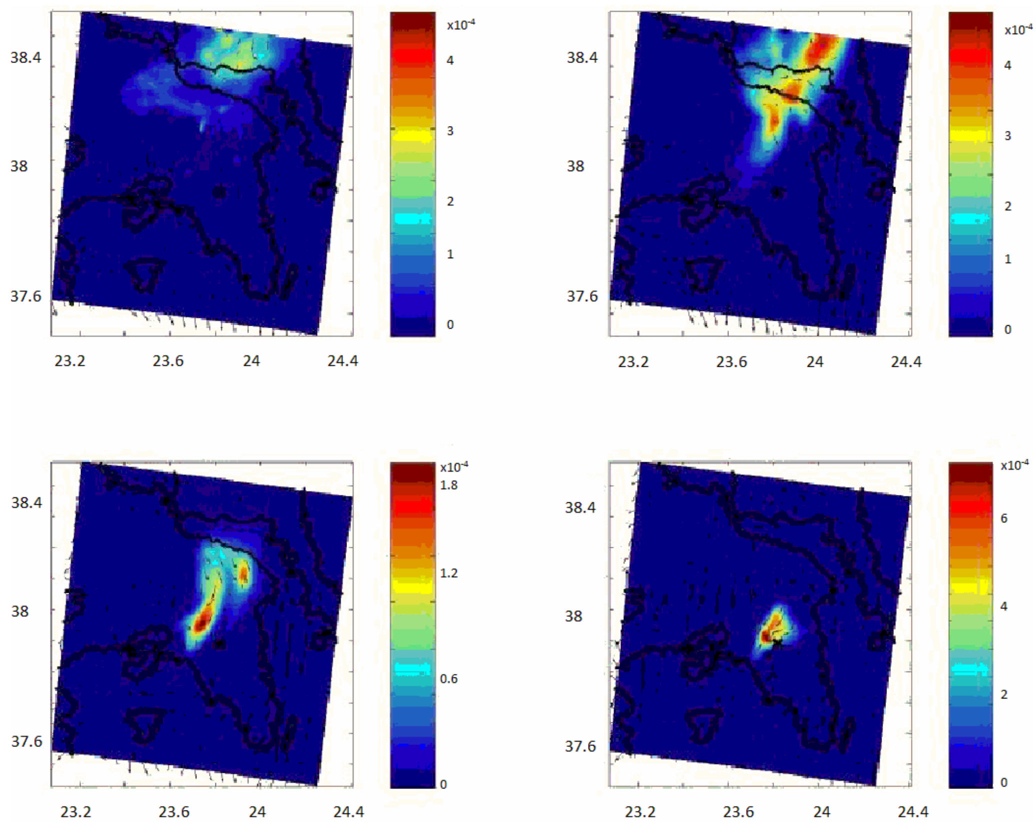

Figure 10. Calculated sensitivities (dO_3/dSO_2) at all model layers (at 3:00, 6:00, 9:00 and 12:00 UTC) (24 June, 2003).

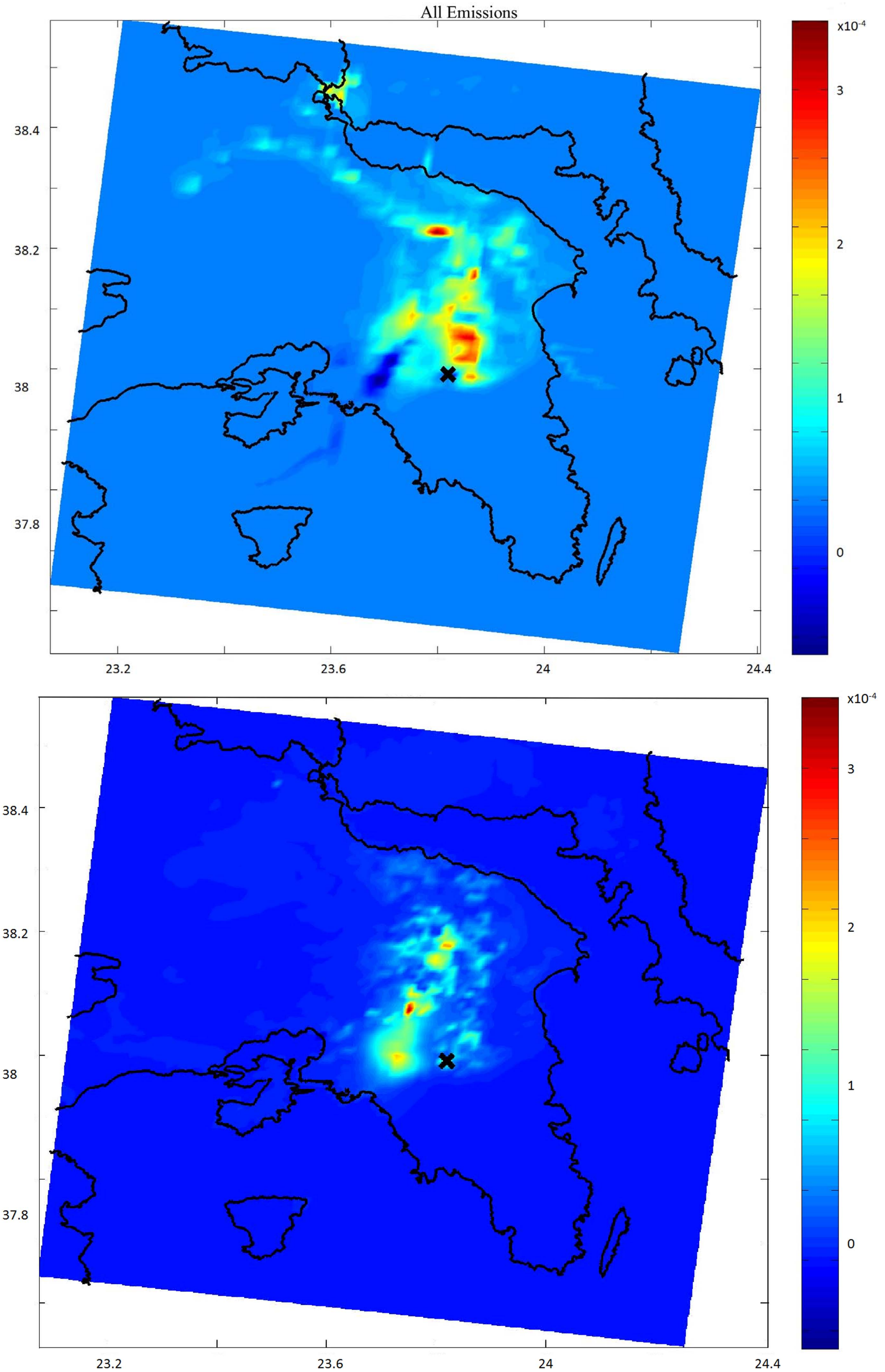

Figure 11. Calculated sensitivities with respect to emissions of NO_2 (dO_3/dNO_2) (left) and NO (dO_3/dNO) (right) at all model layers (at 3:00, 6:00, 9:00 and 12:00 UTC) (24 June, 2003).

4. Conclusion

An adjoint sensitivity study for ground ozone concentrations in Athens has been performed with the adjoint model of CMAQ for the receptor station of Agia Paraskevi (June 24, 2003). The difference on the areas of influence is evident depending on the prevailing wind field. Concerning the weather conditions of wind breeze which correspond to high O_3 levels in the city, the impact of the large emissions sources can be easily traced (city centre/traffic, airport and shipping emissions). Transported pollutant concentrations (O_3, NO_x and SO_2) influence the ozone concentration values at the receptor. The influence of NMVOC emissions on ozone at Agia Paraskevi was not found to be important, although the NMVOC concentrations were high during the particular pollution episode. The study indicated that focus must be placed on the improvement and updating of the high resolution emission inventories particularly that concerning the NO_x emissions. Moreover, since the meteorological influence on the emissions and pollution levels is significant, the meteorological model over the urban canopy must be configured and evaluated against observational data.

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