APPLICATION OF ADJOINT CMAQ CHEMICAL TRANSPORT MODEL IN THE ATHENS GREATER AREA: SENSITIVITIES STUDY ON OZONE CONCENTRATIONS

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Abstract: An operational meteorology and air quality forecasting system is currently under development by the Environmental Research Laboratory of NCSR "Demokritos". The system is based on the meteorological model MM5, the in-house EMISLAB emissions processing system and the chemical transport model CMAQ. It is configured to apply on the Greater Athens Area with a 4-domains nested configuration focusing on a high spatial resolution (1x1 km^2) inner domain. The system produces meteorological and air quality predictions for a 72-hours time horizon with 1 hour time step. This paper uses the output of the operational system to apply the CMAQ adjoint for ozone sensitivity calculations, focusing for the two days of 18 and 19 July 2005.

In the current study, the calculated ground level ozone concentrations at certain defined locations and times are considered as the "response functional". Sensitivities of the response functional with respect to the state variables (species concentrations on the grid points and species emissions, e.g., NO_X, CO, VOCs) are calculated by running the adjoint model backwards in time (reverse mode). The distribution of the sensitivities in the computational domain, obtained for different times, provides essential information for the analysis: isosurfaces of sensitivities delineate influence regions, i.e., areas where perturbations in some concentrations will result in significant changes in the ozone concentrations in the area of interest at the final time.

Key words: Adjoint model, sensitivity analysis, ozone.

1. INTRODUCTION

Air quality models are important tools in air quality management and policy making for regulatory purposes. To evaluate the effectiveness of such decisions in air quality, sensitivity analysis is often undertaken for diagnostic and prognostic calculations. The usual approach in the sensitivity analysis is the forward mode in which, any perturbation in one or more input variables (e.g. initial conditions, emissions) is carried forward in time resulting in the calculation of derivatives at multiple receptors with respect to the perturbed initial and/or model parameters (Hakami et al., 2003). In adjoint (backward) mode, a perturbation in a receptor based metric is propagated backward in time resulting in the calculation of its sensitivities with respect to a large number of perturbed input parameters (Cacuci and Ionescu-Bujor, 2005). The mathematical formulation of the adjoint sensitivity for nonlinear dynamical systems has been presented by Cacuci (1981a, 1981b) and Marchuk et al. (1996). As the adjoint sensitivity method is a potent tool with a strong potential for diverse applications, it has attracted the attention of the atmospheric modellers in the recent years. The mathematical description of the adjoint sensitivity method applied to air transport and chemical models, presenting at the same time a complete set of computational tools for performing three-dimensional adjoint sensitivity studies can be found in Sandu et al. (2005).

The adjoint sensitivity method in air quality models results in a more accurate simulation of the spatial and temporal 3-dimansional fields of the chemical constituents in relation to their sources and sinks. In addition, the adjoint technique can integrate efficiently observational data into the model following a 4-dimensional variational (4D-Var) data assimilation process (Sandu et al., 2005). The method of 4D-Var data assimilation was applied to the analysis of chemically active trace species for the first time, using a Lagrangian stratospheric model, by Fisher and Lary (1995). Elbern and Schmidt (1999) presented the first adjoint of a 3-D Eulerian Chemistry Transport Model (CTM) to include chemistry. In Elbern et al., (2000) a study was presented of the advantages and limits of the 4D-var technique to analyze the emission rates of non-observed precursor constituents of ozone, when only ozone observations are available. A review of the theoretical formulation of the adjoint method in 4D atmospheric chemistry data assimilation was performed by Wang et al. (2001).

These initial works have been followed more recently by similar development and application of adjoint models of several CTMs: e.g. CHIMERE (e.g. Schmidt and Martin, 2003), IMAGES (e.g. Stavrakou and Muller, 2006), the California Institute of Technology urban-scale model (e.g. Martien and Harley, 2006) and DRAIS (Nester and Panitz, 2006). The adjoint of the regional model STEM has also been developed (Sandu et al., 2005) and deployed (Hakami et al., 2006; Chai et al., 2006). Henze and Seinfeld (2006) applied the adjoint of the global chemical transport model GEOS-Chem, focusing on the chemical and thermodynamic relationships between sulfate – ammonium – nitrate aerosols and their gas-phase precursors. Zhang et al., (2008) have performed adjoint sensitivity analysis and 4D-Var data assimilation to investigate the maximum area of influence within the atmosphere on ozone concentrations, using STEM (Sulfur Transport Eulerian Model) over the state of Texas.

2. MODEL CONFIGURATION

This paper presents an attempt to improve our understanding of ozone in the Greater Athens Area (GAA) by performing an adjoint sensitivity analysis at ground level ozone concentrations, in July 18 & 19, 2005. The adjoint version of the Community Multiscale Air Quality, (CMAQ v.4.5), a 3-D atmospheric dispersion and photochemical model, has been employed to conduct the sensitivity analysis. The meteorological predictions are produced by the

MM5 (Mesoscale Model 5) (Penn State University version 3.7.2), which has been parameterized for application to the particular geographical and climatic characteristics of the GAA. Its 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.
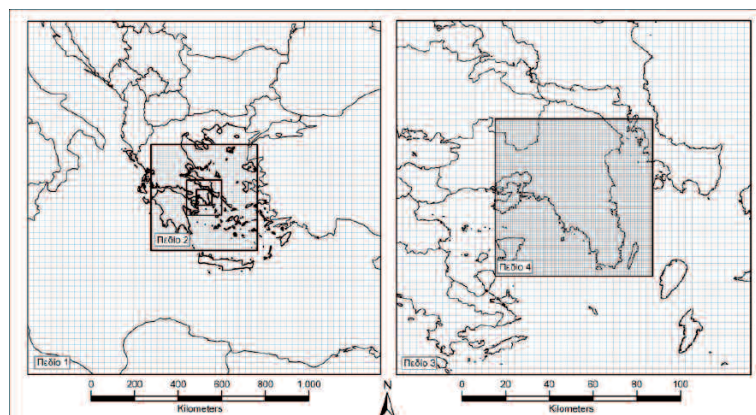

Figure 1. Working Domain specifications.

Table 1. Domain characteristics.

	Cells	Cell size(km)
Domain 1	60 x 60	27 x 27
Domain 2	54 x 54	9 x 9
Domain 3	54 x 54	3 x 3
Domain 4	72 x 72	1 x 1

3. ADJOINT CALCULATIONS

Two consecutive days have been selected in order to study the combined meteorology and chemistry effects on the concentration of O3 in two selected locations in the Greater Athens Area. Two stations have been selected for the analysis which according to the annual report of the Ministry of the Environment exhibit the highest amount of episodic events (i.e. exceedances of maximum 8-h average value) on an annual basis: Thrakomakedones and Agia Paraskevi (location of NCSRD).

JULY 18, 2005

This day is characterized by N–NW surface winds as predicted by the meteorological model MM5. The concentrations that influence the O3 value at 12:00 GMT on the Thrakomakedones area are located on the N–NW part of the area, and more specifically on the industrial zone between neighbouring prefects of Attiki and Biotia. (Fig. 2 and Fig. 3)

JULY 19, 2005

This day is characterized by wind breeze conditions as predicted by the meteorological model MM5. The morning low/moderate wind speeds blowing from the NW direction demonstrate a shift due to sea-land temperature differences in the late morning and afternoon hours from the sea towards inland. The concentrations that influence the O_3 value at 12:00 GMT on the Agia Paraskevi area are diverse and vary according to the strength of the emissions, the meteorological fields and the complex topography of the area.

Figure 4d shows the variation of O3 at 12:00 GMT on the receptor location with respect to O_3 concentration on a 3-h interval backwards in time, which is related mainly to transport. It is important to note the transport of O3 from the sea (both south and east of the receptor). The main emissions are from the city centre, predominantly traffic, the Athens International Airport and shipping portrayed in Figure 5 for the NO_X.

4. CONCLUSIONS

This paper presented the ozone sensitivity analysis for the Greater Athens Area performed using the adjoint version of CMAQ. The adjoint CMAQ estimates the sensitivity of ozone concentrations on user defined locations (receptors) and temporal. Adjoint sensitivity analysis allows us to assess the areas that have the largest impact on a given receptor site. For the purposes of this study two receptor locations were selected on two days with different meteorological conditions. The difference on the areas of influence is evident depending on the prevailing wind field.

Concerning the day with wind breeze conditions that correspond to high O3 levels in the GAA, the impact of the large emissions sources can be easily traced (city center / traffic, airport and shipping emissions)

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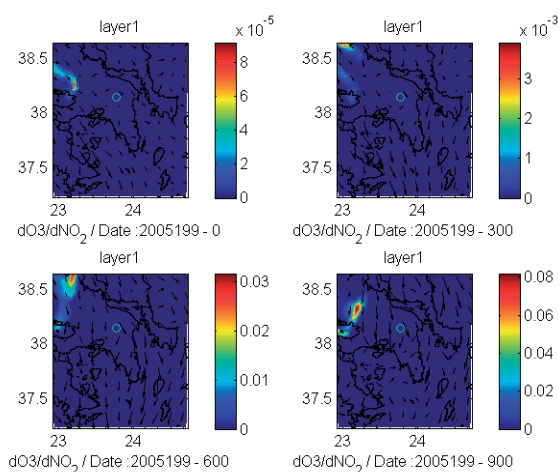
Figure 2. Sensitivity plots for dO3/dNO$_2$ every 3h for receptor placed at Thrakomakedones area (o) at 18/7 - 12:00 GMT.
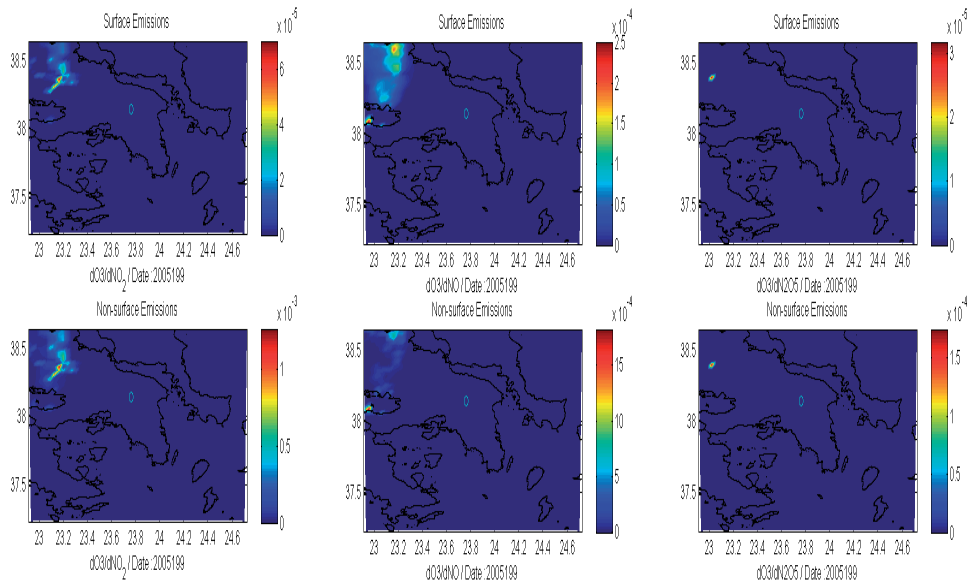
Figure 3. Sensitivity plots for dO$_3$/dNO$_X$ emissions for receptor placed at Thrakomakedones area (o) at 18/7 - 12:00 GMT.
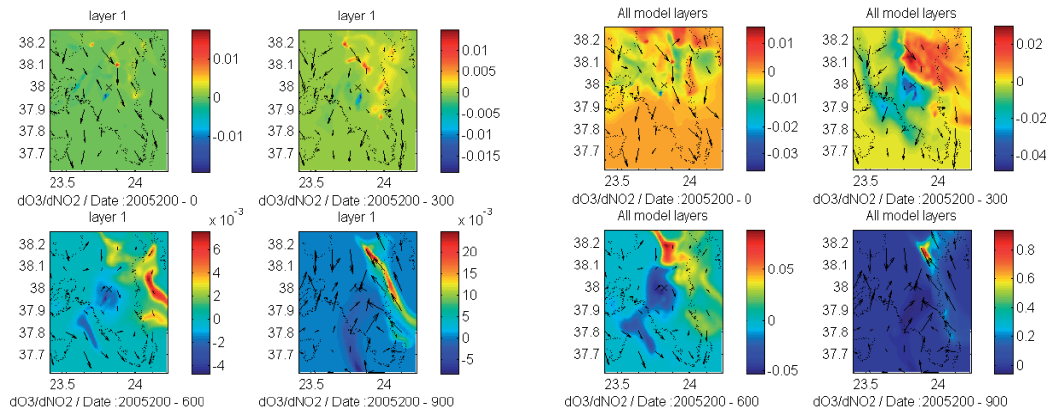

Figure 4a. Sensitivity plots for dO$_3$/dNO$_2$ every 3h for receptor placed at Ag Paraskevi area at 19/7 - 12:00 GMT.
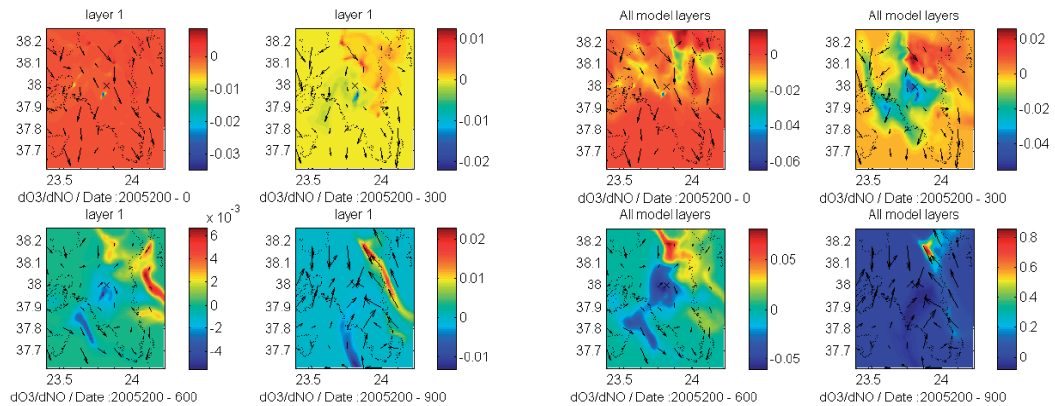

Figure 4b. Sensitivity plots for dO$_3$/dNO every 3h for receptor placed at Ag Paraskevi area at 19/7 - 12:00 GMT.
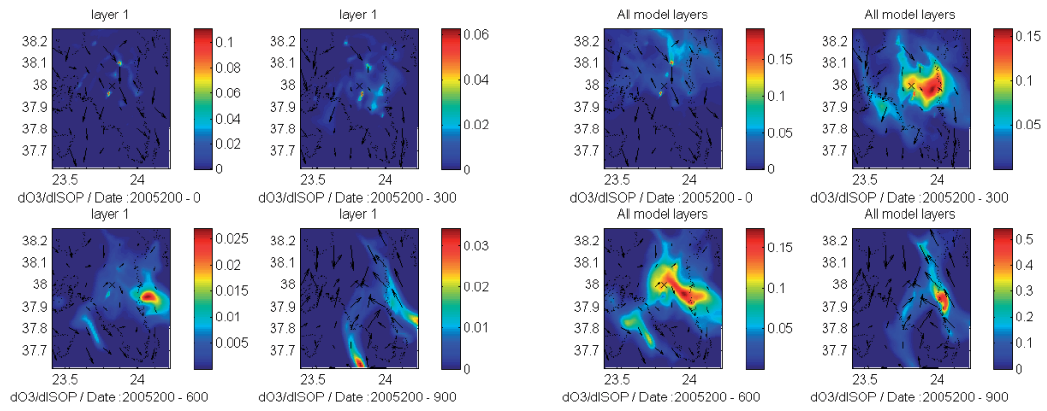
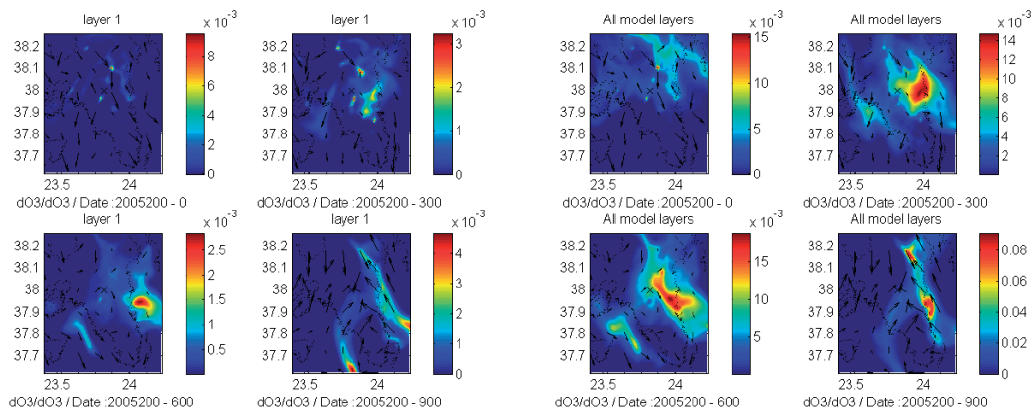Figure 4c. Sensitivity plots for dO3/dISOP every 3h for receptor placed at Ag Paraskevi area at 19/7 - 12:00 GMT.

Figure 4d. Sensitivity plots for dO3/dO3 every 3h for receptor placed at Ag Paraskevi area at 19/7 - 12:00 GMT.
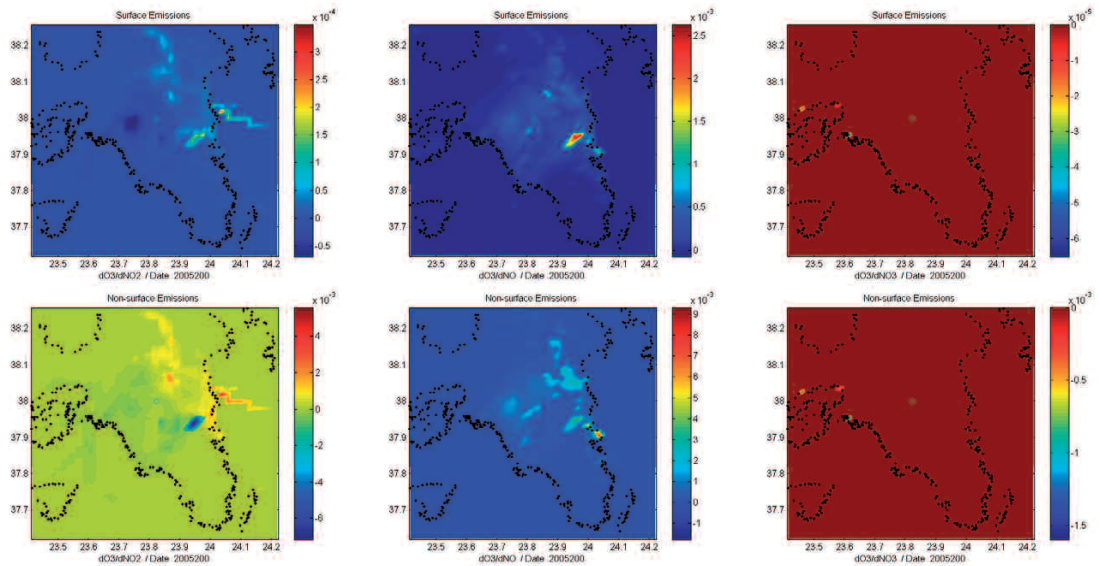

Figure 5. Sensitivity plots for dO3/dNO$_x$ emissions for receptor placed at Ag Paraskevi area at 19/7 - 12:00 GMT.