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Studying the sensitivity of pollutants' concentrations caused by variations of chemical rates

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ABSTRACT

A systematic procedure for sensitivity analysis of a case study in the area of air pollution modeling has been performed. Contemporary mathematical models should include a large set of chemical and photochemical reactions to be established as a reliable simulation tool. The Unified Danish Eulerian Model is in the focus of our investigation as one of the most advanced large-scale mathematical models that describes adequately all physical and chemical processes.

Variance-based methods are one of the most often used approaches for providing sensitivity analysis. To measure the extent of influence of the variation of the chemical rate constants in the mathematical model over pollutants' concentrations the Sobol' global sensitivity indices are estimated using efficient techniques for small sensitivity indices to avoid a loss of accuracy. Studying relationships between input parameters and the model's output as well as internal mechanisms is very useful for a verification and an improvement of the model and also for development of monitoring and control strategies of harmful emissions, for a reliable prediction of the final output of scenarios when the concentration levels of pollutants are exceeded. The proposed procedure can also be applied when other large-scale mathematical models are used.

1. Introduction

Environmental security is rapidly becoming a significant topic of present interest all over the world. It is necessary to carry out many comprehensive scientific studies and to analyze carefully the most important physical and chemical processes during the transport and transformations of air pollutants. An effective performance of such complicated procedures requires a joined research and collaboration between experts in the field of environmental modeling, numerical analysis and scientific computing.

The aim of the present work is to propose a new mechanism for investigating the sensitivity of the calculated concentration levels of important pollutants (like nitrogen dioxide NO_2 and especially ozone O_3) due to a variation of rates of the involved chemical reactions in a real-life scenario of air pollution transport over Europe with the Unified Danish Eulerian Model (UNI-DEM).

In an investigation of various highly complex engineering, physical, environmental, social, and economic systems it is important to measure relations that describe the effect on the output results when the conditions for the input change.

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Sensitivity analysis (SA) is the study of how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model's input [1]. Two classes in sensitivity analysis are considered in the existing literature: local SA and global SA. Local SA studies how some small variations of inputs around a given value change in the value of the output. Global SA takes into account all the variation ranges of the inputs, and apportions the output's uncertainty to the uncertainty in the input factors.

Several sensitivity analysis techniques are available [1]. Most existing methods for providing SA rely heavily on special assumptions connected to the behavior of the model (such as linearity, monotonicity and additivity of the relationship between the input factor and the model's output). Among quantitative methods, variance-based methods are the most often used [2]. The main idea of these methods is to evaluate how the variance of an input or a group of inputs contributes into the variance of the model's output.

Computational tasks arising in the treatment of large-scale air pollution models are enormous, and great difficulties arise even when modern high-performance computers are used. That is why, it is highly desirable to simplify as much as possible the model keeping the needed level of reliability of the models' results. A careful sensitivity analysis is needed in order to decide where and how simplifications can be made. On the other hand, it is important to analyze the influence of variations of the initial conditions, the boundary conditions and/or the chemical rates on the model results in order to make right assumptions about the simplifications which have to be implemented. Such an analysis can give valuable information about the performance of reliable and reasonable simplifications or to identify parameters and mechanisms the accuracy of which should be improved, because the model's results are very sensitive to variations of these parameters and mechanisms. Thus, the goal could be

- improving the model,
- increasing the reliability of the results, and
- identifying processes that must be studied more carefully.

The rest of the paper is organized as follows. A description of the mathematical model used is given in Sections 2 and 2.1. Here we also describe the approach for evaluating Sobol' global sensitivity indices (SI) in Section 2.3. Section 2.4 contains a brief review of two Monte Carlo approaches for small sensitivity indices. Section 3 presents a case study, the proposed scheme for providing sensitivity analysis and some results from numerical experiments. Section 4 contains a discussion about the numerical results obtained. Some concluding remarks are given in Section 5.

2. Mathematical background

2.1. The mathematical model—Unified Danish Eulerian Model

According to the definition, given in [1], sensitivity analysis involves models, model inputs and model outputs.

The focus of our study is in the area of environmental security (air pollution transfer). Contemporary mathematical models of air pollution transport should include a fairly large set of chemical and photochemical reactions to be established as a reliable simulation tool [3]. The investigations and the numerical results that are reported in this paper have been done by using a large-scale mathematical model called the Unified Danish Eulerian Model [4–7].

The Unified Danish Eulerian Model simulates the transport of air pollutants. It has been developed at the Danish National Environmental Research Institute (http://www2.dmu.dk/AtmosphericEnvironment/DEM/). The space domain of the model contains the whole of Europe, the Mediterranean as well as parts of Asia and Africa. The model gives the possibility to study concentration variations in time of a high number of air pollutants, which is important for environmental protection, agriculture, health care. The mathematical model takes into account the major physical processes—advection, diffusion, deposition, emissions, and chemical reactions. It must be emphasized that the main types of pollutants—sulfur pollutants, nitrogen pollutants, ammonia–ammonium, ozone, radicals and hydrocarbons can be studied by this model.

UNI-DEM is described mathematically [4–6] by the following system of partial differential equations:

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} - \frac{\partial (wc_s)}{\partial z} + \frac{\partial}{\partial x}\left(K_x \frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_s}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s}{\partial z}\right) + E_s + Q_s(c_1, c_2, \ldots, c_q) - (k_{1s} + k_{2s})c_s, \quad s = 1, 2, \ldots, q.$$

The number q of equations in this system is equal to the number of chemical species that is studied by the model. The other quantities involved in the model are described below: c_s—concentrations of the chemical species; u, v, w—components of the wind along the coordinate axes; K_x, K_y, K_z—diffusion coefficients; E_s—emissions in the space domain; k_{1s}, k_{2s}—coefficients of dry and wet deposition respectively ($s = 1, \ldots, q$); $Q_s(c_1, c_2, \ldots, c_q)$—non-linear functions that describe the chemical reactions between species.

Chemical reactions play a significant role in the model. The equations in the model are coupled through the chemical reactions. Moreover, both non-linearity and stiffness of the equations are mainly introduced by the chemistry (see [3]). Thus, the motivation to choose UNI-DEM is that it is one of the models of atmospheric chemistry, where the chemical processes are taken into account in a very accurate way. The chemical scheme used in the model is the well-known condensed CBM-IV (Carbon Bond Mechanism; the scheme was proposed in [8], but some enhancements have been obtained in [5] by adding