ENVIRONMENTAL MODELING:
case study

Ivan Dimov

Contents

Chapter 1

APPLICATIONS: MONTE CARLO SENSITIVITY SIMULATIONS TO THE PROBLEM OF AIR POLLUTION TRANSPORT

The aim of this chapter is to develop a special Monte Carlo sensitivity technique in order to study the influence of some input parameters of the atmospheric chemistry to the level of concentrations of pollutants in a real-live scenario of air-pollution transport over Europe.

First, the developed technique is applied on the box-model in order to study the sensitivity of the concentrations of some important pollutants (like NO_2 and O_3). It is shown that the most important parameter (from the point of view of sensitivity simulations) is the rate constant of the reaction producing NO_2 from O_3 and NO. The results are sensitive to small variances of the rate constant.

Second, the developed Monte Carlo simulation technique is applied to the *Danish Eulerian Model*. For running the model to get realistic results for a real-live scenario of air-pollution transport the vector machine CRAY Y-MP C90A is used.

It is shown that the results of the real-life modeling of air-pollution transport are not equally sensitive to different parameters used in the model as input parameters. There are some parameters (like the rate constant of the reaction producing NO_2 from O_3 and NO), which are very important since the results are sensitive to small changes of the values of these parameters. In this sense the Monte Carlo sensitivity simulation could by used as a special "advisor" to physicists, because this simulation permits to find how accurately the input parameters have to be measured, as well as how much theory is needed to describe some of the processes of air-pollution transport.

High concentrations and/or depositions of certain chemical species may cause damages on plants, animals and humans. Such species can be transported over long distances. Therefore areas far away from the large emission sources can also be highly polluted (under certain meteorological conditions, at least). That is why it is

necessary to study the pollution levels on large space domains (e.g. on space domains containing a given continent). Big mathematical models are indispensable tools in the attempts to determine the levels of concentrations and depositions of the harmful air pollutants on very large space domains. Such models are often described by systems of partial differential equations (the number of equations being equal to the number of chemical species studied by the model). Discretization and splitting techniques lead to the solution, over thousands of time-steps, of several very large systems of ordinary differential equations. It is not uncommon that each of these systems contain several million equations. This means that the computational tasks arising in the treatment of large-scale air pollution models are enormous, and great difficulties arise even when modern high-speed computers are used. Therefore, it is highly desirable to simplify as much as possible the model. One way to do this is to apply the simplest physical and chemical mechanisms which will still ensure the achievement of reliable results. A careful sensitivity analysis is needed in order to decide where and how simplifications can be made.

In this chapter the first step in a procedure, related to the sensitivity of the concentrations and depositions to variations of certain chemical rate constants, is described. We started by determining qualitatively a rate constant the variation of which causes big variations of the concentrations of two selected chemical species (nitrogen di-oxide and ozone), which are harmful when their concentrations and/or depositions are high. A simple box model has been used in these tests. After that a big mathematical model for studying air pollution levels in Europe, the Danish Eulerian Model, has been used to study quantitatively the effect of varying the selected chemical rate constant to the concentrations of the two most involved chemical species in different parts in Europe. A Monte Carlo technique has been used in these tests. The results show that the variations of the concentrations in different parts of Europe are different, although the variations of the rate constant were the same at all grid-points in the space domain.

High pollution levels may lead to the destruction of eco-systems and may cause damages on plants, animals and humans. Therefore, the pollution levels must be studied carefully. It is necessary to find out whether the pollution levels are under some critical levels and, if they are, to find reliable control strategies to keep them there. These tasks can be solved successfully by developing and using reliable mathematical models for studying different pollution phenomena. These models must satisfy several important requirements:

1. The mathematical models must be defined on large space domains, because the long range transport of air pollution is an important environmental phenomenon and high pollution levels are not limited to the areas where the high emission sources are located.

2. All relevant physical and chemical processes must be adequately described in the models used.

3. Enormous files of input data (both meteorological data and emission data) are needed.

4. Also the output files are normally very big, and fast visualization tools must be used in order to represent the trends and tendencies, hidden behind many megabytes (or even many gigabytes) of digital information, so that even non-specialists can easily understand them.

If all these requirements are satisfied, then the treatment of the mathematical models will lead to very large computational tasks. Indeed, the application of discretization and splitting procedures leads to several systems of ordinary differential equations. Every system may contain several millions of equations and has to be treated during many time-steps (as a rule several thousand time-steps). It is clear that these computational problems will cause difficulties even when big modern computers are used. That is why it is often necessary to perform some simplifications in the model. Such simplifications must be made so that the output results are still reliable. In order to satisfy the last requirement, one has to investigate how the changes of some parameters or some physical and chemical mechanisms will influence the output results. If the output results are not very sensitive to the variations of certain parameter or mechanism, then this means that the model can be simplified by choosing a simpler algorithm to calculate the parameter under consideration or to describe the mechanism under consideration by a simpler algorithm. If the output results are sensitive to changes in a given parameter of the algorithm, then one must be more careful: the parameter must be calculated in a more accurate way (by a more complicated algorithm), the mechanism must be described by a more advanced (and, again, more complicated) algorithm. This short discussion shows that it is useful to perform some sensitivity analysis in order to understand better the relationships between parameters and/or mechanisms used in the model and the output results.

The chemical reactions that take place under the transport are one of the most important processes. Therefore, we decided to concentrate our attention to the chemical reactions. We shall not present a comprehensive sensitivity analysis of the relationships between changes of the chemical rate constants and the output results, because this is a very difficult task. Instead of this we shall try to determine which reaction is the most important one for two selected chemical species (nitrogen di-oxide and ozone). Then we shall study the influence of changes of the chemical rate constant of this reaction on the nitrogen di-oxide and ozone concentrations. This is done by using a special Monte Carlo sensitivity technique.

The chapter is organized as follows. Short information about the particular mathematical model (the Danish Eulerian Model), which is used in the computations will be given in Section 1.1. The Monte Carlo algorithm used will be presented in Section 1.2. A special simple model, called *the box model*, will be used in Section 1.3 to determine the chemical reaction which is the most important for nitrogen di-oxide and ozone (changes of the chemical rate constant of this reactions lead to great changes of the concentrations of these two species). After that, In Section 1.4, the Monte Carlo algorithm described in Section 1.2 will be used to study the changes of the concentrations of nitrogen di-oxide and ozone in different European area that are caused by changes of the chemical rate constant. Finally, some concluding remarks will be given in Section 1.5.

1.1 The Danish Eulerian Model

The Danish Eulerian Model, (see [Zl95]) is described mathematically by the following system of partial differential equations:

$$\begin{aligned}\frac{\partial c_s}{\partial t} &= -\frac{\partial(uc_s)}{\partial x} - \frac{\partial(vc_s)}{\partial y} - \frac{\partial(wc_s)}{\partial z} \\ &+ \frac{\partial}{\partial x}\left(K_x\frac{\partial c_s}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c_s}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c_s}{\partial z}\right) \\ &+ E_s + Q_s(c_1, c_2, \dots c_q) - (k_{1s} + k_{2s})c_s \quad s = 1, 2, \dots q\ .\end{aligned} \tag{1.1}$$

The number q of equations in this system is equal to the number of chemical species that are studied by the model. This number varies from 10 to 168 in the experiments described in [Zl95]. The other quantities involved in the model can be described as follows (see again [Zl95] for more details):

- the unknowns c_s are concentrations of the chemical species,
- u, v and w are the components of the wind along the coordinate axes,
- K_x, K_y and K_z are diffusion coefficients,
- the emissions in the space domain are represented by the functions E_s,
- k_{1s} and k_{2s} are coefficients of dry and wet deposition respectively ($s = 1, \dots q$),
- the chemical reactions between species are described by the non-linear functions $Q_s(c_1, c_2, \dots c_q)$, where $s = 1, 2, \dots, q$ (the condensed CBM IV scheme that was proposed by [GWKD89], see also [Zl95], is the particular chemical scheme which will be used here).

It is very difficult to treat directly the system (1.1). Therefore, some kind of splitting is to be used. Splitting according to the major physical processes is very popular; see, for example, [Ma85], [MGS84] and [Zl95]. Such splitting procedures lead often to five sub-models which are to be treated cyclicly at every time-step ([Zl95]). These sub-models describe the horizontal advection, the horizontal diffusion, the chemical reactions (1.4) including the emissions, the deposition and the vertical exchange.

$$\frac{\partial c_s^{(1)}}{\partial t} = -\frac{\partial(uc_s^{(1)})}{\partial x} - \frac{\partial(vc_s^{(1)})}{\partial y} \tag{1.2}$$

$$\frac{\partial c_s^{(2)}}{\partial t} = \frac{\partial}{\partial x}\left(K_x\frac{\partial c_s^{(2)}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c_s^{(2)}}{\partial y}\right) \tag{1.3}$$

$$\frac{\partial c_s^{(3)}}{\partial t} = E_s + Q_s(c_1^{(3)}, c_2^{(3)}, \dots c_q^{(3)}) \tag{1.4}$$

$$\frac{\partial c_s^{(4)}}{\partial t} = -(k_{1s}+k_{2s})c_s^{(4)} \tag{1.5}$$

$$\frac{\partial c_s^{(5)}}{\partial t} = -\frac{\partial (w c_s^{(5)})}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_s^{(5)}}{\partial z}\right) \tag{1.6}$$

Five large systems of ordinary differential equations can be obtained from the sub-models (1.2)-(1.6) by applying any space discretization method:

$$dg^{(i)}/dt = f^{(i)}(t, g^{(i)}) \ , \quad g^{(i)} \in \mathcal{R}^{N_x \times N_y \times N_z \times N_s} \ , \quad f^{(i)} \in \mathcal{R}^{N_x \times N_y \times N_z \times N_s} \ , \tag{1.7}$$

where N_x, N_y and N_z are the numbers of grid-points on the grid-lines parallel to the coordinate axes and $N_s = q$ is the number of chemical species involved in the model. The function $f^{(i)}$ is a vector-function whose components are approximations to the concentrations at the grid-points, while $f^{(i)}$ depends on the particular discretization method applied to the corresponding sub-model (see [Zl95]).

The number of equations in any of the five ODE systems in (1.7) is equal to the product of the number of grid-points and the number of species. Thus, if $N_x = 96$, $N_y = 96$, $N_z = 10$ and $N_s = 35$, then every ODE system contains 3225600 equations. Furthermore, the five ODE systems are to be treated numerically during many time-steps (typically several thousand time-steps are needed). This shows that the numerical treatment of large-scale air pollution models leads to very big computational problems. This is why both fast numerical algorithms and high speed computers are to be used.

The chemical sub-model is the most time-consuming part of the model. Therefore, one should be very careful when numerical algorithms for this sub-model are selected. The algorithms chosen must be fast. Furthermore, these must be efficient when high speed computers are used. The difficulties that have to be overcome when the chemical sub-model is treated are discussed in [SZ97]. It is important, however, to emphasize the fact that the chemical sub-model consists of $N_x \times N_y \times N_z$ *independent* ODE systems. Each of these systems contains $N_s = q$ equations and can be rewritten as

$$dg/dt = f(t, g), \qquad g \in \mathcal{R}^{N_s}, \ , \quad f \in \mathcal{R}^{N_s}, \tag{1.8}$$

where g is a vector whose components are approximations to the concentrations at a given grid-point, while the right-hand-side vector f depends on the chemical mechanism which is used in the model (1.1). It is clear now that (1.8) can sometimes be considered (instead of the whole chemical sub-model) in studies of some phenomena which are directly connected to the chemical scheme. The much simpler model (1.8) will be called the box-model. The box model will be used in Section 1.3.

The two-dimensional version of (1.1) is often used in the computations. We shall use the two-dimensional version in Section 1.4.

1.2 An Algorithm for Monte Carlo Simulation

Monte Carlo (MC) simulation algorithms are algorithms for solving problems from different fields of science and engineering by using random variables. In general, the

MC algorithms replace the task of finding an approximation to the exact solution with the task of finding an approximation of the mathematical expectation and some other statistical characteristics of the solution of the problem solved. Let the scalar variable J be the desired solution of the problem or some desired linear functional of the solution. A random variable ξ with a mathematical expectation equal to J must be constructed so that $E\xi = J$. An approximation to J can be computed as a mean value by using n independent values $\xi_1, \xi_2, \ldots, \xi_n$, of ξ,

$$J \approx \frac{1}{n} \left(\xi_1 + \xi_2 + \ldots + \xi_n\right) . \tag{1.9}$$

Monte Carlo simulations are often used to evaluate some important statistical characteristics of the solution, such as the standard deviation, variance, skewness and, so on (see, for example, [So73] for more details)

Very often the Monte Carlo simulation is used to study complicated systems and phenomena when these can be treated as a *black box*. The main idea is to "introduce" some random parameter or random field in the input of the *black box* and to treat the calculated results by using well known statistical algorithms. There are two main problems in a such Monte Carlo simulation:

- how to simulate the input random parameter with a priori given statistical characteristics (mean value, standard deviation, and so on) in order to be sure that the considered realization of the random parameter is "near" to the theoretical one in some measured space

and

- how to handle the output results in order to measure the sensitivity of the *black box* to the considered input parameter?

There are many well known generators of *normally distributed* or *uniformly distributed* random variables, which can be used for producing high quality "input" data with a priori given statistical characteristics. The generator of the uniformly distributed random variables used here is based on a special function $f(x)$, see [So73], which:

- is defined on the interval $[0, 1]$,
- satisfies $0 \leq f(x) \leq 1$,
- its graph is "dense" in the unite cube.

It is necessary to take a linear combination of a large number k of values of the defined above special function $f(x)$ in order to obtain *normally distributed* random variables.

1.3 Finding the Reaction that has Greatest Influence on the Nitrogen Di-oxide and Ozone Concentrations

The box model is defined by the system of ordinary differential equations (1.8) from Section 1.1. This model has been used to find the reaction that has greatest influence on the concentrations of nitrogen di-oxide and ozone. The Monte Carlo algorithm sketched in the previous section is used in the experiments. In each experiment a sequence of N normally distributed random values of the chemical rate constant of one of the chemical reactions was produced by using a random number generator. After that the box model was run for these N random values (in our tests $N = 100$). This procedure has been carried out for all 70 chemical reactions involved in the chemical scheme used in the Danish Eulerian Model; the condensed CBM IV scheme (see [GWKD89] and [Zl95]). This means that N runs were perform per each chemical reaction with normally distributed random values. The standard deviations of the nitrogen di-oxide and ozone concentrations produced when the chemical rate constants were varied as described above were compared. It has been found in this way that the most important chemical reaction for the nitrogen di-oxide and ozone concentrations is:

$$O_3 + NO \implies NO_2 \ . \tag{1.10}$$

This means that small changes of the rate constant of this reaction lead to considerably large changes in the concentrations of nitrogen di-oxide and ozone and, moreover, these changes are larger than the changes, for the same two chemical species, observed when the rate constants of the other chemical reactions were varied by using the same procedure.

1.4 Sensitivity Tests with the Danish Eulerian Model

Consider the reaction (1.10). It is interesting to see what will happen if the experiment with a sequence of N normally distributed random values of the constant rate of reaction (1.10) is performed by using the two-dimensional version of the Danish Eulerian Model (instead of the box model used in the previous section). Several such experiments, each of them consisting of N runs with the Danish Eulerian Model, have been carried out. The standard deviation used for calculating the sequence of normally distributed random values was varied in these experiments. Results obtained when the sequences of $N = 100$ normally distributed random values of the constant rate of reaction (1.10) are produced by using standard deviations $\sigma = 0.5$ and $\sigma = 0.25$ will be presented here, but some other values of the standard deviations were also used.

The results, obtained after performing N runs with normally distributed random

values of the constant rate of reaction (1.10), were used to calculate the standard deviations and the skewness of the nitrogen dioxide and ozone concentrations for every value of the standard deviation σ used in the experiments. The results are presented in Figure 9.3 - Figure 9.8 (where by X and $Y = \sigma$ the mean value and the standard deviation of the randomly generated normalized rate constants are denoted). The following major conclusions can be drawn from this experiment:

- The standard deviations of the ozone concentrations given in Figure 9.3 for $\sigma = 0.5$ and Figure 9.5 for $\sigma = 0.25$ are greatest in the areas where the European emissions are biggest (compare Figure 9.3 and Figure 9.5 with Figure 9.1) and where the nitrogen di-oxide concentrations are highest (compare Figure 9.3 and Figure 9.5 with Figure 9.2).

- The patterns of the distributions of the standard deviations of the nitrogen di-oxide concentrations are not so pronounced (see Figure 9.4 and Figure 9.6, where the results obtained, respectively, with $\sigma = 0.5$ and $\sigma = 0.25$ are given). Nevertheless, it is clear that the effect is opposite to the effect observed when the standard deviations of the ozone concentrations are studied. The standard deviations in the most polluted with nitrogen species areas are smaller than the standard deviation in the areas which are far away from the highly polluted areas; compare Figure 9.4 and Figure 9.6 with Figure 9.1 and Figure 9.2).

- If the standard deviation of the sequences of normally distributed random values of the rate constant of reaction (1.10) is reduced, then the standard deviations of the ozone concentrations are also reduced, but the pattern of the distribution of the highest standard deviations remains the same; compare Figure 9.3 with Figure 9.5. The same is also true for the pattern of distribution of the highest standard deviations of the nitrogen di-oxide concentrations; compare Figure 9.4 with Figure 9.6.

- Results concerning the distribution of the skewness (for the sequence obtained with standard deviation $\sigma = 0.5$) are given in Figure 9.7 for the skewness of the ozone concentrations and in Figure 9.8 for the skewness of the nitrogen di-oxide concentrations. The two plots indicate that here also the effect is opposite: in the areas where the skewness of the ozone concentrations is greatest, the skewness of the nitrogen di-oxide concentrations is smallest.

The main result is that the influence of the rate constant of reaction (1.10) on the ozone concentrations seems to be great in the highly polluted with nitrogen pollutants areas. Therefore an accurate value of this rate constant is needed if the model is to be used on a space domain in which there are highly polluted with nitrogen species areas. On the other hand, if in the space domain of the model there are not areas which are highly polluted with nitrogen species, then the accuracy with which this rate coefficient is determined becomes less important.

1989
NOX EMISSIONS

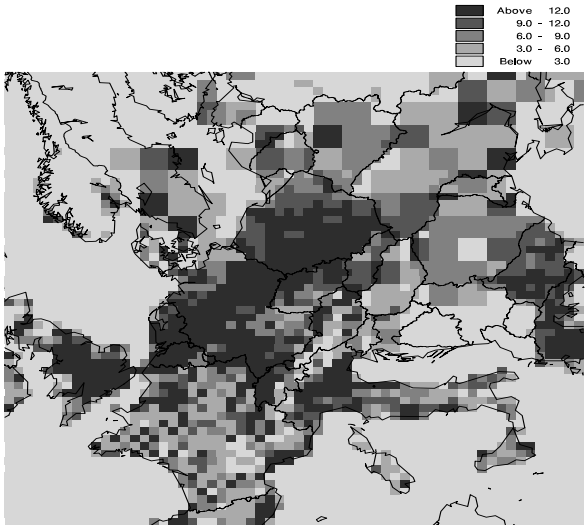

Figure 9.1
European nitrogen oxides emissions

JULY 1989
NO2 ALL EUROPEAN SOURCES

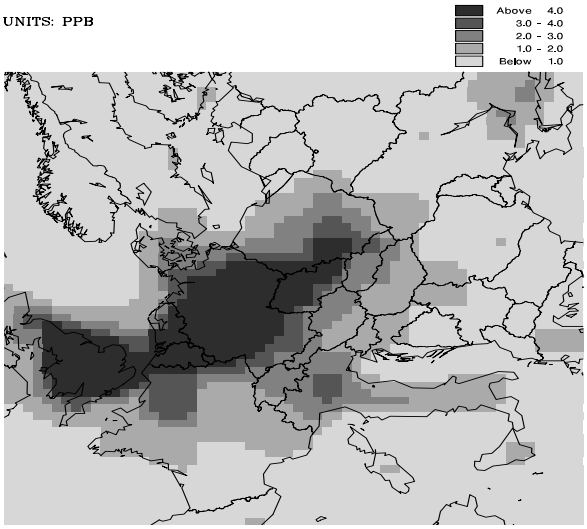

Figure 9.2
Nitrogen di-oxide concentrations in Europe

JUNE 1989
O3 STANDARD DEVIATION X=1.0, Y=0.5)

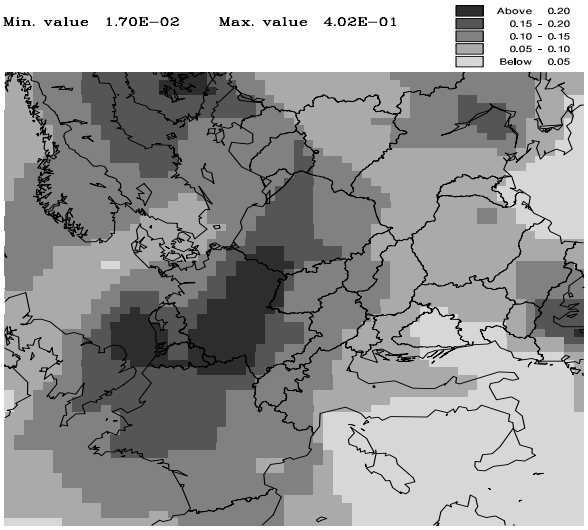

Figure 9.3
Standard deviations of the ozone concentrations (variance 0.50)

JUNE 1989
NO2 STANDARD DEVIATION X=1.0, Y=0.5)

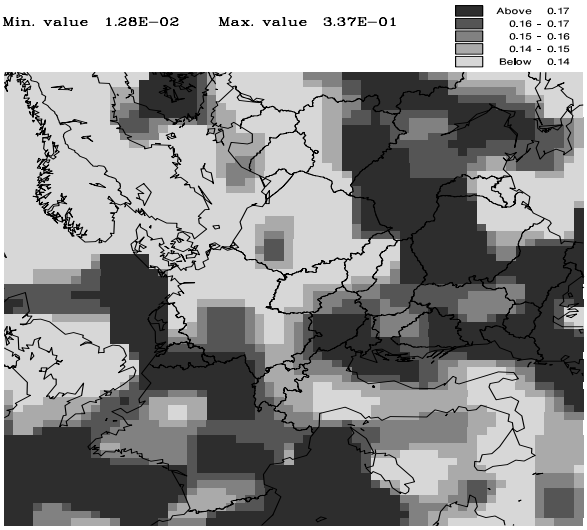

Figure 9.4
Standard deviations of the nitrogen di-oxide concentrations (variance 0.50)

JUNE 1989
O3 STANDARD DEVIATION X=1.0, Y=0.25)

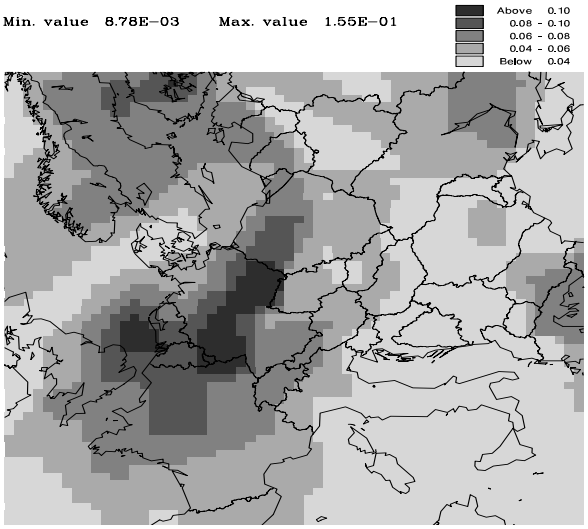

Figure 9.5
Standard deviations of the ozone concentrations (variance 0.25)

JUNE 1989
NO2 STANDARD DEVIATION X=1.0, Y=0.25)

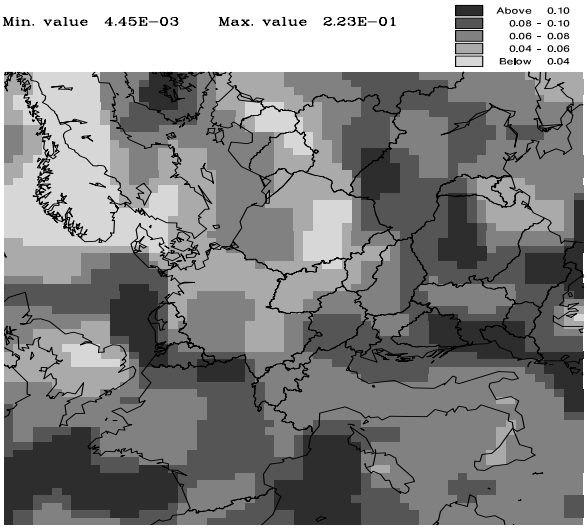

Figure 9.6
Standard deviations of the nitrogen di-oxide concentrations (variance 0.25)

JUNE 1989
O3 SKEWNESS (X=1.0, Y=0.25)

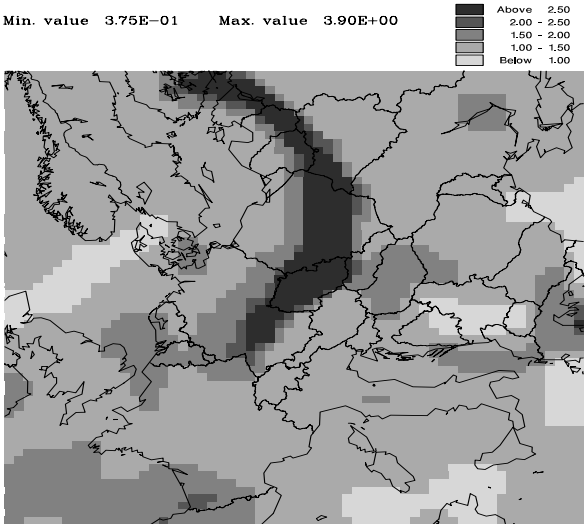

Figure 9.7
Skewness of the ozone concentrations (variance 0.50)

JUNE 1989
NO2 SKEWNESS (X=1.0, Y=0.5)

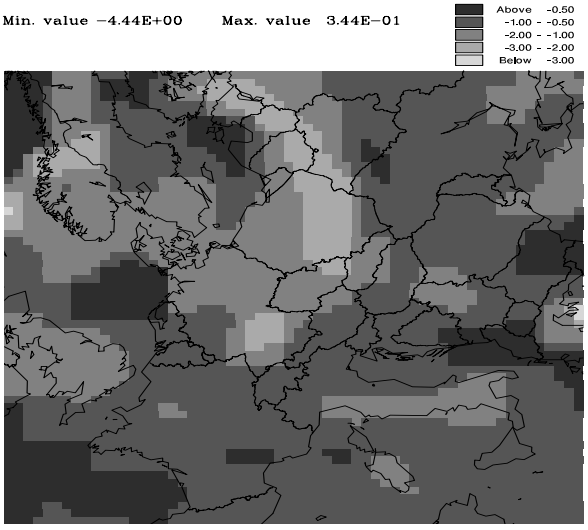

Figure 9.8
Skewness of the nitrogen di-oxide concentrations (variance 0.50)

1.5 Concluding Remarks

It is probably worthwhile to carry out some computations with the three-dimensional version of the Danish Eulerian Model (see [ZDG96]. The experiments presented in this chapter have shown that different areas in the horizontal plane are influenced in a different way when certain constant rates are changed. The experiments with the three-dimensional version of the Danish Eulerian Model may show differences also in the vertical directions. However, such runs are very time-consuming. It will be possible to perform such experiments only if new and faster numerical algorithms are used in the model and, moreover, if bigger and faster computers become available.

It is desirable to use the Danish Eulerian Model in similar experiments, but for some other chemical rate constants. Maybe, one should also test the combined effect of changing simultaneously several chemical rate constants on relevant concentrations and/or depositions.

The sensitivity of the model results to variations of some other parameters (as, for example, the boundary conditions) should also be studied.

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