SOME SOURCE - RECEPTOR RELATIONS STUDIED BY THE DANISH EULERIAN MODEL

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INTRODUCTION

The modern high-performance computer architectures allow the environmental scientists to use operationally large air pollution models (with many pollutants involved, advanced chemical modules with non-linear chemical reactions and an adequate description of the physical processes in the atmosphere). Such a model is the Danish Eulerian Model (DEM) for studying long-range transport of air pollutants over Europe (Zlatev Z, 1995). Four versions of the code of the operational two-dimensional version of DEM for different computer architectures are available now:

- for **vector computers** (*CRAY C92A, Fujitsu*, *etc*.) (Zlatev Z. et al., 1995, 1996);
- for **parallel computers with distributed memory** *(IBM SP, CRAY T3E, Beowulf clusters*, etc.) (Georgiev K., Zlatev Z., 1998, 1999);
- for **parallel computers with shared memory** (*SGI Origin, SUN*, etc.) (Georgiev K., Zlatev Z., 2000);
- for **parallel computers with two level of parallelism** – distributed memory between nodes and shared memory inside the nodes that consist of several processors *(IBM SMP, clusters of multiprocessor nodes*, *etc*.) (Owczarz W., Zlatev Z., 2001, 2002).

The end-user can select an appropriate version of the model, which will allow him/her to exploit in the best possible way the great potential power of the modern supercomputers depending on the available computer architecture. Moreover, each of these four versions of the model can be used with spatial resolution of (*150 km* x *150 km*), (*50 km* x *50 km*) or (*10 km* x *10 km*) depending on the requirements and the power of the computer, which is used for computations. The facts that the high resolution versions of DEM imposes severe storage requirements and the computing time needed for a single run of the code is increased very considerably should be taken into account.

The study of source-receptor relations is of great importance. Particularly, such studies could be used when different trends, concerning the behaviour of the concentrations and depositions of the harmful air pollutants should be illustrated as a function of different emission scenarios. Results about the sensitivity of the concentrations and depositions in Europe to global variations of all emissions are needed from environmental specialists and the decision-makers. The contribution of the emissions of the separate country to the concentrations and depositions in this country and the surrounding this country area is another important problem, which has to be solved in order to reduce the air pollution to the prescribed acceptable levels. These problems are even more important in the sense of the influence of the global climate changes on the pollution levels and the prediction of some dangerous situations for humans, animals and vegetation in the future (see e.g. Dimov I., Geernaert G. and Zlatev Z., 2002).

SHORT ABOUT THE TWO DIMENSIONAL DANISH EULERIAN MODEL

The chemical species, which are involved in the Danish Elerian Model, are: *sulphur pollutants, nitrogen pollutants, ozone, ammonia-ammonium, several radicals* and a large number of relevant *hydrocarbons*. Until now, the model has mainly been used with the well known *CBM IV* chemical scheme containing q=35 species with a few enhancements which have been

introduced in order to make possible to use the model in studies concerning the distribution of *ammonia – ammonium* concentrations. Some experiments with chemical schemes with 56 and 168 species have been carried out. Five processes are involved in the model: *advection, diffusion, emission, deposition* and *chemical reactions*. Mathematically DEM is described by the following system of partial differential equations (Zlatev Z, 1995):

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

The meaning of the quantities in (1) are as follows: c_s – concentration of the s-th species; u and v – components of the wind velocity; K_x and K_y – diffusion coefficients; E_s – emission sources; k_{1s} and k_{2s} – deposition coefficients; Q_s – chemical reactions. The term, which describes the chemical reactions coupled the system and involves nonlinearity in it. As usual in the atmospheric models the system (1) is splited according to the different processes involved using ideas discussed in Marchuk G. (1985) and Mc Rae G. et al (1984) and as result the following four sub-models are solved successively on each time step:

$$\frac{\partial c_s^{(1)}}{\partial t} = -\frac{\partial (u c_s^{(1)})}{\partial x} - \frac{\partial (v c_s^{(1)})}{\partial y}$$

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

$$\frac{\partial c_s^{(3)}}{\partial t} = E_s + Q_s\left(c_1^{(3)}, c_2^{(3)}, \ldots, c_s^{(3)}\right)$$

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

One-dimensional first order finite elements are used during the space discretization of the advection and diffusion parts of the operational two-dimensional DEM. *Predictor-corrector methods* with several different correctors, which are chosen in such a way that the stability of the method is enhanced (Zlatev Z., 1984), are used to solve the systems of ordinary differential equations which appeared after the space discretization there. The QSSA (Quasi-Steady-State Algorithm), which is simple and relatively stable, is used to solve the chemistry-emission submodel while the system of ordinary differential equations which describes the deposition process is linear and it is solved exactly. The size of the systems that arise after the space discretization is enormous, see (Georgiev K., Zlatev Z., 1999). It is clear that such large computational problems can be solved in a reasonable time only if the recent high speed

computers are used and the corresponding algorithms are tuned to exploit as much as possible their great potential power.

SOME SOURCE – RESEPTOR RELATIONS

The emission fields, which are used as input data in DEM, are *sulphur, nitrogen oxides, ammonia – ammonium, anthropogenic hydro – carbons* and *natural hydro – carbons.* Many different emission scenarios have been carried out with DEM. Results obtained in two of them will be reported in this paper. The main goal of the first experiment is to study the sensitivity of the concentrations and the depositions in Europe to global variations of all emissions, excluding the *natural hydro – carbons*. The aim of the second experiment is to obtain results about the contribution of the Bulgarian emissions to the concentrations and depositions in Bulgaria and its surrounding area.

Sensitivity of the concentrations and depositions to emission reductions

The time interval, which is chosen, for the computer simulations, is one month. Five runs with different emission input data were performed. Starting with 100%, i.e. the reported European emissions for the chosen month, in the next four runs the all emissions, excluding the natural VOC (Volatile Organic Compounds) were reduced to 80%, 60%, 40% and 20%, respectively. Let us consider two important *primary* pollutants (*sulphur dioxide* and *nitrogen dioxide*) and two important *secondary* pollutants (*sulphate* and *nitrate*). The output results obtained from the computer runs of the model show that the greatest reductions for the primary pollutants are achieved in the highly polluted areas in Central and Western Europe. For the secondary pollutants just the opposite effect is observed. Moreover, this tendency becomes stronger when the reduction is greater. On the other hand the output results show that the differences between the concentrations in the different emission scenarios are quite different for the different pollutants. They are almost negligible for the *sulphur* pollutants while for the *nitrogen* pollutants they are much greater. The results obtained for the *ozone* concentration show that the reduction of the anthropogenic emissions has no great influence on its concentrations even when this reduction is 80%. However, the reduction of the *maximal daily ozone* concentration is more significant. The output results for another important pollutant, *hydroxyl radical*, show that the range of its variations is increased when the reduction of the European emissions becomes greater. Results about the reduction of the ozone concentrations in Bulgaria and minimal and maximal changes of the *hydroxyl radical* concentrations in the different scenarios are presented in Table 1.

*Table 1. Reductions of O_3 concentrations in Bulgaria and minimal and maximal changes of **OH** concentrations.*

Emission reductions	Ozone	Hydroxyl radical	
	Reduction of concentrations	Minimal change	Maximal change
by 20%	5%	94%	112%
by 40%	9%	86%	130%
by 60%	13%	75%	157%
by 80%	18%	57%	226%

Contribution of the Bulgarian emission sources

One of the great advantages of using large air pollution models is the possibility to study the contributions of the emission sources in a given country to the concentrations and depositions in this country and its surrounding area. Two runs of DEM were used to estimate the contributions due to the Bulgarian emission sources. In the first run, all European emission sources are used. In the second run, all emissions outside Bulgaria, excepting the *natural VOC*, are set to zero.

The output results obtained from these two runs show that the influence of the Bulgarian emission sources in the concentrations of the **primary** compounds is rather considerable both in the territory of Bulgaria and its surrounding area. It has to be seen that this influence is more than 75% in some grid squares for the *sulphur dioxide* and more than 66% in the case when the *nitrogen dioxide* are studied. The influence of the Bulgarian emission sources on the concentrations of the **secondary** pollutants, which are in general transported on longer distances, in Bulgaria and its surrounding area is much less than in the case of the primary compounds. This influence is about 25% in some grid squares for the *sulphate* pollutants, and 8% for the *nitrate* pollutants.

Linear and non-linear effects

Some results about how much the concentrations and depositions of the different pollutants will decrease when the emission in a given area will be reduced or increased by a certain amount are useful for the decision-makers. The experiments performed with different emission scenarios indicate that the effects of varying the emissions on the concentrations and depositions of the *sulphur* pollutants seem to be **linear**. In the case, when **all** emissions are simultaneously reduced with the same amount, the same conclusion can be done for the *ozone* concentrations. But, let us pointed that it is very important all emissions to be changed with the same amount, because when e.g. only *nitrogen* emissions are reduced then the *ozone* concentrations increase in certain areas, i.e. the effect is **non-linear**. On the other hand, the output results of the performed experiments show that the effects of varying the emissions on the *nitrogen* pollution tend to be **non-linear**. The nonlinearity is more promounnced when the emission changes are greater. But if the *total nitrogen depositions* are considered, then the effects are **closer to linear** effects. The effects of varying the emissions on the concentrations of the *hydroxyl radical* are strongly **non-linear** (see: Table 1). There is a clear tendency of increasing of the *hydroxyl radical* concentrations in the highly polluted parts of the space domain (Central and Western Europe) when the emissions are decreased. This explains the behaviour of the *sulphur dioxide* and the *nitrogen dioxide* which concentrations are reduced more in the areas where the concentrations of the *hydroxyl radical* are increased. For the *sulphate* and the *nitrate* pollutants the effect is opposite, i.e. their concentrations are greater where the concentrations of the *hydroxyl radical* are also greater. The conclusions made in this section are valid in the case that **all** European emissions are simultaneously reduced with the same amount. The conclusions can be different if the emissions only in a given region are reduced. The output results obtained in the cases when all European sources are active and when all European sources excluded Bulgarian sources are active, show that there is no linear tendency even for the *sulphur* pollutants.

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