Параллельное программирование

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PARALLEL COMPUTATIONS WITH LARGE-SCALE AIR POLLUTION MODELS

Large-scale mathematical models are very powerful tools in the efforts to provide more information and more detailed information about the pollution levels, especially about pollution levels which exceed certain critical values.. However, the model used must satisfy at least two conditions: (i) it must be verified that the model results are reliable and (ii) it should be possible to carry out different study by using the model. It is clear that comprehensive studies about relationships between different input parameters and the model results can only be carried out (a) if the numerical methods used in the model are sufficiently fast and (b) if the code runs efficiently on the available high-speed computers. Some results obtained recently by a new unified version of the Danish Eulerian Model will be presented in this paper.

1. Need for a Unified Air Pollution Model

It will be possible to apply an air pollution model in many different studies only if it is very flexible. The work on the development of the Danish Eulerian Model (DEM) has been initiated in the beginning of the 80's. Only two species were studied in the first version of the model. The space domain was rather large (the whole of Europe), but the discretization was very crude; the space domain was divided by use of a 32x32 grid, which means, roughly speaking, that 150 km x 150 km grid-squares were used. Both a two-dimensional version and a three-dimensional version of this model were developed. In both versions the chemical scheme was very simple. There was only one *linear* chemical reaction. The two-dimensional version of this model is fully described in Zlatev [27], while the three-dimensional version was discussed in Zlatev et al. [30]. These first two versions were gradually upgraded to much more advanced versions: (i) versions containing more chemical species, (ii) versions discretized on more refined grids and (iii) versions utilizing more advanced numerical algorithms (see Zlatev [28] and Zlatev et al. [29]).

Recently, the different versions of DEM were united in a common model. Several options can easily be specified when the new model is applied in different scientific studies:

- the model can be used both as a 2-D model and a 3-D model,
- different horizontal resolutions can be specified (50 km x 50 km, 16.67 km x 16.67 km and 10 km x 10 km cells can be used in the horizontal planes),
- different chemical schemes can be selected (a scheme with 35 species and a scheme with 56 species being available at present),
- an algorithm for dividing the large arrays into chunks can be applied in an attempt to exploit better the cache memory of the computer used.

The new model is called UNI-DEM.

2. Mathematical Description of UNI-DEM

UNI-DEM is described mathematically, see [28], by a system of partial differential equations (PDEs). The number of equations in this system is equal to the number of chemical species which are treated by the model. Five physical and chemical processes are represented in the model with different mathematical operators. These processes are: (i) horizontal advection (horizontal transport due to the wind), (ii) horizontal diffusion, (iii) chemistry + emissions, (iv) deposition and (v) vertical exchange (vertical advection + vertical diffusion).

The system of PDEs by which these five processes are described in UNI-DEM is of the following type:

$$\frac{\partial c_i}{\partial t} = -\frac{\partial \left(w c_i \right)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_i}{\partial z}\right) -$$

$$-\frac{\partial \left(u c_i \right)}{\partial x} - \frac{\partial \left(v c_i \right)}{\partial y} + \frac{\partial}{\partial x}\left(K_x \frac{\partial c_i}{\partial x}\right) +$$

$$+\frac{\partial}{\partial y}\left(K_y \frac{\partial c_i}{\partial y}\right) + Q_i\left(c_1, c_2, ..., c_q \right) + \qquad (1)$$

$$+E_i\left(x,\ y,\ z,\ t \right) - \left(\kappa_{1i} + \kappa_{2i}\right) c_i,$$

$$\left(x, y, z \right) \in \Omega, t \in \left[0, T\right], i = 1, 2, ..., q,$$

where (i) Ω is the space domain on which the system of PDEs (1) is defined (in the 2-D options of UNI-DEM Ω is a 4800 km x 4800 km square, while a 4800 km x 4800 km x 3 km parallelepiped is the space domain Ω in the 3-D options of UNI-DEM), (ii) $\left[0, T\right]$ is the time-interval (UNI-DEM is normally run over a time-period covering meteorological data for a given year) and (iii) q is the number of chemical species involved in the model.

The unknown functions c_i in (1) are concentrations of the involved chemical species. The quantities u, v and w are wind velocities along the coordinate axes. K_x, K_y and K_z are diffusion coefficients. The chemical reactions are described by the non-linear functions Q_i. The emissions sources in the space domain Ω of the model are represented by the functions E_i. Finally, κ_{1i} and κ_{2i} are deposition coefficients (for dry deposition and wet deposition respectively).

The system of PDEs (1) has to be considered with appropriate initial and boundary conditions. The choice of such conditions is beyond the scope of this paper (some details can be found in Zlatev [28]).

Different air pollution models can be obtained from the generic form (1) of the system of PDEs by using different mechanisms in the description of the underlying physical and chemical processes (More details can be found in Ebel [11] and Zlatev [28]).

3. Applying Splitting in UNI-DEM

It is difficult to treat directly the system of PDEs (1) by which the UNI-DEM is described mathematically. Therefore, different kinds of operator splitting are used in the large-scale air pollution models. Any splitting procedure leads to sub-models, which can be treated by different numerical methods. It is also easier to choose and use standard packages for some of the sub-models. Thus, efficient methods can be selected for each sub-model, which leads to better overall performance when the whole model is handled computationally.

An attempt to simplify the splitting procedure used in [28] is made in UNI-DEM. The big model is split in three sub-models by using this procedure:

- a sub-model containing the vertical exchange operator,

$$\frac{\partial c_i^{(1)}}{\partial t} = -\frac{\partial \left(w c_i^{(1)} \right)}{\partial z} + \frac{\partial}{\partial z}\left(K_z \frac{\partial c_i^{(1)}}{\partial z}\right), \qquad (2)$$

$$i = 1, 2, ..., q,$$

- a sub-model containing the horizontal advection and the horizontal diffusion operators,

$$\frac{\partial c_i^{(2)}}{\partial t} = -\frac{\partial \left(u c_i^{(2)} \right)}{\partial x} - \frac{\partial \left(v c_i^{(2)} \right)}{\partial y} +$$

$$+\frac{\partial}{\partial x}\left(K_x \frac{\partial c_i^{(2)}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial c_i^{(2)}}{\partial y}\right), \qquad (3)$$

$$i = 1, 2, ..., q,$$

- a sub-model containing the chemistry, the emissions and the deposition operators,

$$\frac{\partial c_i^{(3)}}{\partial t} = Q_i\left(c_1^{(3)}, c_2^{(3)}, ..., c_q^{(3)} \right) +$$

$$+E_i\left(x, y, z, t \right) - \left(\kappa_{1i} + \kappa_{2i}\right) c_i^{(3)}, \qquad (4)$$

$$i = 1, 2, ..., q.$$

In the actual computations the three sub-models are treated successively at a sequence of small time sub-intervals of length τ of $\left[0, T\right]$. The three sub-models, (2)-(4), are connected by using appropriate initial conditions (the cou-

pling of the sub-models obtained after applying some splitting procedure are discussed in Zlatev [28]).

The first of these three sub-models is not used when any of the 2-D options is specified.

The particular splitting procedure proposed here, see $(2)-(4)$, is based on ideas discussed in Marchuk [19] and McRae et al. [20]. Other splitting procedures may also be devised. A very popular splitting procedure is that proposed independently in 1968 by Marchuk [18] and Strang [25].

The splitting procedure is in general producing some errors. The order of the splitting procedure described by (2)-(4) is one, i.e. $O(\tau)$. The splitting procedure proposed in Marchuk [17] and Strang [25] is of second order, $O(\tau^2)$. At the same time, it should also be mentioned that the latter splitting procedure is considerably more expensive computationally.

If some assumptions are imposed, then the errors due to the splitting procedure may vanish. Different cases, in which such assumptions are imposed and, as a result of this, the errors due to the splitting procedure disappear, are discussed in Dimov et al. [5] and Lanser and Verwer [17].

4. Numerical Methods Used in UNI-DEM

The sub-models are to be treated by appropriate numerical methods. The particular numerical methods that are implemented in UNI-DEM are listed below.

- The finite elements discussed in Pepper et al. [23] are used to discretize the spatial derivatives in the vertical exchange sub-model (2). The semi-discretized model is handled by the ϑ-method (see Lambert [15] or Samarskii [24]).
- The finite elements from Pepper et al. [24] are used at present also in the discretization of the spatial derivatives in the horizontal advection-diffusion sub-model (3). Many other methods were tried: psedospectral algorithm, finite differences, methods based on the Bott's algorithm, semi-Lagrangian algorithm, etc. The semi-discretized sub-model is treated

by using a set of predictor-corrector (PC) schemes with several different correctors. The major idea is to vary the PC schemes in an attempt both to preserve the stability of the computations and to keep the same time-stepsize (Zlatev [28]).

- The chemistry-emission-deposition sub-model (4) is treated by using an improved QSSA (Quasi-Steady-State-Approximation) algorithm. The original QSSA algorithm, several classical time-integration methods for stiff systems of ODEs and a partitioning algorithm have also been tried, see Alexandrov et al. [1].

5. Need for high-speed computers

The spatial discretization of UNI-DEM leads to huge systems of ordinary differential equations (especially for the fine resolution options and for the 3-D options). This is illustrated in Table 1 and Table 2, where the numbers of equations and time-steps in the advection part for the option with 35 chemical species are given. The numbers of time-steps for the 3-D options of UNI-DEM are the same as the numbers of time-steps for the corresponding 2-D options (which are given in Table 2).

Table 1. **Numbers of equations when six options of UNI-DEM are used**

Spatial resolution (horizontal)	2-D option (1-layer)	3-D option (10 layers)
96x96 grid	322 560	3 225 600
288x288 grid	2 903 040	29 030 400
480x480 grid	8 064 000	80 640 000

Table 2. **Numbers of time-steps when UNI-DEM is used in a one-year run**

Spatial resolution (horizontal)	2-D option (1-layer)
96x96 grid	35 520
288x288 grid	106 560
480x480 grid	213 120

In many studies the model has to be run over many years (in, for example, climatic studies) and/or with many hundreds of different scenarios (when, for example, the influence of the biogenic emissions on high pollution levels is studied).

This short discussion explains why comprehensive air pollution studies can successfully be carried out *only* on modern high-speed computers and when furthermore the code optimized for runs on such computers, which is by far not an easy task.

Moreover, it must be emphasized that the computers which are available for us at present are not sufficiently fast for all options of UNI-DEM. This fact is clearly seen when the results in Table 4 are studied.

6. Organization of the parallel computations

It is very important to apply standard parallelization tools. This is crucial when the code has to be moved from one computer to another (which is often needed in practice).

If a shared memory computer is available, OpenMP [26] can successfully be implemented. It is quite straightforward to use this tool. However one should be careful in the efforts to solve the following task: to identify as large as possible well balanced parallel tasks. While the programming by using OpenMP is relatively simple, the solution of the latter tasks might be difficult.

If the computer is with distributed memory, then one can apply MPI [14] (the Message Passing Interface). The implementation of MPI is a much more complicated task than the implementation of OpenMP. On the other side, the use of MPI leads to dividing the data between the processors, which implies the use of shorter arrays. This very often results automatically in a better utilization of the different cache memories of the computer used.

Very often MPI can be used even on shared memory machines and, moreover, may give good results on such computers, because as mentioned above the caches are utilized in a more efficient way.

6.1. Identification of the parallel tasks when OpenMP is to be used. The first of the two actions is to identify the parallel tasks in the different sub-models

(obtained as a result of applying the splitting procedure used).

Parallel Tasks in the Vertical Exchange Sub-Model. In this sub-model, the vertical exchange of each pollutant along each vertical grid-line can be considered as a parallel task. The number of parallel tasks is equal to the product of the number of chemical species and the number of vertical grid-lines. Since the number of chemical species in UNI-DEM is in fact 32, the numbers of parallel tasks are 96x96x32 = 294912, 288x288x32 = 2654208 and 480x490x32 = = 7372800 for the 3-D options discretized on 96x96, 288x288 and 480x480 grids respectively. The tasks are small. Therefore, it is convenient to group several grid-points as a bigger task in an attempt to improve the performance.

Parallel Tasks in the Horizontal Advection-Diffusion Sub-model. In the horizontal advection-diffusion sub-model, the transport of each pollutant can be considered as a parallel task. The number of species in the UNI-DEM is 35 (see Section 1). However, three of them are linear combinations of other species. Therefore, the number of independent species is 32. The number of parallel tasks in the 2-D options is equal to the number of independent species. This means that the loading balance is not perfect when the number of processors is not a divisor of 32 for the 2-D options. If the 3-D options are used, then the number of parallel tasks become equal to the product of the number of species and the number of layers, i.e. this number is now 320. Again the loading balance will not be perfect when the number of processors used is not a divisor of 320.

Parallel Tasks in the Chemistry-Emission-Deposition Sub-model. In the chemical module, the chemical reactions at a given grid-point can be considered as parallel tasks. This means that the number of parallel tasks is very large and, moreover, the loading balance is perfect. The numbers of parallel tasks are 9216, 82944 and 230400 for the 2-D options discretized on 96x96, 288x288 and 480x480 grids respectively. The numbers

of tasks will be increased by a factor of 10 when the corresponding 3-D options are used. However, in all cases the tasks are small. Therefore it is convenient to group several grid-points as a bigger task. The performance can be improved considerably by a suitable choice of the groups of grid-points. The particular choices of grouping of the small tasks are discussed in detail in Owczarz and Zlatev [21], [22].

6.2. Implementation of MPI options. The approach used when MPI tools are to be implemented is based on dividing the space domain of the model into p sub-domains, where p is the number of processors which are to be used in the run. Two specific modules are needed in the MPI versions:

- a pre-processing module and
- a post-processing module.

Pre-processing Module. The first of these modules performs a pre-processing procedure. In this procedure the data are divided into several parts (according to the nodes that are to be applied) and sent to the assigned for the job nodes. In this way each processor will work on its own data during the whole run.

Post-processing Module. The second module performs a post-processing procedure. This means that every node prepares during the run its own output files. When the run is finished, then the post-processing module collects the output data on one of the nodes and prepares them for future applications (visualizations, animations, etc.).

Benefits of Using the Additional Modules. By the preparation of the two additional modules, one avoids some excessive communications during the run. However, it should also be stressed that not all communications are avoided. The use of the pre-processor and the post-processor is in fact equivalent to the application of a kind of domain decomposition. Therefore, it is clear that some communications are needed along the inner boundaries of the domains. Such communications are to be carried out only once per step and only a few data are to be communicated. Thus, the

actual communications that are to be carried out during the computational process are very cheap.

6.3. Combination of MPI and OpenMP options. On some computer architectures, like IBM SMP, it is efficient to use a combination of MPI and OpenMP options. These computers consist of several nodes. Every node contains several processors which share the same memory. Every mode has its own local memory. Therefore, it is natural to use OpenMP within every node and MPI across the nodes. Some results from runs on such an architecture with a combination of OpenMP and MPI options are presented in Owczarz and Zlatev [22].

7. Parallel runs on SUN computers

The results presented in this section were obtained by running six options of UNI-DEM on 8 processors of SUN computers. The code was also run on many other parallel computers: SGI Origin 2000, IBM SMP, Cray T3E, etc. (see Georgiev and Zlatev [15] and Owczarz and Zlatev [21], [22]).

7.1. Information about the computers used. SUN shared memory computers were used in all runs. These computers are located at the High Performance Centre at the Technical University of Denmark (DTU). The characteristics of the computers used are listed in Table 3. More information about these computers can be found in http://www.hpc.dtu.dk.

7.2. Results obtained by the MPI options and different spatial resolutions. Both 2-D and 3-D options discretized on all grids mentioned above (a 96x96 grid, a 288x288 grid and a 480x480 grid) were used in the experiments. Some results obtained by using these computers are given in Table 4. MPI programming is used in the runs the results of which are shown in Table 4.

The speed-ups were linear (and for the large problems even super-linear). This means that the computing times will be increased with a factor approximately equal to eight if the jobs are run on one processor. The largest job will be completed in more than 286 days if the com-

Table 3. **The computers available at the SUN grid at the Danish Centre for Scientific Computing**

Computer	Type	Power	RAM	Processors
Bohr	SUN Fire 6800	UltraSparc-III 750 MHz	48 GB	24
Erlang	SUN Fire 6800	UltraSparc-III 750 MHz	48 GB	24
Hald	SUN Fire 12K	UltraSparc-III 750 MHz	144 GB	48
Euler	SUN Fire 6800	UltraSparc-III 750 MHz	24 GB	24
Hilbert	SUN Fire 6800	UltraSparc-III 750 MHz	36 GB	24
Newton	SUN Fire 15K	UltraSparc-III 900 MHz	404 GB	72

puter is continuously running in so many days (i.e. no rebooting, no upgrading and no crashes in at least 286 days). On the other hand, if 32 processors are used when the most time-consuming job is run (the 3-D option on a 480x480 grid), then the computing time is 192.08 CPU hours (a speed-up of 4.46 when compared with the corresponding run on 8 processors).

Table 4. **Computing times in CPU hours when 8 processors are used**

Spatial resolution (horizontal)	2-D option (1-layer)	3-D option (10 layers)
96x96 grid	1.41	12.39
288x288 grid	19.56	152.72
480x480 grid	98.72	856.75

It is clearly seen that if the refined options (especially the 3-D refined options) are used, then more powerful processors and more processors are needed when runs over long-time periods are to be carried out and/or when results from many scenarios are to be investigated.

7.3. OpenMP options versus MPI options. It is more profitable to use MPI than OpenMP when the UNI-DEM code is run on SUN computers. Some results, which illustrate this statement, are given in Table 5. Both the OpenMP option and the MPI option were run over a time-interval consisting of 1000 steps and the computing times given in Table 5 are in seconds.

It is seen that the results obtained by the MPI version are better than those obtained by the OpenMP option. This deserves some explanation remarks. In the MPI option the largest arrays are divided to p sub-domains (where p is the number of processors) containing arrays

Table 5. **Computing times in seconds when 8 processors are used to run both the OpenMp option and the MPI option over a time-interval of 1000 steps**

Physical processes (and total time)	OpenMP option	MPI option
Advection-diffusion	2618	457
Chemistry-emission-deposition	1339	688
Total computing time	4011	1281

which are p times smaller. This leads automatically to a reduction of the cache misses and, thus, improves the performance. A general framework and theory to overcome shared memory bottlenecks and to increase performance by meanse of enhanced schemes of data exchanges in multilevel memory systems is presented in [8−10]. In Table 5 we have p = 8. If we increase the number of processors, then the MPI option will perform even better, because the arrays in the sub-domains become smaller. To illustrate that such a statement is true, we performed the same runs (as those in Table 5) on 32 processors. The results are shown in Table 6. The comparison of the speed-ups (which are given in brackets in Table 6) shows that the efficiency of the parallelization is greater for the MPI option.

7.4. Remark about the use of computational grids. Using computational grids might resolve the difficulties arising when the refined options are to be applied in comprehensive air pollution studies (as the studies listed in the next section). If advanced modules for treatment of particles and/or if meteorological forecast models are attached to UNI-DEM in

an attempt to improve the reliability of the results, then the computational work is increased very considerably. Therefore, also here computational grids might be very useful.

Table 6. **Computing times in seconds when 32 processors are used to run both the OpenMp option and the MPI option over a time-interval of 1000 steps. The speed-ups (related to the corresponding results obtained in the runs on 8 processors) are given in brackets**

Physical processes (and total time)	OpenMP option	MPI option
Advection-diffusion	1001 (2.62)	120 (3.81)
Chemistry-emission-deposition	607 (2.21)	171 (4.02)
Total computing time	1771 (2.26)	348 (3.68)

8. Comprehensive Studies with UNI-DEM

UNI-DEM has been used in many comprehensive studies related to air pollution levels in Europe and/or in different specified areas in Europe (as, for example, Ukraine, Denmark, etc.). The most important of these studies are listed below.

- Studying the impact of future climate changes on the pollution levels in Europe, Dimov et al. [6].
- Studying the influence of the biogenic emissions on high ozone levels in Europe, Geernaert and Zlatev [11].
- Economical estimates of losses of crops that are caused by high ozone levels were found in Dimov et al. [7] and Zlatev et al. [31]. Until now results for Denmark and Bulgaria have been obtained. However, the same study can be performed for any other country in Europe.
- Long-term variations of the pollution levels in Europe, Ambelas Skjoth et al. [3], Bastrup-Birk et al. [4], Havasi and Zlatev [15], Zlatev et al. [30].
- Studying the relationship between the human-made emissions and the pollution levels in Europe, Ambelas Skjøth et al. [3], Bastrup-Birk et al. [4], Dimov et al. [7], Zlatev et al. [30].
- Studying the frequency of appearance of pollution levels that exceed the established by EU critical levels [2] (and, thus, might lead to damages on plants, animals and human health), Geernaert and Zlatev [11], Havasi and Zlatev [15].
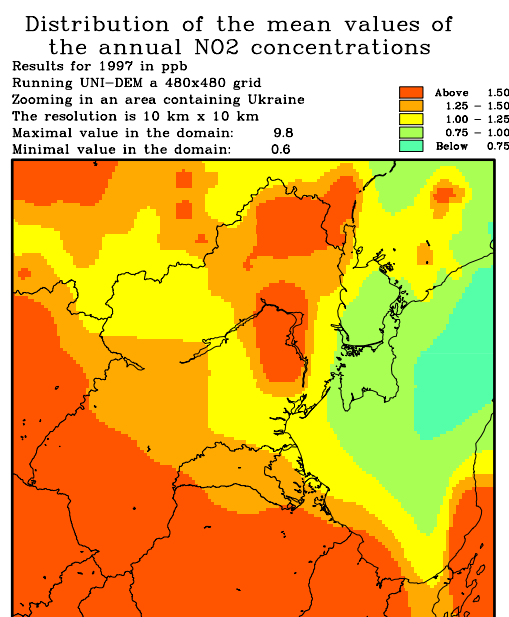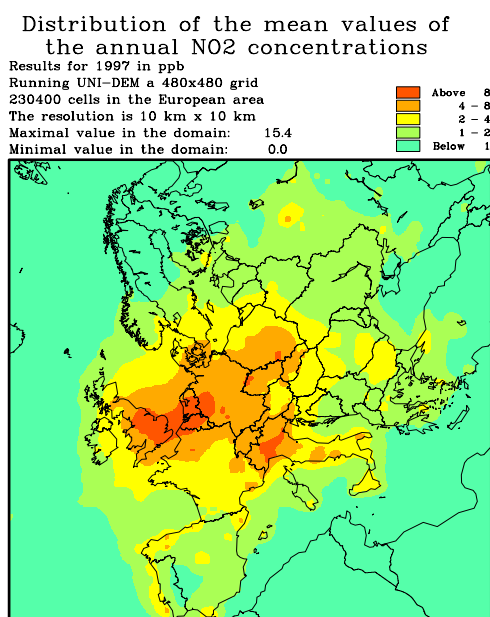- Studying the contribution of emission sources from any given area in

Figure 1. Distribution of the nitrogen dioxide concentrations in Europe (the left-hand-side plot) and in Ukraine (the right-hand-side plot)

Europe to its neighbouring areas (for example, studying the contribution from the European emission sources outside Denmark to the pollution levels in Denmark), Ambelas Skjoth et al. [3], Dimov et al. [7], Havasi and Zlatev [15], Zlatev [28] and Zlatev et al. [30].

9. Some Results from the Studies

The distribution of nitrogen dioxide in Europe is shown, as an example, in the left-hand-side plot of Figure 1. From this plot it is seen that the levels of the NO_2 concentrations in Ukraine are considerably lower than the levels in the most polluted parts of Europe.

The corresponding distribution in Ukraine is given in the right-hand-side plot of Figure 1 (note that the scales in the two plots of Figure 1 are different). Some more details about the levels of the NO_2 concentrations in Ukraine can be seen from this plot. One can see that the levels of the NO_2 concentrations are rather high in the area around Kiev (this should be expected around such a big city).

NH3 + NH4 CONCENTRATIONS

IN THE PERIOD FROM 1989 TO 1998
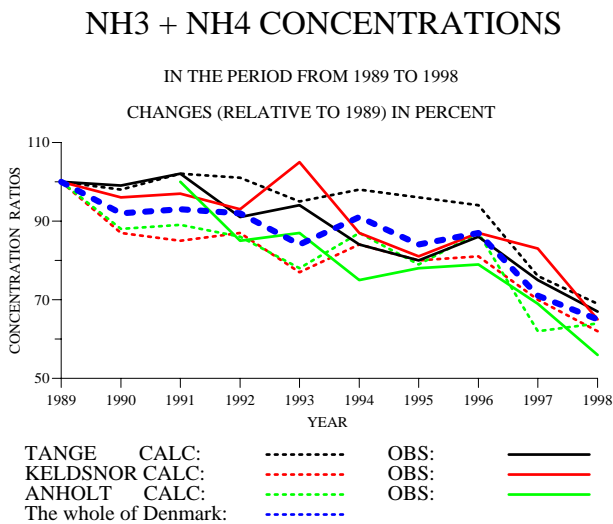
CHANGES (RELATIVE TO 1989) IN PERCENT

Figure 2. Demonstration of the decreasing trend for the Danish ammonia-ammonium concentrations

Some trends of the Danish ammonia-ammonium levels in the ten-year period 1989−1998 are shown in Fig. 2. The reduction of the ammonia-ammonium concentrations is typical not only for Denmark but also for many other countries in Europe in the same time period.

Similar reductions of the concentration levels can be seen also for other species. The reductions of the concentrations are due to reductions of the emissions.

Acknowledgements

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