R E M A P E

REgional **M**odelling of **A**ir **P**ollution in **E**urope

A b s t r a c t s

of the talks and the posters presented

at the First REMAPE Workshop

organized jointly by the University of Copenhagen

and the National Environmental Research Institute (NERI)

September 26 - 27, 1996, University of Copenhagen

Organizing Committee:

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INTRODUCTORY REMARKS

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The talks and the poster submitted to the first REMAPE Workshop (September 26-27 1996, University of Copenhagen) are given in this report. The following remarks are necessary:

(i) The abstracts which have been submitted in plain ascii files and/or latex files are collected (to avoid typing and, thus, some misprints). This means that abstract sent by surface mail or by postscript files are not included in this report.

(ii) The editing work has been reduced to minimum (because of the action explained in the previous paragraph). However, some editing has been performed to unify the style of the presentation. Therefore all speakers are kindly asked to contact Zahari Zlatev if there are misprints in their abstracts. This is necessary because this report will be disseminated to people that may be interested in the topics discussed at our Workshop.

(iii) The abstracts are ordered (alphabetically, with respect to the persons that are giving the talks or the posters).

(iv) The names of the speakers are underlyined.

(v) Only short addresses of the speakers (and the co-authors when appropriate) are given. Full addresses of the speakers (with phone numbers, fax numbers and e-mail addresses) can be found in the list of the participants of the First REMAPE Workshop.

Aerosol modeling in a regional chemistry transport model: status and future development.

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Due to the numerous interactions beetween the gas and the aerosol phase regional chemistry transport models have to take into account particle formation, transport and deposition with respect to aerosol chemistry as well as aerosol dynamics. To fulfill this task MADE (Modal Aerosol Dynamics model for EURAD) has been developed. Aerosol chemistry is treated in the sulfate-nitrate-ammonia and water system and the size distribution of the particles is calculated with a version of the regional particulate model RPM (Binkowski and Shankar, JGR, 1995) that has been modified for European conditions. First results from a coupled model sxstem consisting of MADE and CTM2 (the chemistry transport model of EURAD) will be presented. Additionally we will try to identify the most important needs for the future development of this system in the framework of EUROTRAC2.

Mesoscale and transboundary transport of atmospheric pollutants with consideration for kinetic processes

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A great number of gas- and aerosol-phase chemical species in the atmosphere are subject to a series of physical and chemical transformations through mechanisms of atmospheric photochemistry, particle coagulation and vapor condensation processes. All these mechanisms are closely connected with each other in the combined numerical model describing the dynamics and kinetics of pollutants in the atmosphere. All necessary parameters of flow fields and turbulent characteristics of the atmosphere are determined from the nonhydrostatic mesoscale numerical model.

The photochemical scheme employed here consists of 183 chemical reactions and 36 different chemical species among which are nitrogen oxides (NOx), hydrocarbons (HC), and sulphur oxides (SOx). The coagulation term in the aerosol formation processes is described by using the Smoluchowski equation. To solve the condensation kinetics equation, non-uniform functions of particle-size distribution are utilized. The equation is solved by the help of the method of cells. This model allows one to describe the processes of fluctuating aerosol formation and further growth in the oversaturated vapor, which bring to formation and development of the disperse phase.

Besides, the transboundary transport of sulphur-containing air pollutants in different European regions is simulated using adjoint functions. The pollution considered here results from emissions both in the region itself and transported from other countries or regions. An analysis of results of numerical experiments is provided for both the polluted and unpolluted atmospheres. Also, the formation mechanisms of sulfuric acid aerosol particles in the atmospheric conditions is considered.

Modelling the impact of long-range transported air pollutants on vegetation

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Damages on vegetation are hypothesised to be due to multiple stress factors including anthropogenic stresses from long-transported pollution (e.g. acid deposition and photochemical oxidants) and local sources (e.g. ammonia) as well as natural stresses (e.g.marine salts, drought and storm episodes). The observed effects and their connection to long-range transport of pollutants are the basis for the UN-ECE Convention on Long-range Transboundary Air Pollution resulting in protocols for reduction of emissions. An evaluation of the effects of multi-component stresses is needed to determine the consequences of the actual levels of air pollution, the relative impact of the different stress factors and to develop a tool for evaluation of the effects of different air pollution scenarios on receptors. This can be done by linking long-range transport models to effect models thereby coupling emissions to effects.

A dynamical effect model (TreGro) is under development to examine the mechanisms by which plants regulate their carbon, water and nutrient cycles to mitigate damage caused by pollutants such as ozone and acid rain. The model is used to evaluate the relative impact of the different stress factors (anthropogenic and natural) on vegetation in order to be able to distinguish the effects of acid deposition and photochemical oxidants from e.g. water and nutrients defiencies. As a first step the model has been parameterised for Norway spruce vegetation which is of economical and ecological importance in Denmark. Model runs are compared to experiments in semi-controlled conditions (open-top chambers) and to field experiments in Denmark and Sweden. The next step is to couple the effects of acid deposition and photochemical oxidants and other regional deposition on vegetation to long-range transported air pollution. The used long-range-transport model is the Danish Eulerian Model, DEM. The model is an Eulerian air pollution model describing emission, long-range transport, dispersion, non-linear chemistry and deposition for a space domain covering the whole of Europe.

Studying cumulative ozone exposures in Europe during a seven-years period

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Ozone is one of the most harmful pollutants in the troposphere. High ozone concentrations can damage plants, animals and humans. The damaging effects depend on the magnitude of a critical level of a special parameter, the cumulative ozone exposure. This is why the cumulative ozone exposures must be carefully studied. It is important to determine the relationships between relevant emissions (NO_x emissions, human-made VOC emissions and/or a combination of NO_x emissions and human-made VOC emissions) and cumulative ozone exposures. All these issues are discussed in this paper. Meteorological data from seven consecutive years, from 1989 to 1995, have been used in the experiments with different scenarios for varying the emissions (the NO_x emissions, the human-made VOC emissions as well as both the NO_x emissions and the human-made VOC emissions). The particular air pollution model used in this study is the Danish Eulerian Model. Several hundred runs with different input data (meteorological data and/or emission data) have been performed. Advanced visualization techniques are used to interprete the great amount of digital data collected in these runs and to show clearly different trends and relationships that are normally hidden behind millions and millions of numbers.

Regional differences in tropospheric ozone

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Analysis of ozone-measurements over Europe, as well as modelcalculations do indicate large differerences in the relative importance of the phenomena controlling ozone over different areas in Europe. The ozone budget, consisting of chemistry, deposition, and horizontal and vertical transport shows differences due to differences in emission density and in dry deposition values, the land-sea effect. The reliability of these budget considerations relies heavily on the reliability of the model used. Recently a project has started which is aimed to create a coherent and consistent data set for ozone over the whole troposphere over Europe for the summer of 1997. In this EU-project, which is a cooperation of several European institutes, this data-set will be based on measurements and model results. The measurements will consist of groundlevel measurements, vertical profiles and satellite observations from the Gome-instrument. A data-assimilation technique will be developed which will combine the measurements with the modelresults. This will lead, including a model verification against independent measurements, to a reliable dataset of ozone, also over the sea, which will be used subsequently to analyse the regional differences in Europe.

Long-term national scale modelling on the Italian area

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A preliminary long-term (multiple years) modelling study of acidifying components on the Italian area has been performed. Its main purpose is to support a first assessment of national emission abatement strategies, in connection and coherently with continental scale analyses.

The simulation is based on the integration of emission, meteorological and chemical/transport models, as well as on collection and harmonization of several databases, including the use of measured meteorological and chemical data. Emissions are taken from the CORINAIR database, integrated with information concerning time variability (monthly, weekly and hourly) of activity sectors. The meteorological database has been set up by using a mass-consistent wind field model and proper spatial analysis schemes, fed up with synoptic data, upper-air soundings and ECMWF analysis. Pollutant dispersion is simulated with a Lagrangian back-trajectory model, including a simplified chemical scheme dealing with sulfur and nitrogen (oxidized and reduced) compounds.

The model has been run for two different years (1989 and 1994) and the results have been compared with monitoring data from the national deposition network, showing the combined influence of emission change and meteorological variability. Current work concern the improvement of the Lagrangian model, that is planned to be applied to other years, as well the application of a comprehensive 3D Eulerian model for selected episodes, from which, in perspective, build a simplified long-term model and drive 3D mesoscale photochemical modelling studies over urban areas also ongoing.

Assessment of working life of Buildings and Building Products through Characterization of Degradation Environment and Modelling of Degradation

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The entry into force of the Construction Products Directive puts focus on the need for standards addressing the issue of durability. On the request of CEN/BTS-1 standardization has started within ISO/TC%)/SC3/WG9. This work is based on the considerable body of durability knowledge and data. Insufficient knowledge of the degradation environment is in most cases the major barrier to reliable predictions. The present project focus on the characterization, mapping and classification of the most important environmental degradation factors on the European macro and meso scale, together with the identification and modelling of degradation mechanisms and dose/response functions.Existing environmental dispersion models and environmental data should be used to model the degradation factors. The results should be exhibited in user-friendly Geographical Information Systems (GIS).

This theme is now the subject of the dedicated call for proposals submitted at June 15 from the EU Standards, Measurements and Testing programme. My group have proposed and written the supporting documents for the call, and we are now preparing the proposal.

Modelling long term nitrogen deposition to Danish sea water

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In Danish coastal water, high concentrations of nutrients often lead to a large production of algae. Nitrogen is usually the limiting factor. When the algae die and are deposited at the bottom of the sea they decompose, whereby oxygen is comsumed. This leads to a depletion of the oxygen contained in the water. In worst cases this causes the death of fish and benthic fauna.

In the Danish monitoring programme for marine waters, the atmospheric nitrogen deposition has been estimated from coastal stations through a number of years. In the first years nitrogen depositions were estimated by extrapolation from the coastal stations. In recent years a combination of a monitoring programme and calculations calculations with a mathematical model, the Atmospheric Chemistry and Deposition Model (ACDEP), has stepwize been introduced as a part the programme.

The ACDEP-model is a lagrangian trajectory model, in which a vertical air collumn from ground and up to 2 km is advected along 96 h backtrajectories. The model has 10 vertical layers with a fine mesh at the bottom and coarser towards the free troposphere.

The first use of the ACDEP-model was to compute dry depositions of the gas phase and aerosol phase compounds were estimated from measurements using the dry deposition module. At present the model is used for calculating nitrogen deposition to all Danish waters. These calculations are carefully evaluated towards monitoring data.

The dynamic exchange of pollutants at the air-soil interface and its impact on long range transport

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Emission and deposition rates of volatile substances released at the soil surface are strongly effected by physico-chemical properties of the substance, properties of the soil and meteorological conditions. A multi-layer numerical model is developed to describe the exchange of pollutants between the atmosphere and soil with the following intentions: to study the exchange process and its dynamics, to derive effective emission rates depending on application modes, to derive effective deposition rates, to derive diurnal and seasonal emission patterns and to derive parameterizations for inclusion in LRT models. The model describes the vertical transport and diffusion processes in both soil and atmosphere and the exchange of pollutants between the two compartments in dependence of actual meteorological conditions and soil properties. Although primary intended for the description of the exchange of persistent organic pollutants (POPs), it appears that the model is able to explain observed ammonia emissions and its dynamics to a large extend. The model is applied to calculate 'effective' dry deposition velocities for POPs which are used in a study of the atmospheric inputs to the North Sea. A key result in this is that for some pesticides on the long term the dry flux is upward and thus the net deposition flux smaller than the wet deposition flux. A simplified version of the model will serve as an exchange module in a large scale model for the biochemical cycling of POPs.

The EMEP regional scale multi-layer Eulerian model

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At the Western Meteorological Centre (MSC-W) of EMEP a multi-layer Acid Deposition model (MADE-50 = Multi-layer Acid Deposition model for Europe) has been developed. Basic input are the meteorological data from a Numerical Weather Prediction (NWP) model at the Norwegian Meteorological Institute (DNMI) and emission field estimates based on data submitted officially to the Convention on Long Range Transboundary Air Pollution. The future aim is to use this model calculating annual concentrations and depositions of acidifying compounds under the Convention, supporting the discussions and negotiations for emission reduction protocols. Additionally, a long term goal is to couple the acidification and the photochemical oxidant chemistry and physics to support multi-pollutant protocols. The purpose of this talk is to describe the framework of the model and to discuss model results. The model equations are formulated in the same horizontal and vertical grid as the meteorological data, and the parameterization of the meteorological processes follows as far as possible the same procedure as utilized in the NWP model. The dry deposition, wet deposition and chemistry formulation follows, with some small modifications due to the improved vertical resolution, the parameterization applied in the Lagrangian acid deposition model. The compounds implemented are: NO, NO2, NO3, HNO3, PAN, NH3, NH4NO3, SO2, SO4 and (NH4)1.5SO4. Furthermore, the Eulerian air pollution model has been developed for implementation on massive parallel computers, which now makes it feasible to run the model operationally for long time periods within realistic time-frames. This is also essential in order to make use of the next generation parallel super computing techniques and will make the model applicable to future scenario studies and source receptor calculations. The latest calculations now provide results on sulphur and nitrogen transport and deposition for a whole year. Comparisons of the results obtained for 1992 with the new model correspond quite well with the measurements performed at the EMEP monitoring stations. Two examples of source receptor calculations have been performed for sulphur. Comparing the matrices obtained by the Lagrangian models and MADE-50, it is found that substantial more mass of the emitted pollutants are allocated by the multi-layer model. Furthermore, a larger part of the emissions are deposited both in places far downwind of the emitter and to the emitting country itself. The latter feature may be due to the low accuracy found in the dry deposition flux estimates thus improvements are needed in the description of these processes and in the input data.

Forecasting tropospheric ozone concentrations in Denmark

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A system for operational forecast of ozone concentrations in the atmospheric boun\-dary layer has been developed at DMI. The system is based on the coupling of the chemical routine of he EMEP MSC-W oxidant model and DMI's 3-D Lagrangian transport model utilizing forecast data from DMI's numerical weather prediction model DMI-HIRLAM (High Resolution Limited Area Model). The system is called Danish Atmospheric Chemistry FOrecasting System, **DACFOS**.

The system is set up to make 36 hours forecasts automatically twice a day for selected sites or receptor points within the EMEP-grid covering all of Europe. For a receptor point ten (optional) backwards trajectories (96 hours) arriving at different heights within the atmospheric boundary layer are calculated including the meteorological parameters needed for the chemistry model. For each trajectory the concentrations of the chemical species are calculated independently of the other trajectories, assuming total mixing in the boundary layer.

The analyses of ozone forecasts for Jægersborg in Denmark for a two-months period in summer '95 show that the model reproduces many of the observed features.

Linear Gauss-Seidel iterations in stiff solvers for atmospheric chemistry.

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The integration of the atmospheric chemistry part is a time consuming task in three dimensional transport modelling. Our favorite solver is a second order BDF--method where the the solution of the linear systems is done by a fixed number of Gauss--Seidel iterations. Here we will describe how implicit Runge--Kutta--like methods behave if the direct solver is replaced by the Gauss--Seidel method. The comparision is done with known gas phase mechanisms under different emission scenarios.

Mesoscale model estimation of soil acidity in the St.-Petersburg region.

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Investigated area called St.-Petersburg region includes Leningrad region and some parts of another regions and countries. This territory is limited by 9 EMEP grids (150km*150km) and is divided into 324 small grids (25km*25km). The estimations were done with the help of Eulerian - Lagrand model (MSC- E, Moscow).

The main goal of this work is to determine the role of external and internal sources of SO2 emissions and their influence on natural ecosystems.

The results show that in average the external influence on Leningrad region is 52% from total SO2 deposition. However, in different parts of the region this influence is inequal and decreases to 35% in locations with powerful internal sources. Critical loads on forest soils were determined also on mesoscale level.

Comparisons were made between results obtained by micro- and mesoscale model estimations (150km*150km and 25km*25km). The temporal variability of SO2 depositions and exceedings were investigated in 1990-1994. The results demonstrate that at present decrease in SO2 emissions in St.-Petersburg region leads to exponential reduction of exceedings.

THE DIRECT AND INDIRECT RADIATIVE EFFECT OF ATMOSPHERIC SULFATE AEROSOLS: COMPARISON OF GLOBAL AND REGIONAL MODEL RESULTS

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Atmospheric aerosol particles, such as sulfate aerosols, have been identified to modify solar radiation in two ways. In clear-sky condition they scatter UV-radiation back to space, reducing solar irradiance and photolysis rates at the ground (direct effect). The capability of sulfate particles to act as cloud condensation nuclei, thus influencing cloud droplet number concentration,cloud albedo and the development of precipitation is referred to as indirect effect. Evidence has been presented that sulfate aerosol climate forcing is sufficiently large to reduce significantly the positive forcing by anthropogenic greenhouse gases. We have used a computationally efficient off-line analysis tool (d-Eddington approximation, 18 wavelength intervals between 0.2 and 5.0 mm) to determine the direct and indirect shortwave radiative effect of natural and anthropogenic sulfate aerosols as simulated by the global chemistry-circulation model ECHAM on the one hand side, and by the regional chemistry-transport-model of the EURAD system on the other hand side. Relating microphysical and optical properties of sulfate aerosols - in dependence of the ambient relative humidity - and the effective radii of cloud droplets to sulfate aerosol mass concentration, the shortwave radiative forcing can be obtained. A comparison of global and regional model results will be shown together with the influence of natural and anthropogenic sulfate aerosols for the European domain.

Regional scale atmospheric chemistry modelling at the Swedish Meteorological and Hydrological Institute

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Over the last five years SMHI has developed an Eulerian atmospheric transport and chemistry modelling system called MATCH (Mesoscale Atmospheric Transport and Chemistry model). MATCH is an off-line model and is coded to be flexible with regard to horizontal and vertical resolution and caters for common vertical and horizontal grid systems. The MATCH system is used in a range of applications from high resolution assessment studies for sulfur and nitrogen compounds in regions of Sweden to continental scale studies in developing parts of the world as well as emergency response applications over Europe. Depending on the required horizontal resolution, time period and study area we use meteorological input data from ECMWF, HIRLAM or from a specially designed mesoscale objective analysis scheme. The temporal resolution of the meteorological input data is usually three or six hours. Currently a photochemical submodel is developed and the intention is to use MATCH as a tool for assessing the importance of different sources of pollutants to the levels of photochemical oxidants over Sweden and to study control strategies. This will involve nesting of a European scale model with a higher resolution model over Sweden. Once the model becomes operational the intention is to focus on seasonal modeling although detailed study of episodes will of course be required to establish the quality of the modelling system. The development of a photochemical module opens up several interesting research areas related to REMAPE. In particular we think data-assimilation of chemical data, forcasting and nesting of models are areas where we would like to contribute.

Analytic methods of compressing gas-phase chemical mechanisms

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The number of hydrocarbons in the real atmosphere can be very large (typically hundreds, Middleton et al., 1990). Gas-phase mechanisms used in regional pollution models (eg. ADOM, RADM, EuroRADM) are typically simplified by combining hydrocarbons through parameterizations known as "lumping". However, these parameterizations are formulated on unrealistic assumptions about the gas-phase system. These assumptions can lead to substantial errors in comparison to the original detailed reaction mechanism results. A new mathematical technique for reducing the size of a regional model's chemistry mechanism is presented. Simple operations on the detailed mechanism's differential equations leads to a compressed system with fewer variables than the earlier "lumped" mechanisms, while retaining the accuracy of the original mechanism to machine precision. The "lumped" mechanisms are shown to make substantial errors in simulation predictions, for some sets of initial conditions. The new method is easily extended to include oxidation by other species in addition to the hydroxyl radical (unlike earlier methods), allowing accurate simulation of organic radical production during the night as well as during the day. Results from several numerical tests will be presented, and compared to results using one of the earlier parameterizations (Integrated Reactivity Weighting, used in the RADM mechanism).

Budget calculations of photo-oxidants and their precursors in Europe

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The concentration of ozone and other photo-oxidants is determined by different processes as photochemical reactions, transport due to large-scale atmospheric circulation systems and small-scale turbulent exchange, cloud processes, and deposition. The contribution of these processes to the formation of photo-oxidants and its precursors is investigated for a summer-smog episode in July/August 1990 using the regional-scale model EURAD.

Numerical experiments has been performed to analyse the impact of different treatment of initial/boundary conditions and the effect of emission scenarios on the results of the budget calculations.

Regional scale modelling in Belgium: state-of-the-art and future prospects

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Unlike to other subprojects of EUROTRAC, the Belgian contribution towards regional scale modelling of air pollution in Europe has been very limited so far. This should change however, since the federal and regional governments in Belgium have given priority to the use of air quality models to provide policy support in assessing the environmental quality.

For these purposes VITO has evaluated and compared six regional scale transport models operational in Europe [1], focusing on acidification and photochemical smog on a regional scale. As a result the Lagrangian OPS model [2] was selected and implemented to compute concentration and deposition fields for SO2, NOx and NH3 on a 5 km x 5 km grid. For photochemical smog modelling, the EUROS model [3] was chosen to be implemented. EUROS is an Eulerian model with variable space resolution which can be obtained by means of local grid refinement. Through this nesting technique, in combination with a limited vertical resolution (4 layers) and the use of very fast numerical solvers, the model has become very efficient for seasonal and long-term modelling of photochemical smog. In order to satisfy the immediate urge to address the effect of photochemical abatement strategies on a European scale, ozone computations were ordered to be performed by TNO using the LOTOS model. Runs with different scenario's concerning VOC and NOx emissions were carried out.

In the summer of 1997 model validations will be carried out by means of a STAAARTE project, which has been approved now by the EU. Flight measurement will be performed along the borders of Flanders at which ground measurement stations are located, allowing an estimation of transboundary fluxes and a validation of model computations.

Along this line of work VITO wants to contribute to further improvements of advanced computational tools by participating in an interactive network in which different model parts running at different locations can be connected. The possibilities, requirements, problems and pitfalls of such a network have to be assessed. Experimental runs and tests of the network system have to be carried out, including tests of communication and file transfer protocols and an evaluation of memory and CPU requirements needed for computation and communication. Proposed is a also a coupling of the results of prediction models like SMOGSTOP (1-D casuistic prediction model with a high accuracy for short term (24h-48h) predictions on a local scale) with those of regional scale Eulerian models like EUROS, LOTOS or EURAD. The idea is to find out if and how the more accurate short term predictions by models like SMOGSTOP can be included into Eulerian models.

The workshop presentation will give an overview of the state-of-the-art on regional scale modelling in Belgium, discussing briefly some of the results. In combination with the future prospects for Belgium, the expected contributions to REMAPE will be discussed as well.

References

[1] C. Mensink, A critical evaluation and comparison of six European models for regional scale applications, poster presented at the EUROTRAC Symposium '96, Garmisch-Partenkirchen, 25-29 March 1996.

[2] J.A. van Jaarsveld, Modelling the long-term atmospheric behaviour of pollutants on various spatial scales,PhD thesis, University of Utrecht, October 1995.

[3] M. van Loon, Numerical methods in smog prediction, PhD thesis, University of Amsterdam, June 1996.

EVALUATION OF THE MODEL SYSTEM KAMM/DRAIS

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The model system KAMM/DRAIS consists of the meterological model KAMM and the dispersion model DRAIS. It is designed to simulate the transport, diffusion, deposition and chemical transformation of the relevant species in a mesoscale area. Comparisons with measurements in a lot of studies have shown that the models provide realistic results, but a systematic model evaluation has not yet been done. In order to do this evaluation for both partial models data will be taken from the SANA experiment, 1994, the TRACT experiment, 1992 and a sommer smog episode in 1994. Different kinds of comparisons with the observations will be performed:

- graphic comparison by time series
- scatter diagramms
- frequency distributions of the differences between measured and simulated data
- correlation coefficients

If possible, the evaluation is carried out with partial data collectives in order to distinguish between:

- time periods of the day
- height above ground
- rural and urban areas.

The main problem will be the assessement of the results and the definition of reliability measures. This definition will be done together with other groups carrying out similar studies in the frame of the German Troposheric Research Programme and hopefully in the frame of REMAPE.

MODEL NETWORK FOR THE SIMULATION AND FORECAST OF THE AIR POLLUTION - MESOSCALE SIMULATION

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Aim of this projekt is the disposition of the efficient mesoscale model system KAMM/DRAIS in a model network in order to provide real-time forecasts of the relevant air pollutants in mesoscale areas. This project is part of the model network project SICHTROZ initiated by the EURAD group. Modern networks are able to combine different models by the exchange of model results during the simulations. To realize this exchange a fast data transfer and well defined interfaces between the models in the network are necessary. Modifications in the models have to be performed to minimize the data transfer. The model network will be build up in two main steps:

1. Realization of the model network on the basis of the present models

In order to realize the network, modifications in the structure of the model system KAMM/DRAIS are necessary. Mainly the coupling procedures between the EURAD model and the model system have to be incorporated as subprogramms to avoid unnecessary data transfer. The data structure of the emission data has to be changed too. The model network will be tested by carrying out simulations which are necessary for the model evaluation project. Episodes of the SANA experiment, 1994, the TRACT experiment, 1992 and a sommer smog period in 1994 are selected for these test calculations.

2. Further development of the models in the network

The performance of real-time forecasts requires greater changes in the model system KAMM/DRAIS. In order to minimize the transfer of the emission data, part of the emission model has to be implemented into the system. In this phase of the project the mesoscale meteorological data are provided by the German Weather Service. This requires a modification of the coordinate system in the DRAIS model. Aditionally a parallelization of the code is necessary to use the new generation of parallel computers.

Modeling Atmospheric Transport and Deposition of Heavy METals in the KATowice Province in southern Poland (Project METKAT).

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A large part of Poland's heavy industry, notably hard coal mining, ferrous and non-ferrous metallurgy and power generation is located in the Katowice Province. Therefore, this heavy industrialized region, which is populated by some four million people, experiences considerable problems with air pollution. Atmospheric emissions, concentrations and depositions of arsenic (As), cadmium (Cd) and zinc (Zn) are among the highest in Europe.

In the METKAT study launched by the International Institute for Applied Systems Analysis (IIASA), we try to model the atmospheric transport and deposition of As, Cd, Zn and lead (Pb) in the region by using the Mesoscale Dispersion Modeling System (MDMS) developed by Uliasz. The version of MDMS that we used, was composed of the mesoscale meteorological model named MESO and a Lagrangian Particle Dispersion and Deposition (LPDD) model. The input data for MDMS namely meteorological, emission and land use data were provided by Polish collaborators. The results of mesoscale simulations performed for 150km x 150km domain with grid spacing of 5km were compared with Cd deposition calculated with the aid of Bartnicki's long range transport models HMET150 and HMET50.

The preliminary deposition calculations for the entire year of 1992 show that results depend primarily on the quality of emission data (magnitude and spatial distribution). Also land use data seem to be relatively important when estimating the location and magnitude of peak depositions. Meteorological variability for longer time periods (seasons to years) seems to be less important. In general the simulations show some potential to reproduce local maxima in the deposition fluxes.

However, very high Cd deposition values observed in the region cannot be reproduced by the model with available emission inventory even when emission from selected sources was increased by two orders of magnitude. The model calculations do not consider re-emission of particulates from post-mining areas and waste dumps, which may contribute considerably to ambient concentrations. A receptor-oriented modeling approach based on an influence concept is proposed as a tool to investigate contributions of different potential emission sources to the observed depositions.

The representation of boundary-layer convection in atmospheric chemistry models

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Boundary-layer convection is usually represented in atmospheric chemistry models with first-order closure schemes like simple and modified K-closures. In the simple K-closure scheme the flux at each height is parametrized as the product of the local (positive) value of K and the local gradient of the transported species. An example of the modifications proposed is the decomposition of the local gradient in a bottom-up and a top-down part which relate to the local flux via bottom-up and top-down K-profiles, respectively. Typically for bottom-up species the K-values can become negative due to countergradient transport. Another example is the inclusion of an explicit countergradient term in the flux-gradient relationship in order to have physically well-behaved (i.e., positive) K-profiles.

In this study another approach than first-order closure is followed to parametrize vertical transport of reactive species in the convective boundary layer. The motive that led to this alternative parametrization was the following problem with typical first-order closure models: it has been found that simple K-closure schemes completely fail to reproduce boundary-layer budgets and profiles of species in the simple chemistry scheme consisting of only one binary one-way reaction of a bottom-up and a top-down species with a chemical time scale equal to the convective turbulence time scale. The alternative closure proposed here to solve this problem is the mass flux scheme, which is a higher-order (but not fully second-order) closure. In the mass flux scheme the availability of two prognostic variables offers the possibility to model horizontal segregation effects in atmospheric chemistry. These effects are expected to be of importance in modelling correct boundary-layer budgets and fluxes of species like nitrogen monoxide (NO), isoprene (C5H8), and ozone (O3), in regions of high emissions. In the near future an implementation of the mass flux scheme will be developed that can be incorporated in mesoscale and global chemistry models. Results will be presented of an evaluation of the mass flux approximation for transport of chemically reactive species in the convective boundary layer. The evaluation makes use of Large-Eddy-Simulations of the chemistry cases studied.

Efficient treatment of chemical rate equations in Air Quality Models

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As Air Quality Models evolve, their complexity grows and so does the need for: (i) flexibility in updating/changing the chemical mechanism and (ii) robust integration of the chemical rate equations using (semi) implicit methods. Both points can be addressed by using KPP (the Kinetic PreProcessor) - a specialized software environment intended to assist the development of air pollution modeling codes. KPP takes as input a description of the chemical mechanism (from its own library or user-supplied), an integration routine (library or user-supplied) and a driver and produces ready-to-run optimized C or FORTRAN code describing the evolution of the chemical system.

Despite their excellent stability properties, the overhead associated with linear algebra calculations often precluded the use of (semi) implicit methods in air quality models. (Semi) implicit methods may be useful, though, if one carefully exploits sparsity. Once the chemical mechanism is specified, all the interactions among the species are known; thus, the entries in the Jacobian which are structurally zero can be detected at preprocessing stage. KPP performs automatically this analysis, reorders the species to minimize the fill in and generates the sparsity data structures, as well as the routines needed for sparse decomposition and back-substitution. These routines are fast, as no extra data manipulation is required at run time.

Are sparse (linearly) implicit methods timely competitive to be used in Air Quality Simulations? Dr. Jan Verwer's (CWI, Amsterdam) presentation on Benchmarking Stiff ODE Solvers provides a thorough answer to this question based on the the joint CGRER - CWI research [3,4].

References:

[1] V. Damian-Iordache and A. Sandu: KPP - A symbolic preprocessor for chemical kinetics - User's guide, CGRER, The University of Iowa, internal report, 1995.

[2] A. Sandu, F.A. Potra, V. Damian-Iordache and G.R. Carmichael: Efficient implementation of fully implicit methods for atmospheric chemistry, J. Comp. Phys., to appear.

[3] A. Sandu, J.G. Verwer, M. van Loon, G.R. Carmichael, F.A. Potra, D. Dabdub and J.H. Seinfeld: Benchmarking stiff ODE solvers for atmospheric chemistry problems I: implicit versus explicit, Atmospheric Environment, to appear.

[4] A. Sandu, J.G. Verwer, J.G. Blom, E.J. Spee and G.R. Carmichael: Benchmarking stiff ODE solvers for atmospheric chemistry problems II: Rosenbrock methods, submitted to Atmospheric Environment.

Study of different deposition parameterizations on an atmospheric mesoscale Eulerian air quality model: Madrid case study

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The importance of an adequate parameterization of the deposition processes for simulation of three dimensional pollution fields in a mesoscale context is out of any doubt. An accurate parameterization of the deposition flux is essential for having a precise determination of the flux removal and also for allowing longer simulation periods of the atmospheric processes. Also, more accurate deposition patterns will allow a much more precise diagnostic of the different impact of different pollutants on the different types of terrain which are present in complex environments such urban ones and its environs. In this contribution we have implemented a complex resistance deposition model in the Air Quality System (ANA) which is applied over the Madrid Metropolitan area and surroundings (80 x 100 km). The ANA model is composed on four different modules: a meteorological module which solves numerically the Navier-Stokes ewuations and predicts the wind, temperature and humidity in a three dimensional domain every time step; the emission module is a high spatial and temporal resolution model (one hour and 250 m x 250 m) and with land use information for the natural or biogenic processes which is obtained by the LANDSAT-5 satellite information (30 m x 30 m resolution); The CBM-IV chemical mechanism is solved by the SMVGEAR numerical method. Two deposition modules are used, the Wesely (1989) and the Erisman et al. (1994). Results show a high sensitivity to the deposition parsmeterization. Erisman et al. (1994) approach seem to simulate more properly the air concentrations at different monitoring stations.

Integration of Partitioned Stiff Systems of Ordinary Differential Equations

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Stiff systems of ODEs require implicit integration formulas for efficient numerical integration. The solution of the resulting algebraic system by Newton iteration involves the computation of a Jacobian and the solution of systems of linear equations. With a system of N differential equations, these steps require $O(N^2)$ - $O(N^3)$ operations and become very expensive for large systems.

Assume that the system of ODEs can be partitioned into q subsystems of n=N/q equations. Assume further that each sub-system of the partitioned system can be discretized *independently* by the backward Euler formula using solution values from the other subsystems corresponding to the previous time step. Then the dominant complexities become $O(qn^2)$ and $O(qn^3)$\$, resulting in savings by a factor q - q^2.

Besides the savings in arithmic operations, this so-called decoupled implicit Euler method is ideally suited for parallel computers. With one or several sub-systems allocated to each processor, information only has to be exchanged after completion of a step but not during the solution of the nonlinear algebraic equations.

This talk presents the condition for monotonic max-norm stability which guarantees the stability of the decoupled implicit Euler discretization. It also considers strategies and techniques for partitioning a system into a monotonically max-norm stable system and presents error bounds to be used in controlling stepsize, relaxation between sub-systems and the validity of the partitioning. Finally an example is presented based on the condensed CBM IV scheme for simulating the chemical reactions in the Danish Eulerian air pollution model.

On the TRAP advection scheme - description, tests and applications

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A new created advection scheme will be presented and discussed. It is developed especially for the Bulgarian Eulerian dispersion model. The model development was provoked by the needs of the Environmental authorities of more detail description of the acid loads in the region. The model is PC-oriented because of the broad distribution of this computers in the Eastern European Countries and the limited possibilities of using more powerful machines. So, special attention was paid on time and space optimization of different schemes.

The new advection scheme, called TRAP, is an explicit, positively definite and conservative scheme with limited numerical dispersion and good transportability. It is specific combination from Bott's scheme and Lurner and Roussel's slope-scheme. The TRAP scheme is tested using the standard rotational test as well as some other tests. The results are compared with those of some other well known schemes. It occurs, that having almost the same properties as Bott's scheme, TRAP scheme is some times faster then it.

The TRAP scheme is used in the new developed dispersion model EMAP. It is realized using log-linear terrain following Z-coordinate system. The simplest 2-order time forward explicit scheme is used for description of horizontal diffusion. The vertical diffusion block uses implicit scheme accounting for the dry deposition as bottom boundary condition. A proper SL parametrization allows to have the first computational level at the top of the surface layer. In the S-version of the model only two species - SO2 and SO4 - are involved and a simple transformation rate approach is used to parameterize the chemistry. The wet scavenging is parameterized by proper wash-out rates, depending on precipitation intensity and type. The model is used for estimation of sulphur deposition in the region of East-Southern Europe in a grid 25 km x 25 km. The aerosol version of the model, which is now under verification, is used for calculation of lead dispersion in the same region, as well as over the 50-km EMEP grid.

Benchmarking Stiff ODE Solvers for Atmospheric Chemistry Problems

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In the numerical simulation of atmospheric transport-chemistry processes, a major task is the integration of the stiff systems of ordinary differential equations describing the chemical transformations. It is therefore of interest to systematically search for stiff solvers which can be identified as close to optimal for atmospheric applications.

In this contribution we report on a comparative investigation based on a set of box-models used in present day transport models. A wide range of integration techniques has been tested, including explicit methods (QSSA, CHEMEQ, TWOSTEP), implicit (BDF,DIRK) and linearly implicit ones (Runge-Kutta-Rosenbrock). In the presentation the focus is on Rosenbrock solvers. These turn out to be very well suited when they are provided with highly efficient sparse matrix techniques to economize on the linear algebra. Within the class of explicit methods TWOSTEP is the clear winner [1,2,3].

The benchmarking project [1,2] is a joint activity between the CWI and the University of Iowa. Adrian Sandu (University of Iowa) will present a talk on the preprocessor KPP developed at the University of Iowa. KPP not only generates production and loss terms from a given set of chemical reactions, but also analyses the sparsity pattern of Jacobian matrices and generates sparse linear algebra routines which are used by the implicit and linearly implicit methods.

References

[1] A. Sandu, J.G. Verwer, M. van Loon, G.R. Carmichael, F.A. Potra, D. Dabdub and J.H. Seinfeld: Benchmarking stiff ODE solvers for atmospheric chemistry problems I: implicit versus explicit, Atmospheric Environment, to appear.

[2] A. Sandu, J.G. Verwer, J.G. Blom, E.J. Spee and G.R. Carmichael: Benchmarking stiff ODE solvers for atmospheric chemistry problems II: Rosenbrock methods, submitted to Atmospheric Environment.

[3] J.G. Verwer, J.G. Blom, M. van Loon, and E.J. Spee: A comparison of stiff ODE solvers for atmospheric chemistry problems, Atmospheric Environment 30:49-58, 1996.

See **http://www.cwi.nl/cwi/projects/nw1.4.html** for preprints and related work.

Comparison of the numerical efficiency for different chemical mechanisms in a chemistry-transport model.

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An explicit-implicit time integration method is presented for the solution of three-dimensional advection-diffusion-reaction equations which describe the transport and chemical transformation of atmospheric pollutants. Vertical transport processes (advection, diffusion, deposition) and chemical kinetics are treated in every horizontal grid point implicitly and simultaneously. The time-integration is performed by the second-order BDF scheme. For horizontal advection an up-wind scheme is implemented. The advection time step is restricted by the CFL-criterion. The resulting fluxes from horizontal advection are handled as "artificial" sources during the integration of columns.

In our approach the chemical reaction system is given as a data file. Therefore changes within the chemical mechanism or the replacement of the whole chemistry can be performed in a simple and comprehensive way. For testing in real-live scenarios our code is coupled with the mesoscale meteorological model METRAS.

In this paper we compare the numerical efficiency for the chemical reaction mechanisms "Euro-RADM", "RADM2" and "CHEMSAN". The test scenario describes a summer episode over Saxonia. The modeling area has a horizontal extension of 160km x 140km. The horizontal grid size is fixed at 4 km. In the vertical direction the grid consists of 27 non-equidistant layers. The time-dependent emission data with diurnal and seasonal variations are separated into point and area sources.

The three-dimensional version of the Danish Eulerian Model

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The two-dimensional version of the Danish Eulerian Model has been developed during the 80'ies. More than 70 chemical reactions (some of them photochemical) are involved in the model. The space domain of the model covers the whole of Europe. It has been discretized by using a (32 x 32) equidistant spatial grid. The concentrations and the species calculated by the model were compared both with measurements taken over land and with measurements taken over sea. The model has also been run by using finer grids; as, for example, a (96 x 96) grid. The experiments indicated that in general the model calculates rather reliable results. However, it is also clear that the results might be improved if a three-dimensional version of the model is developed. Three-dimensional air pollution models are very time-consuming. Therefore the development of a reliable three-dimensional version of an air pollution model is a very challenging task. The efforts to solve some of the numerical problems arising during the development of a large three-dimensional air pollution model (with non-linear chemical reactions) will be discussed in this paper.