NUMERICAL MODELLING OF AIR POLLUTION ON REGIONAL AND LOCAL SCALES

A. Ebel[1], T. Davitashvili[2], H. Elbern[1], D. Gordeziani[2],
H. J. Jakobs[1], M. Memmesheimer[1] and I. Tavkhelidze[2]

[1]I.Rhenish Institute for Environmental Research
and University of Cologne (RIU),
Aachener Str. 201 - 209, 50931 Cologne, Germany.
e-mail: eb@eurad.uni-koeln.de

[2]I.Vekua Institute of Applied Mathematics
Tbilisi State University
380043 University Street 2, Tbilisi, Georgia
e-mail: tedav@viam.hepi.edu.ge

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Abstract

The development and application of numerical regional and local chemistry transport models (CTMs) is discussed. Introductory remarks address the motivation for the employment of these models in atmospheric and environmental science. Furthermore, it is stated that there is a strong need for application of CTMs to environmental policy and planning and air quality forecasts as an important factor for the reduction of health risks. The fundamentals of CTM design are addressed, thereby emphasizing the necessity of grid adaptation in regional models for the treatment of smaller scale and local air pollution problems. Going to very high resolution it is convenient to couple regional models with models especially designed for specific local conditions. An example of such a model chain is the planned coupling of the European Air Pollution Dispersion model system (EURAD) with the Tbilisi Air Pollution model (TAP). Practical aspects of the treatment of boundary and initial conditions are discussed. Examples of model applications are given exploiting the experience gained with the EURAD system. Model evaluation studies have not been included in the paper, but it is emphasized that they are an important and demanding part of air pollution model development and application.

Key words and phrases: Decomposition method, Operator split, Semigroup, Trotter formula, Cauchy abstract problem, Rational approximation.

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Introduction

Numerical models have proven as indispensable tools for the treatment of the composition of the Earth's atmosphere regarding long-term global changes and their impacts on climate and biosphere on the one hand and short- to medium-term changes and their role for air quality, human health, agriculture and socio-economic issues on the other hand. Numerical environmental models are widely employed for the treatment of scientific and applicational problems, yet at the same time they are under permanent development with respect to their physical and chemical content, improvement of numerical algorithms and extension to new fields of application. They offer a multitude of challenges to specialized and interdisciplinary research and application. This paper is concerned with the development and use of numerical chemistry transport models (CTMs) for the study of air quality problems generated by human activities on regional and local scales, i. e. in regions with the extension of small continents (like Europe) down to areas with the size of a city. It is outlining the structure, i. e. the main components, of air pollution models, which have to deal with meteorology, chemical reactions and fluxes of minor atmospheric constituents and emissions of anthropogenic and natural gases and aerosols. Attention is also given to the treatment of initial and boundary conditions and to the application of zooming or nesting methods, i. e. the use of variable resolution and grids. Though air quality and its changes are governed by a unique system of meteorological and chemical processes a rather large variety of models has been developed due to different aims of model application and availability of computational resources. Depending on the way how transport is treated one finds two principal types of models, namely Lagrangean and Eulerian ones. The tendency of increasing physical and chemical complexity in most advanced models may require massive parallel processing instead of sequential calculations. Various methods of grid adaptation for the treatment of processes on scales ranging from local to regional to global may be chosen. The following sections are based on the experience gained from the development and application of a specific regional Eulerian chemistry transport model (the European Air Pollution Dispersion Model System "EURAD" [1]) and a local model (Tbilisi Air Pollution model "TAP" [3]).

1. Fundamentals of model design

Subsection 1.1 Basic equations. The chemistry transport model basically consists of a set of continuity equations for the sample of minor constituents which play a role for the composition of the lower atmosphere in general and air pollution and its changes in particular. The set of equations is complimented by boundary conditions for each transported species which are usually formulated in flux form. For a species (or tracer) named "i" with mixing ratio C_i one has

$$\frac{\partial}{\partial t}C_i = P_i - L_i + E_i + \nabla\left(K \nabla C_i\right) - \nabla\left(C_i v\right). \tag{1.1}$$

P_i, L_i and C_i represent the production, loss and emission (by elevated sources), respectively, of the species i in the atmosphere. The last two terms describe the divergence of the turbulent flux and advection by the mean wind, respectively. The turbulent flux is parameterized by the turbulent diffusion tensor K. In general, only the vertical component of turbulent flux needs to be considered, particularly in the planetary boundary layer, so that the approximation

$$\nabla\left(K \nabla C_i\right) \approx \frac{\partial}{\partial z} K_{zz} \frac{\partial}{\partial z} C_i \tag{1.2}$$

holds where Kzz is the vertical eddy diffusion coefficient. The total (vertical) flux of the tracer at the earth's surface (F_T) usually consists of two components, namely dry deposition (F_D) and emission from surface sources (F_E):

$$F_T = F_D + F_E$$

The emissions may be of anthropogenic and natural origin. Both types play a role for the generation of primary and secondary atmospheric pollutants.

Subsection 1.2. Model structure. A convenient way of model design is the treatment of air pollution in a system of sub-models dealing with meteorology, chemistry and emissions. In many applications it is sufficient to treat chemistry and transport off-line, i. e. decoupled from meteorological calculations. A modular structure for the representation of different processes guarantees flexibility with respect to the degree of complexity of a model. Models of such design are described in [2].

Subsection 1.3. Processes and parameterizations. A considerable number of processes which control atmospheric composition changes ($\partial C_i / \partial t$ in (1)) cannot be resolved in grid models or can only vaguely be described with respect to their dependence on general meteorological parameters. Radiative flux and boundary layer turbulence are prominent examples. Their detailed treatment is out of the scope of this article. The reader is referred to the relevant literature (e. g. [7]).

Fig. 1. Schematic of nesting procedure

Subsection 1.4. Nesting. Historically, the development of CTMs started with rather coarse horizontal resolution (80 to 150 km). The increasing computer performance enabled a considerable improvement of the resolution also for larger domains of integration. Yet the challenge of local air quality problems was a strong motivation to proceed to even smaller grid sizes in small sub-domains of larger regions. For correct treatment of boundary conditions it proved necessary to embed these sub-domain models in larger scale models. A convenient way is subsequent nesting of the same model going from larger grid sizes, i. e. scales, to smaller grid sizes in smaller sub-domains. Fig. 1 exhibits an example for Central Europe where a coarse grid integration is carried out for the main part of Europe with a coarse resolution of $\triangle x = 125$ km in nest 0 (N0) and subsequent simulations are performed with increasing resolution in N1 ($\triangle x = 25$ km) and N2 ($\triangle x = 5$ km). The parameterizations used in a specific model, e. g. for clouds, depend on the scale it may be necessary to change them with increasing resolution or to use another model designed for local calculations. As an example, regional calculations could be carried out with the EURAD model for the Black Sea, Caspian Sea and Caucasus area and then gradually be nested down to a smaller domain around Tbilisi, where the local Tbilisi Air Pollution model finally could be applied.

Subsection 1.5. Boundary and initial conditions for the CTM. Boundary and initial conditions need to be carefully formulated for the regional integration of chemistry and transport. As regards topographical data increasing precision is needed with increasing resolution for the description of the earth's surface as the lower boundary. Whereas gross features of a terrain can easily be described for larger scales, accurate surface modelling has to be carried out for the micro-scale range, e. g. for street canyons or small valleys. The type of surface has to be prescribed since parameterizations of surface effects on meteorology and chemistry depend on it. For long-term calculations seasonal changes must be taken into account. Limited area CTMs pose a problem with respect to lateral and upper boundaries since fluxes of all transportable chemical species through them have to be defined. Observations can rarely help since they are usually sparse or not available for a large group of chemically relevant species. A solution can be the nesting of a regional CTM into a hemispheric or global one. Unfortunately, not all the constituents needed for regional integration are provided by the global model. Another way is to put the borders of the model domain far enough away from the polluted area and carry out a spin-up integration to generate reasonable fields of concentrations of air pollutants which then are used for model initialization. These large domain calculations can then provide initial and time dependent boundary conditions. To avoid negative effects from ill-defined upper boundary conditions (usually zero flux condition) it is advisable to move this boundary to larger heights far enough from the highest level of interest. (The upper boundary of the EURAD model is usually put at 100 hPa around 16 km altitude). Evidently the situation for the formulation of regional CTM boundary and initial conditions is fundamentally different from that for meteorological models which can be nested into global weather analyses and models.

The success and reliability of air pollution simulations crucially depends on the quality of emission data.. Considerable work has been done to derive reliable data sets with gridded time dependent emission values for primary atmospheric pollutants and the precursors of the secondary ones [4]. (For instance, ozone is a secondary pollutant in the atmospheric boundary layer.) Anthropogenic emission inventories which are usually only available for larger areas, longer time intervals (annual estimates) and, in the case of volatile organic components (VOCs), groups of components have to be scaled down to the needed spatial and temporal resolution and decomposed into individual species according to the chemical mechanism used in a CTM. Natural (biogenic) emissions may be parameterized with time-dependent surface (land use) data.

For the initialisation of CTMs new methods resulting from strong progress in the field of chemical data assimilation are beginning to develop [5]. This is a promising step forward to higher accuracy of simulated chemical fields and its changes in the atmosphere.

2. Treatment of processes

The continuity equation of matter in the atmosphere (1) describes a complex system of interacting processes whose complete treatment by numerical methods would cause serious problems regarding availability of computer resources, stability of the numerical system and reliability of results. Therefore, it has to be decided what processes should be taken into account. About one decade ago most modellers still believed that aerosol effects could be left out in the simulation of photo-oxidants. Now aerosols have become a major challenge for environmental modelling - not only because of their impact on chemical gas phase reactions, but also and even more due to their relevance to human health and climate. Their treatment is now feasible in advanced chemical transport models up to a certain degree due to the advancement of computer technology. This has decreased the model formulation uncertainty. Nevertheless, it still holds that a minimum of uncertainty below the point of maximum executable processes - resulting in higher input uncertainty - exists as shown by the schematic in Fig. 2 [10], [11]. The gain of information obtained by numerical simulation studies may still somewhat increase beyond the point of minimum uncertainty but certainly not too far as anticipated in the figure.

Fig. 2. Schematic view of the relationship between uncertainty of model formulation, input uncertainty, resulting total uncertainty and possible gain of information. Uncertainty curves adopted from Irwin [10]

The terms P_i and L_i contain gains and losses of a constituent C_i in a given volume (grid box) of the domain under consideration. They are generated by chemical as well as physical processes. On the chemical side one has gas phase, heterogeneous (on aerosol surfaces) and wet (in droplets) reactions. A physical process is the dissociation of minor constituents due to incoming solar radiation, which is the main driver of atmospheric chemistry. Consequently, CTMs need an efficient module for the treatment of solar radiative fluxes and photolytic effects relevant for atmospheric chemistry. Physical processes like coagulation, nucleation, condensation and evaporation control the distribution of aerosols in the atmosphere to a high degree. On the other hand aerosol formation is also influenced by chemical processes as demonstrated in Fig. 3 by the interaction scheme for a specific aerosol model (MADE used in the EURAD system [6], [12]). Aerosols may change the actinic flux (i. e. flux of the photolytic component of solar radiation) in the atmosphere. This forms a complex (non-linear) system of processes with efficient feed back mechanisms. The system is not yet well understood, nor are the feed back mechanisms comprehensively simulated until now. It is evident that clouds and rain can efficiently influence atmospheric chemistry which in turn may modify cloud formation via its influence on aerosol processes. They cause losses of pollutants through washout, are shielding lower levels from solar radiation and cause vertical transport, i. e. vertical redistribution,

Fig. 3. Modal aerosol dynamics module MADE developed for and used in EURAD

of minor constituents. Since cloud modelling is an extremely demanding task many models avoid to simulate them and are therefore only applicable to fair weather conditions. The input of pollutants from elevated emission sources (term in (1)) is also interrelated to other processes treated in the CTM. Elevated sources are formed by stacks. The behaviour of their outflow is mainly controlled by meteorological parameters, preferably the stability of the stratification of the lowest levels of the atmosphere. Here, in the so-called planetary boundary layer (PBL), the efficiency of the vertical transport of pollutants and other properties of air (heat, momentum, water vapour) depends on the intensity of irregular fluctuations of the atmosphere, i. e. turbulence. Turbulent transport as described by (2) in parameterized form is week when the ABL is stably stratified (at night), and it is strong when irregular vertical convective motions are generated by insolation (during the day). Under fair weather conditions this causes a pronounced change of ABL conditions with little vertical exchange in a flat stable boundary layer during night, strong vertical mixing in an extended convectively unstable boundary layer, called mixing layer, and short periods of transition between these states in the morning and afternoon [7]. Boundary mixing and turbulent transport is caused by sub-grid wind fluctuations which need to be parameterized. A great variety of parameterization schemes is available. Their generalization for application to all relevant ABL conditions still has to be achieved. Reliable ABL parameterization is indispensable for high quality simulations of air pollution in the ABL. A parameter which can be observed and is useful for the evaluation of ABL modules is the mixing layer height. In off-line calculations the wind field needed for the calculation of advective transport given by the last term in (1) can be generated by meteorological simulations employing a separate meteorological model (as done in the EURAD system), it can be taken from meteorological analyses like those of the ECMWF or can be derived from observations. A part of the lower boundary fluxes (3) is also characterized by interactive processes. Deposition of pollutants to the surface is the ultimate cleaning process for the atmosphere. Deposited materials may change surface properties which are relevant for the deposition process, e. g. physiological conditions of plants, fertility of the ground (which can be changed by NO_2 deposition) or modifications of ecosystems by acid deposition, and may change the deposition flux intensity in the short or long run.

3. Simulation studies

Application of CTMs are motivated by a broad range of goals. These may be solving of scientific problems related to air pollution, support of environmental policy, control and forecasting of air quality or treatment of emergency cases. The planned joint employment of EURAD and TAP is mainly aiming at the treatment of control and emergency problems in the Caucasus region and elsewhere. Among those problems are the impact of traffic and industry on air quality, possible pipeline accidents and nuclear power plant emissions. In order to demonstrate the applicability of the envisaged model system some simulation studies carried out with the EURAD model system are briefly discussed in this section.

Subsection 3.1. Some details of the EURAD model The EURAD model system consists of a meteorological (MM5), chemistry transport (EURAD-CTM) and an emission (EEM: EURAD Emission Model) part. The design of the EURAD-CTM has been based on the Regional Acid Deposition Model (RADM) by Chang et al. [7]. The gas phase chemical mechanism RADM2 [8] is employed together with MADE (see Section 2) for the treatment of aerosols. Anthropogenic emissions are derived from the EMEP emission inventory or provided by the GENEMIS emission project [4]. The Eulerian approach is used for the calculation of air pollutant distributions. The standard version of the CTM contains a variable number of levels (usually 23) in the vertical between the earth's surface and 100 hPa with maximum resolution near the ground in the PBL. The lowest layer is about 80 m thick, but smaller values may and have been employed in special applications. The horizontal resolution may be chosen between about 50 km for the coarse grid and 1 km for high degree sequential nesting. The model is used for regular air quality forecasts in this configuration. They may be found on the internet under www.eurad.uni-koeln.

Subsection 3.2. Analysed events and problems Some applications of the EURAD system which may be helpful and can be exploited for our future cooperative work are briefly mentioned in this section. During the development phase of the model, simulations of the spread of the radioactive cloud after the Chernobyl accident were carried out. The possible transport of soot from oil fires in the Persian Gulf region have been studied on the occasion of the last two Iraq wars. This demonstrates the applicability of the model system to emergency events causing emissions into the atmosphere. Several simulation studies were concerned with the impact of complex terrain on atmospheric chemistry and transport. The behaviour of polluted air in urban areas and possible ways of air quality improvement have been analysed. This includes the investigation of effects resulting from complex emission reduction scenarios. Two particularly relevant applications are the downscaling of the calculations from regional to local domains by nesting and studies of the transport and chemistry in mountainous regions. The are discussed in the following subsection.

Fig. 4. Example of subsequent nesting. Simulation of photo-oxidant episode in Central Europe, July 1994. Ozone mixing ratios (in ppbV) are shown for the lowest model layer of the EURAD system (0 - 70 m). Resolution of nest 3 with Berlin in the centre is 3 km

Fig. 5. Net chemical production rates of ozone , 20 July 1998, 14:00 UTC, around Berlin. Nested calculation, lowest model layer (0 - 40 m)

Subsection 3.3. Examples of episodic simulations Fig. 4 shows results from an analysis of ozone formation around a densely populated area (Berlin). The wind is roughly blowing from NW to SE. A city plume of polluted air can be found in the downwind direction from the city. It is marked by increased levels of ozone. Rather fine details can be resolved by nesting as demonstrated for the same domain during a different episode in Fig. 5 by the ozone production rates. They are clearly influenced by strong NO emissions along the highways around and in the city. The role orographic barriers can play is highlighted by a simulation of a photo-oxidant episode in northern Italy. Apparently, the Alps form an efficient obstacle for the flow of polluted air from SE to NW during the simulated episode (Fig. 6A). The distribution of ozone at 700 hPa is significantly different from the one which would be found in the case of flat terrain (Fig. 6B). Air crossing the mountain range is lifted up to larger heights thus carrying pollutants from the planetary boundary layer to free tropospheric levels as shown for NO_x in Fig. 6C. This causes enhanced production of ozone at higher elevations which than can be transported over large distances in the free troposphere (Fig. 6D). This phenomenon is therefore relevant to problem of trans-continental transport of primary and secondary anthropogenic pollutants and the question of global atmospheric and climate change. The Caucasus range - like other mountain ranges - is expected to generate similar effects which still need to be investigated

Fig. 6. Simulation of air pollution in a mountainous region (Alps) with the EURAD system, 13 May 1998, 12 UTC. Results for the 700-hPa constant pressure level are shown. A. Simulation taking into account the complex orography. B. The same, but flat terrain assumed. C. NOx distribution over the mountains indicating upward transport of boundary layer air due to the air flow over the Alps from SE to NW. D. Modelled net production of ozone at 700 hPa

4. Conclusion

The discussion of general aspects of air pollution modelling and the presentation of specific model applications employing a special advanced chemical transport model show the broad range of problems to which numerical simulations of the state and development of the atmospheric environment can be applied. For the sake of brevity the discussion of model evaluation strategies and evaluation results has been omitted. Yet it is strongly emphasized that CTM evaluation is an extremely important and demanding task of model design and application. The cooperation between our institutes is motivated by the aim to fulfil the societal need of further work for the solution of local and regional environmental problems. The benefit of such applications for the society will be a reduction of health risks due to air pollution. Furthermore, contributions to the analysis of regional impacts on the global climate resulting from anthropogenic emissions will become possible with a high degree of reliability. Such studies are still underrepresented in the discussion of global change though they are strongly needed for the development of mitigation strategies concerning harmful impacts of global atmospheric change [9].

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