

Simulation Models for Air Quality Management

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Abstract Air quality models are extremely valuable for environmental planning and management, as they may be used to study complex source/receptor relationships. The aim of this paper is to present a survey of atmospheric simulation models and its applications for air quality management in different model scales. To provide an example for the usability of an air pollution simulation system, the DYMOS system is described. Air quality management systems based on DYMOS permit an integrated quantitative and qualitative analysis of the air quality in urban and industrial areas. In particular it supports historical investigations, prediction of trends and planning issues. Applications of the DYMOS system as basic module of different management decision support systems for different purposes will be presented. These applications are mainly performed in the frame of European cooperation projects.

1. HISTORY AND TASKS

During the past decade atmospheric modelling and air quality analysis have been significantly improved by developing comprehensive 3D simulation models describing the transport and chemical transformation of air pollutants, taking into account complex flow and dispersion characteristics. The model domain ranges from microscale (street canyon, flow around buildings) over mesoscale (urban and industrial areas) to macroscale applications (continental pollutant transport, global climate research). In recent years, increasing computing capacity (and its use by parallel programming) made it possible to run realistic scenario analyses in an acceptable time and to enable smog predictions at all (computation time less than simulation period). Nowadays two developments in atmospheric research can be observed:

1. efforts for building air quality management systems, e.g.
 - enlargement of existing model systems in order to include models for controllable parts like traffic;
 - integration of software environments into existing model systems for the automation of experiments like Monte Carlo algorithms, sensitivity analysis, etc.;
 - integration of software environments into existing model systems for result verification and decision support like GIS, statistics, expert systems.
2. efforts for building forecast systems connected with monitoring networks for meteorological data and emission and background concentrations. Through the World Wide Web, forecast results can be presented to the broad public.

In the following sections air quality management applications based on the use of the DYMOS system will be presented. These applications are mainly performed in the frame of European cooperation projects.

2. THE SIMULATION SYSTEM DYMOS

At GMD FIRST the DYMOS system has been developed (Sydow 1996), a parallelly implemented air pollution simulation system for mesoscale applications. The DYMOS system consists of different meteorology/transport models for various application purposes including an air chemistry model for the calculation of photochemical oxidants like ozone. The core of the model system is formed by a hydrostatic mesoscale Eulerian model with a low vertical resolution for fast operational forecast tasks (enhanced version of REWIMET - Heimann 1985) and a non-hydrostatic mesoscale Eulerian model with a high vertical resolution and complex parameterization facilities (enhanced version of GESIMA - Kapitza and Eppel 1992). The air chemistry model (Gery, Whitten and Killus 1988) involves 34 species in 82 reaction equations for simulating the photochemical processes in the lower atmosphere. The model system takes into account surface uptake processes as well as biogenic emissions. The current version of DYMOS also contains a mesoscale Lagrangian model (Gerharz, Mieth and Sydow 1996).

In addition to the implemented models, the DYMOS system includes a database for model input and simulation results and a graphic user interface visualizing data in spatial relations. The simulated air pollutants concentrations can be displayed either as a two-dimensional raster images or in the form of a helicopter flight. In the latter case, an altitude profile is overlaid with a satellite picture of the earth surface. Concentration ranges of air pollutants are visualized using a colored transparent layer (Walter 1997).

Figure 1 shows the functional organization of the DYMOS system, including database, visualization software and the integration of two additional simulation models for traffic flow (DYNEMO) and traffic emissions.

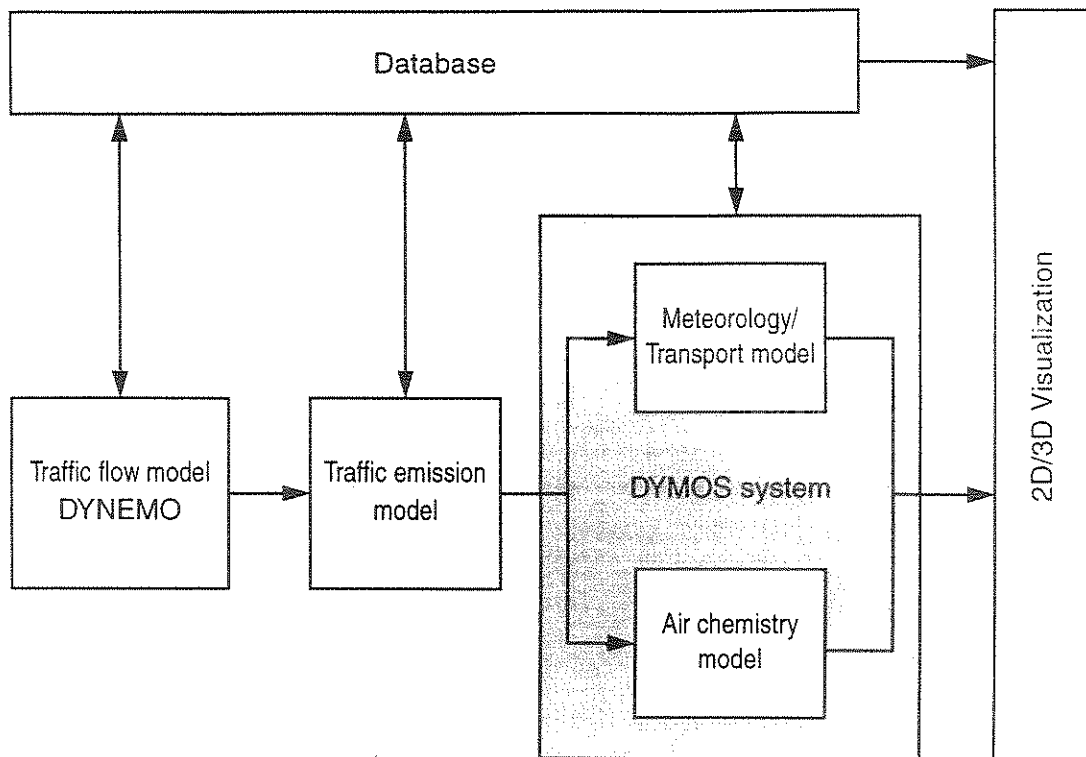


Figure 1. Structure of a simulation system consisting of DYMOS and two additional models

3. REGIONAL OZONE ANALYSIS AND FORECAST

Various case studies of summer smog conditions in urban areas have been carried out using the DYMOS system. The Department of the Environment of the Berlin State Government and the Ministry for Environment of the State Brandenburg commissioned different summer smog analyses accompanying a measuring campaign carried out in July 1994 (Mieth and Unger 1996). Greenpeace commissioned an analysis of the influence of emissions caused by traffic in Munich on the ozone concentration in the Munich area. The analysis was performed for a typical mid-summer day in 1994 (Smid 1996). In order to inform the public about ozone concentrations, the DYMOS system is currently in its test phase for the operational daily forecast of near surface ozone concentrations in the Berlin-Brandenburg region. Figure 2 shows typical raster images for an ozone forecast as in the near future (next summer period) to be found on the WWW pages of a Berlin radio station. The further development and application of the DYMOS system is characterized by two main factors:

- the integration of new models into DYMOS and
- the use of DYMOS (or parts of DYMOS) as component of air quality management systems developed within the frame of European cooperation projects.

4. DEVELOPMENT OF AN INTEGRATED ENVIRONMENTAL MONITORING AND SIMULATION SYSTEM

The ECOSIM project (funded by the European Commission in the Telematics Applications Programme) builds up a prototype of an environmental monitoring and simulation system including advanced visualization and analyzing capabilities for urban areas. Its main features are designed for planning, analyzing and forecasting within the field of air quality management and decision support. It is based on the idea of connecting air quality models with geographical information systems (GIS) and monitoring networks (Fedra 1995). Public authorities in Berlin (Germany), Athens (Greece) and Gdansk (Poland) will provide day-to-day feedback to the ECOSIM developers and will apply the system to their current environmental problems. In the ECOSIM system, DYMOS is coupled with MEMO, an Eulerian mesoscale atmospheric model (Moussiopoulos 1989) calculating the wind field and all important meteorological parameters (e.g. temperatures, stability, pressure, solar radiation). Due to advanced parameterizations, MEMO is able to describe wind fields in complex terrain, e.g. sea breeze effects.

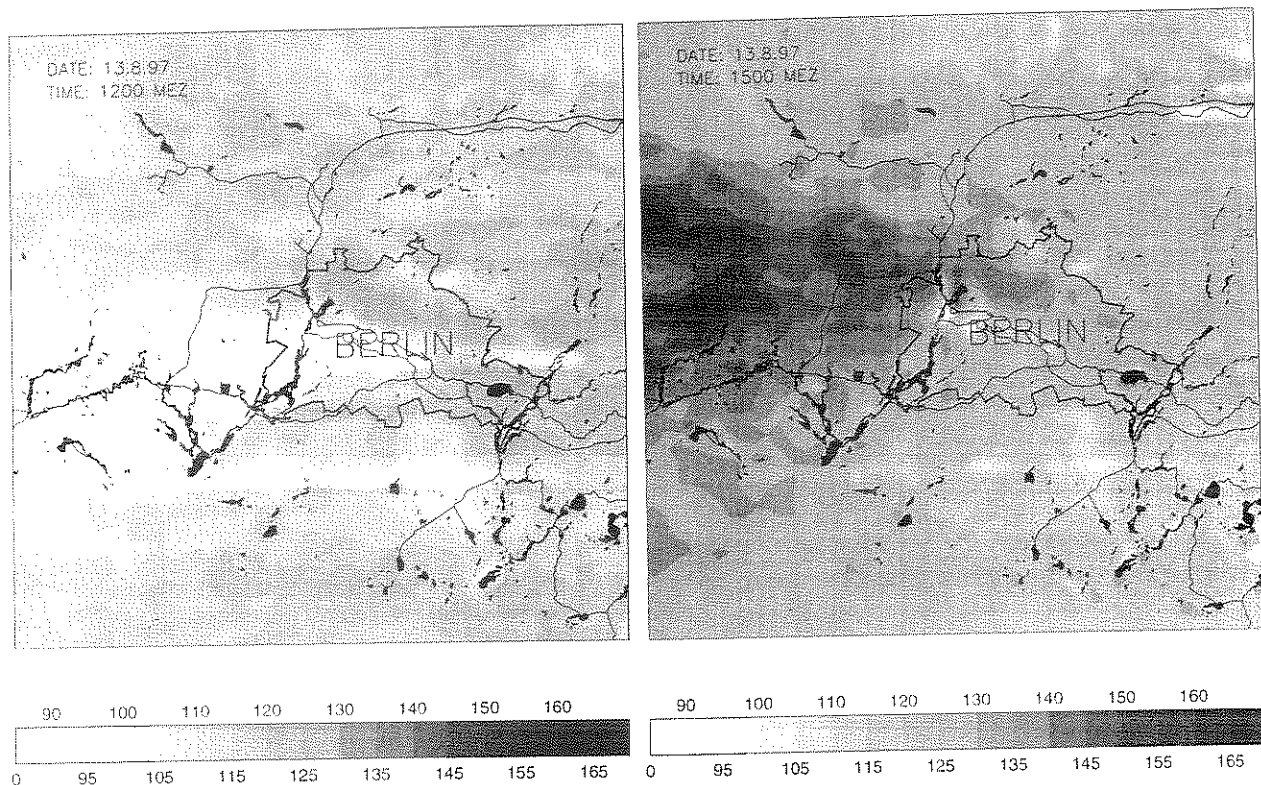


Figure 2. Predicted surface-near ozone concentrations for a typical mid-summer day in 1997 in the Berlin-Brandenburg region with wind from East (left: forecast for 1200 CET, right: forecast for 1500 CET)

5. ENVIRONMENTAL RISK MANAGEMENT

The HITERM project (funded by the European Commission in the ESPRIT Programme) aims at reaching better-than real time performance for the simulation of accidental release of hazardous substances into the atmosphere, ground and surface water. The HITERM system integrates various simulation models (partly from the DYMOS system) for describing technological risk and emergency situations. In particular HITERM includes:

- models for chemical spills or runaway/undesirable reactions, leading to (i) atmospheric dispersion of a toxic gas or evaporating liquid; (ii) fires and explosions of a gas, liquid or evaporating liquid; (iii) transport and dispersion in soil, groundwater and surface water systems;
- pre-processor codes such as 3D diagnostic wind field models and source models such as spill/pool or tank evaporation models;
- routing algorithms for transportation risk analysis;
- impact models.

The demonstrator applications of the HITERM system cover:

- dynamic adaptive routing:
The route optimization of the vehicle fleet (tanker trucks with hazardous cargo) of a Portuguese oil company through its distribution (road) network will be performed

taking into account dynamically updated environmental risk criteria.

- transportation accident simulation:
The case study will address transportation risks (roads and railways) of hazardous goods in the Canton of Uri which is part of the Gotthard alpine transit corridor linking France and Germany with Italy.
- chemical process and storage plant accidents:
The case study for process plant accidents will be carried out in Ponte San Pietro near Bergamo, Northern Italy.

6. TRAFFIC FLOW AND EMISSION MODELLING

In order to obtain an comprehensive picture of pollutant concentrations in the urban area and its surroundings and to simulate the effects of different traffic control measures, an integrated simulation system for traffic flow, traffic emissions and air quality must be available. The project SIMTRAP (funded by the European Commission in the ESPRIT Programme) aims at the development of such a system integrating mesoscale models for traffic flow, traffic emissions, meteorology, air pollutants transport and air chemistry. To this end the DYMOS system will be coupled with the traffic flow model DYNEMO (Schwerdtfeger 1984), using a traffic emission model as interface. Following the demonstrator implementation, first test applications and case

studies are planned for three conurbations in Europe. In addition to the region of Berlin (Germany), the regions of Vienna (Austria), Milano (Italy) and Maastricht (The Netherlands) are involved in this project.

7. TRANSBOUNDARY AIR POLLUTION

The DYMOS group is also interested in studying the long-range transport of air pollutants and the environmental effects in different areas of Europe in order to assess alternative control strategies. In this field a cooperation exists with the International Institute for Applied Systems Analysis (IIASA), Laxenburg, Austria and EMEP's Meteorological Synthesizing Centre - West (MSC-W) at the Norwegian Meteorological Institute, Oslo. Here, the employed model is the MSC-W ozone model, a single-layer Lagrangian trajectory model calculating concentrations of photochemical oxidants every six hours for a set of up to 740 arrival points covering all Europe (Simpson *et al.* 1997). In order to carry out large numbers of scenario runs in an acceptable time, the MSC-W model has been parallelized resulting in a significant decrease of computing time (Unger 1996).

8. EARTH OBSERVATION DATA CONVERSION WITH APPLICATION TO AIR QUALITY FORECAST

In order to use model systems for scenario analysis or air pollution forecast, various kinds of input data of the model domain are necessary:

- digital elevation map
- information about land use
- data for the parameterization of surface effects
- vegetation types
- data characterizing meteorological conditions
- data characterizing air pollution situation
- emission inventory.

The use of image processing for converting earth observation data offers the possibility to update simulation input data more dynamically, e.g. using current maps and taking into account the seasonal change of the vegetation pattern. Furthermore, there exists a variety of model parameters which can be determined in a more objective manner by means of satellite images. Various meteorological input quantities are often only sparsely available from surface observations, but can be detected with a high spatial resolution from remote sensing data. Moreover, new opportunities are available in model evaluation procedures by the usage of earth observation data.

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10. REFERENCES

- Fedra, K., From Spatial Data to Spatial Information: GIS, Environmental Models and Expert Systems, Proc. Joint European Conference and Exhibition on Geographical Information, The Hague, The Netherlands, March 26-31, 1995, 264-278.
- Gerharz, I., P. Mieth, and A. Sydow, A Model to Identify Sources of Particles in Air, Proc. Computational Engineering in Systems Applications - CESA'96 IMACS Multiconference, Part: Modelling Analysis and Simulation, Lille, France, July 9-12, 1996.
- Gery, M.W., G.Z. Whitten, and J.P. Killus, Development and testing of the CBM-IV for urban and regional modeling, US Environmental Protection Agency, EPA-600/3-88-012, USA, 1988.
- Heimann, D., Ein Dreischichten-Modell zur Berechnung mesoskaliger Wind- und Immissionsfelder über komplexem Gelände, Ph.D. thesis, University of Munich, Germany, 1985.
- Kapitza, H., and D.P. Eppel, The Non-Hydrostatic Mesoscale Model GESIMA. Part I: Dynamic Equations and Tests, *Beitr. Phys. Atmosph.*, Vol. 65, pp. 129-146, May 1992.
- Mieth, P., and S. Unger, Estimation of the Influence of Anthropogenic Emissions of the City of Berlin on the Ozone Production, Proc. 5th International Conference on Atmospheric Sciences and Applications to Air Quality, Seattle, WA, June 18-20, 1996.
- Moussiopoulos, N., Mathematische Modellierung mesoskaliger Ausbreitung in der Atmosphäre, *Fortschr.-Ber. VDI, Reihe 15, No. 64*, 1989.
- Schwerdtfeger, Th., DYNEMO: A Model for the Simulation of Traffic Flow in Motorway Networks, Proc. 9th International Symposium on Transportation and Traffic Theory, 1984.
- Simpson, D., K. Olendrzynski, A. Semb, E. Storen and S. Unger, Photochemical oxidant modelling in Europe: multi-annual modelling and source-receptor relationships, EMEP/MS-CW Report 3/97, 1997.
- Smid, K., Cities Cause Ozone Smog in Rural Areas, GMD-Spiegel, Special: Simulation Models, Sankt Augustin, 1996.
- Sydow, A., Smog Analysis by Parallel Simulation", GMD-Spiegel, Special: Simulation Models, Sankt Augustin, 1996.
- Unger, S., Parallelisation and Optimisation of EMEP's Transboundary Air Pollution Model, Proc. International Conference HPCN challenges in Telecomp and Telecom: Parallel Simulation of Complex Systems and Large-Scale Applications, Delft, The Netherlands, June 10-12, 1996, Elsevier, Amsterdam, 467-474.
- Walter, B., Combining Ozone Visualization with Atmospheric Light Scattering, Proc. International Congress on Modelling and Simulation MODSIM 97, Hobart, Australia, Dec 8-11, 1997.