Chemical and dynamical characterization of air pollution episodes using a 3-D Eulerian modeling system

Contribution to subproject GLOREAM

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Summary
The European Air Pollution Dispersion Model EURAD has been used to calculate the concentration and deposition of air pollutants for several episodes of specific interest. The paper focus on nesting applications for Berlin (first intensive measurement campaign during the Berlin Ozon Experiment (BERLIOZ)) and the Federal State of North Rhine-Westphalia. BERLIOZ aimed on the understanding of photochemical processes in the urban plume of Berlin. Calculated concentrations and chemical indicators as H_2O_2/HNO_3 are used to characterize the chemical regimes of the episodes. The processes (e.g. net chemical production, flux divergence due to turbulent exchange and large scale transport) contributing to the concentration changes are used as an additional tool to characterize the dynamical and chemical state of the atmosphere. The results can be used to analyse the impact of different emission scenarios on the air quality in Europe.The calculations performed for NRW include the Modal Aerosol Dynamics Model for Europe and aims on the formation and transport of aerosols. Within a long-term simulation for the year 1997 the current situation in Europe and in NRW with respect to the EU directives 96/62 and 99/30 has been investigated. Details for the results of the long-term results can be found in the contributions by Friese et al. and Feldmann et al. (this issue). The model design used for the NRW case is also used for air pollution forecast available under http://www.eurad.uni-koeln.de (see also Jakobs et al., this issue).

Introduction
Regional-scale air quality models are an important tool to understand the physical and chemical processes controlling the concentrations of atmospheric pollutants and their deposition to the surface. Furthermore the results of model calculations can be used to fill the gaps in measurement networks and to estimate the current and future status of air quality. Model evaluation (Ebel et al., 2000) is important for the reliability of the model results. Photochemical processes as well as the treatment of the atmospheric aerosol is of growing interest with respect to recently established EU directives (96/62, 99/30) in particular for long-term and climatotological aspects.
The EURAD modeling system (Jakobs et al., 1995; Hass et al., 1997; Memmesheimer et al., 1997) is a comprehensive air pollution modeling system which has been used for scientific applications and environmental planning studies for the troposphere over Europe. It consists of the metoerological model MM5, the chemical transport model CTM and an emission model EEM. Gas phase chemistry is handled by the RADM2 or RACM mechanism, aerosols are treated by the MADE model (Ackermann et al., 1998). It can be used with different horizontal and vertical resolutions. Horizontal grid size is in the range of 1 to 125 km, the typical vertical extent is from the surface up to 100 hPa (about 16 km; 23 layers) with about 15 layers below 3000 m to account for the processes in the polluted atmospheric boundary layer.

Objectives

The main goals are the further improvement of the EURAD modeling system as a tool for the short-term forecast of air pollution (Jakobs et al., 2001), the application to future emission scenarios and the support of field experiments. Specific scientific objectives are the analysis of photochemical reactions over Europe and in urban plumes, e.g. BERLIOZ (Becker et al., 2001; Corsmeier et al., 2001). For air pollution planning strategies aiming on the reduction of ozone concentration it is important to know if a region is VOC- or NO_x-sensitive. This can be analysed partly by indicators as H_2O_2/HNO_3 (Sillmann, 1999; Vogel et al., 1999).

Activities

The EURAD modeling system has been used with its nesting option to simulate the European scale down to local/urban scales. The emphasis in this contribution is laid on photochemical processes in the urban plume of Berlin. Other applications performed during the year aim on the strongly polluted area of North Rhine-Westphalia (NRW). In the NRW case a long-term run with the complete system including atmospheric particles has been done covering the year 1997. This run for the year 1997 has been analysed for gaseous pollutants (see Feldmann, this issue, contribution from GLOREAM to TOR-2) and particles (see Friese, this issue, contribution from GLOREAM to AEROSOL). Another special application is the quasi-operational use for the prediction of air pollutants from the European scale to the local scale (in this case NRW) done during the year 2001 (see Jakobs et al., this issue). The data generated during the forecast available in the internet can be used by other groups active in the field of atmospheric sciences, in particular participants of the recently established atmospheric research programme AFO2000 of the BMBF.

Results

Figure 1 show the H_2O_2/HNO_3 ratio for July 20, 1998, 10 UTC (12 CEST) for all nest levels of the EURAD-BERLIOZ simulation. The VOC sensitive regions identified by this indicator are in the plume of the central/western Europe, Northern italy, southern Poland, Moscow and along the mediterranean coast (coarse grid simulation). Also southward of Berlin (Saxonia) a larger area of low rations can be identified. The values in Saxonia are clearly lower as those in the urban plume of Berlin. The air masses near the frontal system approaching Berlin in the morning of July 21, 1998 is also characterized by small H_2O_2/HNO_3 ratios (not shown here). Details for the general results the long-term run for 1997 can be found in the abstracts by Friese et al., Feldmann et al. (this issue) and for the forecast, in Jakobs et al. (this issue).

Conclusions

The H_2O_2/HNO_3 ratio show strong variations in space and time which has to be investigated in the future together with emission scenario runs and other indicators. Interpretation of the ratio also depends on the importance of deposition (dry and wet) and aqueous phase chemistry during the transport of the air masses. The impact of these processes also have to be considered in the future (Sillman, 1999).

A long-term run for the year 1997 has been sucessfully completed and was analysed for gaseous pollutants and atmospheric particles. This gives a contribution from GLOREAM to the subprojects TOR-2 and AEROSOL(see Feldmann et al.; Friese et al., this issue). The results have been analysed with respect to EU directives 96/62 and 99/30. In particular the number of days with average PM_{10} concentrations of more than 50 ug/m^3 exceeds the limit value of 35 days per year for large areas in Europe. The quasi-operational short-term predictions has been done during the year 2001 for gases and atmospheric particles. Further improvementof the system is planned for the future by an evaluation and update of the chemical mechanism in close cooperation with the ICG-II, Research Centre Jülich (Atmospheric Simulation Chamber SAPHIR; Dorn et al., this issue). A set of typical episodes will be selected in close cooperation with the DWD based on its operational prediction with the aim to identify climatological significant standard scenarios (Klein and Zimmermann, this issue). These scenarios will be used for further process analysis for different regions and seasons in Europe to improve the scientific basis of the modeling systems with respect to air pollution forecast and the development of air pollutant abatement strategies.

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Aims for next year and list of publications in 2001

The numerical simulation of several emission scenarios and their analysis is planned for the next year. The chemical mechanism will be evaluated and updated for applications within the EURAD modeling system in close cooperation with the ICG-II, Research Centre Jülich. A set of typical episodes will be selected in close cooperation with the DWD based on its operational prediction with the aim to identify climatological significant standard scenarios These scenarios will be used for further process analysis for different regions and seasons in Europe to improve the scientific basis of the modeling systems with respect to air pollution forecast and the development of air pollutant abatement strategies.

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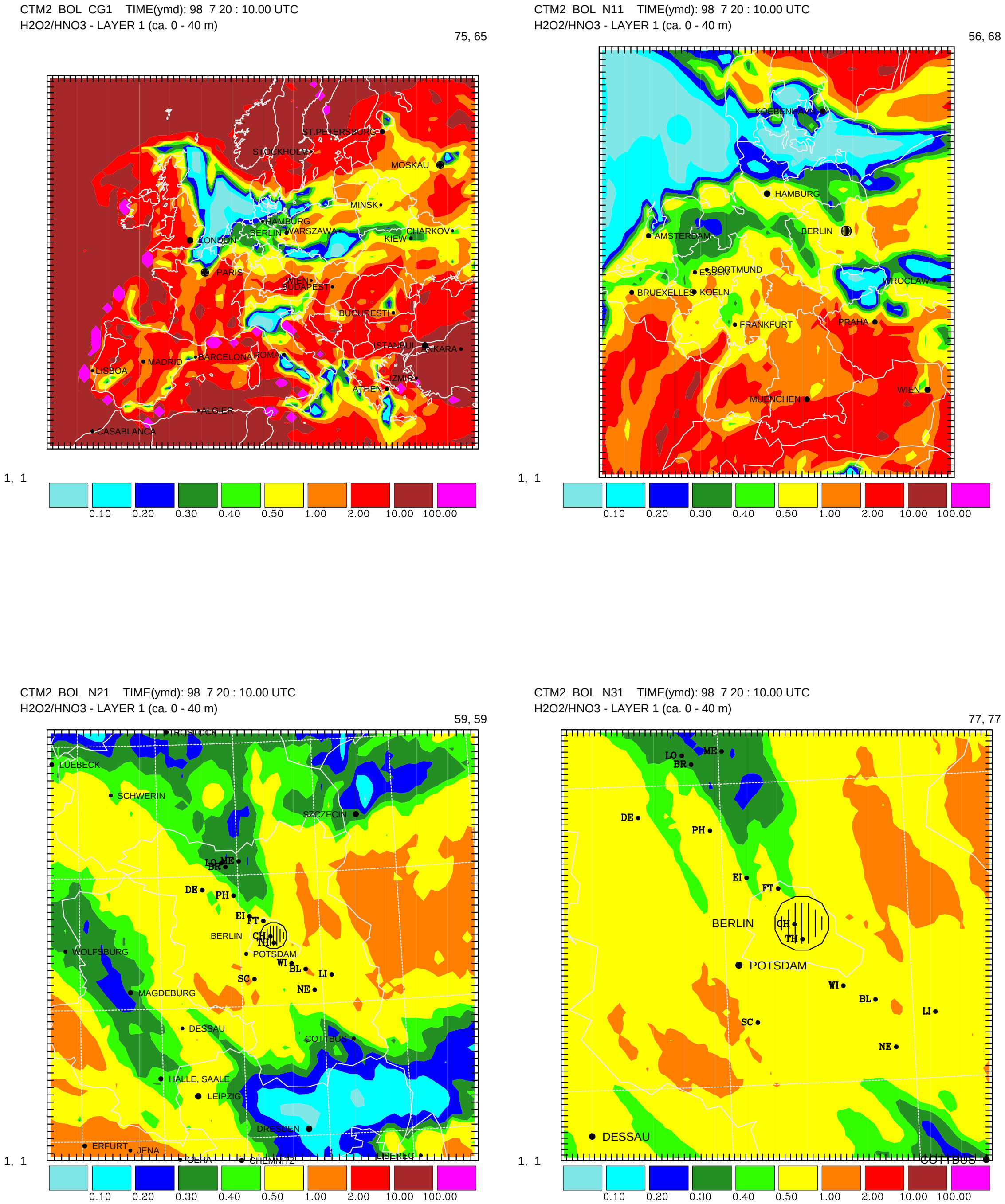

Figure 1: The „sillman-indicator“ H_2O_2/HNO_3 for all nest levels of the EURAD simulation for July 20, 10 UTC (12 CEST). Upper left show results for the mother domain with a horizontal grid size of 54 km, upper right for the first nest level (25 km grid size). The lower panel shows the results for the N2-domain (6 km grid resolution) and the highly resolved N3-domain (2 km grid size).