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NUMERICAL SIMULATION OF THE INTERACTION OF TRANSPORT, DIFFUSION AND CHEMICAL REACTIONS IN AN URBAN PLUME

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ABSTRACT

A model system is presented that takes into account the main physical and chemical processes on the regional scale here in an area of 100x100 km^2. The horizontal gridsize used is 2x2 km^2. For a case study it is demonstrated how the model system can be used to seperate the contributions of the processes advection, turbulent diffusion and chemical reactions to the diurnal cycle of ozone. In this way typical features which are visible in observations and are reproduced by the numerical simulations can be interpreted.

1 INTRODUCTION

Concentration levels of reactive trace gases observed in nature at any specific point of time and space are determined by a number of physical and chemical processes. In the case of a cloud free atmosphere these processes are the transport by the mean wind field, the diffusion caused by atmospheric turbulence and the chemical reactions. The mean wind field and the atmospheric turbulence field are remarkably influenced by the topography on the regional scale. Chemical reactions make the set of differential equations describing the temporal and spatial variation of the different air constituents nonlinear. The nonlinearity of the chemical reactions rises a number of problems. One is that it is impossible to derive simple emittor-receptor relations.

If in a highly industrialized region the behaviour of trace gases is to be studied, it is necessary to achieve a high temporal and spatial resolution, a requirement which can be fullfilled by measurements only during short periods. Such measuring activities were carried out e.g. by Becker et al. (1979) and during the TULLA-experiment (Fiedler, 1987).

Another possibility to study the involved processes with the relevant resolution in space and time arises by the use of a numerical simulation model.

In order to be able to apply a model for realistic conditions the most important processes must be included. In addition it also should be tested against measurements of a variety of atmospheric conditions.

With respect to atmospheric research there exist two main areas of interest. The first is connected to air quality studies where the most important problem is to keep concentration levels below a certain value or to reduce concentration levels. In this sense numerical simulation models can be used to develop efficient strategies for emission reductions.

The second area of interest, which will be focused on in this paper, is devoted to studies of the interaction of the different processes (advection, diffusion and chemical reactions) and to quantify the contributions of these processes to the time and spatial variation of the ozone concentration. The seperation of the different processes from measurements alone is rather troublesome and is often not possible due to the lack of information. This is especially true if only measurements are available at a specific point and no information about the spatial variation of the variables is given. In many cases this lack of information is the reason for speculative interpretations.

Therefore models can be used to support the interpretation of measurements and to better understand the observed features.

2 THE MODEL SYSTEM

The nonhydrostatic mesoscale model KAMM (Adrian, Fiedler; 1991) coupled with a diffusion model and the RADM chemical transformation mechanism (Chang et al., 1987; Stockwell, 1986) is used to calculate the time variation of the three-dimensional distribution of the meteorological variables wind, temperature, humidity and turbulence and a number of chemical species on the regional scale. The model

system which takes into account the topography and the different land use includes a soil-vegetation model (Schädler, 1990) and a detailed parameterization of the dry deposition (Baer, Nester; 1992). With a method developed by Adrian (1987) it is possible to determine the basic state and the forcing of the model system from operational numerical weather forecast. Results of the model system were already compared with observations, for example by Vogel,H. (1991). Figure 1 shows the structure of the model and the input data which are necessary.

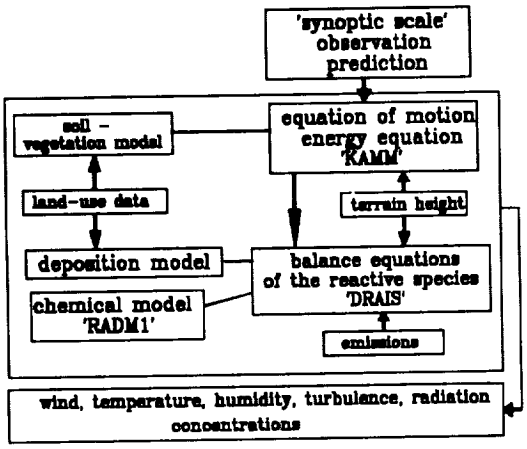

Figure 1. : The structure of the mesoscale model system developed at the 'Institut für Meteorologie und Klimaforschung' in Karlsruhe.

For this case study, only the emissions of the area sources of Heilbronn, a small city in the southwestern part of Germany, are taken into account. The emission area is indicated by a rectangular in Figures 2-6. The emission data were taken from the emission data base determined for the time period of the TUL-LA experiment (Obermeier et al. 1989). The emission data are available with a spatial resolution of 1x1 km^2 and a temporal resolution of one hour. For the initial background concentrations, measurements are used. The horizontal grid size is 2 km, the vertical grid size differs from 18 m close to the surface up to 600 m at the top of the model which is 8 km above sea level. A geostrophic wind from north-west with 7.5 m/s is chosen for this simulation. Two complete diurnal cycles are calculated for a typical summer day.

In order to better understand the observed diurnal cycles the model is used to calculate the contributions of the relevant processes (advection, turbulent diffusion and chemistry) to the spatial and temporal variation of the O_3 concentration and to study their interaction.

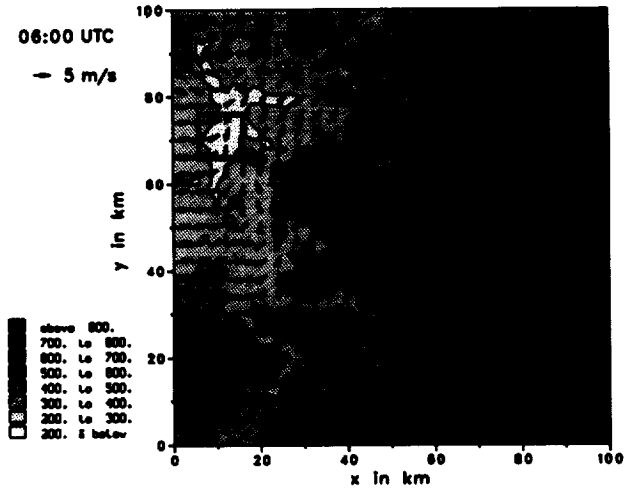

Figure 2: Topography and simulated windfield 18 m above ground (day 2, 06:00 UTC). The rectangular shows the area where the emissions are taken into account.

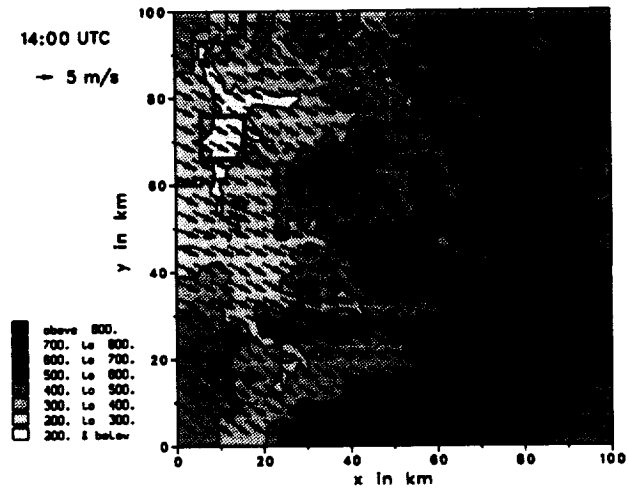

Figure 3: Topography and simulated windfield 18 m above ground (day 2, 14:00 UTC).

3 RESULTS

- The results show a strong modification of the flow field during the diurnal cycle caused by the topography. Therefore the city plume is also remarkably influenced (Figures 2-6).
- The simulated diurnal cycles of ozone show typical features for urban and rural areas (A,B in Fig. 7) which are in good agreement with measurements. These features are: First, concentrations close to zero are found during night in urban areas and therefore a high amplitude of the diurnal cycle. Second, much higher concentrations during night are found in rural areas and therefore a small amplitude of the diurnal cycle.

- There is a buildup region of ozone due to chemical reactions in the city plume about 50 km behind the source area (Fig. 6).
- At points A and B, the total hourly variations of ozone are in the same order of magnitude in spite of the fact that the order of magnitude of the single processes at both points are quite different (Fig. 8 and 9).
- In the urban area (Point A) the increase of ozone between sunrise and the early afternoon is mainly caused by turbulent diffusion (Fig. 8).
- The simulation shows that the secondary maximum of the ozone concentration after midnight at point A is caused by reduced chemical destruction and the advection of ozone from outside into the city (Fig. 8). Such a secondary maximum commonly can be recognized in the observations of many urban stations.
- During night the ozone distribution close to the surface is controlled by the interaction of turbulent diffusion and dry deposition (Figures 10-11). Low turbulence together with low windspeed results in low ozone concentrations (Point C). In contrast at elevated sites enhanced turbulence compensates the deposition (Point D).

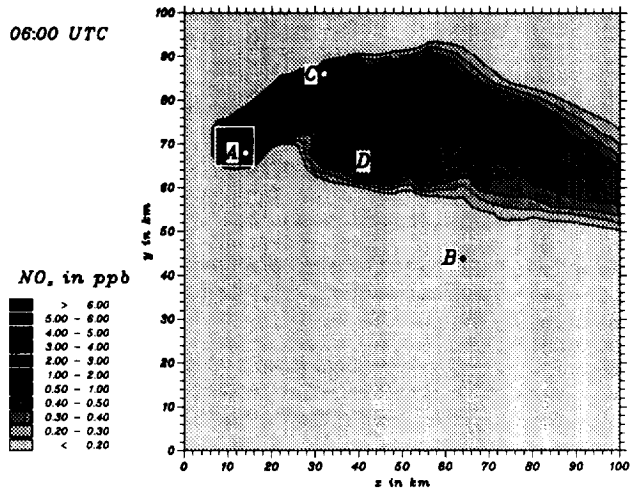

Figure 4: Simulated NO_x –distribution 18 m above ground (day 2, 6:00 UTC).

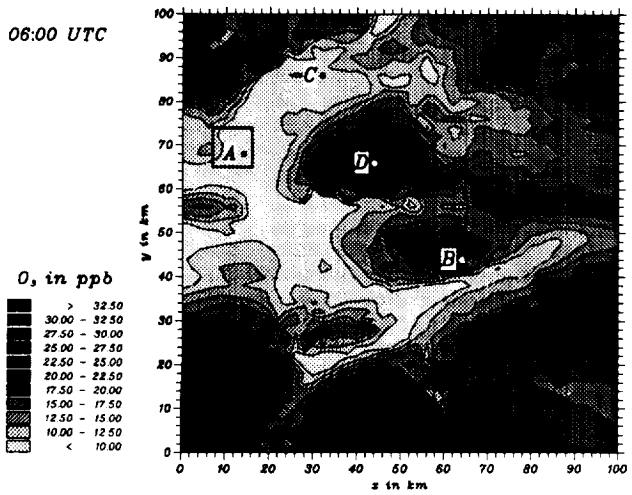

Figure 5: Simulated O_3 –distribution 18 m above ground (day 2, 6:00 UTC).

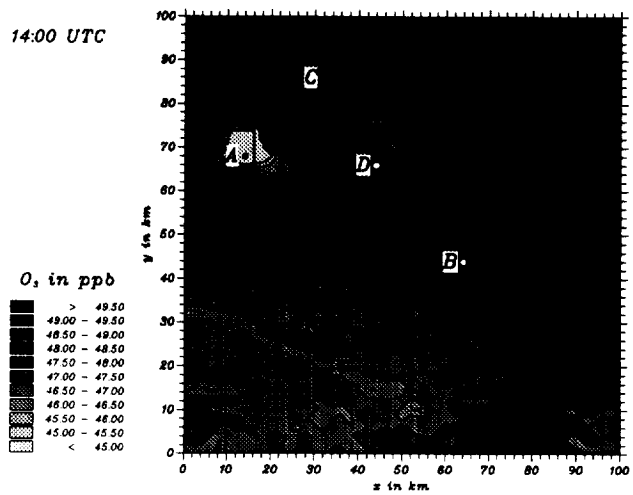

Figure 6: Simulated O_3 –distribution 18 m above ground (day 2, 14:00 UTC).

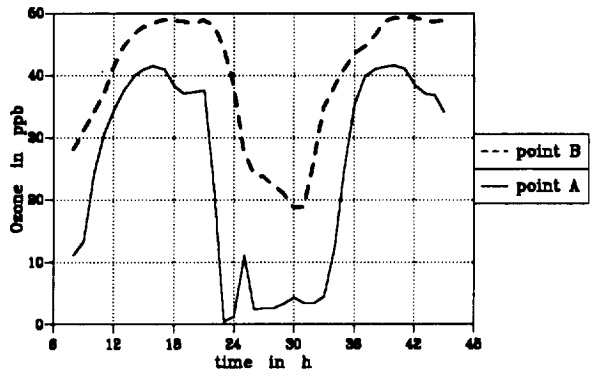

Figure 7. : Simulated diurnal cycles of the ozone concentration 18 m above ground at points A and B.

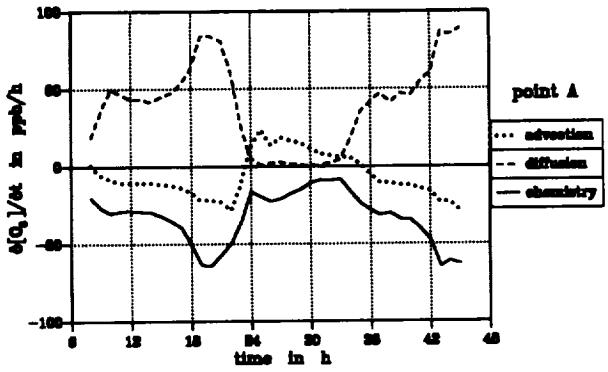

Figure 8. : Contributions of the different processes to the hourly variation of the ozone concentration 18 m above ground at point A.

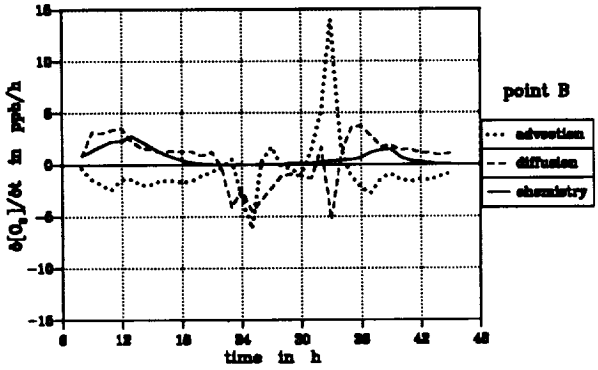

Figure 9. : Contributions of the different processes to the hourly variation of the ozone concentration 18 m above ground at point B.

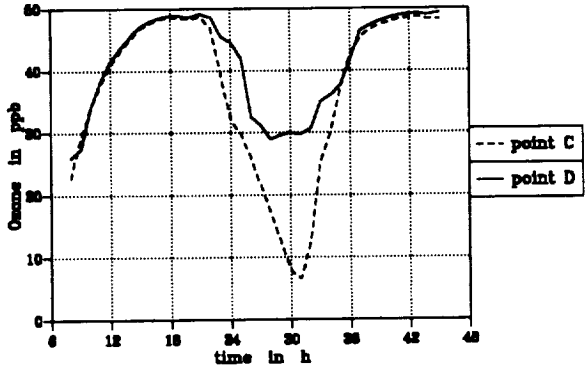

Figure 10. : Simulated diurnal cycles of the ozone concentration 18 m above ground at points C and D.

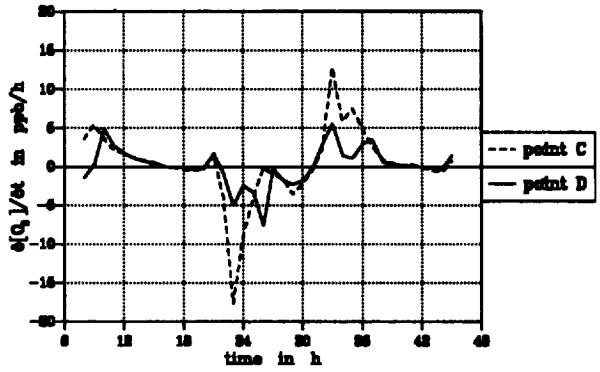

Figure 11. : Contributions of the turbulent diffusion including dry deposition to the hourly variation of the ozone concentration at the surface at points C and D.

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