Modelling Tropospheric Ozone Formation in Hungary using an Adaptive Gridding Method

A contribution to subproject TOR-2

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Summary

Previous EUROTRAC investigations have shown that some of the highest regional ozone concentrations in Europe can be observed in Central Europe, including Hungary. Computational models are important tools in the management of photochemical smog episodes because they can be used for testing the effect of various emission control strategies. High spatial resolution of such models is very important to reduce the impact of numerical errors on predictions. Within a UK-Hungarian co-operation project a regional air quality model has been developed that describes the transport and chemical transformation of photochemical oxidants across Central Europe using an adaptive gridding method to achieve high resolution. The basic coarse grid covers a wider Central European region and a nested finer resolution grid covers Hungary. Further refinement of the unstructured triangular grid is invoked during the simulation at intermediate time-steps using spatial error estimators based on the comparison of high and low order numerical solutions of the atmospheric diffusion equation. Using this method, grid resolutions of the order of 20 km can be achieved in a computationally effective way within a domain of 1540 km × 1500 km.

Introduction

Background monitoring stations in Hungary frequently observe high ozone concentrations during hot summer periods. Budapest and Vienna are large cities in this region and emit significant amount of ozone precursors. Until now, no simulation model has been available for Hungary capable of studying regional photo-oxidant pollution with high spatial resolution. Within a UK-Hungarian co-operation project such a computational model was constructed (Hart et al., 1998; Lagzi et al., 2001) that can calculate the concentration of several pollutants from emission statistics and meteorological data.

Objectives

The objective of the project was to construct an air quality simulation code that calculates the photo-oxidant concentrations for any region of Hungary. To obtain good results even at the borders of Hungary, the simulated area must cover a large region of Central Europe. The model is required to reproduce the measured air pollution concentrations from available monitoring stations and to give good spatial resolution within acceptable turnaround times.

P.M. Midgley, M. Reuther (Eds.)
Proceedings from the EUROTRAC-2 Symposium 2002

Activities

The model describes the spread of reactive air pollutants in several vertical layers. The modelled area is a 1540 km × 1500 km region of Central Europe with Hungary in the centre. The model describes the horizontal domain using a Cartesian co-ordinate system through the stereographic polar projection of a curved surface onto a plane. The dispersion of species in the horizontal domain are described by the atmospheric transport-reaction equation in two space dimensions:

$$\frac{\partial c_s}{\partial t} = -\frac{\partial (uc_s)}{\partial x} - \frac{\partial (vc_s)}{\partial y} + \frac{\partial}{\partial x}(K_x \frac{\partial c_s}{\partial x}) + \frac{\partial}{\partial y}(K_y \frac{\partial c_s}{\partial y}) + R_s(c_1, c_2, ..., c_n) + E_s - (k_{1s} + k_{2s})c_s,$$

where c_s is the concentration of the s'th compound, u, w are horizontal wind velocities, K_x and K_y are eddy diffusivity coefficients and k_{1s} and k_{2s} are dry and wet deposition velocities respectively. E_s describes the distribution of emission sources for the s'th compound and R_s is the chemical reaction term, which may contain non-linear terms in c_s. For n chemical species an n dimensional set of partial differential equations is formed describing the rates of change of species concentration over time and space, where each is coupled through the non-linear chemical reaction terms. The four vertical layers of the model are the surface layer (extending to 50m), the mixing layer, the reservoir layer and the free troposphere layer. At night the mixing layer extends to the height determined by the midnight radiosonde data, then it is assumed to rise smoothly to the height determined by the noon radiosonde measurement. The reservoir layer, if it exists, extends from the top of the mixing layer to an altitude of 1000 m. Vertical mixing and deposition are parameterised according to the vertical stratification (Van Loon, 1996). Deposition velocities are assumed to be constant across the whole domain. The eddy diffusivity coefficients for the x and y directions were set to 50 m^2s^{-1} for all species. The local wind speed and direction, relative humidity, temperature, Monin-Obukhov length and cloud coefficient were determined by the meteorological model ALADIN (Horányi et al., 1996) with a time resolution of 6 hours and spatial resolution of 0.1×0.15 degrees for each of the four layers. Wind data were interpolated to obtain data relevant to a given spacial point on the unstructured grid using conservative methods. The emissions of precursor species into the domain were described by the EMEP emissions inventory for 1998 based on a 50km × 50km resolution grid. The emissions data have to be interpolated onto the unstructured mesh following each change to the mesh during refinement. This is achieved using the mass conservative method of overlapping triangles. The EMEP data is therefore split into triangular grid cells and the proportion of each EMEP triangle that overlaps each mesh triangle calculated. In the present simulations the GRS chemical scheme (Azzi and Johnson, 1992) was used, although the model also allows the utilisation of larger reaction schemes. Photolysis rate constants are calculated as described by Derwent and Jenkin (1990) and are expressed as mth order rate constants with units (molecule cm^3) $^{m-1}s^{-1}$. Temperature dependent rate constants are represented by standard Arrhenius expressions.

The basis of the numerical method is the spacial discretisation of the partial differential equations derived from the atmospheric transport-reaction equation on unstructured triangular meshes using the software SPRINT2D. This approach, (known as the 'method of lines'), reduces the set of partial differential equation in three independent variables to a system of ordinary differential equations in one independent variable, time (Berzins and Ware, 1995). The system of ordinary differential equations can then be solved as an initial value problem. Unstructured triangular meshes are commonly used in finite volume/element applications because of their ability to deal with general complex geometries. They have advantages for air quality models in that they are capable of achieving high levels of mesh refinement in regions of high spatial structure where concentration gradients are steep. Examples of such structures in the atmosphere include urban and point source plumes and fronts. A method of lines

approach with the above spatial discretisation scheme results in a system of ordinary differential equations, which is integrated using code SPRINT. The Theta method of SPRINT has been invoked since it is specially designed for the solution of stiff systems with moderate accuracy and controls the local error automatically in time (Berzins et al. 1992). Operator splitting is carried out at the level of the non-linear equations formed from the method of lines by approximating the Jacobian matrix. Full details of the method can be found in Tomlin et al. (1997). The initial unstructured meshes used in SPRINT2D are created from a geometry description using the Geompack mesh generator (Joe and Simpson, 1991). These meshes are then refined and coarsened by the Triad adaptivity module. Low and high order solutions are obtained for each species and the difference between them gives a measure of the spatial error (Tomlin et al. 1997). The algorithm can choose to refine in regions of high error by comparison with a user-defined tolerance for one or the sum of several species. An original triangle is split into four similar triangles by connecting the midpoints of the edges. These may later be coalesced into the parent triangle when coarsening the mesh.

Results

The model was tested for the simulation of a photochemical oxidant episode that took place in Hungary in August 1998. The simulation period was from midnight on the 1st August 1998 to midnight 6th August 1998. Measured and simulated ozone concentrations were compared at the K-puszta monitoring station of the Hungarian Meteorological Service (46°58'N, 19°33'E, 125 m asl), which is located 70 km south-south-east of Budapest. The initial mesh was refined in this area. The initial conditions for the most important species were 20.0 ppb for NO_2, 0.4 ppb for NO, 30.0 ppb O_3 and these were constant throughout the whole domain. Figure 1 shows the initial grid structure and the refined grid after five simulation days.

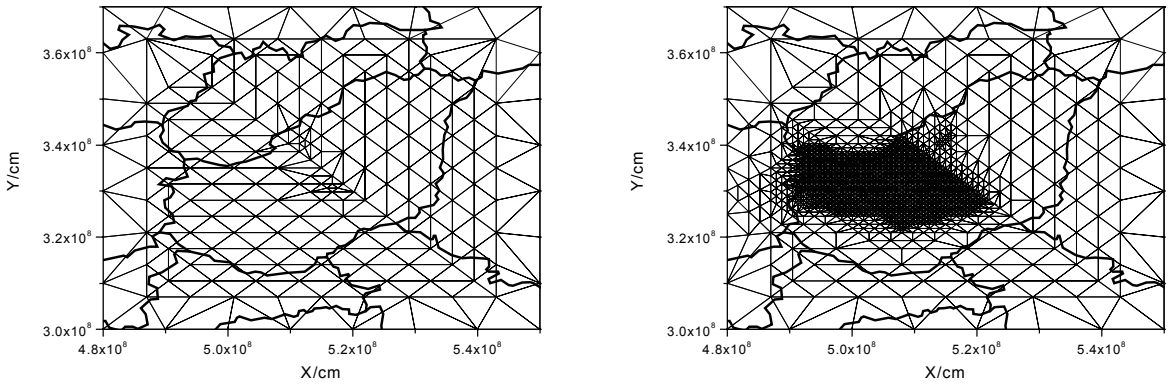

Figure 1. The structure of initial and final triangular grid.

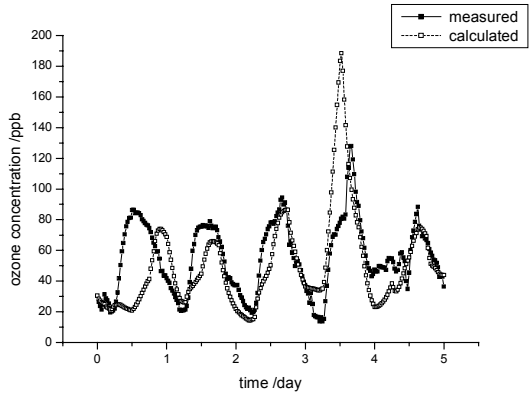

Figure 2: Calculated ozone concentration in ppb after three days simulation of 17.00 on 3 August, 1998 and a comparison of model predictions and measured ozone concentrations at the K-puszta EMEP monitoring station for the simulation period.

Figure 2 shows the simulated and measured ozone concentrations at K-puszta station. The simulated ozone concentrations agree very well with the measured ones.

Conclusions

An adaptive grid model that describes the formation and transformation of photochemical oxidants, based on triangular unstructured grids has been developed for the Central European Region including Hungary. The model automatically refines the grid in regions where higher numerical error is predicted. Using an adaptive method it is therefore possible to achieve grid resolutions of the order of 20 km without excessive computational effort on a modelled area of 1540 km × 1500 km.

Acknowledgements

The authors acknowledge the support of OTKA grant T025875 and UK-Hungarian co-operation grant GB50/98.

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