Unexpected Vertical Profiles over Complex Terrain due to the Incomplete Formulation of Transport Processes in the SAIMM / UAM-V Air Quality Model

A contribution to subproject GLOREAM

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Summary

The air quality model package SAIMM / UAM-V (Systems Applications International Mesoscale Model / Urban Airshed Model with Variable grid) was applied to a domain with complex topography including Switzerland. We simulated the 3-dimensional mixing ratios of pollutants with UAM-V for the summer smog period of July 28-29, 1993. Unexpected features were detected: the values tended to increase with height above the surface and with surface elevation above sea level. The Swiss topography was mirrored in the mixing ratio fields. By using CO as a quasi-inert tracer, it became evident that transport phenomena such as advection and diffusion did not consider expansions or compressions due to pressure and temperature variations. After the conversion of the concentrations to a common reference pressure and temperature before the calculation of transport, these strange topographic features in the mixing ratios vanished completely. The CO mixing ratio was underestimated by 10 to 15 ppb (7 to 10 %) in the lowest layer over the Swiss Plateau due the omission of compression or expansion. For O_3 and NO_2, the differences were 0 to 5 ppb (0 to 10 %) and 0 to 0.2 ppb (0 to 15 %), respectively.

Introduction

The air quality model package SAIMM / UAM-V has been developed by Systems Applications International (SAI). The main modules are the meteorological pre-processor SAI Mesoscale Model (SAIMM) (SAI, 1995), the Urban Airshed Model with variable grid (UAM-V) (SAI, 1999) and a set of utility programs for input preparation and data conversion between SAIMM and UAM-V. Both programs have variable grids and grid nesting capabilities. The pollutants are simulated on the basis of the Carbon Bond Mechanism, CBM-IV. There are two output files: the mixing ratios (in ppm) of the lowest layer averaged over 1 hour, and the instantaneous, 3-dimensional concentrations (in µmol m-3). To obtain mixing ratios for all vertical layers, the concentrations have to be converted to ppm or ppb.

In the past, the model package was used by many institutions. The topography was mostly flat or smooth. For Switzerland, we applied the model to a more complex topography. The model domain had a 5km resolution, 74 x 57 grid cells, and 8 vertical layers up to 3000 m a.g.l. Simulations were performed for July 28-30, 1993. Preliminary tests showed surprising vertical ozone profiles: the mixing ratio of ozone in the upper layers increased with height above ground. To separate chemistry from transport, we focused on CO, a low reactive trace gas. Outside areas of high CO emissions, we observed strange patterns of the CO mixing ratios:

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- for a given location the mixing ratio increased with height above ground.
- for a given layer (i.e. a given altitude above ground), the mixing ratio increased with topographic height and the spatial pattern mirrored the topography.

Objectives

The objectives are

- to describe the unexpected patterns in detail,
- to find the reasons for this behaviour, and
- to report modifications of the model algorithms, which lead to improvements of the simulation results.

Activities

The model was run for a domain including Switzerland. The unexpected 3-dimensional CO patterns were analysed. A closer look at the routines that simulate the transport processes of pollutants showed that the compression and expansion of trace gases due to pressure and temperature variations are not correctly taken into account. The routines were modified and the influence of these changes on the mixing ratio pattern and the mass balance were investigated.

Results

The model run was initialised at 12:00 CET (Central European Time) with 160 ppb CO in layer 1 and 140 ppb in the layers 2 to 8. The mixing ratio was kept at a constant value of 140 ppb at the top of the domain. The results of the simulation at 12:00 and 15:00 for the layers 1 (0-50 m a.g.l.) and 6 (1500-2000 m a.g.l.) are shown in Figure 1. At 12:00 the horizontal distributions are constant and the vertical profile is equal to that of the initial data. After 1 hour of simulation (not shown) the *mixing ratio* increased up to 170 ppb in the upper layers. In addition, the Swiss topography is mirrored in the horizontal CO distribution. With progressing simulation time, the mixing ratio in the upper layers further increased and exceeded 200 ppb. This behaviour contradicts the reality. For instance, the mixing ratios of a homogeneous mixture of inert atmospheric species should not change when the air is moving over a complex topography. Due to the atmospheric pressure and temperature changes, only the density (concentration) vary.

The pattern of the simulated *concentration* field (in μmol m-3) (not shown) differs from the field of the mixing ratio (in ppb) shown in Figure 1. At the initialisation, it is obvious that the concentration decreases with altitude. With progressing time the distribution becomes more homogeneous. In other words, apart from increases due to emissions, the molecular density depends only weakly on the height above ground. In addition, for a given layer, there are only small spatial variations regardless of the altitude above sea level. Hence, for lower air pressure values, the proportion of CO, i.e. the mixing ratio increases with height. This phenomenon and the fact that the topography is mirrored in the pattern of the mixing ratio let us suspect that altitude dependent quantities, in particular air pressure and temperature must have an influence.

Hence, we converted the trace gas concentrations of each grid cell to a common pressure and temperature before the mixing processes due to vertical and horizontal turbulent exchange, advection and entrainment occur. After these modifications the pressure and temperature dependence of the mixing ratios disappeared (Figure 2).

The mass balance on the basis of the fluxes of pollutants through the domain boundaries is reported in the UAM-V diagnostic file. After the software modifications, these fluxes are no

longer balanced. The residual flux can be attributed to an additional CO flow through the lateral boundaries due to the expansion when an air parcel is lifted to higher levels.

Conclusions

Simulations with the SAIMM / UAM-V package were performed for a domain including Switzerland. The topography is rather complex, the altitude ranging from about 170 to 4800 *m a.s.l.* Hence, the pressure and the temperature vary by about 430 hPa and 30 ^{0}C, respectively. We detected that the mixing ratios of the species tend to increase with both height above the surface and surface elevation above sea level. The Swiss topography was mirrored in the mixing ratio fields. By using CO as a quasi-inert tracer, it became evident that transport phenomena such as advection and diffusion do not consider expansions or compressions due to pressure and temperature variations. After the conversion of the concentrations to a common reference pressure and temperature before the transport occurs, the strange topographic features in the mixing ratios vanish.

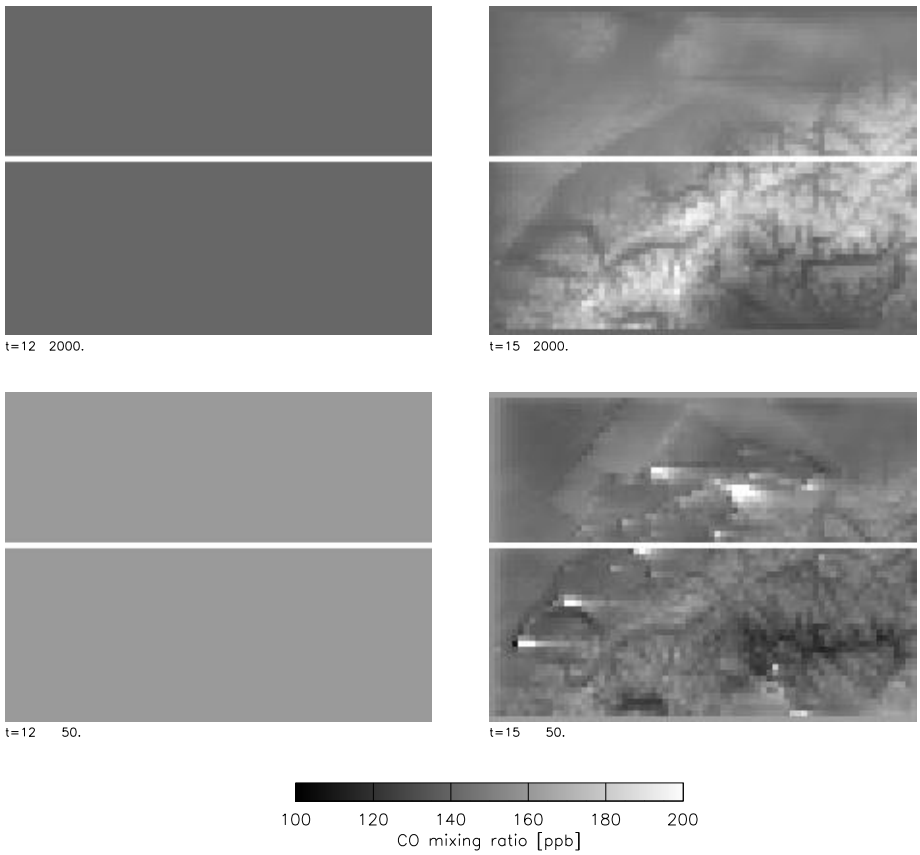

Figure 1. Instantaneous CO mixing ratio (in ppb) of layers 1 (0-50 m a.g.l.) and 6 (1500-2000 m a.g.l.) at 12:00 (left) and 15:00 hours CET (right) on July 28, 1993. The simulation started at 12:00 with a constant mixing ratio of 160 ppb in layer 1 and 140 ppb in the layers 2 to 8. The white horizontal line indicates the location of the vertical profiles (not shown)

In the Swiss Plateau, the mixing ratio of CO in the bottom layer is underestimated by the original UAM-V version by 10 to 15 ppb. For O_3 and NO_2, the differences are 0 to 5 ppb and 0 to 0.2 ppb, respectively. At higher altitudes, the mixing ratios are generally overestimated. Ozone, for instance, is 5 to 10 ppb higher when calculated with the original version.

As far as we know, there are no studies dealing with these unexpected features of UAM-V. Ozone simulations with UAM-V were mostly performed over nearly flat terrains. Because no

significant pressure and temperature changes are involved in the horizontal advection and diffusion processes, the compression or expansion of the air is negligible.

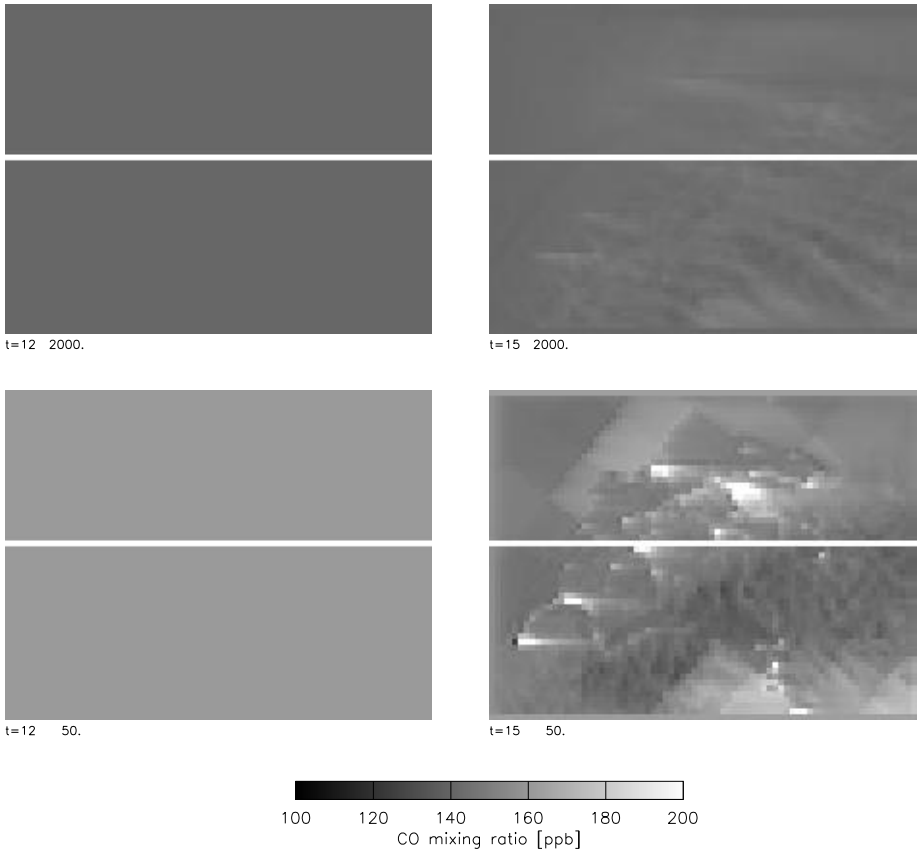

Figure 2. Instantaneous CO mixing ratio (in ppb) of layers 1 and 6 corrected for *p/T* effects. The mixing ratio was calculated taking into account spatial pressure and temperature variations in the advection, diffusion and entrainment scheme (see text). For further information see Figure 1.

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