Uncertainty of Modelled Urban NO_x and CO Emissions for the City of Augsburg evaluated from Mass Budget Simulations with the KAMM/DRAIS Model

A contribution to subproject GLOREAM

K. Nester and H.-J. Panitz

Institut für Meteorologie und Klimaforschung
Forschungszentrum Karlsruhe / Universität Karlsruhe; Postfach 3640; D-76021 Karlsruhe
klaus.nester@imk.fzk.de

Summary

The Augsburg field experiment (EVA) campaigns had been carried out in 1998. The aim of this experiment was the evaluation of the urban emissions of NO_x and CO being calculated with the emission model of IER, University of Stuttgart. Using a mass balance technique, the real emissions have been estimated from advective flux measurements of NO_x and CO, thereby neglecting other processes like deposition, turbulent transports, and chemical transformations. From the results of the KAMM/DRAIS model simulations using the mass budget module, it could be deduced that about 85% of the NO_x emissions and about 95% of the CO emissions can be determined only from these fluxes.

In order to estimate the uncertainty of the modelled urban emissions, three evaluations have been compared, using I) the KAMM/DRAIS model results including the emissions from the IER emission model; II) the KAMM/DRAIS wind field and NO_x and CO concentrations being measured by the IBUF aircraft; and III) only the experimental data. From the results of the evaluation cases I and II it can be concluded that the modelled CO emissions can be about a factor of two lower than the real ones and the modelled NO_x emissions correspond to the real ones within an uncertainty of about 50%. This result cannot be generalized because the uncertainty is probably caused by discontinuously emitting point sources. The difference in the fluxes of the cases II and III indicate the sensitivity of the derived emissions to the flow field.

Introduction

Emission data belong to the most uncertain input data for Chemistry-Transport-Models (CTM) but only a few studies exist dealing with the assessment of the reliability of emission inventories (e.g. Vogel et al. 2000). One emission model has been developed at the IER, University of Stuttgart (Kühlwein and Friedrich 2000), which provides highly resolved emissions for CTMs. In order to perform a systematic evaluation of the IER emission model, experimental campaigns named EVA (Evaluation of Highly Resolved Emission Inventories) have been carried out in March and October 1998 in the area of the city of Augsburg (Germany). One aim was the evaluation of modelled CO and NO_x emission data of the city using a mass balance technique. The basic idea of the experiments was to derive the CO and NO_x emissions of Augsburg solely from measured advective CO and NO_x fluxes (Kalthoff et al. 2002). If only advective fluxes are measured, steady state meteorological and emission conditions are required. Therefore, the mass balance experiments took place between the late morning and the early afternoon hours. Furthermore, it has been assumed that chemical transformation, deposition, and turbulent fluxes through the boundaries could be neglected. Using ground-based and aircraft measuring systems the horizontal advective fluxes have

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been determined along flight tracks surrounding the city (Fig. 1). The vertical advective fluxes of CO and NO_x through the ceiling of the experimental box were calculated by the experimentalists using an average vertical wind that has been estimated from the continuity equation of the air masses, and average CO and NO_x concentrations derived from the aircraft measurements.

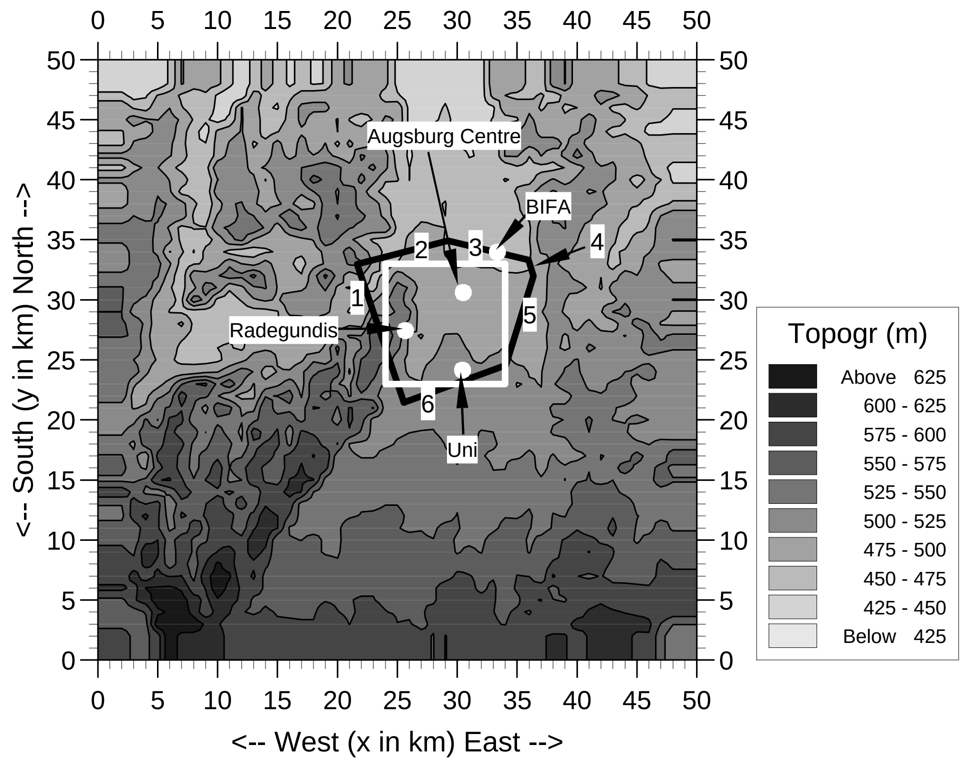

Figure 1. Topography (m ASL) of model area and flight pattern of IBUF aircraft (black pentagon). The white square indicates the horizontal boundaries of the volume for the mass budget calculations.

Objectives of the simulations

Because it could be expected that the assumption of steady state conditions was not ideally fulfilled and in order to estimate the importance of those processes which have not been measured, CTM simulations have been carried out with the model system KAMM/DRAIS in order to estimate the influence of these effects. Furthermore, the uncertainties of the CO and NO_x emissions that were input data for the CTM are assessed. For this purpose modelled horizontal advective fluxes along the flight tracks have been analysed in the same manner as it has been done by the experimentalists.

Performance of the simulations with the model system KAMM/DRAIS

The mesoscale CTM KAMM/DRAIS possesses a mass budget module that calculates the individual contributions of emissions, advective and turbulent fluxes, deposition and chemical transformation in predefined volumes for each species being considered (Panitz et al. 1997).

For the simulations a model area of 50 $*$ 50 km^2 has been chosen enclosing the city of Augsburg (Fig. 1). The horizontal resolution is 1 $*$ 1 km^2. The model domain extends vertically up to 4 km above sea level (ASL) and is divided into 35 vertical levels with a resolution of about 12 m near the ground and 200 m at the top. The emission data have been provided by IER, University of Stuttgart. The simulations are performed for October 21st and October 22nd, separately.

Results and conclusions

During both experimental time periods on October 21st (11:00 UTC –13:00 UTC) and October 22nd (10:00 UTC and 14:00 UTC) south-westerly winds prevailed. The wind speed increased from about 2-3 m/s near the ground to about 8-10 m/s at the top of the PBL. The model KAMM could reproduce the wind field within an uncertainty of about 10%. From the measured vertical profiles of the potential temperature it can be deduced that the maximum height of the boundary layer (mixing layer) was between 400 m and 600 m above ground, which is comparable with the model results. Several simulations have been carried out in order to get an acceptable agreement (less than 5%) of the NO_x and CO concentrations at the measuring stations and along the flight tracks upwind of the city.

Mass budgets of CO and NO_x have been calculated in an integration volume whose horizontal size was 10km∗10km (white square in Fig. 1). The heights of 1050 m ASL (about 550 m above ground) and 1350 m ASL have been chosen as top of the integration volume for

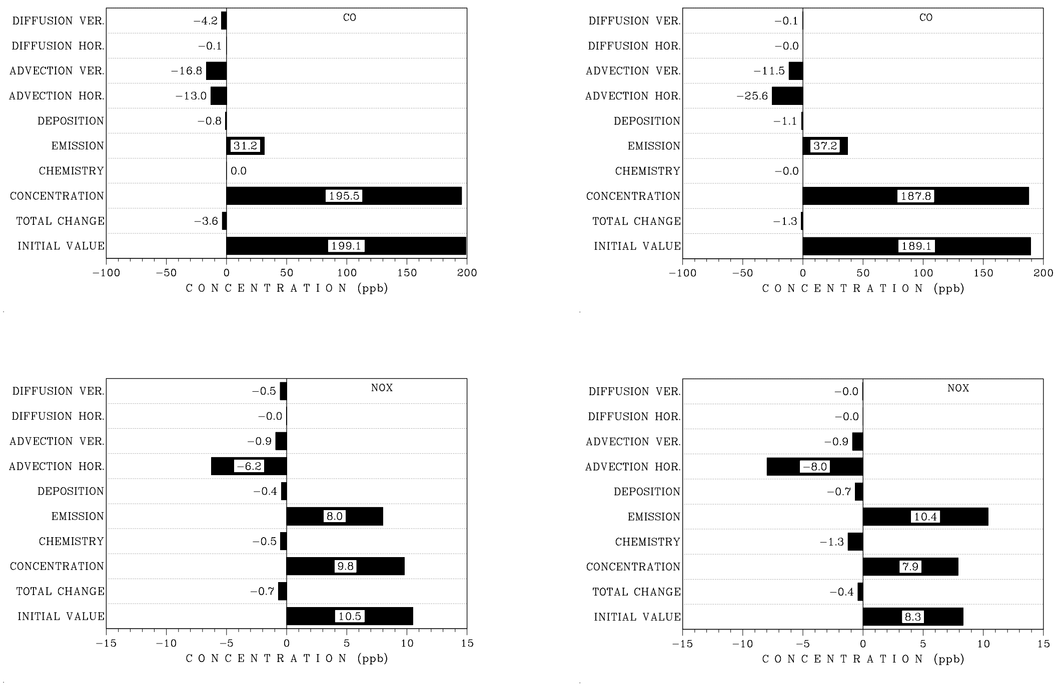

Figure 2: Mass budget components for October 21st (left) and October 22nd (right)

October 21st and 22nd, respectively. The mass of a species is defined as the spatial integral of the concentration over a defined volume. In the KAMM/DRAIS model this mass has been divided by the size of the volume. This value defines a volume-averaged concentration in terms of mixing ratio. The mass budget components are treated in the same manner. They are shown in Figure 2 for October, 21st, and October, 22nd. On both days about 85% of the NO_x emissions can be explained by the advective NO_x fluxes. For CO this value increases to about 95%. But the results also clarify, that a reliable determination of the vertical advection is essential, especially for the estimation of the CO emissions from advective flux measurements.

Because most of the emissions of the city can be explained by the advective fluxes through the lateral and vertical boundaries of a volume around the city, a further analysis applying the mass balance concept is justified. Using different databases, the fluxes through the vertical planes defined by the six flight legs (Fig. 1) and the top of the corresponding volume have been calculated for both days. Three different cases have been considered:

I. KAMM/DRAIS: only the results of the KAMM/DRAIS simulations have been used;
II. KAMM/IBUF: fluxes are calculated using the flow conditions that have been modelled with KAMM and the concentrations measured by the aircraft;
III. IBUF: wind and concentrations measured by the aircraft have been used.

The results of these evaluations are given in Figure 3, where negative net fluxes correspond to the emissions. Summarising the results of the evaluation cases I and II, it can be concluded, that the modelled CO emissions are about a factor of two lower than the real ones, and that the modelled NO_x emissions correspond to the real ones within an uncertainty of about 50%. The underestimation of the CO concentrations is probably caused by the emissions of special point sources. The real emissions from these sources are discontinuous and their temporal description by the emission model cannot be realistic, because only annual averages of the emissions are available. Thus, it has to be concluded that the conditions might be different on other days and that the results being described in this paper are restricted to the two days, which have been analysed. They cannot be generalized. They only indicate that uncertainties in the emission inventory as described above may occur. The differences between the cases II and III vary considerably from one day to the other. This result indicates how sensitive the emission estimation by advective fluxes depends on the flow field.

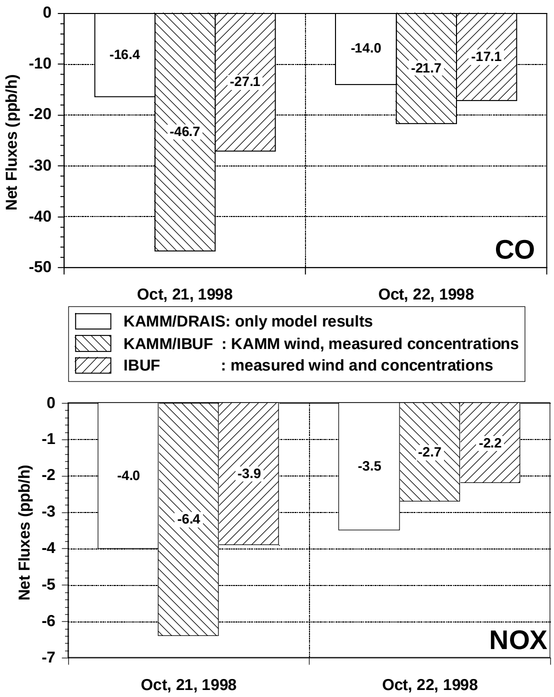

Figure 3. Comparison of the net CO and NO_x advective fluxes of the three cases for October 21^{st} and October 22^{nd}.

Acknowledgement

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