MODEL BASED SOURCE ESTIMATION OF ROADSIDE CONCENTRATION OF NO_2 AT STUTTGART, GERMANY

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ABSTRACT

Monitoring results at heavy traffic sites show that the present NO_2 ambient air concentrations are clearly higher than the annual limit value for NO_2 air quality of 40 µg/m³ coming into effect in 2010 even though a distinct decline of NO_x concentration has been observed at heavy urban traffic sites over the last years. This is attributed to the steep abatement of NO concentrations, whereas the NO_2 concentration declines far slower or even stays unchanged. A box model has been designed to analyse the behaviour of NO_2 in a street canyon without complex three-dimensional dynamic chemistry simulations.

Simulations with a box model with comprehensive chemistry show the fractional contribution of NO_2 to total NO_2 at Stuttgart for a heavily trafficked street location.

Keywords: *NO_2-increase,roadside measurements, chemical box modeling.*

1. INTRODUCTION

Monitoring results at heavy traffic sites show that the present NO_2 ambient air concentrations are clearly higher than the annual limit value for NO_2 air quality of 40 µg/m³ coming into effect in 2010 even though a distinct decline of NO_x concentration has been observed at heavy urban traffic sites over the last years. This is attributed to the steep abatement of NO concentrations, whereas the NO_2 concentration declines far slower or even stays unchanged.

At a heavily trafficked street in Stuttgart, Germany a modelling exercise was performed for the year 2005 and part of 2006 with an observationally constrained box model where the processes chemistry, traffic emission and advection are considered. The model simulates the hourly concentrations at the measuring station Stuttgart-Straße with an annual mean NO_2-concentration of 73 µg/m³. Hourly concentrations measured at Stuttgart Bad-Cannstatt provide the urban background level of NO_2, NO and ozone. A detailed emission calculation to assess not only daily NO_x emission strength, but also the NO_2/NO_x-ratio of traffic emission provides the essential details (Lambrecht 2008). In this companion paper results of model calculations for the years 2010, 2015 and 2020 are discussed in depth.

2. DESIGN OF EXPERIMENT

Transport and transformation of reactive species in the microscale environment of a city were calculated with a box model. The box model incorporates the description of:

- Wind driven advection along one direction with diurnal wind speed
- Emissions of NO_x, VOC, SO_2 and CO
- Chemical reactions between species in the gasphase
- Solar radiation

The gasphase chemistry is described by 161 (140 thermal and 21 photolytic) reactions considering 56 species as given in the atmospheric reaction system RADM2 [5]. Heterogeneous, aqueous and aerosol chemistry as well as deposition and turbulent mixing have not been considered. The time scale, at which these effects would contribute distinctively to the results is larger compared to the time scale in which gasphase reactions and transport through the street canyon take place. This argument might not hold for the effects of turbulent mixing,

however, inclusion of turbulent effects entails knowledge on threedimensional diurnal variations of turbulent mixing parameters in street canyons as well as the addition of one or more upper mixing layers with a known concentration gradient at the upper level. Although this would add more details, it will also add additional uncertainties, as there is no validated dataset available, which applies to the model setup selected in this study.

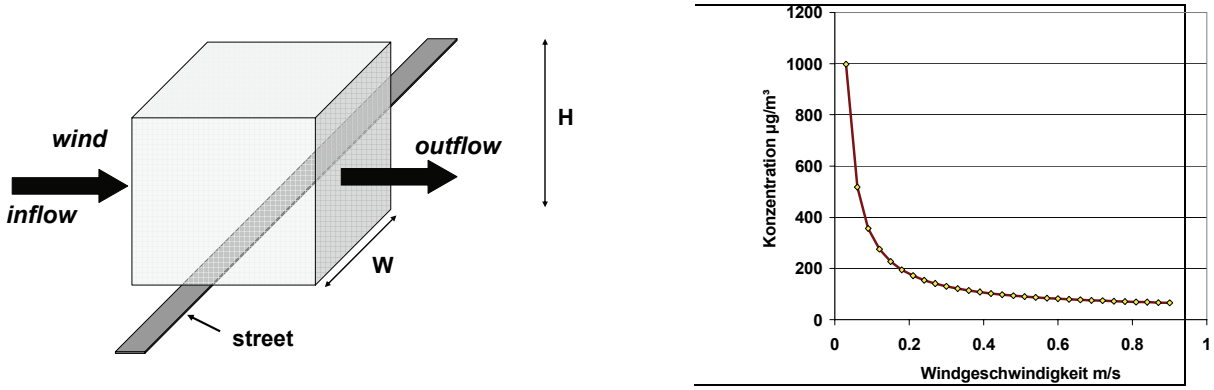

Figure 1: Left: Boxmodel with inflow and outflow. Right: Concentration vs. wind speed for a boxmodel with a passive species

The model consists of one box with a height of 20m respectively. The length along the wind direction is 20m and the length along the street direction is implicitly given by the length of the emission length. (***Figure 1*** left)

The system of differential equation resulting from the description of chemistry is solved with an implicit-explicit solution algorithm (Verwer, 1996) with a variable time step ranging from fractions of a second to minutes. The photolysis frequency is modelled according to observed incident radiation.

A calibration procedure for daily NO_x mean for the year 2005 concentration has been set-up to adapt the box model to the complex street properties and to reflect the influence of wind from different directions. After the calibration runs modelled daily mean NO_x at the street level must reflect the daily mean concentration observed at the traffic station (***Figure 1*** right). In order to follow this observational constraint the wind speed is adapted in several steps by a correction factor for each day. This factor is stored for each day and applied to all scenarios with meteorology of the given year.

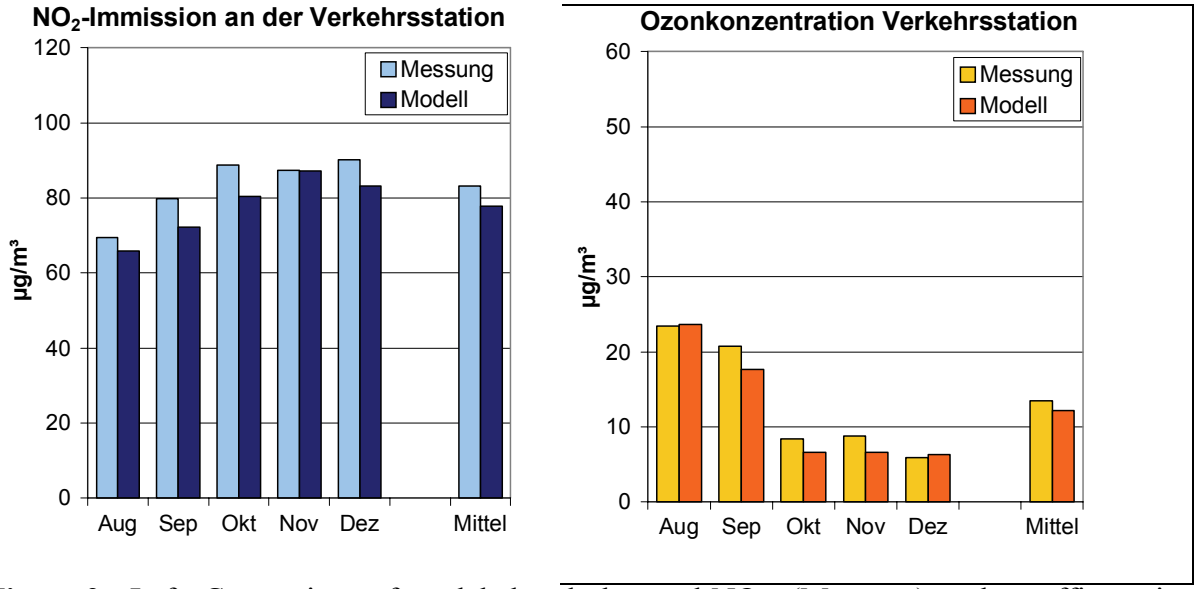

Figure 2: Left: Comparison of modeled and observed NO_2 (Messung) at the traffic station Stuttgart-Straße and Ozone-concentration at the traffic station (right) for five months in 2006

3. CONCLUSIONS

Model results are in good agreement with annual NO_2- and NO-concentration in 2005 and also ozone titration is close to ozone observations at Stuttgart-Straße during a five month period in 2006 (***Figure 2***). Selective deactivation of processes (chemistry, direct emissions of NO_2 from traffic and all traffic emissions) allows estimating the contribution of processes to the NO_2 measured at the road site.

Results will be presented regarding the allocation of NO_2 to three sources, namely:

- Urban background NO_2 on roadside NO_2 concentration.
- NO_2 from traffic emissions: Which part of roadside NO_2 is caused by road traffic and how much of this part could be avoided (e.g. prescribing a maximum NO_2/NO_x-ratio of vehicle NO_x emissions)?
- Which part is allocatable to chemistry, i.e. the titration of NO by ozone?

The results will cover the baseline scenario 2005 as well as a period in 2006.

The computing time for a year with hourly time resolution is manageable even for several scenarios, whereas fully three-dimensional chemistry simulations with a prognostic wind field are prohibitively expensive considering the small domain of analysis and its necessary companion i.e. the small grid size.

4. ACKNOWLEDGEMENT

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5. REFERENCES

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