

# Effects of uncertainties in emission modelling on results of ozone simulation

Burkhard Wickert<sup>1</sup> · Rainer Friedrich<sup>1</sup> · Michael Memmesheimer<sup>2</sup> · Adolf Ebel<sup>2</sup>

<sup>1</sup>Institute of Energy Economics and the Rational Use of Energy, University of Stuttgart, Germany

<sup>2</sup>Institute of Geophysics and Meteorology - EURAD, University of Cologne, Germany

## Introduction:

Anthropogenic emissions contribute to a large extent to the deterioration of air quality in Germany and Europe. In this context emissions of ozone precursor substances are of special interest, since in summer months with suitable meteorological boundary conditions they are responsible for high ozone concentrations. Scientific research can contribute to understand the causal processes of ozone formation and to analyse possibilities for the decrease of ozone production by emission control. However, the uncertainties, which are inherent in model-supported air quality studies, are mostly unknown.

Sensitivity analyses with a coupled emission and chemistry transport model can contribute to examine the effects of uncertainties in the emission model on results of atmospheric modelling.

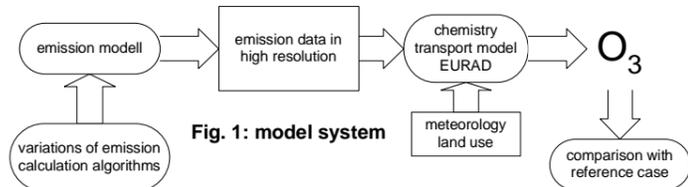


Fig. 1: model system

For this, a complex emission model for Germany was developed to be able to supply the required data sets of highest possible accuracy. Variations of the emission model supply input data for chemistry transport model EURAD, which simulates near-surface ozone concentrations for the sensitivity analyses from emissions, land use, orographical and meteorological data for three domains of Germany in different spatial resolution. Two days of the FLUMOB measurement campaign over Berlin was chosen as modelling period (July 25th - 26th 1994).

## Evaluation parameter:

For the comparison of near-surface layer ozone concentrations from the prevailing sensitivity case with those from the reference case, the 0.95 quantiles of concentration differences are used. The derivation of this parameter is shown in Figure 2: First, for each hour and grid cell the difference between the sensitivity case and the reference case is calculated. Then, these differences are sorted.

The 0.95 quantile is the difference value which is not exceeded by more than 95 % of all differences.

That means: In the case of switching off anthropogenic emissions in Germany an error of 60.01  $\mu\text{g}/\text{m}^3$  has to be accepted, if 95 % of all simulated near-surface ozone concentrations should match the reference case

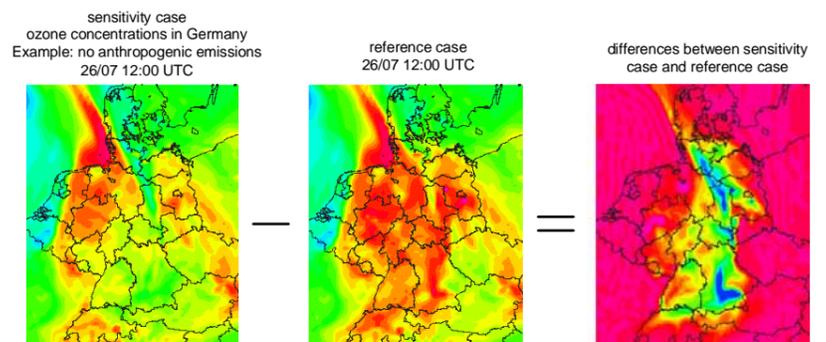
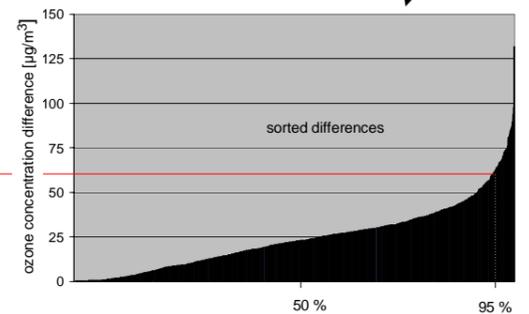


Fig. 2: evaluation parameter

0.95 quantile (here: 60,01  $\mu\text{g}/\text{m}^3$ ): 95 % of all differences do not exceed 60,01  $\mu\text{g}/\text{m}^3$ .



## Reference case:

In the reference case, the emission model was applied without changes. Altogether 38,170 emission sources (30,756 point sources), 270 hourly time curves, 4380 spatial allocation vectors, and 206 VOC profiles were included. The share of biogenic NMVOC emissions calculated by the CTM for the 2-days period was 60 % up to 70 %. In Figure 3 the NO emissions on 25th July, 12:00 UTC, are shown.

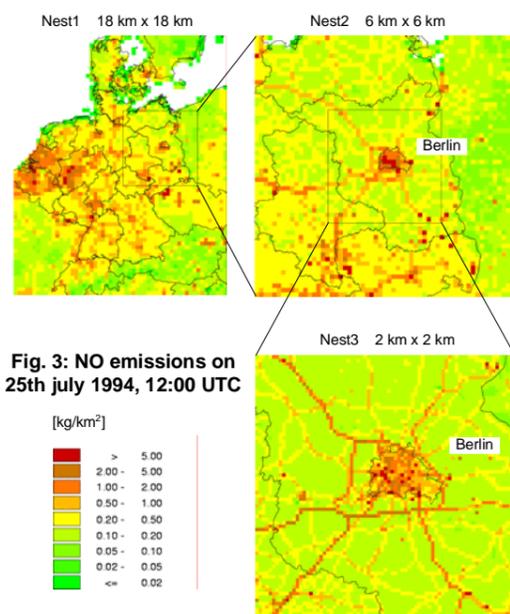


Fig. 3: NO emissions on 25th July 1994, 12:00 UTC

## Sensitivity test cases:

The variations in emission calculation algorithms can be classified according to their effects on the emission model's results:

- variation of emission totals ( $\text{NO}_x$ , NMVOC)
- variation of spatial allocation
- variation of time curves
- variation of VOC splits

### Sensitivity cases:

REF: reference case, no changes  
 OANT: no anthropogenic emissions  
 OBIO: no biogenic emissions  
 BIO[z]: decrease or increase of biogenic NMVOC totals by a factor of z  
 NM[x]N[y]: decrease or increase of anthropogenic NMVOC totals by a factor of x and of  $\text{NO}_x$  totals by a factor of y  
 OLANU: no land use data for allocation of area sources  
 OLIN: OLANU + no road network for allocation of road traffic  
 OPKT: OLIN + no coordinates for allocation of point sources  
 TMINUS: emissions 1 hour earlier  
 TPLUS: emissions 1 hour later  
 TSIMPLE: simple rectangular time curve for hourly emissions  
 NMSIMPLE: only one standardized VOC profile

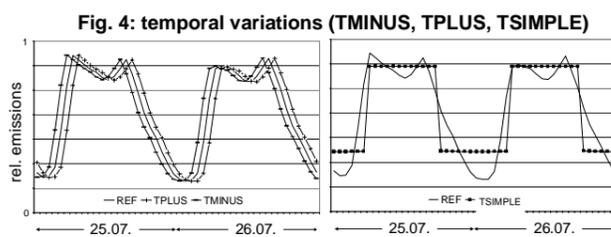


Fig. 4: temporal variations (TMINUS, TPLUS, TSIMPLE)

### Fig. 5: spatial variations (OLANU, OLIN, OPKT)

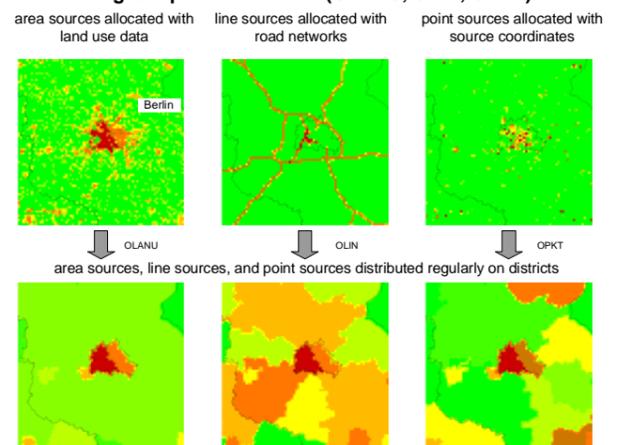
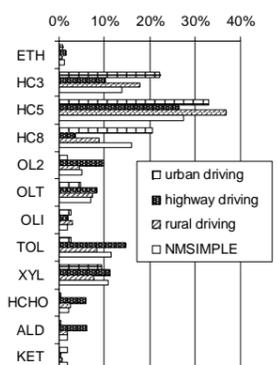


Fig. 6: standardized VOC profile (NMSIMPLE)

Three NMVOC profiles for road traffic are compared with the mean annual NMVOC profile for all emission processes in Germany 1994 (NMSIMPLE). The NMVOC emission classes are arranged according to the RADM2 chemical mechanism which is used for the EURAD CTM ozone simulations.



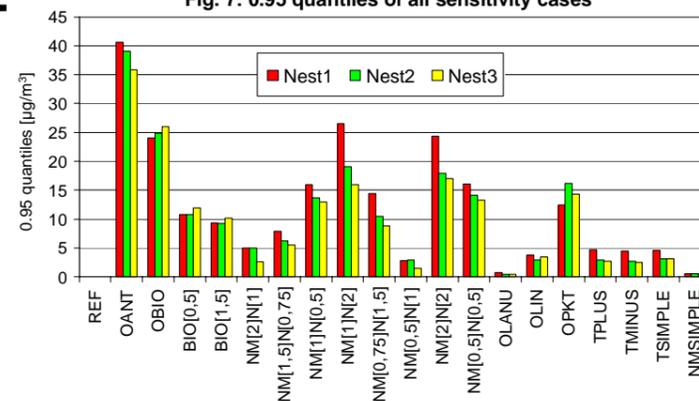
## Results and Conclusions:

In Fig. 7 the effects of variations in emission calculations on the results of atmospheric modelling are shown. Switching off all anthropogenic emissions (OANT) has major influence on near-surface ozone modelling with a 0.95 quantile of 35 - 41  $\mu\text{g}/\text{m}^3$  while the application of one standardized NMVOC profile for all anthropogenic NMVOC emission sources hardly affects the simulation results (NMSIMPLE).

A detailed analysis leads to the following conclusions for this sensitivity study:

- Variations of anthropogenic  $\text{NO}_x$  emissions have more influence on ozone simulation results than anthropogenic NMVOC emissions ( $\text{NO}_x$  limitation, analysis of OANT, NM[x]N[y]).
- Variations of biogenic emissions have more influence than variations of anthropogenic emissions of the same magnitude (analysis of OBIO, BIO[z], NM[2]N[1], NM[0.5]N[1]).

Fig. 7: 0.95 quantiles of all sensitivity cases



- The application of land use data to distribute area source emissions from district level less effect than the inclusion of road networks and point source coordinates (analysis of OLANU, OLIN, OPKT).
- The effects of time curve variations are all in the same order. The application of one rectangular time curve for each pollutant leads to similar 0.95 quantiles as the shift of the time curves one hour earlier or later (analysis of TPLUS, TMINUS, TSIMPLE).
- For ozone simulation with the RADM2 chemical mechanism the use of one annual VOC profile hardly affects the near-surface layer concentrations (analysis of NMSIMPLE).

Contact:

IER / University of Stuttgart  
 Heßbrühlstr. 49a  
 70565 Stuttgart, Germany  
 e-mail: rf@ier.uni-stuttgart.de