QUALITY CONTROL IN DISPERSION MODELING: VALIDATION OF A SCREENING MODEL FOR PM10 AND NO_2

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Abstract: The validation of the screening model IMMIS^{luft} with recent measurement data from the German federal state of North Rhine-Westphalia is described. The aspect of statistically deriving NO_2 values from NOx model results is discussed in the light of increasing NO_2 direct emissions.

Key words: *air quality, screening, modelling, validation, EC Directives, road traffic, NO_2 direct emissions.*

1. INTRODUCTION

European air quality guidelines require gathering information about air quality at locations where the population is affected or possibly affected by high concentrations. High concentrations are often found in densely built up streets with high traffic loads. In order to identify these hot spots and to assess possible measures to improve the situation, screening models are widely applied in current air quality planning. Besides accomplishable data requirements, the main request for such models is to produce reliable results. The screening model IMMIS^{luft} is being widely applied throughout Germany to assess air quality in cities, e. g. for the entire Ruhr area with over 5 million inhabitants. The validation of the model has recently been updated in a study based on data from several years for 15 continuous measurement stations for PM10 and NO_2 and additional 31 diffusive samplers for NO_2 in North Rhine Westphalia. As a screening model's main task is to identify hot spots, the relevant quality criterion is the hit rate. A hit is defined as the situation where the model correctly predicts the compliance with or violation of the respective limit values. The rate is the ratio of hits to the total number of examined situations. In its first part, this paper describes the data sets used for the model validation and shows that the model is adequate for its task together with the limits of its application. In the second part, the paper addresses the issue of deriving reliable NO_2 values based on NO_X.

2. SCREENING MODEL

Studies conducted in the German federal state of North Rhine-Westphalia (NRW) revealed a large number of street sections where limit value exceedances of the pollutants PM10 and NO_2 may occur (Hartmann and Geiger, 2003; Hartmann and Geiger, 2005). The evaluation of the exposure situation for the entire street network of such a large area only by measurements is impossible due to practical and financial limits. One approach to get an overall assessment of the exposure situation is the application of a screening model. Screening models are computer models that give an estimate of air quality parameters (e. g. daily or annual mean values) for various substances. The calculation of these parameters is mainly based on the traffic load and the building situation along the streets. These data are relatively easy to acquire.

The screening in North Rhine-Westphalia was carried out with IMMIS^{luft} (IVU Umwelt, 2005a). This screening model has been implemented to calculate traffic-induced air pollution in urban streets. It is based on the CPB model (Yamartino and Wiegand, 1986) for street canyons and a box model for open building structures.

3. VALIDATION

In an earlier study, it was shown that IMMIS^{luft} succeeded well in identifying exceedances of and compliance with the limit values for benzene, soot and NO_2 valid at that time (Diegmann and Mahlau, 1999). These findings have been confirmed through recent investigations for PM10 and NO_2 (Hartmann and Diegmann, 2006). Deviations of the model results from the measurements are within the data-quality objectives defined in Directive 1999/30/EC Annex VIII (EC, 1996), and the model shows high prediction accuracy for the occurrence of limit value violations. The input data and the results of the latter study are summarised in the following sections.

Input data

The study includes data of 15 traffic-related measurement stations from the North Rhine-Westphalian observational network. Measurements were generally available for the years 2003 to 2005. Due to incompleteness, 33 datasets out of 45 were employed for the annual mean value of NO_2 and 35 datasets for the annual mean value and the daily limit value of PM10 (Geiger and Romberg, 2004; Geiger 2005). To calculate the emissions and subsequently the air pollutant concentrations within the street canyons, traffic data including the fleet composition are needed. Hence, only measurement locations with sufficient traffic data were included in the study. The traffic data were mainly based on the information collected in traffic censuses in the context of clean air management and action planning. In cases where no measured traffic data was available, the state-wide emission inventory of road traffic was used.

Results

Figure 1 shows a scatter plot comparing measured and modelled NO_2 and PM10 concentrations. Values above the diagonal indicate an overprediction, values below the diagonal an underprediction of the measurements. Additionally, the NO_2 and PM10 annual limit values of 40 µgm^{-3} and the zone meeting the data-quality objectives for NO_2 as defined in Directive 1999/30/EC Annex VIII is marked. The required accuracy for model calculations is 30 % for NO_2 annual mean values and 50 % for PM10 annual mean values. Following these specifications, IMMIS^{luft} provides good results both for PM10 and for NO_2. The PM10 model results even outperform the requirements, fulfilling for the larger part the 30 %-criterion. The few pairs of variates outside the data-quality objective zone can be attributed to three measurement stations and will be discussed below. A comparison of the PM10 and NO_2 values in Figure 1 shows that for the case discussed here, the model performs better with PM10 than with NO_2 which on average is slightly underpredicted. One reason for this is that even in street canyons the PM10 concentrations are influenced to a large degree by the larger scale or background PM10 concentrations. Hence, PM10 shows less sensitivity than NO_2 concerning the uncertainties in predicting the traffic-induced part of the pollutant load. Another reason may be found in the underestimation of direct NO_2 exhaust emissions (IVU Umwelt, 2005b) which are not included in the statistical relationship used to derive NO_2 concentrations from NO_X. This issue is addressed in the second part of this paper.

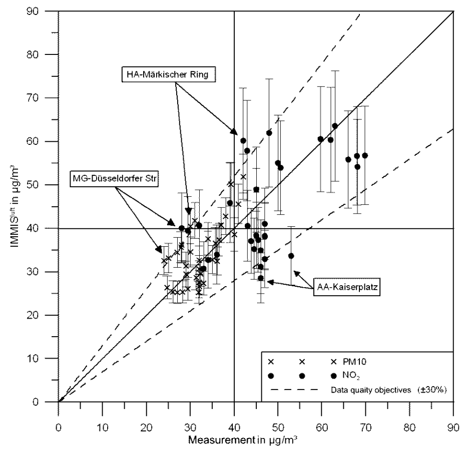

Figure 1. Scatter plot comparing measured (x-axis) and modelled (y-axis) annual mean values for PM10 and NO_2 (2003-2005). Dashed line indicates data-quality objectives for NO_2 as defined in Directive 1999/30/EC, Annex VIII. Annual limit value of 40 µgm^{-3} for PM10 and NO_2 is marked. Model results are displayed with an error bar of 10 % for PM10 and 20 % for NO_2. Outliers are indicated and discussed in the text.

To evaluate the model's ability to predict exceedances of and compliance with the given limit values, a hit rate is introduced. A hit is counted either if a measured limit value exceedance is predicted correctly with IMMIS^{luft} or if the measured and the modelled value comply with the limit value. The hit rate is the ratio of hits to the total number of examined situations. Table 1 summarises the hit rates for NO_2 and PM10 for the annual limit value of 40 µgm^{-3} considering an error tolerance of 20 % for NO_2 and 10 % for PM10 as shown in Figure 1. Additionally, Table 1 gives the hit rates for the PM10 annual mean of 32 µgm^{-3} which indicates that the allowed number of daily means above 50 µgm^{-3} is most probably exceeded (Brandt et al., 2006). The total hit rate for the three investigated years amounts to 79 % for the NO_2 and to 86 % for the PM10 annual limit value. The hit rate for the PM10 annual mean value of 32 µgm^{-3} corresponding to the PM10 daily limit value evaluates to 71 %.

Table 1. Hit rates for the investigated years and the annual limit values of 40 µgm^{-3} for NO_2 and PM10 and for the annual mean value of 32 µgm^{-3} for PM10 indicating the possible exceedance of the allowed number of daily means above 50 µgm^{-3}. Error tolerances of 20 % for NO_2 and 10 % for PM10 are considered (Hartmann and Diegmann, 2006).

Year	NO_2 (40 µgm^{-3})	PM10 (40 µgm^{-3})	PM10 (32 µgm^{-3})
2003	78 %	89 %	67 %
2004	77 %	86 %	64 %
2005	82 %	83 %	83 %
2003-2005	79 %	86 %	71 %

The presented comparison demonstrates the ability of IMMIS^{luft} to predict exceedances of and the compliance with the limit values for PM10 and NO_2 in streets. Deviations are registered for only three measurement stations in this study. It has been shown that these stations are not suitable for model verification as they do not comply with the model assumptions (Hartmann, U. and V. Diegmann, 2006). They were kept in this paper to demonstrate the range of applications for IMMIS^{luft} and to show that measurement stations may not catch the highest concentration in the street canyon due to inadequate placement. Neglecting the three stations leads to hit rates of 90 % for both substances.

Two of the three outliers will be discussed here in more detail. The situation at the third station HA-Märkischer Ring closely resembles the situation at MG-Düsseldorfer Str. It has to be kept in mind that IMMIS^{luft} has a clearly defined area of application. It calculates the emissions from road traffic and the corresponding contribution to the pollutant concentration in street canyons with the scope of detecting street sections of likely limit value exceedances. Prerequisites of IMMIS^{luft} calculations are a homogeneous distribution of the buildings and homogeneous emission conditions. At the measurement station AA-Kaiserplatz in Aachen (Fig. 2), IMMIS^{luft} underpredicts the measured NO_2 values more than 30 %. The station is located near a large crossroad. The measurements are affected by emissions of the crossing roads which are not considered in the model calculations. This leads to the observed underestimation of the measured values. Additionally, the chosen street section does not comply with the IMMIS^{luft} specification that the length of a street section should be at least twice the distance between the opposite buildings on both sides of the street.

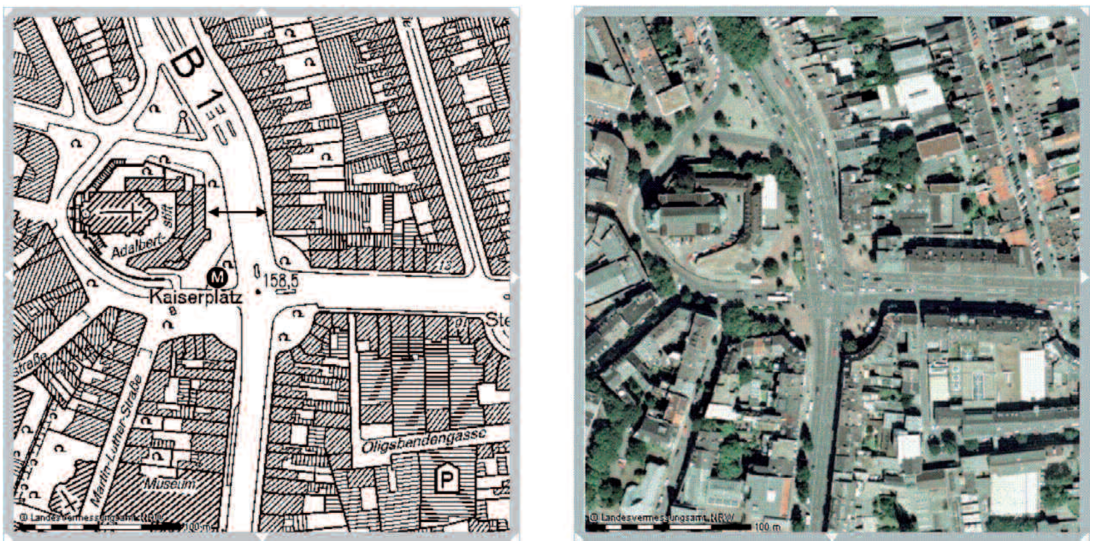

Figure 2. Site map and aerial view of measurement station Aachen Kaiserplatz (station location marked with M, IMMIS^{luft}-cross section marked with an arrow). Topographical map and aerial view provided by Landesvermessungsamt NRW.

The opposite is found at the measurement station MG-Düsseldorfer Str. in Mönchengladbach (Fig. 3). Düsseldorfer Straße is in parts a typical street canyon with closely lined-up buildings on both sides. The measurement station is located on a grass strip with a lower building density and better ventilation. Consequently, IMMIS^{luft} overpredicts the measurements. If the station was located in the canyon-type part of the street, measurements might be higher and thus, much closer to the model results.

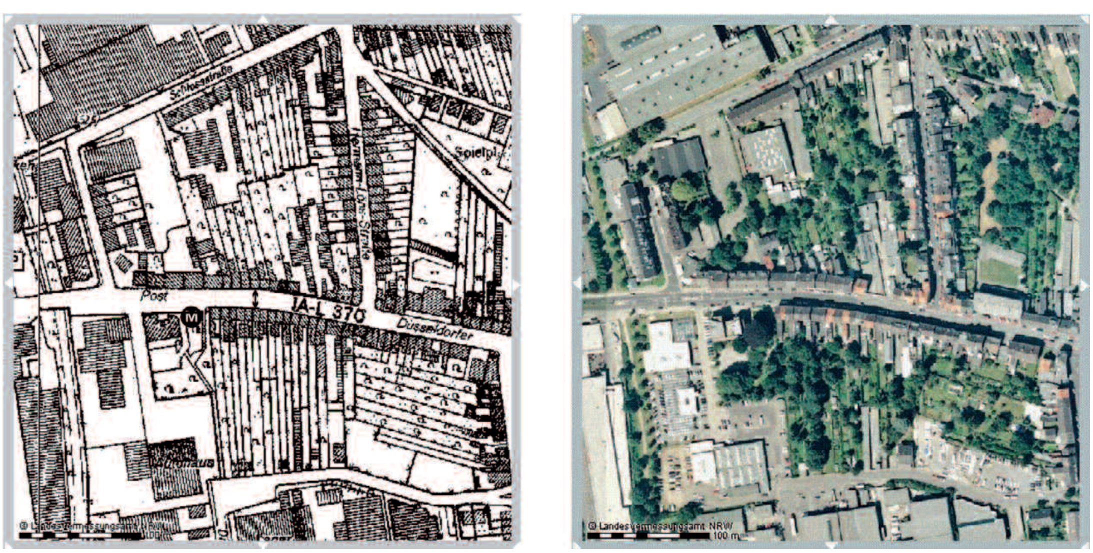

Figure 3. Site map and aerial view of measurement station Mönchengladbach Düsseldorfer Straße (station location marked with M, IMMIS^{luft}-cross section marked with an arrow). Topographical map and aerial view provided by Landesvermessungsamt NRW.

4. DERIVING NO_2 FROM NO_X

Validating the NO_2 annual mean values for the years 2003 to 2005 in the previous section showed a slight underestimation of the measured data. These findings were confirmed when comparing model results with data measured in North Rhine-Westphalia in 2006 at 31 diffusive samplers for NO_2 (Figure 4, left). The model shows a good overall performance with respect to the data-quality objectives for NO_2 as defined in Directive 1999/30/EC, Annex VIII. The hit rate evaluates to 77 % without and 100 % with the error tolerance of 20 % as described in the previous section. Nevertheless, the mean value of all observations (52.7 μgm^{-3}) is underpredicted with $IMMIS^{luft}$ by 10 % (47.5 μgm^{-3}).

NO_2 is a photochemically active substance which is related to NO and O_3 via processes mainly depending on temperature and solar radiation. While the equilibrium reaction itself is well known, the necessary input data for a detailed calculation are not. Emission data are usually available for NOx, which is the sum of NO_2 and NO, and detailed O_3 values are rarely available. So far, models which do not account explicitly for photochemical processes generally derive NO_2 concentrations by calculating the NOx annual mean values and estimating the NO_2 values from NOx using statistical approaches (e. g. Romberg et al., 1996; IVU Umwelt, 2002). Such approaches are based on the evaluation of measured NO_2/NO-relationships. Exemplarily, Figure 4, right, shows NO_2 versus NOx annual mean values from 1956 to 1998 for urban measurement sites with the corresponding regression function and 95 % prediction interval. Thus, a NOx annual mean value of e. g. 200 μgm^{-3} results in an NO_2 annual mean value of 61.5 μgm^{-3} ± 7.5 μgm^{-3} at a confidence level of 95 %.

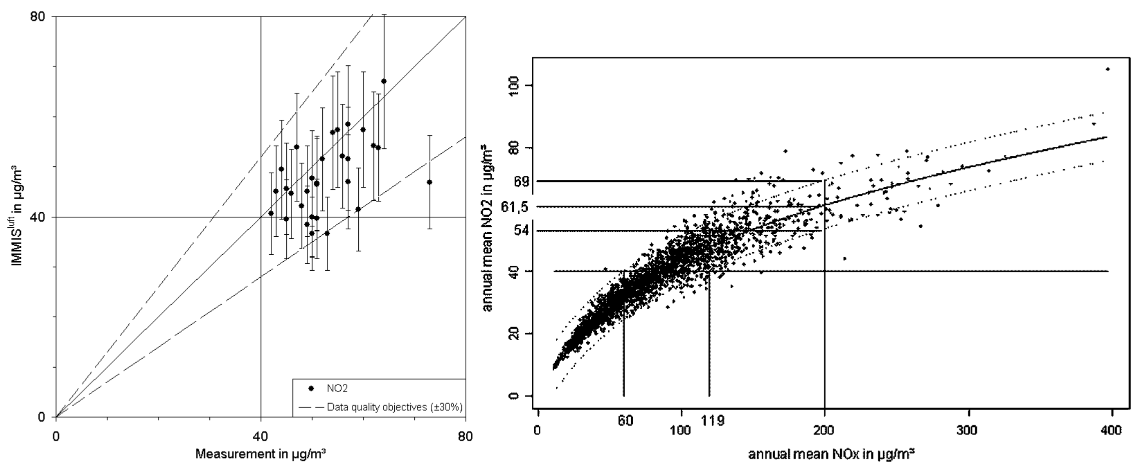

Figure 4. Left: Scatter plot comparing measured (x-axis) and modelled (y-axis) annual mean values for NO_2 (2006). Dashed line indicates data-quality objectives for NO_2 as defined in Directive 1999/30/EC, Annex VIII. Annual limit value of 40 μgm^{-3} for NO_2 is marked. Model results are displayed with an error bar of 20 %. Right: NO_2 versus NOx annual mean values 1956 – 1998 for urban measurement sites (IVU Umwelt, 2002). Black line represents regression function deriving NO_2 annual mean value from NO_X. Dashed lines indicate 95 % prediction interval.

In recent years, it has been observed that while NO_X emissions were reduced considerably, NO_2 concentrations decreased only slightly or even increased. Inspection of the available data revealed that new exhaust emissions reduction technologies, namely the emission standards Euro 3 and higher for diesel passenger cars, result in NO_X emissions containing several times as much NO_2 as petrol engine cars and diesel engine cars with older emission standards (Görgen and Lambrecht, 2008). These increased NO_2 direct emissions are so far not considered with statistical approaches which may lead to underestimated NO_2 results. Figure 5 shows annual mean values of NO_2 versus NO_X for the years 2000 – 2002 (left) and 2003 – 2006 (right) from stations in Germany where NO_2 exceeded the annual limit value of 40 μgm^{-3}, compared to the Romberg-Lohmeyer function (Romberg et al., 1996) and assumed error margins of 10 % and 20 %. While the earlier values are reasonably well described, the latter values are generally underestimated with the Romberg-Lohmeyer approach.

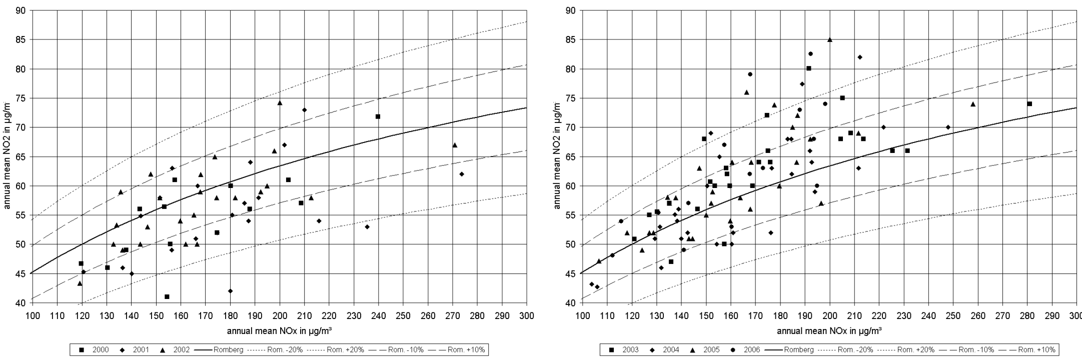

Figure 5. NO_2 versus NO_X annual mean values for stations in Germany (exceedance of 40 μgm^{-3} only). Black line represents Romberg-Lohmeyer function. Dashed lines indicate 10 %, dotted lines 20 % error margin. Left: Data 2000 – 2002. Right: Data 2003 – 2006.

5. CONCLUSIONS

The screening model IMMIS^{luft} for calculating concentrations of air pollutants in inner-city roads is very well suited to identify hot spots where exceedances of limit values according to EC Directives are to be expected. This was validated in a study comparing modelled and measured values for three years at 15 measurement sites in the German federal state of North Rhine-Westphalia.

Statistical approaches to derive NO_2 from NOx and their basic assumptions were discussed. The importance of giving a prediction interval together with the results of statistical approaches was shown. Recent measurements illustrated that the increasing level of NO_2 direct emissions necessitates the improvement of the existing approaches. A first step would be to update and validate the statistical functions with data from recent years. Further improvement will arise from quantifying and parameterizing the influence of NO_2 direct emissions and implementing and considering their effects in micro-scale models.

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