H14-104

IMPROVEMENT OF A SIMPLE DISPERSION MODEL FOR CALCULATIONS OF URBAN BACKGROUND CONCENTRATIONS

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Abstract:A simple dispersion model for calculation of urban background concentrations, similar to the one used for Copenhagen in Denmark, has been developed for Sweden (SWE-BUM). The model calculates concentration on a 1 x 1 km^2 grid and is, within the national Air Quality system SIMAIR, operationally applied for 150 cities in Sweden. In this study, a simple stability parameterisation is implemented in the calculation of the vertical dispersion parameter, since stability plays an important role for Swedish conditions with cold climate and small towns. Furthermore, the meteorology is corrected in order to represent urban conditions. The model is evaluated against monitoring data from 13 cities in Sweden. The performance is improved in the new model version; when comparing the calculated NO_2 concentrations with measurements, 95 % of the data points are within ±50 % for the new model version in comparison with 41 % for the original model. However, the improved model still doesn't succeed to fully reproduce the highest daily and hourly peaks of concentrations.

Key words: *Air Quality,urban background model, model evaluation,cold weather conditions, parameterisation of* σ_z*.*

1. INTRODUCTION

The Air Quality in Sweden is strongly influenced by the climate in Northern Europe. The cold winters cause a need for space heating and anti-skid treatment of roads which, in turn, are important emission sources of particles (Omstedt et al., 2011).Furthermore, the cold climate affects the atmospheric stability and thus the dispersion of air pollutants; stable conditions, low wind speeds and inversions, causing high levels of air pollutants, are commonly experienced during winter in Sweden (Johansson et al., 1994).

SIMAIR (Gidhagen et al., 2005; Omstedt et al., 2011) is a national web based Air Quality system that can be used by all Swedish municipalities to assess their air pollution levels and how they compare with the EU Air Quality Directive targets. It is a coupled model system using models on regional, urban and local scales. The intension is also to use SIMAIR for calculations of individual exposure to specific air pollution components in epidemiological studies. The model has recently been applied to estimate annual average PM10 levels in more than 25 000 residential addresses from different part of Sweden, separating PM contributions on three different scales: the regional, the urban and the local traffic contribution. The urban background concentrations contribute to an important part of the total exposure (Gidhagen et al., 2011).

Urban contributions are simulated with a spatial resolution of 1 x 1 km^2, using emission data from the Swedish Database for Emissions to the Environment (SMED; http://www.smed.se). Calculations are made operationally for approximately 150 cities in Sweden, corresponding to 62% of the total Swedish population. The fundamental concept of the simple urban dispersion model is similar to the model developed for Copenhagen in Denmark (Berkowicz, 2000a). In the Danish model,neutral conditions are assumed motivated by the fact that Copenhagen is a rather large city. However, for Swedish conditions with a cooler climate and also with many small towns, the stability plays a more important role for the urban Air Quality. Thus, an important step is to include stability in the model.

In this study, the Swedish urban background dispersion model (SWE-BUM) will be described andimprovements,including the parameterisation of the vertical dispersion parameter, will be presented. Furthermore, the model results (both the original and the improved model version) will be validated against monitoring data from 13 cities, located in different parts of Sweden.

2. METHODOLOGY

2.1 Model description

2.1.1 Original version

Contributions from ground-level emission sources are calculated by a simple trajectory model using an adjoint approach, similar to that developed for Copenhagen in Denmark (Berkowicz, 2000a), while the dispersion of stack emissions are treated in a Gaussian point source model (Omstedt, 1988). In the trajectory model, all emissions are aggregated to the final concentration within an influence area as follows

$$\begin{cases} C = \frac{1}{2\Delta\theta}\int_{-\Delta\theta}^{\Delta\theta}\int_{0}^{x} f(\theta)\,\frac{Q(x,\theta)}{u\sigma_z(x)}\,dxd\theta \\ \qquad f(\theta) = sin\left(\pi\,\frac{\Delta\theta+\theta}{2\Delta\theta}\right) \end{cases} \tag{1}$$

where$C$ is the concentration, u the wind speed, x the distance at a central line upstream the trajectory, Q is the emission intensity per square meter (g s^{-1}m^{-2}) and the angular shift $\Delta\theta$ is calculated by

$$\Delta\theta = \max\left(\frac{0.5}{u};0.25\right) \tag{2}$$

Thus, $\Delta\theta$ varies between 57° (when u is low, 0.5 m s^{-1}) to 14° (when u> 2 m s^{-1}).

The vertical dispersion parameter σ_z is assumed to grow with the distance x, asymptotic from an initial dispersion height, h_0, corresponding to the height of the well-mixed layer (approximately the average height of the buildings), to the mixing height,h_{mix}

$$\sigma_z(x) = h_0 + (h_{mix} - h_0)\left(1 - e^{-\frac{\sigma_W \cdot x}{u(h_{mix} - h_0)}}\right) \tag{3}$$

This formulation slightly diverges from the formulation by Berkowicz(2000a); its advantage is that it gives a smooth variation with distance.

The vertical turbulence parameterσ_w is assumed to be stability and height dependent according to

$$\begin{gathered} z < 0.1 \cdot h_{mix}\sigma_w = \sqrt{1.2{u_*}^2 + 1.54{w_*}^2 \cdot \left(\frac{z}{h_{mix}}\right)^{\frac{2}{3}}} \\ z \geq 0.1 \cdot h_{mix}\sigma_w = \sqrt{1.2{u_*}^2 + 0.33{w_*}^2} \end{gathered} \tag{4}$$

where$u_*$is the friction velocity and w_* it the convective velocity scale. This is a slight modification from Berkowicz(2000a);the formulation is more general based on the formulation used in the Danish OML model (Berkowicz et al., 1986). These parameters are calculated by methods from van Ulden and Holtslag (1985), Holtslag et al. (1995) and Zilitinkevich and Mironov (1996). Meteorological data used are from the routine objective analysis system Mesan (Häggmark et al., 2000).

Nitrogen dioxide is calculated using a simple chemical model similar to that applied in OSPM (Hertel and Berkowicz, 1989; Berkowicz, 2000b). Background concentrations such as NO, NO_2 and O_3 are given by the regional model integrated in SIMAIR's coupled model system. To prevent double counting, regional background concentrations for a given city are calculated excluding emissions in that city. This procedure is done for all 150 Swedish cities used by the SIMAIR system today.

2.1.2 Improved version

The original SWE-BUM model has been further developed, with a special focus on improving the calculations for low boundary layer height conditions. There are, however, some other minor changes that have been implemented as well. The lower limit of the vertical turbulence intensity (the vertical turbulence parameter divided by wind speed) has been decreased from 0.05 to 0.016 based on Briggs(1973) formula for strong stable open-country conditions. Furthermore, the height of the well-mixed layer $h_0$has been decreased to 10 m for communities with less population than 50 000; for larger cities 20 m is used except for Stockholm where 40 m is used.

The meteorological data from the routine objective analyses(Mesan)can be regarded as representing rural meteorological conditions. Hence, it was found important to adopt a correction of the meteorology to represent urban conditions. This is done by means ofMonin-Obukov's similarity theory

$$u(z)_{urban} = \frac{u_{*urban}}{k}\left(\ln\left(\frac{z}{z_{0\,urban}}\right) - \Psi_m\left(\frac{z}{L_{urban}}\right) + \Psi_m\left(\frac{z_{0\,urban}}{L_{urban}}\right)\right) \tag{5}$$

where k is von Karmans constant, $L$is Monin-Obukov's length and Ψ_m is the stability function, calculated in accordance with Dyer (1974) for unstable conditions ($L < 0$) and Holtslag and de Bruin (1988) for stable conditions ($L > 0$). $u_{*\,urban}$is calculated by assuming that the wind speed at a certain height above an urban area (e.g. 100 m) is the same as the wind speed given from Mesan for that area (rural area) and corrected for differences in surface roughness (z_0 correction).

A sensitivity study of the model has been carried out, which points out the vertical dispersion parameter σ_z as the most important parameter affecting the concentrations of NO_2in the dispersion calculations. The original parameterisation of σ_z in SWE-BUM (Eq. 3),which isa modification of the formulation inBerkowicz (2000a), is shown in Figure 1 (left hand side). In the calculations, meteorology from Umeå in northern Sweden in January 2005 is used. As can be concluded from the figure, the variation of$\sigma_z$with distance is rather similar to Brigg's formulas for open country conditions (Briggs, 1973). However, for a winter month in a town in northern Sweden,more stable conditions are expected. Thus, a simple stability parameterisation is introduced in the formulation of σ_z, by including a stability dependent parameter βin Eq. (3).

$$\sigma_z(x) = h_0 + (h_{mix} - h_0)\left(1 - e^{-\frac{\beta \cdot \sigma_W \cdot x}{u(h_{mix} - h_0)}}\right)$$

$$L \leq 0 \quad \beta = 1 \tag{6}$$

$$L > 0 \quad \beta = \frac{1}{1+\frac{20z}{L}}$$

The effects of implementing this formulation arevisualised in Figure 1 (right hand side). The vertical dispersion parameter tends to be shifted to more stable conditions. How this affects the calculated concentrations of NO_2 can be found in Section 3. For Stockholm we decide to keep the original parameterisation ($\beta = 1$), since Stockholm is a large Swedish city with a population of 2.1 million in the metropolitan area (1.4 million in the urban area). Hence, neutral conditions are likely a good assumption.

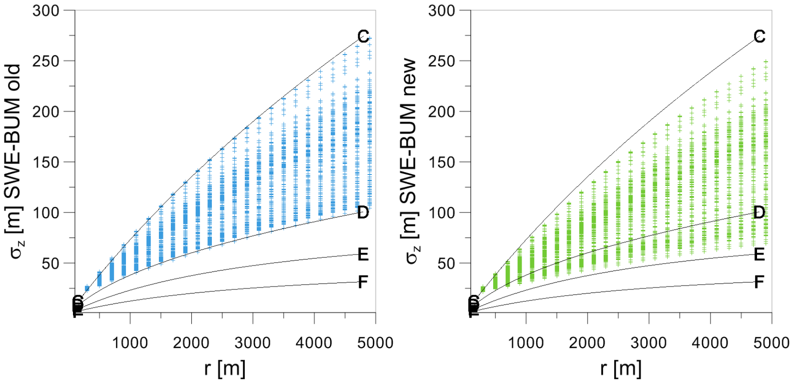

Figure 1. Vertical dispersion parameter σ_z calculated at different distances from the receptor point. On the left hand side results are shown for the old parameterisation (according to Eq.3) and on the right hand side results are shown for the improved parameterisation (according to Eq.6). The curves C-F relate to Pasquill stability classes consistent with Brigg's formulas for open country conditions (Briggs, 1973). The calculations are made for meteorology in January 2005 forUmeå in northern Sweden.

2.2 Measurements

The calculated concentrations of $NO_2$are validated against urban backgroundmeasurements from 13 cities in different parts of Sweden. In Table 1, thesemonitoring stations are listed from south to north. The measurements have been carried out by the municipalities and data are available from the data hosting of Air Quality in Sweden (IVL, 2011). The stations are consistently located in the central parts of the cities; however, the height above ground varies from a few meters up to rooftop level. Measurements only covering winter half-year have been included;many stations in Sweden only perform measurements during winter half-year when the concentrations peak (Persson et al., 2010). Furthermore, NO_X measurements are rather uncommon in Sweden, since only standards for NO_2 are defined in the EU Air Quality Directive.Thus, only concentrations of NO_2 are analysed within this study.

Table 1.Urban background monitoring stations included in the model validation, sorted from south to north. The monitoring data have been downloaded from the data hosting of Air Quality in Sweden (IVL, 2011).

City	Station name	Location	Instrument type	Measuring period
Malmö	Rådhuset	Rooftop	Active	2005, calendar year
Jönköping	Hoppetstorg	3 m above ground	Passive	2005, winter half-year
Göteborg	Femman	Rooftop	Active	2005, calendar year
Norrköping	Rosen	Rooftop	DOAS	2005, calendar year
Stockholm	T. Knutssonsg.	Rooftop	Active	2005, calendar year
Karlstad	Rådhuset	3 m above ground	Passive	2005, winter half-year
Västerås	Stadshuset	Rooftop	DOAS	2005, calendar year
Falun	Folketshus	Rooftop	DOAS	2005, calendar year
Sundsvall	Stadshuset	Rooftop	DOAS	2005, calendar year
Östersund	Z-gränd	3 m above ground	Passive	2005, winter half-year
Örnsköldsvik	Centrum	3 m above ground	Passive	2005, winter half-year
Umeå	Stadsbiblioteket	Rooftop	Active	2004, 2005, 2007, calendar year
Luleå	Stadshuset	Rooftop	DOAS	2005, calendar year

3. RESULTS

In the scatterplots in Figure 2, the calculated concentrations of NO_2 in SWE-BUM are compared to monitoring data from the 13 Swedish cities given in Table 1. Concentrations are defined in terms of annual/winter half-year average and 98 percentile of daily and hourly average, respectively, in consistence with the definitions in the EU Air Quality Directive. Results are shown both for the original and improved version of SWE-BUM. As can be concluded from the figures, the new model is able to reproduce better annual average concentrations and especially 98 percentiles of daily and hourly average; when compared to measured concentrations, 41 % of the data points are within ±50 % for the original model, while the corresponding result for the improved model is 95 %.

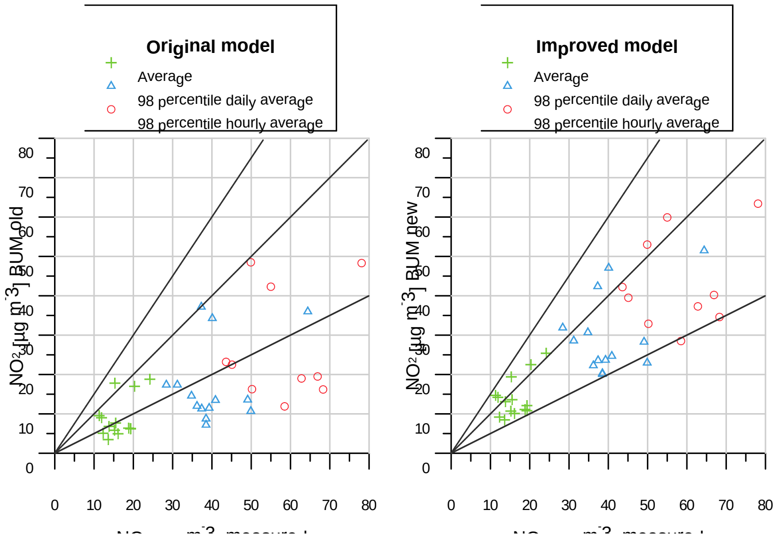

Figure 2. Comparison of measured and modelled NO_2 concentrations (µg m^{-3}) expressed in terms of Air Quality levels defined in the Swedish legislation and the EU Air Quality Directive, for urban background stations in13 cities in Sweden (see Table 1). The broken line indicates ± 50 % modelling uncertainty. On the left hand side, calculations with the original model version of SWE-BUM are shown while the calculations on the right hand side show the improved model version.

A more detailed analysis for one monitoring station (Umeå in northern Sweden), is shown in Figure 3. In the upper figure, the seasonal variation of NO_2 (monthly average concentrations) is plotted for the year 2004, while the lower figure shows the variation of daily average concentrations of NO_2 for the year 2007.In general, the correlation between modelled and measured concentrations increases, and the time variation is considerablybetter captured in the new model version.Note that the regional background concentration of NO_2 is low. For 2007 the yearly mean concentration of NO_2 at the regional background station Vindeln (about 48 km northwest of Umeå) is 0.72 µgm^{-3} which can be compared to 14.0 µg m^{-3} measured at the urban background station inUmeå.However, the improved model still doesn't succeed to fully reproduce the highest daily and hourly peaks of concentrations.

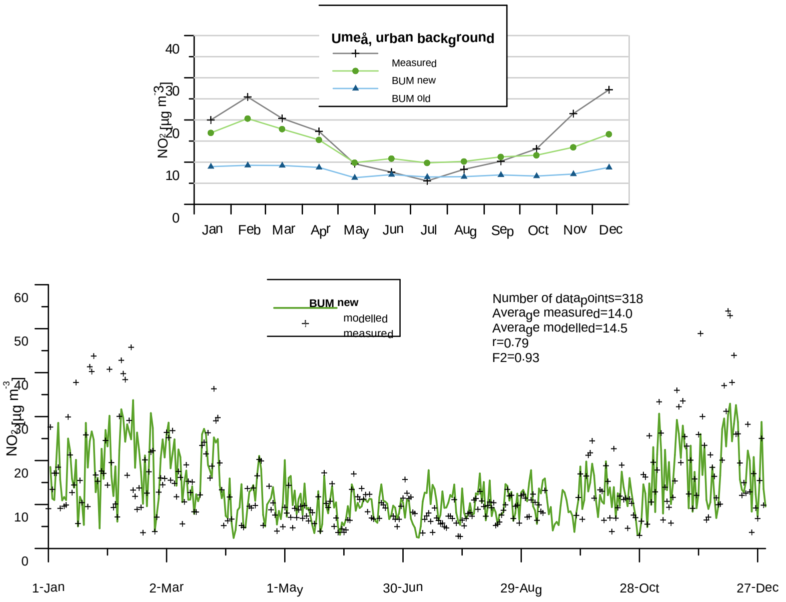

Figure 3.Measured (+) and modelled (solid line) urban background concentrations of NO_2 for Umeå in northern Sweden. The upper figure shows the seasonal variation of NO_2 (monthly average) for the year 2004 (the modelled concentrations are divided into the old and new model version), while lower figure shows daily average of NO_2 for the year 2007. r is the correlation coefficient and F2 is the fraction of data points within a factor of 2.

In Table 2 the model is validated in terms of Relative Percentile Error (RPE) and Relative Directive Error (RDE) which are the mathematical interpretations of the quality objectives in the EU Air Quality Directive (Denby et al., 2010).Regarding both RPE and RDE, the new model version yields improved performance; for annual average the maximum value of RPE decreases from 0.69 to 0.41, while corresponding values for RDE are 0.33 to 0.19. Overall, RDE values for annual average are lower than RPE, reflecting the fact that the concentrations, in general, are far below the limit values in the EU Air Quality Directive.

Table 2.Relative Percentile Error (RPE) and Relative Directive Error (RDE). Results are shown for the original (old) and improved (new) model version, respectively, and presented as maximum and median value. 10 % of the monitoring stations with the highest values are excluded when calculating maximum value (consistent with the quality objectives in the EU Air Quality Directive).

		NO_2 annual average		NO_2 98 percentile daily average		NO_2 98 percentile hourly average	
		old	new	org	new	old	new
RPE	max	0.69	0.41	0.79	0.48	0.76	0.49
	median	0.55	0.27	0.67	0.33	0.59	0.27
RDE	max	0.33	0.19	0.81	0.54	0.79	0.44
	median	0.19	0.08	0.63	0.34	0.64	0.39

4. DISCUSSION AND CONCLUSION

The modifications implemented in the urban background model SWE-BUM, including the new simple stability parameterisation for the vertical dispersion parameter, significantly improve the model performance. When comparing the calculated NO_2 concentrations with monitoring data from 13 cities in different parts of Sweden, 95 % of the data points are within ±50 % for the improved model in comparison with 41 % for the original model. The correlation increases and the seasonal variation is better captured in the new model version. Furthermore,the new model version yields better RPE and RDE values for both annual average and daily and hourly concentrations of NO_2. However, the improved model still doesn’t succeed to fully reproduce the highest daily and hourly peaks of concentrations.

It should be emphasized that there are difficulties when comparing point measurements with modelled concentrations on 1x1 km^2; the representativeness of the measurements varies between the sites andthe location of the monitoring station is very crucial for the results.In a model validation point of view,rooftop measurements are likely most representative, since the influences of local emission sources are minimized.Other possible error sources in the calculations are the emission data; more detailed emission inventories might improve the results further. Infuture follow up studies, it would alsobe interesting to evaluate the model performance for other compounds, for example NO_X, benzene and PM10.

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