Chapter 6

Extension of an Operational Short-Range Dispersion Model for Applications in an Urban Environment[*]

Abstract—When operationally modelling dispersion of air pollutants over a city, ‘conventional’ dispersion models are often used with modifications in some of the parameters such as the roughness length. However, the presence of a roughness sublayer (RS) is usually neglected, although its turbulence structure is different from that in the surface layer. Therefore, in the present work a roughness sublayer for urban applications is introduced. The principle of the modification has already been tested by simulating two tracer experiments using a Lagrangian particle model and it was shown that the introduction of an RS clearly improves the model performance for both experiments. In this paper, it is shown that the same holds for the introduction of the RS in the multi-source/multi-receptor Gaussian OML model. Its performance is furthermore investigated for the city of Zurich in the year 1990, when a detailed emission inventory and observations at 29 stations are available. It is concluded that the introduction of the RS increases the physical significance of the model in urban environments and thus the credibility of its predictions.

Keywords: dispersion modelling, urban turbulence, rough surfaces, urban air pollution, roughness sublayer

6.1 INTRODUCTION

Air pollution modelling in urban areas suffers from the discrepancy between the explicit need for dispersion simulations due to the high emission densities on the one hand, and a deficit concerning the knowledge on the flow and turbulence structure due to the complicated building structure on the other hand. The presence of tall roughness elements (buildings, trees, etc.) with irregular spacing leads to the formation of a roughness sublayer (RS), which ranges from the physical surface up to 2–5 times the average roughness element height (Raupach *et*

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[*] this chapter has been published as:
de Haan, P., Rotach, M. W., and Werfeli, M. W. (1998): Extension of an operational short-range dispersion model for applications in an urban environment. *Int. J. Vehicle Design*, **20**, 105–114

al., 1991), i. e. it includes the urban canopy layer (see Fig. 1). Within this RS the flow and turbulence structure is different from that of the surface layer (Högström *et al.*, 1982; Rotach, 1993a, b; Roth and Oke, 1993; Roth, 1993; Oikawa and Meng, 1995), which latter usually constitutes the lowest part of applied (operational) dispersion models.

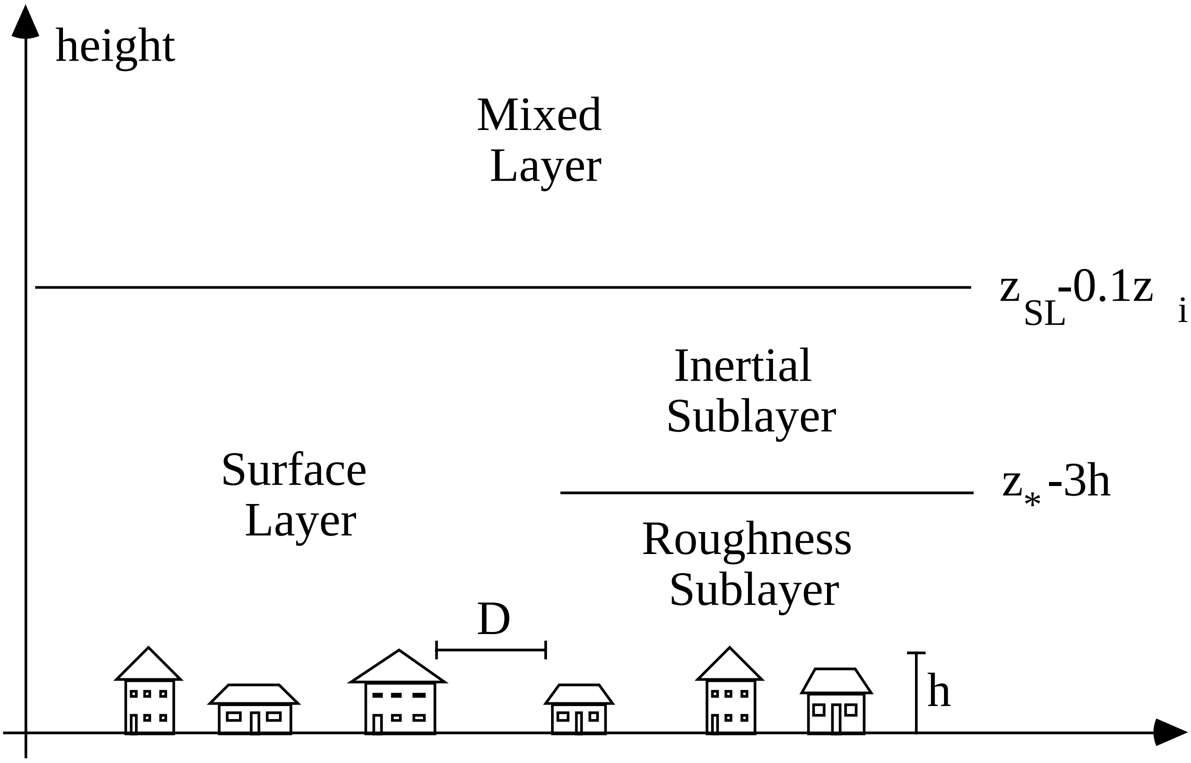

Figure 1 Conceptual sketch of the lowest layers within the boundary layer over an urban surface. The left hand side of the figure shows the situation as it is conventionally used in applied dispersion models (‘non-urban’ in the present terminology), while the right hand side depicts the actual situation with a roughness sublayer adjacent to the surface (referred to as ‘urban’ in the text).

The most striking difference is the fact that the turbulent fluxes of momentum (and heat) are not constant with height (cf. the identification of the surface layer as a ‘constant flux layer’). For momentum, Rotach (1993a) hypothesised that the non-constant turbulent flux within the urban RS is most likely due to a mean horizontal pressure gradient, as it is characteristic for a flow over a warm (cf. the urban heat island) and rough surface. The non-constant Reynolds stress within the RS leads to a smaller gradient of mean wind speed as compared to the ‘logarithmic profile’ of the surface layer (Rotach, 1993a) and the necessity to revise the scaling concept for the turbulence statistics such as velocity variances (Rotach, 1993b). Both these features are likely to modify dispersion characteristics and hence surface concentrations over urban surfaces, and this modification may be severe due to the relatively large vertical extension of an urban RS.

In a recent comparison study, the performance of five operational dispersion models was compared with respect to three tracer data sets (Olesen, 1995). Two of these tracer experiments were conducted in the cities of Copenhagen (Gryning and Lyck, 1984) and Lillestrøm (Haugsbakk and Tønnesen, 1989), i. e. over (sub)urban surfaces. The intercomparison showed that in both cases all the participating operational models underestimated the surface concentrations on average (Olesen, 1995). Using a Lagrangian particle dispersion model, Rotach (1997b), for a hypothetical near-surface source and Rotach and de Haan (1997), for the tracer experiment of Copenhagen showed that this underestimation is likely to be due to neglecting the flow and turbulence structure of the urban RS. In both these studies the model is run in an ‘urban’ mode and in a ‘non-urban’ mode: the former takes into account the effect of the rough surface by explicitly using the turbulence characteristics of the RS (corresponding to the right side of Fig. 1) and the latter uses surface layer characteristics at the bottom of the model domain (cf. the left side of Fig. 1) as it is common for essentially all applied dispersion models.

In the present contribution it is investigated how the modified turbulence structure for simulating dispersion over an urban surface can be introduced into an operational dispersion model. It is shown that the modification improves the model performance for the case of the (‘ideal’) tracer experiments (Section 6.2). When simulating yearly averages of pollutant concentrations from ‘real sources’ (traffic, domestic and industrial heating) over the area of a whole city (Section 6.3) a similar improvement is observed, but other effects such as the treatment of plume rise tend to mask the improvement of the physically more consistent ‘urban’ type simulation.

6.2 THE MODIFICATION OF AN OPERATIONAL MODEL

6.2.1 The OML Model

The so-called OML is the basic atmospheric dispersion model for environmental impact assessments in Denmark. Besides the scientific multi-source/multi-receptor version used in the present work, OML-Multi, a single-source version for regulatory purposes is available (OML-Point). The OML is a Gaussian plume model, but in contrast to many regulatory models its physical description is not based on the traditional discrete stability categories (Pasquill-Turner stability classes). Instead, the model uses basic boundary layer scaling parameters (see below). It is intended to be used for distances up to about 20 km from the source. It requires information on emission and meteorology on an hourly basis, and returns a time series of concentrations calculated at user-specified receptor points. For a more detailed description of the model and the associated meteorological preprocessor, see Olesen *et al.* (1992). The lower boundary of the model domain in vertical direction equals the roughness length, z_0. Perfect reflection without deposition is assumed. This is done by placing a mirror source below the ground.

6.2.2 Modification for urban environments

In the OML model the determination of the standard deviations of the plume dimensions in cross-wind and vertical direction, σ_y and σ_z, respectively, is based on a simplified Lagrangian theory. As input parameters, some of the boundary layer turbulence statistics are required and these, in turn, are parametrised based on similarity theory with the friction velocity, the convective velocity scale and the Obhukov length as scaling variables. This part of the OML is called its meteorological preprocessor. In our modification of the OML for urban environments, the parametrisations in the lower part of the surface layer, i. e. the roughness sublayer, are modified according to the observations which were briefly introduced in Section 6.1. Specifically, this means that due to the decreasing Reynolds stress (in connection with the concept of local scaling) the velocity variances become smaller than they would be in a surface ('constant flux') layer, and the same is true for the gradient of mean wind speed. Additionally, the lower boundary of the modelling domain is lifted up to the zero plane displacement *d* in order to avoid the physically dubious use of a Gaussian dispersion model between the roughness elements.

The 'urban modification' of the OML model only requires one additional step, which slightly modifies the results of its meteorological preprocessor. This is, in general, the simplest way of modifying operational dispersion models for urban environments. No major changes are needed in the code of the program itself. It is important to notice that our distinction between 'urban' and 'non-urban' has nothing to do with the possible contrast between urban and rural. 'Urban' in our context simply means that the RS turbulence structure is correctly taken into account, while 'non-urban' denotes a simulation in which this is not the case. More details about the modification of the meteorological input to dispersion models for application in urban environments can be found in Rotach (1997a).

6.2.3 ‘Urban’ vs. ‘non-urban’ simulations

The modification of the OML is validated using the two tracer experiments in Copenhagen and Lillestrøm (see Section 6.1). These tracer experiments are widely used for the validation of models for regulatory purposes. Here, the results of two different simulations of the Copenhagen and Lillestrøm experiments are presented. In the ‘non-urban’ version, all meteorological input parameters are used as in the original papers (for Copenhagen: Gryning and Lyck, 1984; for Lillestrøm: Haugsbakk and Tønnesen, 1989). For the Copenhagen experiment, mixing layer depths are available from radio soundings; for the Lillestrøm experiment, however, no measurements of the inversion layer height are available, so that a parametrisation has to be used. In this study the formulation of Zilitinkevitch (1972) with a proportionality constant of 0.28 is applied. (Note that since no details on the parametrisation employed are provided in Olesen (1995), we are unable to *exactly* reproduce these results for the ‘non-urban’ case.)

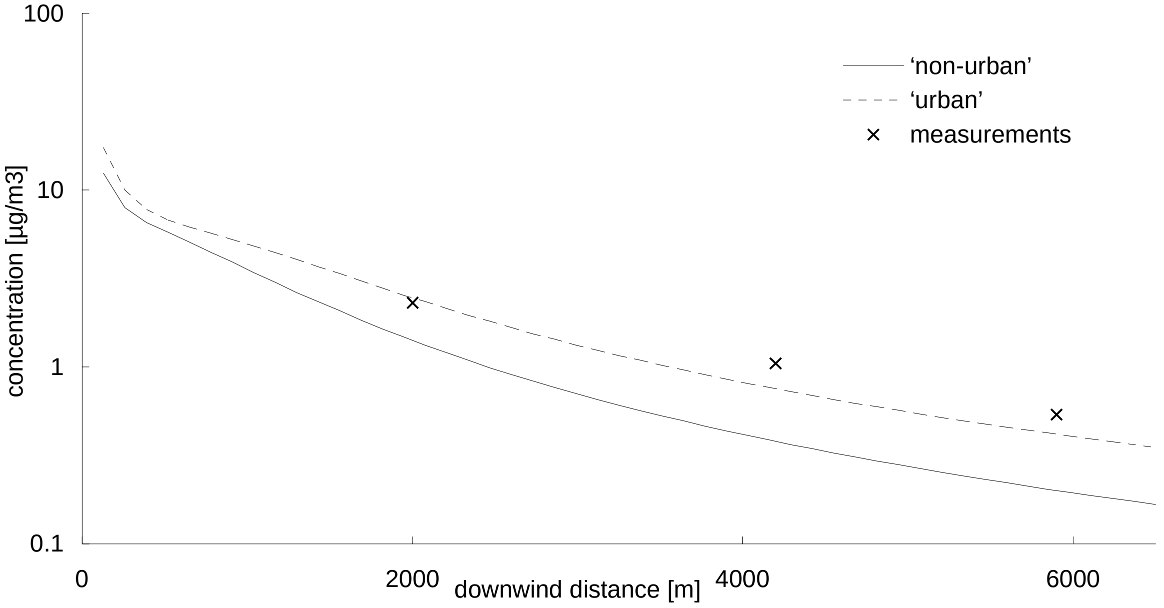

Figure 2 Example of the plume centre line concentration at 2 m above the ground for the ‘original’ (i. e., ‘non-urban’) version of the OML and the ‘urban modification’. Crosses depict the measurements (Copenhagen experiment from April 30, 1979).

For the ‘urban’ simulations, the zero-plane displacement has to be estimated from the available information on the average building height and the density of the roughness elements (for details see Rotach, 1997a). For Copenhagen and Lillestrøm, these estimated values for the zero-plane displacement height are 1.0 m and 0.9 m, respectively. In both experiments the friction velocity was measured (or determined from other measurements) at a nominal height of 10 m, i. e. within the RS. Therefore, the parametrised profile of Reynolds stress within the RS (Rotach, 1997a) was used to determine a friction velocity for the inertial sublayer, u_*^{IS}, and this value was input to the OML.

The main effect on the surface concentrations of the modification of the OML with the urban preprocessor is illustrated in Fig. 2. The profile of Reynolds stress within the RS and the associated profiles of the velocity variances give rise to a reduced dispersion as compared to a surface layer assumption (‘non-urban’ in our notation), thus leading to larger ground-level concentrations downwind of the maximum concentration.

In Table 1 the following statistical measures are compared for the two different simulations of the two tracer experiments:

FB the fractional bias: $FB = \left(\overline{C}_{\mathrm{obs.}} - \overline{C}_{\mathrm{pred.}}\right) \Big/ \left(0.5\left(\overline{C}_{\mathrm{obs.}} + \overline{C}_{\mathrm{pred.}}\right)\right)$

NMSE the normalised mean square error: $NMSE = \overline{\left(C_{\mathrm{obs.}} - C_{\mathrm{pred.}}\right)^2} \Big/ \left(\overline{C}_{\mathrm{obs.}}\overline{C}_{\mathrm{pred.}}\right)$

COR the correlation coefficient: $COR = \overline{\left(C_{\mathrm{obs.}} - \overline{C}_{\mathrm{obs.}}\right)\left(C_{\mathrm{pred.}} - \overline{C}_{\mathrm{pred.}}\right)} \Big/ \left(\sigma_{\mathrm{obs.}}\sigma_{\mathrm{pred.}}\right)$

FAC2 percentage of simulations within a factor of two of the measurement

Here, $C_{\mathrm{obs.}}$ is the observed concentration and $C_{\mathrm{pred.}}$ the simulated one. These statistical measures are calculated for the maximum concentration (plume centre line) measured on an arc of receptors placed cross-wind at a constant distance from the source, at 2 m above the ground, and for the cross-wind integrated concentration, CIC.

		arcwise maximum conc.				cross-wind integrated conc.			
		NMSE	COR	FAC2	FB	NMSE	COR	FAC2	FB
Copenhagen	Observations	0.00	1.000	100%	0.000	0.00	1.000	100%	0.000
	OML ‘non-urban’	1.03	0.798	22%	0.743	0.49	0.852	57%	0.577
	OML ‘urban’	0.37	0.737	87%	0.247	0.41	0.836	74%	0.519
Lillestrøm	Observations	0.00	1.000	100%	0.000	0.00	1.000	100%	0.000
	OML ‘non-urban’	0.47	0.811	47%	0.427	2.10	0.572	37%	0.960
	OML ‘urban’	0.38	0.751	58%	0.131	1.15	0.502	58%	0.514

Table 1 Comparison of statistical measures for the ‘urban’ and ‘non-urban’ simulations for the two tracer experiments from Copenhagen and Lillestrøm.

As can be seen from Table 1, the results of the OML are improved when using the ‘urban’ modification. In the case of the Copenhagen experiment, all statistical measures show a clear improvement, with the exception of the correlation coefficient, which slightly decreases but still remains relatively high. In general, the improvements are more pronounced in the statistical measures for the arcwise maximum concentration than for those of the CIC.

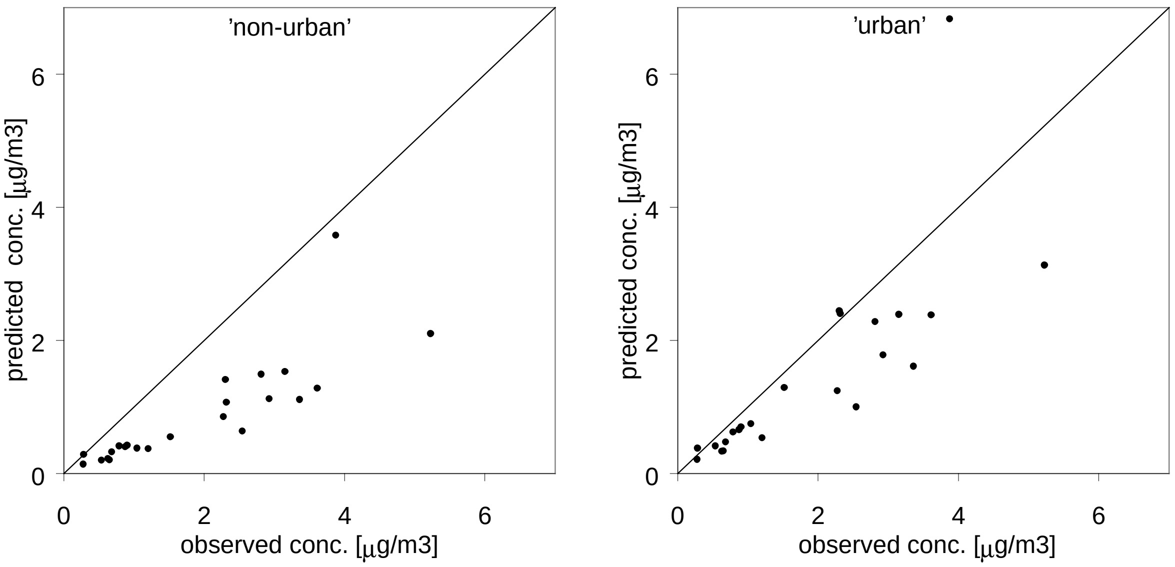

Figure 3 Scatter plot of all observed arcwise maximum concentrations vs. predictions (Copenhagen experiment). Total number of data points is 23. a) ‘non-urban’ simulation, and b) ‘urban’ simulation.

A scatter plot of observed vs. simulated arcwise maximum concentrations for the Copenhagen experiment is presented in Fig. 3. As can be seen, the underprediction from the non-modified version of the OML is clearly reduced. Only in one case the ‘urban’ modification causes a previously underpredicted value to become overpredicted. For all other observed values, the predictions improve when using the ‘urban modification’. This leads to the significantly improved statistical measures in Table 1, with the most remarkable changes for the ArcMax predictions, with the FB and NMSE measures becoming almost three times smaller. For the Lillestrøm experiment, the statistical measures show similar improvements, but are most pronounced for the CIC predictions, with FB and NMSE dropping by almost 50%. Again, the correlation coefficient shows a slight decrease. With the ‘urban modification’, however, the performance of the OML becomes comparable to the performance of more advanced scientific dispersion models (Olesen, 1995).

6.3 APPLICATION TO THE CITY OF ZURICH, 1990

In the previous section, the importance of the roughness sublayer turbulence structure was demonstrated for an ‘ideal’ setting of a tracer experiment. For this type of experiment the source is well defined and its strength is exactly known, no effects of plume rise have to be taken into account and the receptor density is usually high. In contrast, when using an operational dispersion model such as the OML for the simulation of, e. g., the spatial distribution of the annual mean surface concentrations over the area of a whole city, these conditions are not fulfilled. In the following we present first results from such an attempt, namely the simulation of the surface concentration of NO_x in the year 1990 for the city of Zurich. For this year a detailed (100 m x 100 m resolution) emission inventory was constructed (Werfeli, 1995). It takes into account traffic (number of vehicles per day and estimated speed on the 152 largest roads of the city; additionally, estimates of short-distance traffic not using major roads), domestic and commercial heating and the 35 largest industrial sources (treated as point sources in the model).

This emission inventory sums up to over 4300 SO_2 sources and over 4300 NO_x sources, where the line sources (roads) are split up and added to area sources. To simulate the time dependence of source strength, the amplitude of the traffic sources is modulated according to the hour of the day and the day of the week, and the strength of the heating sources depends on the hour of the day and on the month. The emission data of the heating sources was collected very carefully (0.01% missings in the number of sources) and the traffic emissions were modelled using numerous results from actual traffic census data. The emission factors used for the calculation of the overall emissions for each source type and pollutant were checked with in-site monitoring measurements. With this procedures the overall accuracy of the emission data is estimated at ±5% for heating sources (SO_2 and NO_x) and at ±20% for NO_x and ±25% for SO_2 for emissions from traffic sources. This amounts to a total maximum estimated error in the emission data of 6.3% for SO_2 and, due to the larger contribution of traffic sources, of 14.3% for NO_x. For details concerning the emission inventory see Werfeli (1999).

In addition, for the year of 1990, a total of 29 stations spread all over the city, yielded observational data of surface pollutant concentrations for comparison to the simulations. Besides from five continuously monitoring stations (hourly averaged concentrations for the whole year), pollutant concentrations were measured over shorter time periods (covering all seasons) at the remaining 24 stations, from the results of which annual average concentrations were estimated by statistical means.

For the configuration of the model and the definition of the required model input, one has to be aware that several assumptions are likely to have a significant influence on the resulting ground level concentrations. The approaches chosen for the most sensitive parametrisations are outlined in the following:

- Plume rise plays an important role in determining surface concentrations for real sources. The commonly used plume rise schemes of Briggs (1984) are designed for large point sources. For the present purpose, these schemes are translated for use in connection with domestic heating and traffic area sources by choosing average stack heights above roof level and above the street level, respectively. Instead of specifying values for vertical exit velocity and source radius, averaged buoyancy fluxes are assigned to the individual sources depending on the source strength (being a function of time and of space). The temperature of the emissions is set to a constant level and not to an constant excess with respect to the ambient temperature. This has been done in order to reflect the more or less constant burning temperature of engine vehicles and of heatings.
- The well known Gaussian plume solution to atmospheric dispersion does not apply close to the source, since all parametrisations of the vertical and lateral plume standard deviation, $\sigma_y(x)$ and $\sigma_z(x)$, respectively, approach zero near the source. This causes the ground level concentration prediction of Gaussian plume models to approach infinity for $x \rightarrow 0$, since both $\sigma_y(x)$ and $\sigma_z(x)$ appear in the denominator of an exponential expression. Therefore, Gaussian plume models only apply for $x > 100\,\mathrm{m}$ (Briggs, 1973). Hence, Gaussian dispersion models tend to overestimate the surface concentrations close to the source. To circumvent the problem that typically small sources, which are located in the vicinity of any receptor in an urban environment, promote an average (potentially large) overestimation due to this flaw of Gaussian dispersion models, the groundlevel concentration predictions caused by the individual sources is set to zero for the near-field $(x < 100\,\mathrm{m})$ (note that for the tracer experiments discussed in the previous section the closest measurement arc was far enough from the source so that this problem did not occur).

- The definition of the model surface is another key factor in determining the model performance. In order to avoid the use of a (relatively simple) Gaussian model for dispersion estimates *between* the roughness elements, where its application can certainly not be justified, a model surface corresponding to the zero displacement height (see Rotach, 1994) rather than the physical surface $(z = 0)$, is used.

First results of the simulation of the annual mean NO_X surface concentrations for 1990 for the city of Zurich at the 29 measurement stations are shown in Fig. 4. The simulation with the parametrisations and the set-up as outlined above, is denoted 'non-urban' (see Fig. 4a). This 'non-urban' simulation results in a fractional bias of 0.17, i. e. an underestimation of 17% (Fig. 4a). As for the tracer experiment in the previous section, the 'urban' simulation improves the performance (Fig. 4b). In particular, the fractional bias is reduced, and does not any more differ significantly from zero on a 5% level, whereas the scatter (the normalised mean square error) and the correlation coefficient do not change significantly.

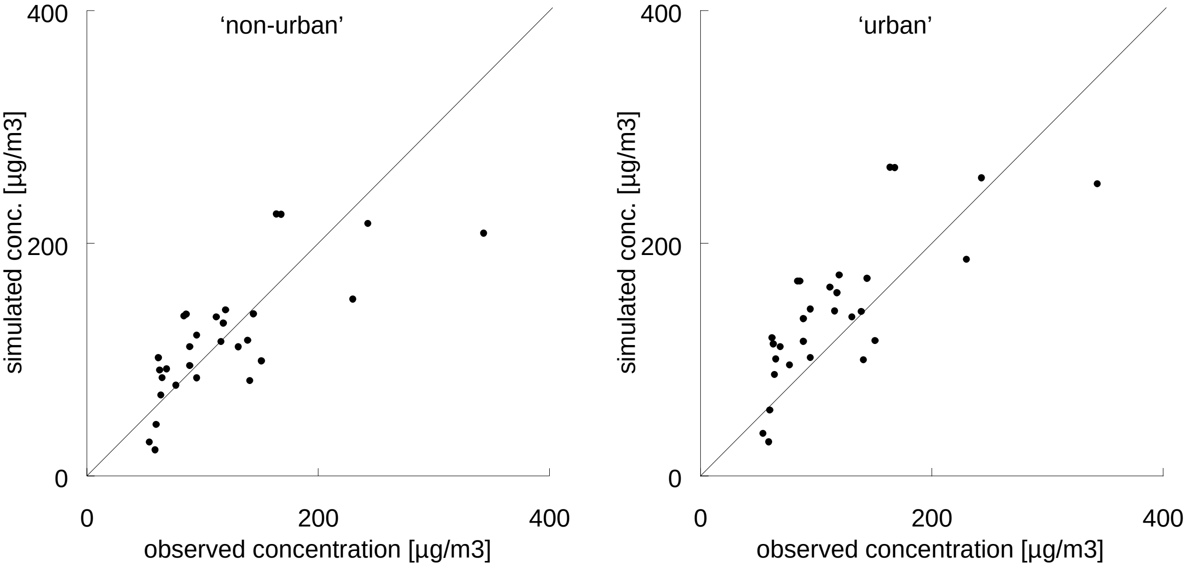

Figure 4 Comparison of observed vs. modelled yearly averages of NOx groundlevel concentration in at 29 surface observation stations in the city of Zurich (1990). a) 'non-urban' simulation, and b) 'urban' simulation.

In future work, an attempt for further refinements will be made, especially concerning the improvement of the near-field correction of the Gaussian plume model. Additionaly, the background concentration of SO_2 and NO_X in the city of Zurich will be assumed to consist of two contributions: firstly, the natural concentration measurable at remote rural stations, and, secondly, the contribution from sources near the city of Zurich, but not accounted for in the emission inventory, which only covers sources within the community of Zurich, and not the whole urban agglomeration. Nevertheless, the preliminary results presented here show clearly that the main effect of introducing a RS in a conventional Gaussian dispersion model leads to higher annual average ground level concentrations of between 10–20%, thus compensating the underestimation most models show over urban environments. The other statistical performance measures of the modified dispersion model in question, the OML, remained approximately unchanged for the case of a real emission scenario over an European city.

6.4 SUMMARY AND CONCLUSIONS

To obtain a proper modification of operational (Gaussian) dispersion models for use within urban environments, the concept of an urban meteorological preprocessor has been introduced. Its basic principle is to use similarity theory based on local fluxes for the parametrisation of the turbulence structure within the urban roughness sublayer. The first validation step of this concept has been reported on elsewhere (Rotach and de Haan, 1997) and was performed by use of a Lagrangian particle dispersion model (research model) for the simulation of two tracer experiments, which took place in (sub)urban environments. A clear improvement of the predictability was the result. This indicates that the urban preprocessor is able to better take into account the rough character of the surface at the sites where these experiments took place. As a second validation step the performance of the operational Gaussian multi-source dispersion model OML for these two experiments also shows an improvement of the correspondence between the simulated and the measured concentrations if the urban preprocessor is applied. Therefore, the concept of the urban preprocessor can be used within operational Gaussian dispersion models to improve the model's prediction ability over urban surfaces. First results for the case study of the surface pollution concentration (NO_x) in the city of Zurich in the year 1990, for which a very detailed emission inventory (100 m x 100 m resolution) is available, also show an improved model performance after introduction of the roughness sublayer.

Acknowledgements-The present work was partly financed by the Swiss Federal Department of Education and Sciences (BBW) and the Swiss Federal Department of Environment, Forest and Landscape (BUWAL) through a project in the framework of COST 615 (citair), and by the Swiss National Science Foundation through Grant Nr. 21-46849.96.

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