THE EFFECT OF SOURCE TREATMENT ON POLLUTANT DISPERSION IN AN IDEALISED URBAN ROUGHNESS IN NUMERICAL SIMULATIONS USING THE STANDARD k-ε TURBULENCE CLOSURE MODEL

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Abstract: The need for accurate model predictions in urban air quality assessment studies during the past decade has led to the ever increasing use of Computational Fluid Dynamics (CFD) models in order to resolve the various local scale inhomogeneities which dominate flow and dispersion and are usually encountered in urban areas. Towards the aim of improving model predicted dispersion via the use of CFD models, a numerical study was undertaken in order to investigate the effect of different techniques applied for treating the sources of emissions on the near source behaviour of the models, as well as on the actual predicted concentrations at locations away from the vicinity of the sources under consideration. A series of 3D numerical simulations were performed for the wind tunnel model geometry of the Mock Urban Setting Test (MUST) field experiment of the University of Hamburg, Meteorological Institute, Division of Technical Meteorology, which was made available within the frame of COST Action 732. Overall in conclusion, results show that depending on the type of source, the intensity of the vertical component of the emissions exit velocity at the source and the mesh refinement close to source boundaries predicted concentrations can deviate significantly from the wind tunnel measurements. However, it is possible to partially improve the performance of a CFD model in urban dispersion problems, mainly via the application of the proper combination of these parameters.

Key words: *Source treatment, exit velocity, pollutant dispersion, roughness, turbulence.*

1. INTRODUCTION

Flow patterns around buildings have a strong influence on pollutant dispersion from sources located in urban areas. The prediction of ground-level pollutant concentrations is important for assessing the impact of existing sources both on human health and on the environment. Recently, Computational Fluid Dynamics (CFD) models have become an attractive and useful tool for the accurate prediction of air pollution levels in urban areas, since they can resolve the complex effects of the various urban structures such as buildings. However, according to several recent studies, the application of many CFD models for urban dispersion modelling purposes is prone to large uncertainties, mainly due to their inability to take into account the dependency of the turbulent diffusivity on the distance from the source. In addition, the ability of CFD models to accurately predict pollutant dispersion in urban areas largely depends on the turbulent Schmidt number, which is the dominant parameter that characterizes the relative diffusion of momentum and pollutant mass due to turbulence (Flesch et al., 2002). Several studies have suggested that for urban dispersion problems, depending on the density of the main urban structures, a Schmidt number between 0.4 and 0.7 should be used. However, within the frame of COST Action 732, apart from the Schmidt number, there are also other parameters which may influence dispersion and the accurate prediction of the concentration levels within urban areas.

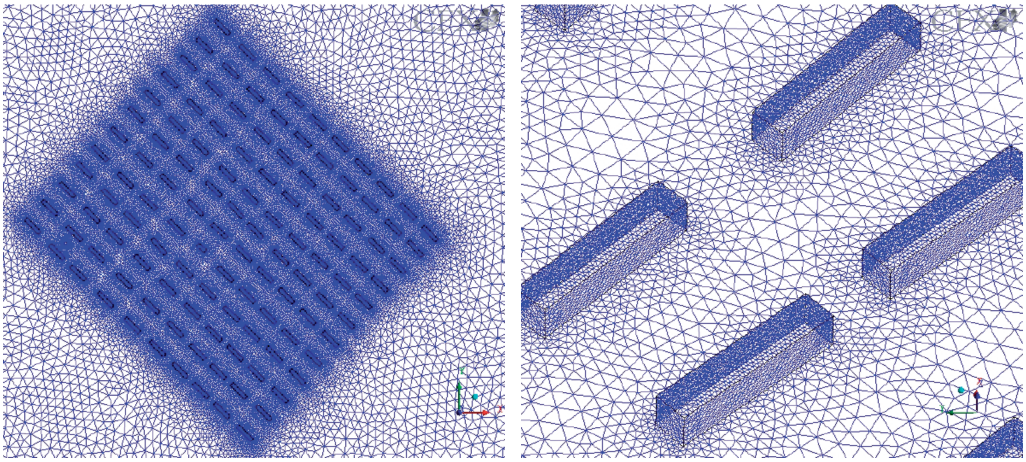
The present work was realized within the frame of COST Action 732 in an effort to gain an insight on the effect of the type and geometry of the sources under consideration, the mesh refinement close to the sources and the vertical component of the exit velocity of the emissions on the predicted concentrations for urban dispersion problems. Towards this aim, a series of detailed 3D numerical simulations of the wind tunnel model of the Mock Urban Setting Test (MUST) field experiment were performed, using different types of sources of emissions, namely a point source and an area source and different source strengths for a specific type of source. The objective was to determine whether it is possible to improve the performance of CFD models, through proper treatment of the sources under consideration during an urban dispersion problem.

2. METHODOLOGY

Computational domain and mesh

The MUST field site was composed by a total of 120 commercial cargo containers, placed in a nearly regular array of 10 by 20 containers. The average distance between two consecutive obstacles was 12.9 m in the longitudinal direction and 7.9 m in the lateral direction. Each container was 12.2 m long, 2.42 m wide and 2.54 m high, with the exception of the so-called VIP container, serving as collection point for sampled wind and concentration data, which is located in the geometrical centre of the array and was 6.1 m long, 2.44 m wide and 3.51 m high. Detailed description of the geometry of the MUST field site can be found in Biltoft (2001). A model of the MUST field site under a scale of 1:75 was placed in a boundary layer wind tunnel and detailed meteorological and concentration measurements for various approaching wind directions were performed. The small irregularities in the alignment of the containers that comprised the MUST field site array were accurately reproduced in the wind tunnel model (Bezpalcova and Harms, 2005). For the needs of our study, the wind tunnel model of the MUST field site was approximated via an unstructured mesh, which was generated using the ANSYS™ ICEM grid generating code.

Due to the complexity of the modeled area and the expected large number of grid cells it was decided to use an unstructured, tetrahedral mesh rather than a typical, structured, hexahedral mesh. The resulting grid comprised of a total of 5.5×10^6 cells (Fig. 1a) with sufficient refinement near the buildings and the ground in order to resolve the important features of the flow (Figure 1b). The selected expansion rate between two consecutive cells was set to 1.2 in regions of high gradients. The inlet boundary of the domain was placed at a distance of $5H_{max}$ upstream of the containers array, the outlet boundary at a distance of $7H_{max}$ downstream of the container array, the lateral boundaries on both sides at a distance of $5H_{max}$ and the top boundary at a height of 6H from the ground, where H_{max} is the height of the VIP container.



(a) **(b)**

Figure 1. (a) Computational domain and overall mesh of the MUST array and (b) mesh refinement close to the containers.

Discretisation scheme and turbulence modelling

The current numerical study was conducted using the commercial ANSYS™ CFX 5.7.1 general purpose CFD code. It uses a flexible multi-block grid system and an automatic unstructured hybrid element mesh generator with an adaptive mesh refinement algorithm. The conservation equations for mass, momentum and scalar quantities like temperature, turbulent kinetic energy and any number of species are solved. The model employs a first-order in time and a second-order in space discretisation scheme based on the Finite Volume approach. The basic discretisation technique adopted is a conventional Upwind Difference Scheme (UDS) with Numerical Advection Correction (NAC) for the advection terms in the momentum and energy equations (Raw, 1994). Proper modelling of turbulence plays a crucial role in providing accurate microscale wind fields, necessary for the reliable prediction of the transport and dispersion mechanisms of pollutants in the vicinity of buildings. The Reynolds stresses and turbulent fluxes of scalar quantities can be calculated by several linear and nonlinear turbulence models. For the needs of the study the standard k-ε two equations turbulence closure model in conjunction with the standard wall functions for the near wall treatment was chosen (Launder and Spalding, 1974). The specific turbulence model was chosen because it is widely used and has been tested for various similar cases with very satisfactory results, as it has proved to provide stable solutions.

Boundary conditions

During all cases, the inflow boundary conditions were the same. More specifically, in all simulations that were performed wind tunnel measurements for the vertical profiles of the velocity components and the turbulence kinetic energy of the approaching atmospheric boundary layer were used as inflow boundary conditions, with an approaching wind direction of -45°. Also, during all simulations the ground inside the container array as well as the container walls were treated as smooth, in accordance with the wind tunnel model conditions, while the ground surrounding the container arrays was treated as rough, with a roughness length of z_o=0.017 m. It should be noted, that during all cases the approaching atmospheric boundary layer was neutrally stratified. Furthermore, in all cases no heat transfer effects were taken into account, as the flow was treated as isothermal.

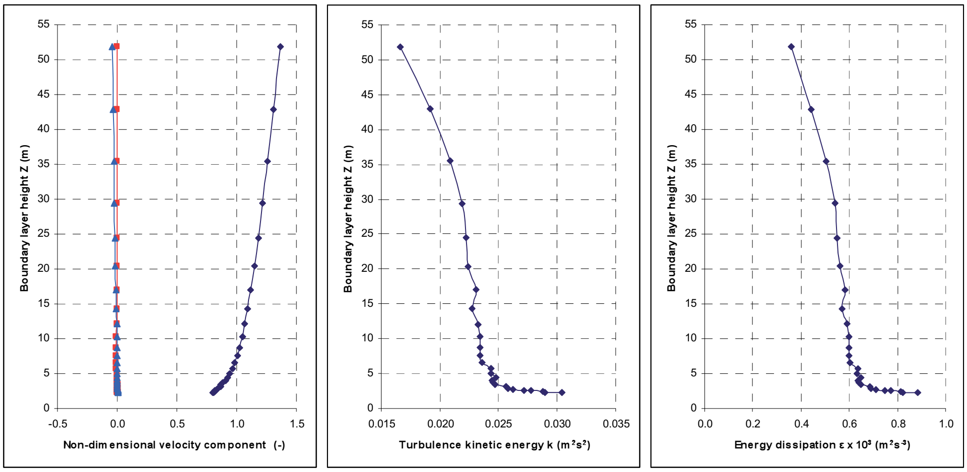
Furthermore, in all cases considered, the inflow boundary conditions were set at the same location as in the wind tunnel, namely at a distance of $3.5H_{max}$ of the container array. The corresponding profile for the energy dissipation ε, was calculated assuming that:

$$\varepsilon = \frac{C_{\mu}^{3/4} k_{in}^{3/2}}{\kappa z} \tag{1}$$

where k_{in} is the turbulent kinetic energy at inflow and κ is von Karman's constant with κ = 0.4. The inflow boundary conditions which were used are presented on Figure 2.

For the needs of the study, three simulations were performed. During the first, the source of emissions was treated as a point source with a volumetric source strength $Q = 2.78\times10^{-7}$ m^3s^{-1}. During the second, the source was treated as an area source, with an area equal to the area of the source used during the MUST field experiment and a source strength

$Q = 2.78\times10^{-6}$ m^3s^{-1} while during the third simulation, the source was also treated as an area source with the same dimensions compared to the second simulation, but with a source strength $Q = 8.34\times10^{-6}$ m^3s^{-1}.



(a) **(b)** **(c)**

Figure 2. Inflow boundary conditions for the three cases considered (a) non-dimensional velocity components, (b) turbulent kinetic energy and (c) energy dissipation vertical profiles.

3. RESULTS AND DISCUSSION

Results for the non-dimensional concentration at selected locations between the three cases that were simulated and wind tunnel measurements were compared. It should be noted at this point that during the second simulation, the area of the source was ten times higher compared to the first simulation. However, since the source strength was also ten times higher, the resulting vertical component of the exit velocity of the emissions was the same. Therefore comparison of results between the first two simulations and the wind tunnel data would offer the opportunity to gain an understanding of the effect of the type of source on the modelled dispersion. Furthermore, the area of the source in the third simulation was equal to the area of the source during the second simulation. However, the intensity of the source in the third case was three times higher compared to that during the second case. Therefore, the corresponding vertical component of the exit velocity of the emissions was also three times higher and as a result, a comparison of results between these two cases and the wind tunnel measurements was made in order to qualitatively identify the impact of the source strength on dispersion. The calculated mean concentrations are presented as non-dimensional concentration K, via the following formula:

$$K = \frac{CU_{ref}H_{\max}{}^{2}}{Q_{emitted}} \qquad (2)$$

where C is the calculated concentration in kgm^{-3}, U_{ref} is the reference wind speed in ms^{-1} and H_{max} is the height of the VIP container in m and $Q_{emitted}$ is the massflow emitted from the source in kgs^{-1}. Figure 3 illustrates a qualitative comparison of the calculated non-dimensional concentration fields at a horizontal level at half the height of the containers, between the first and the second cases. The comparison reveals small differences in the horizontal growth of the plume between the two cases. More specifically, emitted pollution in the first case spreads over a smaller region compared to the second case. Furthermore, the direction of the calculated growth of the plume between the two cases also presents a difference, with the plume in 2nd case forming a steeper angle with respect to the longitudinal axis, compared to the corresponding angle of the plume in the 1st case.

A similar comparison between the second and the third cases did not reveal any significant differences in the horizontal growth of the plume and therefore these results are not shown here. Although there is no evidence to support why these differences in the plume growth between the two cases exist, the fact remains that compared to the second and third cases, depending on the distance from the source, the predicted non-dimensional concentrations from the simulation with the point source show larger deviations from the wind tunnel measurements compared to the two simulations with the area sources. Figure 4 shows a comparison between the predicted concentrations for the three cases which have been simulated and the wind tunnel measurements. The comparison takes place at horizontal profiles along the longitudinal axis of the domain (Y) which extend from the origin of the coordinate system at the centre of the domain close to the VIP car towards the negative lateral direction. Four locations towards the positive direction of the longitudinal axis have been selected, namely at distances from the source of 35 m, 65 m, 87.5 m and 102.5 m.

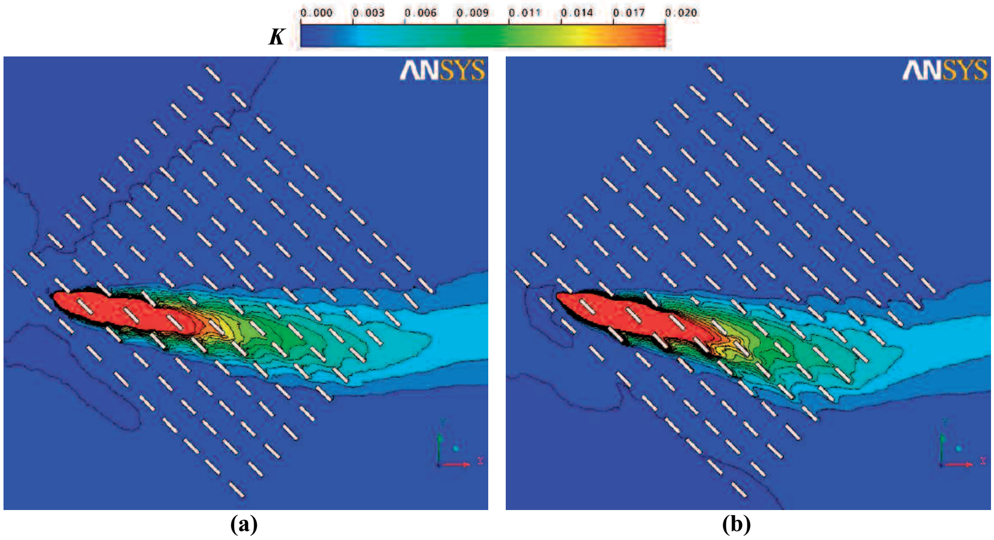


Figure 3. Horizontal plume growth at z = 1.25 m for (a) point source case and (b) for an area source case.

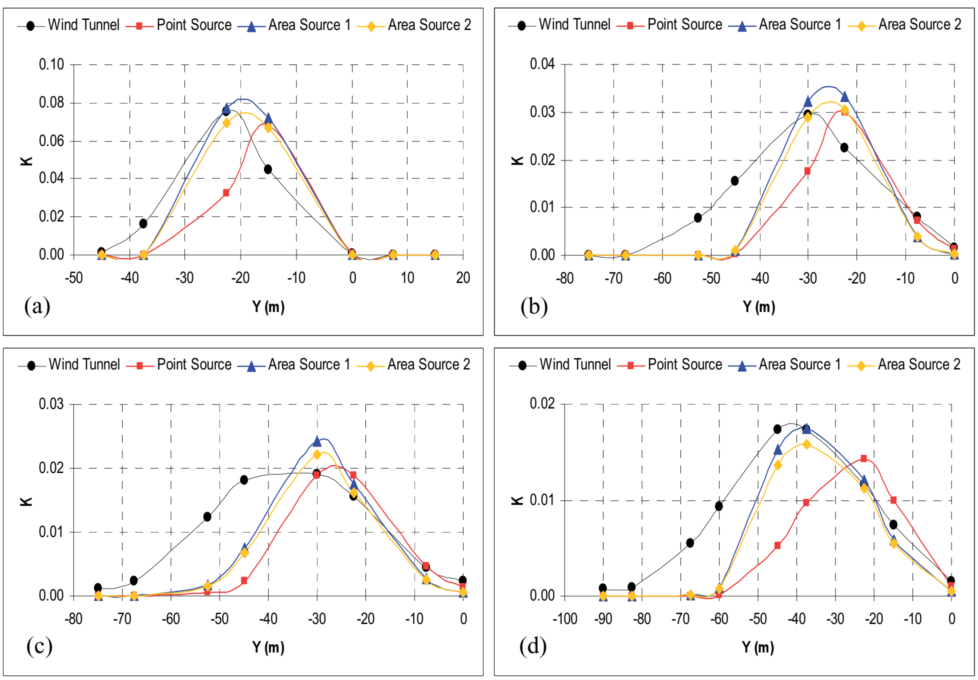


Figure 4. Non-dimensional concentrations along the x- axis of at distances of (a) 0 m, (b) 15 m, (c) 30 m and (d) 67.5 m from the source.

The results shown in Figure 4 show that compared with the two area source cases, the first case presents the larger disagreement with the wind tunnel measurements at all locations and in particular away from the source. It should be borne in mind that in the first case the source was treated as a point source, while in the other two cases as an area source, with significant mesh refinement near the boundaries of the source. Therefore, the fact that close to the source the second and third cases have performed better could be attributed to a more uniform diffusion of the pollutant mass to the area near the immediate vicinity of the source.

Furthermore, it should be noted that in all three cases the disagreement with the wind tunnel results is smaller closer to the source and that it increases depending on the distance from the source towards the direction of the plume growth. This could be attributed to the fact that as the flow progresses well inside the container array, the dispersion mechanism is dominated by the aerodynamic effects of the flow around the containers and the resulting generation of additional turbulence due to the interaction of the turbulent structures generated between consecutive containers (Hanna et al., 2002, Martilli and Santiago, 2007).

Finally, comparison of results between cases two (Area Source 1) and three (Area Source 2), shows that in the latter case the predicted non-dimensional concentration is closer to the wind tunnel measurements. The only difference between the second and third simulations lies in the vertical component of the exit velocity of the emissions: In the third case it was three times higher compared to that in the second case. Hence, emissions are dispersed more rapidly in the vicinity of the source, and as a result, although small, there is a slight underestimation of the predicted concentration levels between the numerical simulations and the wind tunnel results.

4. CONCLUSIONS

Within the frame of the current study we investigated the effect of the geometry of a source, the type of a source and the vertical component of the exit velocity on the results of CFD model simulations for urban dispersion problems. Comparison with wind tunnel measurements reveals that even when comparing non-dimensional concentrations, both the type of the source and the prescribed source strength can have an influence of the numerical results.

However, it is indeed possible to at least partially improve the performance of CFD models for urban dispersion problems by applying proper modelling techniques for the sources under consideration, both taking into consideration the actual geometrical characteristics of the source and refining properly the mesh close to the source boundaries.

Last but not least, further investigation of this particular problem is deemed necessary, in order to establish specific standard set of guidelines for modellers and enhance the capabilities of CFD models for urban dispersion problems.

Acknowledgements: *The authors greatly acknowledge support from COST Action 732.*

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