MUST EXPERIMENT SIMULATIONS USING CFD AND INTEGRAL MODELS

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ABSTRACT

Flow patterns around buildings have a strong influence on pollutant dispersion in urban areas. Computational Fluid Dynamics (CFD) methods are increasingly used to provide solutions to the fundamental fluid dynamics equations at spatial scales smaller than the typical urban ones. CFD models are frequently used to predict concentration fields near buildings in an operational context, but validations are still needed. Gaussian-type modelling still is the most used and reliable tool for the prediction of pollutant concentration in urban areas. In this paper, we compare CFD numerical simulations provided by FLUENT with predictions from the well validated Gaussian-type model ADMS-Urban. In particular, we analyse the effect on dispersion due to the presence of a buildings array as performed in the MUST experiment.

INTRODUCTION

Air quality is one of the main concern in most cities. This has lead to the development of suitable atmospheric dispersion models that can be easily used for urban air quality management (*Holmes, N. and L. Morawska*, 2006). Integral flow and dispersion models belong to that class of models which have been widely used for regulatory purposes. This is because of their low computational time, their requirements for routinely available input data, and more importantly for their possibility of accounting for a large number of emission sources. Computational Fluid Dynamics (CFD) models have recently received much attention as they allow to consider the effect of complex building arrangements and morphology. Up to now, CFD model applications to large urban dispersion studies are isolated cases. Limited work has been done to check the performance of these kinds of models for routine air pollution studies and still there is not in place a standardization of modelling practise for atmospheric applications. During our research experience, we have compared predictions from the commercial code FLUENT (*FLUENT 6.2*, 2005) with wind tunnel data and results from the well-validated commercial atmospheric dispersion model ADMS-Urban (*CERC*, 2006). We have investigated flow and dispersion from point and line sources in different configurations from the simplest boundary layer to isolated street canyons and small groups of buildings (*Di Sabatino, S. et al.*, in press). We have found that the standard *k-e* model within FLUENT reproduces well the flow pattern in street canyons, while dispersion predictions in street canyons tend to overestimate both wind tunnel measurements and ADMS-Urban concentration results. Thus, CFD calculations may require a lower turbulent Schmidt number (Sc_t) to increase plume dispersion. Here we extend the analysis to the effect on dispersion due to the presence of building arrays with two different frontal area density, by simulating the MUST (Mock Urban Setting Test) field experiment (*Yee, E. and C.A. Biltoft*, 2004). The objective is to evaluate the performance of CFD model, to compare results with an operational urban dispersion model and to suggest an approach for the two widely used commercial codes of different nature when used in urban air quality studies.

THE BUILDING ARRAY CONFIGURATION

The building array considered here consists of 120 standard size shipping containers set up in a nearly regular array of 10 by 12 obstacles. This set up is the same of the Mock Urban Setting Test (MUST) experiment (Fig. 1), an extensive field campaign carried out on a test site of the US Army in the Great Basin Desert in 2001. We modelled the exact geometry in

GAMBIT. Table 1 summarizes the grid and the computational domain extent used for the CFD simulations, based on the verification and validation assessment performed in *Buccolieri, R. and S. Di Sabatino* (2007). Two wind directions are considered (0° and -45°) as approaching flow conditions. For both cases, the wind direction has been aligned along the x-axis; so that for the -45° approaching flow case the geometry has been opportunely rotated. As pollutant concentration results were not still available, we choose to "activate" the point source (1.8 m high) shown in Fig. 1 (labelled with source 29 in the MUST wind tunnel data documents available from the COST 732 Action).

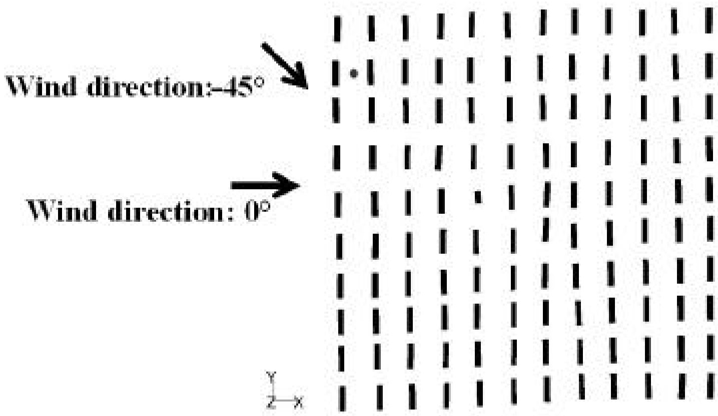

Fig. 1; Schematic view of the experimental setup. The point source is positioned along the axis of the first street canyons line.

Table 1. Computational domain and grid used in CFD modelling. L: distance from the inlet plane to the first buildings, Y: distance above the ground, H_{max}=3.51m: height of the tallest building. d_{xmin}, d_{ymin} and d_{zmin} refer to the size (normalised with H_{max}) of the smallest grid spacing in x, y and z directions, respectively

Domain	L	O	Y
	$5H_{max}$	$15H_{max}$	$5H_{max}$
Grid	Cells	d_{xmin} d_{ymin}	d_{zmin}
	~1.300.000	0.28	0.05

DISPERSION MODELLING

FLUENT setup

Simulations are carried out by considering a neutral boundary layer. We use the same inlet conditions as in *Buccolieri, R. and S. Di Sabatino* (2007) for the inlet wind speed, turbulent kinetic energy and dissipation rate profiles, specified as follows:

$$\frac{U(z)}{U_{ref}} = \frac{u_*}{k}\ln\left(\frac{z}{z_0}\right) \qquad (1)$$

$$k = \frac{u_*^{\,2}}{\sqrt{C_m}} \qquad (2)$$

$$e = \frac{u_*^{\,3}}{k(z+z_0)} \qquad (3)$$

where *U(z)* is the average wind speed at the height *z* above the ground, U_{ref} =5.5 m/s is the reference wind speed (undisturbed flow), z_0=0.017 m (only upwind ground floor) is the roughness length, u_*=0.36 m/s is the friction velocity, C_μ=0.09 is a coefficient used to define the eddy viscosity in the *k-e* model and *k* is the von Karman's constant. The remaining boundary conditions (surface roughness representation, symmetry conditions etc.) are those specified in *Di Sabatino, S. et al.* (in press). For dispersion simulations we use the advection-diffusion (AD) module. In FLUENT the diffusion term in the pollutant transport equation is modelled using

$$J = -\left(rD + \frac{m_t}{Sc_t} \right) \nabla Y \qquad (4)$$

where D is the diffusion coefficient for the pollutant in the mixture, $\mu_t=½(C_\mu k^2/e)$ is the turbulent viscosity, Y is the mass fraction of the pollutant, r is the mixture density. $Sc_t=\mu_t/(½D_t)$ is the turbulent Schmidt number, where D_t is the turbulent diffusivity. The source has been simulated by separating a volume in the geometry at the required discharge position and by setting a source term for this volume. The emission rate Q is set at 10g/s; mean concentrations are expressed as dimensionless values K which are defined as:

$$K = \frac{CU_{ref}H_{ref}^{\ 2}}{Q} \qquad (5)$$

where C is the calculated concentration.

ADMS-Urban setup

To simulate the point source in ADMS-Urban we used the same emission rate Q =10g/s used in FLEUNT. To model this case we do not explicitly model the individual buildings as in CFD modelling, but we replace the area occupied by the buildings with a single value of surface roughness. We use the same z_0=0.017m as in the CFD modelling in the area upwind of the array of buildings, while we use z_0=0.094m and z_0=0.269m in the area occupied by the array for the 0° and the -45° approaching flow cases, respectively. These values of z_0 are calculated using the morphometric method proposed by *Macdonald, R.W. et al.* (1998) using the following equations (6) and (7):

$$\frac{z_d}{H} = 1 + a^{-l_p}(l_p - 1) \qquad (6)$$

$$\frac{z_0}{H} = \left(1 - \frac{z_d}{H}\right) \exp\left\{ -\left[0.5b \frac{C_D}{k^2} \left(1 - \frac{z_d}{H}\right) l_f \right]^{-0.5} \right\} \qquad (7)$$

where equation (6) indicates the zero-plane displacement height normalized with the building height H, C_D is the drag coefficient (1.2), a is an empirical coefficient (4.43) and ß a correction factor for the drag coefficient (1.0). l_p and l_f are the plan area index and the frontal area index, respectively. The estimated value of l_p for our case is 0.095. While l_p is independent of the incident wind direction, l_f is not. For the 0° approaching flow case l_f has been estimated to be equal to 0.101, while the estimated value of l_f for the -45° approaching flow case is equal to 0.085. This has been calculated by projecting the frontal areas of the buildings along the wind direction axis. We refer to those flow configurations as the larger frontal area density (0° approaching flow case) and as the lower frontal area density (-45° approaching flow case).

RESULTS

We analyse the dispersion from a point source focusing on the effect of the l_f parameter due to the change of incident wind direction on the same MUST building array. Overall, CFD simulations of plume spread and horizontal concentrations match ADMS-Urban predictions.

Fig. 2 shows the horizontal profiles (along the x axis) of the dimensionless concentration K for the larger frontal area density case (left) and for the lower frontal area density one (right) plotted at z=1.5H. We note that FLUENT concentration results are consistent with ADMS-Urban results both qualitatively and quantitatively. In particular, for the lower frontal area density case FLUENT results obtained with Sc_t=0.7 are in good agreement with ADMS-Urban ones. When l_f increases (larger frontal area density case), a value of Sc_t=0.4 in FLUENT modelling seems to be the most appropriate choice, as the CFD results agree better with ADMS-Urban. Fig. 3 shows contour plots obtained from ADMS-Urban (left) and FLUENT (right) at the same height. For these cases we used Sc_t=0.7 for the lower frontal area density and Sc_t=0.4 for the larger frontal area density, for which again it has been necessary to increase diffusion in the CFD model to achieve a closer agreement with ADMS-Urban.

CONCLUSIONS

In this paper, we presented two different approaches for modelling the pollutant dispersion from a point source within complex geometries. We used a building-resolving CFD model (FLUENT) which simulates detailed features of urban flow, such as urban canyon effects and in-canyon eddies. We analysed its performance in comparison with the performance of the well validated integral atmospheric dispersion model ADMS-urban. CFD model run time requirements have been much larger than the ADMS-urban ones. An important goal of this work was to provide useful suggestions for the use of general-purpose CFD models in the operational context. Also it intended to contribute to the development of helpful guidelines to support future application of CFD code for simulating pollutant dispersion in large cities. In particular we investigated dispersion characteristics in terms of the l_f parameter. This study further showed that an important model parameter is the turbulent Schmidt number, which characterizes the relative diffusion of momentum and pollutant mass due to turbulence (*Flesch, T. et al.*, 2002). It is essential to choose the most adequate Sc_t, even if it is difficult to assign a specific value for dispersion in presence of various building arrangements. Nevertheless, we found that a good agreement between the CFD and the integral model is achieved by using a turbulent Schmidt number of 0.7 for the lower frontal area density case (l_f=0.085) and 0.4 for the larger frontal area density one (l_f=0.101). Our results also suggests that the application of the *k-e* turbulence model seem to be satisfactory to simulate plume dispersion within complex geometries. However, the CFD modelling in routine atmospheric studies could become common after establishing a standard practice guideline and using and parallel computing.

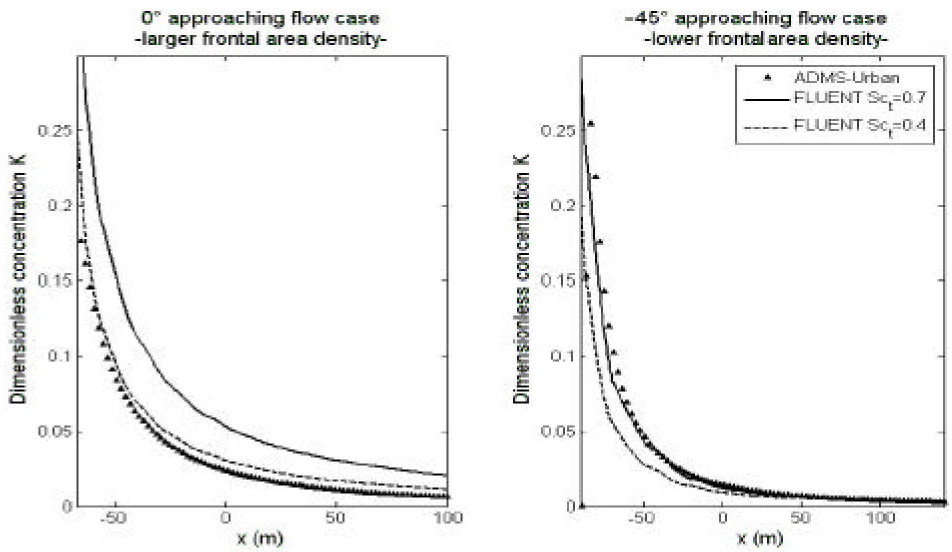

Fig 2; Dimensionless concentration horizontal profiles at z=1.5H.

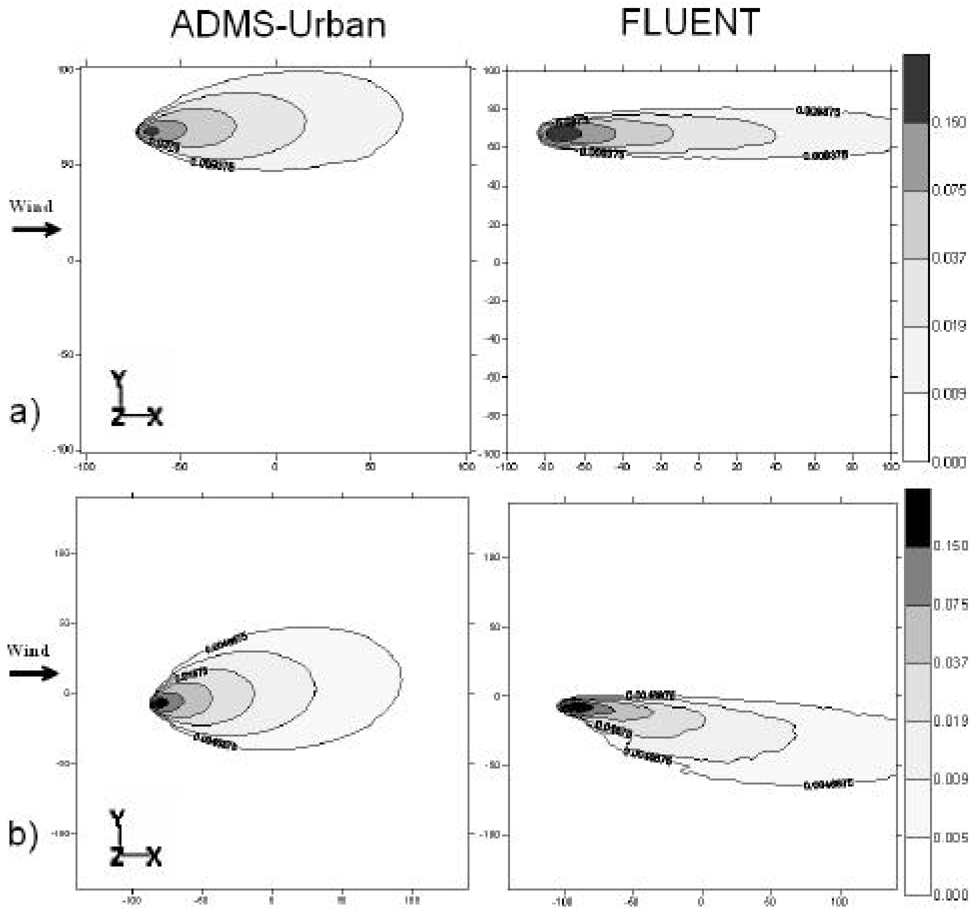

Fig 3; Contours of dimensionless concentrations at z=1.5H. The wind originates along the positive x axis. a) 0° approaching flow case (l_f = 0.101), b) -45° approaching flow case (l_f=0.085).

REFERENCES

Buccolieri, R. and S. Di Sabatino, 2007: Flow and pollutant dispersion in urban arrays for the standardization of CFD modelling practise. *Proc. 11th conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Cambridge, UK, July 2-5.*

CERC, 2006: ADMS-Urban, USER Guide. *Available from Cambridge Environmental Research Consultants, Cambridge, UK.*

Di Sabatino, S., R. Buccolieri, B. Pulvirenti and R. Bitter, in press: Flow and pollutant dispersion modelling in street canyons using Fluent and ADMS-Urban. *Environmental Modelling & Assessment.*

Flesch, T., J. H. Prueger and J. L. Hatfield, 2002: Turbulent Schmidt number from a tracer experiment. *Agricultural and Forest Meteorology*, **111**, 299–307.

FLUENT 6.2, 2005: User's Manual. *http://www.fluent.com.*

Holmes, N. and L. Morawska, 2006: A review of dispersion modelling and its application to the dispersion of particles: An overview of different dispersion models available. *Atmospheric Environment*, **40**, 5902–5928.

Macdonald, R.W., R.F. Griffiths and D.J. Hall, 1998: An improved method for estimation of surface roughness of obstacle arrays. *Atmospheric Environment*, **32**, 1857-1864.

Yee, E. and C.A. Biltoft, 2004: Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. *Boundary Layer Meteorology*, **111**, 363-415.