CFD simulation of heavy pollutants in urban areas: the case study of Messina

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1. Introduction

In many instances hazardous materials are to be transported across urban areas, e.g. with road tankers or railway tanks, as no viable alternatives exist. The high threat to human health that may result makes it important to develop methods for its quantification and assessment. Due to the semi-confined nature of the dispersion site (a network of city roads with buildings on their sides) simplified models are unsuitable. The problem then arises of developing complex models in order to quantify the extent of the area affected by dangerous concentrations during cloud dispersion.

Among the others, Computational Fluid Dynamics (CFD) has the potential to provide realistic simulations for geometrically complex scenarios (Scargiali *et. al*. 2005, Gilham *et al*. 2000, M.A. McBride *et al*., 2001) since the heavy gas dispersion process is described by basic conservation equations with a reduced number of approximations.

In a recent work an effective simulation procedure for dense cloud dispersion able to exploit a general purpose CFD code has been developed and applied to a simplified geometry mimicking a urban canopy (Scargiali *et al*. 2008). Results confirmed that the presence of buildings strongly affects the dispersion phenomenon. In particular, comparative results obtained by neglecting the real geometry, i.e. assuming the terrain to be flat, were found to be conservative from the point of view of maximum ground concentrations (which were slightly overestimated), but not from that of the area interested by the release (which was greatly underestimated).

In the present work the same CFD model is applied to the simulation of heavy pollutants dispersion in a real urban canopy, namely the "Viale Boccetta" of Messina located in Sicily (Italy), with the aim of showing the potential and drawbacks of CFD tools for the above detailed risk assessments.

Notably the territory of Sicily is characterised by a high concentration of chemical plants, mainly petrochemical and refineries, for this reason it is an area with a great risk of industrial accidents; in addition to this there are several natural risk sources. There is an over-production of chemicals compared to the regional needs, for this reason a large part of these substances is exported and thus the region is characterised by an inflow of raw materials and an outflow of final products. As a consequence there are urban areas subject to an intense traffic of hazardous materials, an example is the city of Messina due to its geographical location. In the past years

many researcher (Milazzo *et al. 2002,* Antonioni *et al. 2004*) have been directed towards the risk analysis in the transports of dangerous substances and, in particular, towards the use of risk analysis methodologies as a support for territorial management. Milazzo *et al. 2002* show the problem associated with the transport of toxic substances, in particular when an a release happens in an urban area.

2. Numerical simulation

The constitutive equations solved during the simulation runs are the Reynolds-averaged mass, momentum and scalar transport equation. These can be written in conservation form as:

$$\frac{\partial \rho}{\partial t} = -\left(\nabla \cdot \rho \mathbf{U}\right) \tag{1}$$

$$\frac{\partial \rho \mathbf{U}}{\partial t} = -\left[\nabla \cdot \rho \mathbf{U}\,\mathbf{U}\right] - \nabla p + \nabla \cdot \left[\rho\left(\nu + \nu_t\right)\left(\nabla \mathbf{U} + \left(\nabla \mathbf{U}\right)^T\right)\right] + \rho \mathbf{g} \tag{2}$$

$$\frac{\partial \rho Y}{\partial t} = -\nabla \cdot \rho \mathbf{U} Y + \rho\left(D + \frac{\nu_t}{\sigma_Y}\right)\nabla^2 Y \tag{3}$$

The turbulent kinematic viscosity ν_t is obtained from the Prandtl-Kolmogorov equation:

$$\nu_t = C_\mu \frac{k^2}{\varepsilon} \tag{4}$$

where k (turbulent kinetic energy) and ε (its dissipation rate) are computed by solving appropriate transport equations:

$$\frac{D\rho k}{Dt} = \nabla \cdot \left[\rho\left(\nu + \frac{\nu_t}{\sigma_k}\right)\nabla k\right] + \rho\left(G + G_k\right) - \rho\varepsilon \tag{5}$$

$$\frac{D\rho \varepsilon}{Dt} = \nabla\left[\rho\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + C_1 \frac{\varepsilon}{k}\rho\left(G + C_3 G_k\right) - C_2 \rho \frac{\varepsilon^2}{k} \tag{6}$$

Here, G is turbulence production due to shear whereas G_k is turbulence generation associated with buoyancy, which in the k-ε model are usually expressed as:

$$G = \rho \nu_t \nabla \mathbf{U} \cdot \left(\nabla \mathbf{U} + \left(\nabla \mathbf{U}\right)^T\right); \qquad G_k = -\frac{\nu_t}{\sigma_k} g \nabla \rho = -\frac{\nu_t}{\sigma_k} \alpha \rho_a g \nabla Y \tag{7}$$

where $\alpha = (\rho_Y - \rho_a)/\rho_a$ is a density coefficient due to concentration, ρ_Y and ρ_a being the densities of the dense gas and background fluid, respectively.
The parameter values used in all simulations are as follows:

$C\mu = 0.09$; $C_1 = 1.44$; $C_2 = 1.92$; $C_3 = 0.50$; $\sigma_k = 1.0$; $\sigma_\varepsilon = 1.3$

The so called "weakly compressible approximation" (CFX 4.4 User Manual, 1999) was adopted for the buoyancy treatment instead of the simpler Bussinesque simplification employed elsewhere (Scargiali *et al*. 2005), in view of the strong density gradients in the proximities of the dense plume. The main hypothesis behind this approximation is that density variations are related only to the mean molecular weight and/or temperature changes in the fluid, while density is assumed to be independent of the pressure field. Density is in practice expressed by the following equation of state:

$$\rho = \frac{P_{ref} W_m}{RT} \tag{8}$$

Hence a constant reference pressure is assumed for the estimation of fluid density; as a consequence, no sound waves are possible (i.e. sound speed is infinite). Also the fluid kinetic energy is assumed to be negligible with respect to its internal energy, and any transfer between kinetic and internal energy is ignored. This is achieved by ignoring the kinetic term in the total enthalpy. The reference pressure P_{ref} was always set at 1 atm in the present case.

The dense gas dispersion model here adopted has already been validated by comparison with literature experimental data (Scargiali *et al*., 2004a). The simulations there performed concerned the experiments carried out by Ayrault *et al*., 1998, in an atmospheric wind tunnel. Simulation results were found to correctly predict the swap from the Gaussian profile characterizing neutrally buoyant dispersions and the bi-modal pattern experimentally observed with negatively buoyant plumes. This remarkably good agreement between simulation results and experiment may be regarded as a confirmation of the model soundness.

3. Simulation procedure

A sketch of Messina Map, including Viale Boccetta is reported in Fig. 1. The whole avenue is about 2 km long and presents a slight slope between 5 – 7 % depending on the specific zone. In order to obtain a satisfying discretization of the computational domain only a portion of the entire map had to be chosen as area of interest for the simulation exercise (black square in Fig. 1) as trying to include the entire area in a sole computational domain would have required an unusual large number of cells.

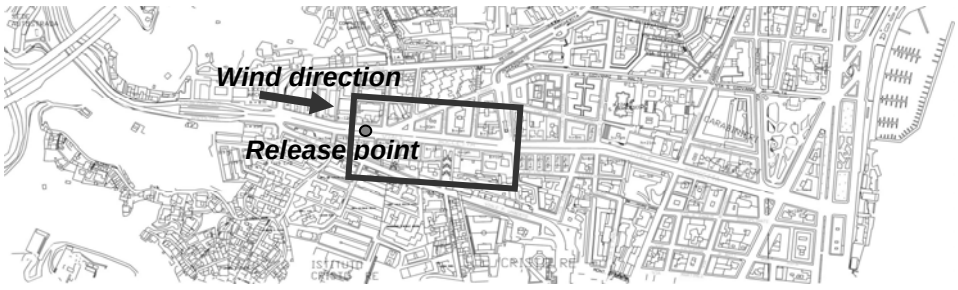

Fig. 1: *Messina, Viale Boccetta plan.*

This area allows simulating the dispersion dynamics of a heavy pollutant in the first minutes after the release highlighting possible critical areas of gas stagnation or preferential escape routs. It becomes clear that an in-depth study of the whole site would include the subsequent simulations of more than one sub-area depending on of wind speed, wind direction and the release point.

The computational grid employed was denser to the ground and encompassed 163x46x44 = 329 912 cells. The minimum cell size was 2x2x1m in the volume between the buildings with the total volume of the computational domain 350x92x210 m^3 (Fig. 2). In order to reproduce the 7 % slope of the site, the gravity vector was suitably inclined in the *x*-*z* plane. The simulation of each release event was conducted in two steps: (i) the first step was devoted to the generation of the flow field before the release, (ii) the second step dealt with the heavy pollutant release simulations.

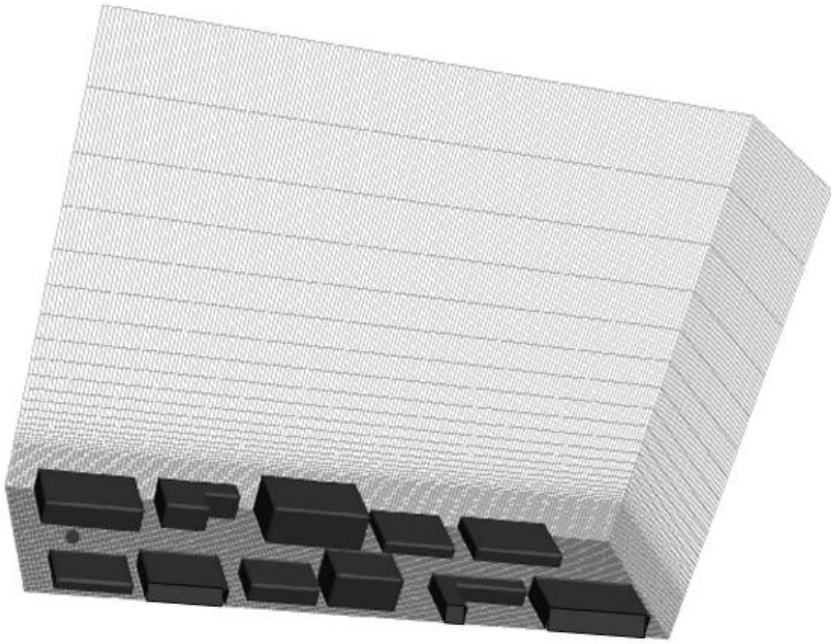

Fig. 2: Computational grid

3.1 Before release flow-field simulations

The before-release simulations were conducted in order of obtaining a fully developed wind-field which took into account the presence of all the other buildings surrounding the computational domain. This was obtained by imposing appropriate boundary conditions to the computational domain. In particular, periodic boundary conditions were imposed on the two vertical planes orthogonal to wind direction, thus mimicking the repetition of an identical geometry behind and in front of the computational domain. For the same reason the remaining two vertical planes (parallel to wind direction) were set as symmetric planes. Wall boundary conditions were imposed on all solid surfaces while a constant wind speed of 5 m/s was imposed at the

top boundary of the domain, i.e. 210 m above ground level. The simulations were carried out in steady state conditions for 15000 iterations to guarantee that fully converged results had been achieved. The "first-step" procedure here adopted has already been validated by comparison with literature experimental data (Scargiali *et al.* 2004, 2008). The simulations there performed concerned the experiments carried out by Hanna *et al.*, 2002 in a water channel with a scaled down geometry with the same area coverage and normalized buildings height. Simulation results were found to predict very well the experimental vertical velocity profiles both in the wake behind buildings and in the gap between buildings.

3.2 Simulation of pollutant release and dispersion

The flow and turbulence fields predicted in the first step of the simulation procedure were used as initial and inlet boundary conditions for the heavy pollutant dispersion simulations in the same domain. At the downstream boundary, a "mass flow" boundary condition was specified, which fixes the total mass outflow to be the same as that entering the domain from all sources. At the two lateral vertical sizes of the domain, symmetry conditions were specified, which constrain the bulk flow to be parallel to the lateral boundaries at the locations. At the upper surface of the domain, quite far from ground level, a symmetry condition was also specified, to ensure that velocity stayed horizontal through the simulation and that all quantities had zero gradients across the boundary. The simulations of after-release chlorine dispersion process were carried out in transient conditions until the gas cloud had exited the computational domain. The time step was chosen in order to obtain in all cells a Courant number smaller than one. The heavy pollutant suddenly released was assumed to be chlorine which has a molecular weight 2.5 times that of air. The instantaneous quantity of chlorine released was assumed to be 100 kg.

4. Results and discussion

4.1 Before release flow-field

Examples of vector plots obtained respectively over a horizontal plane 5 m above ground level and on a vertical plane across the right row of buildings, are reported in Figs. 3 and 4 respectively.

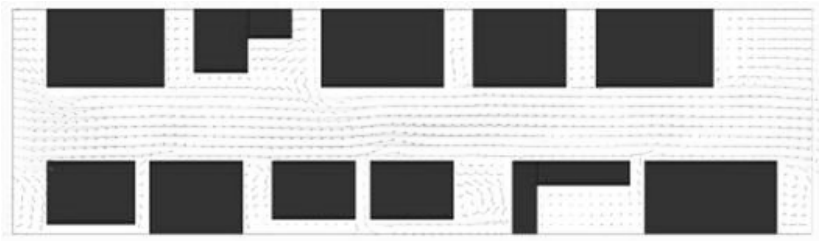

Fig. 3: Vector plot over a horizontal plane 5 m above ground level.

As it can be seen, simulations highlight the presence of flow recirculation rings between subsequent buildings both in the vertical plane and in the horizontal plane, a characteristic that is bound to affect the dispersion process. Typical values for the velocity module between buildings are between 0.25 - 2 m/s while in the lateral streets is of the order of 0.5 m/s.

4.2 Heavy pollutant dispersion

The simulation results obtained are reported in Fig. 5 as three dimensional views of iso-surfaces of chlorine concentration at defined time steps, namely 10, 60, and 300 seconds after the release. The outer iso-surface refers to a chlorine concentration in air of 25 ppm wt. This surface may be regarded as a safe external cloud boundary in view of the reference concentration of ~25 ppm wt (10 ppm vol), which is currently considered as "Immediately Dangerous to Life or Health" (IDLH) by the NIOSH (Pocket Guide to Chemical Hazards,1997).

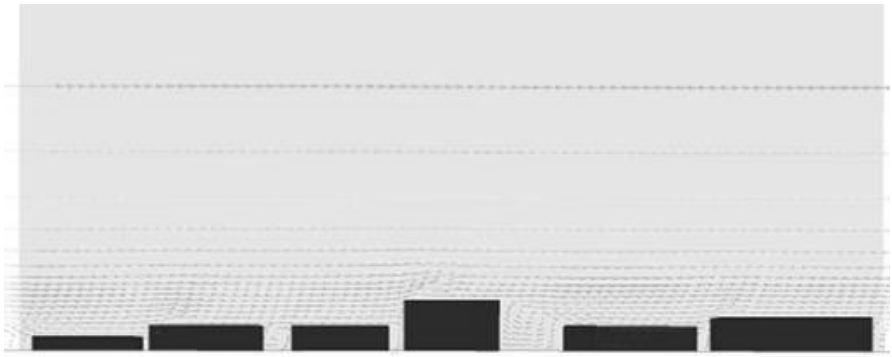

Fig. 4: Vector plot on a vertical plane across the right row of buildings.

As it can be seen, shortly after the release (Fig. 5 *a* and *b*), the cloud is homogeneously dispersed by turbulence while is slowly advected horizontally between the buildings due to the low velocities present there. Above the buildings the advection is much faster due to the higher wind velocities. This results in the unobvious shape observable after 30 s (Fig. 5 *c*). The cloud portions that emerge above the buildings are much faster advected due to the higher horizontal velocities there present (Fig. 4) resulting in somewhat unexpected cloud shapes visible in Figs. 5 *c – e*. After 5 minutes (Fig. 5 *f*), cloud core has already gone over the computational domain, though zones with a chlorine concentration higher than the IDLH are still present in side streets.

5. Conclusions

A simulation procedure for dense cloud dispersion able to exploit a general purpose CFD codes has been applied to the real urban canopy of Messina.

Results indicate that the presence of buildings strongly affects the dispersion phenomenon, as expected. The results obtained in this work may be employed for the assessment of risk mitigation strategies, and/or for the production of “pseudo

experimental" data aimed at analyzing and validating the simplified models available in the open literature.

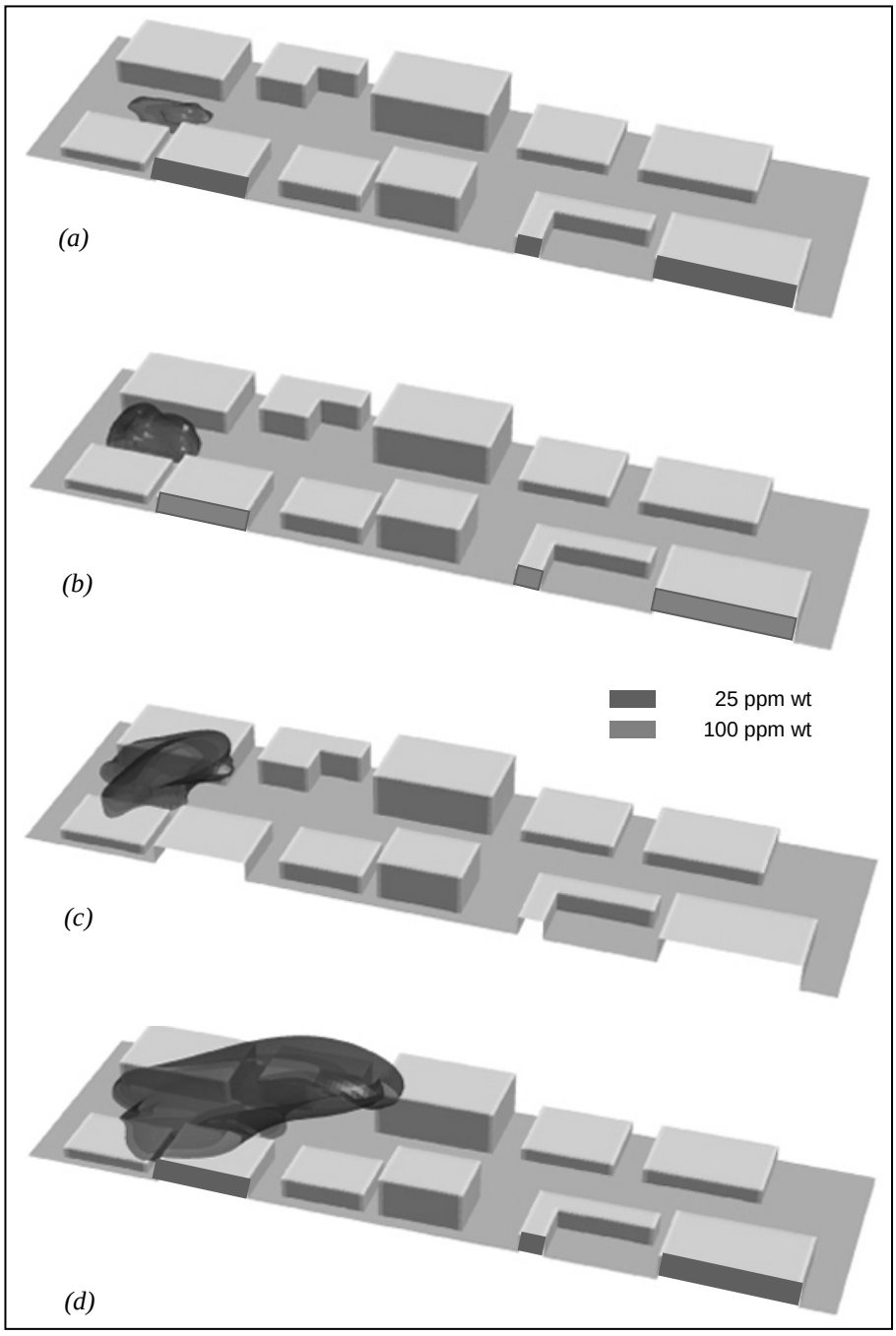

Fig. 5: a- d (continues in next page)

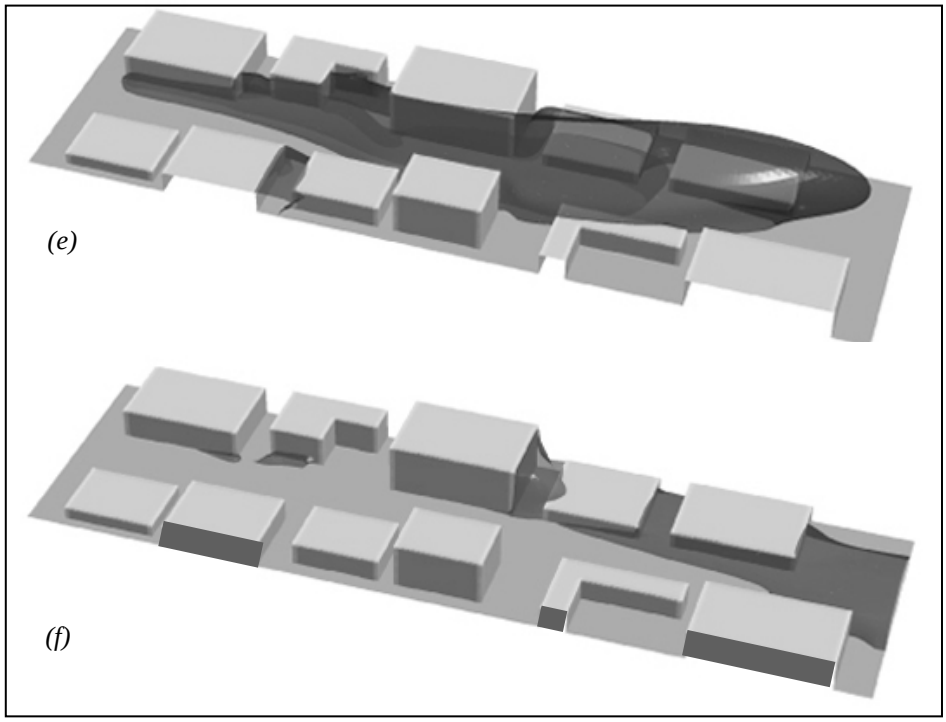

Fig. 5: Constant Chlorine concentration iso-surfaces at 1 (a), 10 (b), 30 (c), 60 (d), 180 (e) and 300 (f) seconds after the release

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