Journal of Hazardous Materials 197 (2011) 285–293

Contents lists available at SciVerse ScienceDirect

Journal of Hazardous Materials

journal homepage: www.elsevier.com/locate/jhazmat

Modeling and simulation of dense cloud dispersion in urban areas by means of computational fluid dynamics

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ARTICLE INFO

Article history:
Received 6 July 2011
Received in revised form
21 September 2011
Accepted 22 September 2011
Available online 29 September 2011

Keywords:
Heavy clouds
Urban canopy
CFD
Dispersion modeling
Complex terrain

ABSTRACT

The formation of toxic heavy clouds as a result of sudden accidental releases from mobile containers, such as road tankers or railway tank cars, may occur inside urban areas so the problem arises of their consequences evaluation.

Due to the semi-confined nature of the dispersion site simplified models may often be inappropriate.

As an alternative, computational fluid dynamics (CFD) has the potential to provide realistic simulations even for geometrically complex scenarios since the heavy gas dispersion process is described by basic conservation equations with a reduced number of approximations.

In the present work a commercial general purpose CFD code (CFX 4.4 by Ansys®) is employed for the simulation of dense cloud dispersion in urban areas. The simulation strategy proposed involves a *stationary pre-release* flow field simulation followed by a *dynamic after-release* flow and concentration field simulations.

In order to try a generalization of results, the computational domain is modeled as a simple network of straight roads with regularly distributed blocks mimicking the buildings. Results show that the presence of buildings lower concentration maxima and enlarge the side spread of the cloud. Dispersion dynamics is also found to be strongly affected by the quantity of heavy-gas released.

1. Introduction

Heavy clouds are gaseous mixtures of air and hazardous materials characterized by a density larger than the environment. The dispersion dynamics of such negatively buoyant mixtures can be quite different from that of neutrally or positively buoyant mixtures, depending on the initial cloud Richardson number R_{i0}, as gravity keeps them close to the ground where the threat to human safety is highest. R_{i0} is dependent on the initial cloud mass or the mass flux, the relative density excess of the cloud, the representative size of the cloud, and the ambient wind speed.

Quantitative risk analysis for loss prevention purposes demands successful simulation of possible accidental events, which is usually carried out by means of simplified empirical models. For example the so-called "box-models" developed in the past (SLAB, DEGADIS) are widely used in risk analysis procedures [1,2]. Although they show satisfactory agreement with available field observations at several sites, including some with obstacles [3] these models would have problems in areas with large terrain obstacles especially when the irregular topography of the site plays an important role [4–6]. This is the case of toxic heavy cloud formation inside urban areas, as a result of sudden accidental releases from mobile containers, such as road tankers or railway tank cars.

In this field, computational fluid dynamics (CFD) may provide the answer as it allows the simulation of complex physical processes by describing heat and mass transport phenomena with fully developed mathematical models. CFD simulations of pollutant dispersions in the atmospheric boundary layer (ABL) have been carried out in the past using the k–ε turbulence model with encouraging results both for neutrally buoyant pollutants [7] and for heavy gas dispersion processes [8–10]. Koopman and Ermak [11] reported a comprehensive review of the methodologies available to describe the dispersion of liquefied natural gas (LNG) in the ABL and stated that "Navier–Stokes models provide the most complete description of the flow and dispersion of cold, denser than air cloud in the atmosphere and are well suited for ... dispersion simulations over complex terrain".

As concerns gas dispersions in confined or semi-confined areas, CFD tools have been largely applied to describe neutrally buoyant pollutant dispersions inside urban canopies, using both RANS [12–15] and Large Eddy Simulations [16,17], or to assess a building canopy model for urban climate planning [18–20].

CFD techniques were also used to model the release and mixing process of a dense gas within buildings using RANS [5,6,21–23] and

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doi:10.1016/j.jhazmat.2011.09.086

Nomenclature

BRFFS	Before-Release Flow Field Simulation
C_1	parameter in k–ε model (Eq. (6)), dimensionless
C_2	parameter in k–ε model (Eq. (6)), dimensionless
C_3	parameter in k–ε model (Eq. (6)), dimensionless
C_μ	constant in k–ε model (Eq. (4)), dimensionless
CRDS	Cloud Release and Dispersion Simulation
D	molecular diffusivity of chlorine in air, $m^2\,s^{-1}$
G	turbulence production due to viscous forces, $J\,m^{-3}$
G_k	turbulence production due to buoyancy forces, $J\,m^{-3}$
H	buildings height, m
IDLH	concentration "Immediately Dangerous to Life or Health", ppm
P_{ref}	reference pressure, Pa
R	ideal gas constant, $Pa\,m^3\,K^{-1}\,kmol^{-1}$
S	buildings face to face distance, m
T	temperature, K
$\mathbf{U}$	vector of velocity field, m/s
U_∞	wind velocity at 200 m above ground level, m/s
$\mathbf{U}_H$	wind velocity at top building height (H), m/s
U_x	wind velocity along wind direction (x), m/s
W	buildings width, m
M_w	mean molecular weight of the gas mixture, $kg\,kmol^{-1}$
Y	chlorine mass fraction, dimensionless
f	building fractional area coverage, dimensionless
$\mathbf{g}$	acceleration gravity, $m\,s^{-2}$
k	turbulent kinetic energy, $m^2\,s^{-2}$
p	pressure, $N\,m^{-2}$
x	distance from the release point, m

Greek symbols

ε	dissipation of turbulent kinetic energy, $m^2\,s^{-2}$
μ	viscosity, Pa s
μ_T	turbulent viscosity, Pa s
ν	kinematic viscosity, $m^2\,s^{-1}$
ν_t	turbulent kinematic viscosity, $m^2\,s^{-1}$
ρ	fluid density, $kg\,m^{-3}$
ρ_Y	dense gas density, $kg\,m^{-3}$
ρ_a	background fluid density, $kg\,m^{-3}$
σ_k	k–ε model parameters, dimensionless
σ_ε	k–ε model parameters, dimensionless
σ_Y	turbulent Schmidt number, dimensionless

LES [16,23]. Results showed reasonable agreement with flow field and gas dispersion experimental data, confirming that CFD may be an effective tool for understanding wind flow and tracer dispersion in urban areas.

The aim of the present work is that of setting up a CFD based simulation strategy for modeling dense (as well as neutrally buoyant) cloud dispersion in urban environments. The simulation strategy proposed involves a stationary pre-release flow field simulation followed by a dynamic after-release flow and concentration field simulations.

In order to generalize the results, the computational domain was modeled as a simple network of straight roads with regularly distributed blocks mimicking the buildings. Influence of building fractional area coverage and normalised height, wind velocity and release quantity on the dispersion phenomenon, was also investigated.

2. Numerical simulation

For all numerical simulations of the present work, advantage was taken from the use of the commercial CFD code CFX-4.4 by Ansys®.

2.1. Basic equations and buoyancy treatment

The simulation runs solve the Reynolds-averaged mass, momentum and scalar transport equations. If the k–ε model [24] is used for turbulence, these can be written as:

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

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

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

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:

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

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

Here, σ_k and σ_ε are turbulent Prandtl numbers for k and ε, respectively.

G is the turbulence production terms due to shear:

$$G = \rho \nu_t \nabla \mathbf{U} \cdot (\nabla \mathbf{U} + (\nabla \mathbf{U})^T); \tag{7}$$

whereas G_k is the turbulence production term associated with buoyancy. In the present case density gradients are practically entirely related to concentration gradients, as thermal gradients contribution is negligible in the relatively short (200 m) domain height. The relevant generation term was therefore computed as:

$$G_k = -\frac{\nu_t}{\sigma_k} g \nabla \rho = -\frac{\nu_t}{\sigma_k} \alpha \rho_a g \nabla Y \tag{8}$$

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 the "consensus" values for k–ε model:

$$C_\mu = 0.09; \quad C_1 = 1.44; \quad C_2 = 1.92; \quad C_3 = 0.50; \quad \sigma_k = 1.0;$$

$$\sigma_\varepsilon = 1.3$$

The so-called *weakly compressible* approximation (CFX 4.4 User Manual) was adopted for the buoyancy treatment instead of the simpler Boussinesq approximation employed elsewhere [8], 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:

$$\rho = \frac{P_{ref} M_w}{RT} \tag{9}$$

Hence a constant reference pressure is assumed for the estimation of fluid density; as a consequence, no sound waves are possible (*i.e.*