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CFD dispersion modelling for emergency preparadnes

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ABSTRACT

Chemical plants, storage houses, transportation, these are some of the most potential sites for accidental release of dangerous materials into the surroundings. After releasing such gas, it will disperse in air. Air quality models predict the transport and the turbulent dispersion of gases or aerosols after they are released into the atmosphere. The Computational Fluid Dynamic (CFD) approach has been taken that natural account for dispersion process in urban areas.

This paper provides a comparison of the results obtained by the FLADIS field experiments and the results of CFD modelling by Fluent 6.2. FLADIS experiments were carried out by the Risø National Laboratory. Experimental trials were done with pressure liquefied ammonia. Meteorological conditions and source strength were determined from the experimental data and simulated using the CFD approach. The initial two-phase flow of the released ammonia was also included. The liquid phase was modelled as droplets using discrete particle modelling, i.e. Euler–Lagrangian approach for continuous and discrete phases.

1. Introduction

Potentially hazardous gases are very common in industrial and also in domestic use. The term 'hazardous' means gas toxicity to the public or environment or flammability of the gas. These gases are usually stored in liquefied state at ambient temperature in highly pressurized vessels. If an accident happens and the stored gas is suddenly depressurized the resulting jet will consist of a gaseous vapour phase and a liquid phase containing particle droplets mixed with air. Concentrations of the released gas are then predicted by various types of models and the values obtained are used in the hazard and risk assessment studies or by authorities (e.g. fire department) in case of an accident.

The most used models are simplifications of the conservation equations for mass, momentum and energy. The models used in the mentioned area can be distinguished on basis of the density of the gas released into light gases (the density is equal to that of air) and heavy gases (the density is much higher than that of air). As an analytical solution for light gas dispersion, Gaussian models were derived from the diffusion equation and from observations made by the experimental work, i.e. the concentration of released gas is following the Gaussian distribution (Lees, 1996). The dispersion coefficients were derived from experiments (Barrat, 2001). Heavy gas dispersion was modelled mainly by box models. In a simple box model the gas is assumed to be a pancake-shaped cloud with properties uniform in the crosswind and vertical directions. The model contains relations describing the growth of the radius and height of an instantaneous release, or the crosswind width and height of a continuous release, presented for example in Spicer and Havens (1989). These simplifications do not allow to model complex geometries, they are derived for a flat plane geometry with no obstacles or for a two-dimensional model with a simple obstacle.

Another possibility is the CFD approach, i.e. simultaneous solution of balance equations (Eqs. (1)–(4)) of mass, momentum and energy (Bird, Stewart, & Lightfoot, 2002). The results obtained by CFD modelling are more accurate because the wind velocity is completely resolved in comparison to the simpler models where velocity is a single value or a function of height. This is clearer in an area with high obstacles. Using the CFD set of equations, any real hazardous situation including gas release in the presence of buildings can be modelled (Venetsanos, Huld, Adams, & Bartzis, 2003). Moreover, in the CFD model, the second phase can be included. The gaseous phase (air – toxic gas) is modelled by the mentioned balance equations, and the liquid phase (droplets generated by a sudden pressure drop of the superheated liquid) can be modelled by a multiphase approach. This means that the second phase is modelled by the same equations as the first phase or the droplets are modelled as discrete particles (Crowe, Sommerfeld, & Tsuji, 1998).

Numerical simulations are very important for the verification of models with measured data. Delaunay (1996) performed numerical simulations of tracer gas experiments carried out at Porte Maillot in Paris. Hanna, Hansen, and Dharmavaram (2004) used FLACS

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Notation

A_p	surface of droplet particle, m^2
c_p	specific heat capacity, $J\,kg^{-1}\,K^{-1}$
C	molar concentration, $mol\,m^{-3}$
C_o	observed concentration of ammonia, $mol\,m^{-3}$
C_p	calculated concentration of ammonia, $mol\,m^{-3}$
$C_{n,s}$	concentration of ammonia in liquid phase, $mol\,m^{-3}$
$C_{n,\infty}$	concentration of ammonia in gas phase, $mol\,m^{-3}$
D	diffusion coefficient, $m^2\,s^{-1}$
D_t	turbulent dispersion coefficient, $m^2\,s^{-1}$
d_p	diameter of droplet particle, m
G_k	generation of turbulence kinetic energy, $kg\,m^{-1}\,s^{-3}$
f	vapour fraction, 1
h	specific enthalpy, $J\,kg^{-1}$
Pr	Prandtl number, 1
Re	Reynolds number, 1
Nu	Nusselt number, 1
Sc	Schmidt number, 1
Ri	Richardson number, 1
H	thickness of the layer, m
S_m	mass source, $kg\,m^{-3}\,s^{-1}$
S_h	enthalpy source, $J\,m^{-3}\,s^{-1}$
S_u	momentum source, $kg\,m^{-2}\,s^{-2}$
S_n	species source, $kg\,m^{-3}\,s^{-1}$
J	species diffusion flux, $kg\,m^{-2}\,s^{-1}$
L	Monin–Obukhov length, m
N_n	molar flux of vapour, $mol\,m^{-2}\,s^{-1}$
$\dot{m}$	release rate, $kg\,s^{-1}$
m_p	mass of droplet particle, kg
m_v	mass in vapour phase, kg
m_l	mass in liquid phase, kg
P	static pressure, Pa
Y	species mass fraction, 1
Sc_t	turbulent Schmidt number, 1
T	temperature, K
T_0	ambient temperature, K
T_p	temperature of droplet particle, K
T_b	boiling temperature, K
u	local velocity, $m\,s^{-1}$
w	release velocity, $m\,s^{-1}$
u_{10}	average wind velocity at 10 m, $m\,s^{-1}$
u_*	friction velocity, $m\,s^{-1}$
n	coefficient in Eq. (13), 1
v_p	droplet velocity, $m\,s^{-1}$
$\Delta_v h$	specific evaporation heat, $J\,kg^{-1}$
F_D	defined as $\frac{18\mu}{\rho_p d_p^2}\frac{C_D Re}{24}$, s^{-1}
C_D	drag coefficient, 1
$\vec{F}$	additional acceleration, $m\,s^{-2}$
x	co-ordinate, m
y	co-ordinate, m
z	co-ordinate, m
z_{10}	z direction with the elevation of 10 m, m
α	convective heat transfer coefficient, $W\,m^{-2}\,K^{-1}$
λ	thermal conductivity, $W\,m^{-1}\,K^{-1}$
λ_t	turbulent thermal conductivity, $W\,m^{-1}\,K^{-1}$
k	von Karman constant, 1
k_c	mass transfer coefficient, $m\,s^{-1}$
k	kinetic turbulent energy, $m^2\,s^{-2}$
ϵ	dissipation of turbulent kinetic energy, $m^2\,s^{-3}$
ρ	density, $kg\,m^{-3}$
ρ_p	density of droplet particle, $kg\,m^{-3}$
μ	viscosity, Pa s
μ_t	turbulent viscosity, Pa s

software to simulate the MUST experiment, Venetsanos, Huld, Adams, and Bartzis (2003) worked on the modelling of the Stockholm hydrogen gas explosion. All these works validated the application of the CFD approach as a useful tool for predicting gas dispersion in the vicinity of buildings.

In the present work the dispersion of the liquefied ammonia release was simulated by the CFD approach using the commercial software package Fluent 6.2. Ammonia was chosen because it is toxic and increasingly used in the industry. Ammonia is usually stored in the liquid phase in pressurized vessels. After its release, a two-phase flow occurs near the release point forming an ammonia cloud which is denser than the ambient air. The temperature and density gradually approach values of the ambient air and the cloud exhibits signs of a neutral or even a lighter type of gas dispersion.

The dispersion of ammonia was modelled using a full set of numerically solved conservation equations with additional equations for turbulence and a discrete particle model for liquid particle droplets. The mixture phase composed of air and ammonia vapour was modelled by the Eulerian approach. The liquid phase consisting of particle droplets with different diameters is modelled by the Lagrangian approach to the discrete phase.

Data obtained by mathematical simulation were compared to the experimental data from the FLADIS (Nielsen et al., 1997) field experiment. In this field experiment the release rates were approximately $0.5\,kg\cdot s^{-1}$ unlike the most well-known field experiment, Desert Tortoise Series (Goldwire at al., 1985), with release rates about $100\,kg\cdot s^{-1}$, these are much higher than those presented in the FLADIS experiment. However, smaller amounts of ammonia release occur more frequently in practical situations. Other differences are a lower ambient temperature and higher humidity, which are more representative for the European climate, comparing to the Desert Tortoise Series. The FLADIS experiment was also chosen because of its perfectly organized data, and the free access to them on the webpage (Rediphem database, 1996).

2. Governing equations

The following Reynolds averaged Navier–Stokes equations (RANS) of mass, momentum, energy and species balances with mass S_m, enthalpy S_h, momentum S_{u_i} and species source S_m, were used in CFD modelling in all three directions x, y, z (Fluent, 2005) as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = S_m \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho g_i + S_{u_i} \tag{2}$$

$$\frac{\partial}{\partial t}(\rho c_p T) + \frac{\partial}{\partial x_j}\left[u_j(\rho c_p T)\right] = \frac{\partial}{\partial x_j}\left[(\lambda + \lambda_t)\left(\frac{\partial T}{\partial x_j}\right) - \sum_i h_i \vec{J_i}\right] + S_h \tag{3}$$

$$\frac{\partial}{\partial t}(\rho Y_n) + \frac{\partial}{\partial x_j}\left[u_j(\rho Y_n)\right] = \frac{\partial}{\partial x_j}\left[\rho(D_{n,m} + D_t)\frac{\partial Y_n}{\partial x_j}\right] + S_n \tag{4}$$