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CFD simulations of ammonia dispersion using "dynamic" boundary conditions

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A B S T R A C T

Ammonia is stored in liquid form at ambient temperature and under high pressure. During an accident, ammonia will flash out of the vessel and disperse in the surrounding area. This paper provides a comparison of the results obtained by the FLADIS field experiments and those of CFD modeling by Fluent 6.3. FLADIS experiments were carried out by the Risø National Laboratory using pressure liquefied ammonia. Time series of meteorological conditions as wind speed, wind direction and source strength were determined from the experimentally measured data and used as the inflow boundary conditions. Furthermore, for more realistic simulation of air flow in the computation domain for the desired atmospheric stability, periodic boundary conditions were used on both side boundaries. The initial two-phase flow of the released ammonia was also included. The liquid phase was modeled as droplets using discrete particle modeling, i.e., the Euler–Lagrangian approach for continuous and discrete phases.

Keywords: CFD modeling; Gas dispersion; Ammonia release; Emergency preparedness

1. Introduction

In many industrial installations (storages, pipelines, reactors), hazardous materials can be released accidentally as vapor, gas or liquid and are dispersed in the atmosphere.

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).

Simplified dispersion models such as the well know 'box-models' or Gaussian models were derived and they are widely used in risk analysis procedures, providing fast dispersion estimations and usually reliable results when describing unobstructed gas flow over flat terrain (Hanna and Drivas, 1987; Hanna and Strimaitis, 1988; Reynolds, 1992). On the other hand, the simplifications used in these types of models do not allow to model complex geometries, they are derived for 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 et al., 2002). Advances in the speed of modern computers, and more significant recent advances in the CFD techniques have made CFD modeling tractable for complex environmental problems. The results obtained by CFD modeling are more accurate because the wind velocity is completely resolved in comparison to the simplified models where velocity is a single value or a function of height. This is more obvious in an area with high obstacles and real hazardous situations including gas release in the presence of buildings which can be modeled using this approach (Delaunay, 1996; Gavelli et al., 2008; Hanna et al., 2004; Scargiali et al., 2005; Venetsanos et al., 2003). Moreover, in the CFD model, the second phase can be included. The gaseous phase (air–toxic gas) is modeled using the mentioned balance equations, and the liquid phase (droplets generated by a sudden pressure drop of the superheated liquid) can be modeled using a multiphase approach. This means that the second phase is modeled using the same equations as the first phase or that the droplets are modeled as discrete particles (Crowe et al., 1998; Kiša and Jelemenský, 2009).

Studying the atmospheric dispersion of ammonia was motivated due to two reasons. Firstly, ammonia is one of the most extensively used industrial chemicals. Secondly, ammo-

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Nomenclature

c_p	specific heat capacity ($J\,kg^{-1}\,K^{-1}$)
C	molar concentration ($mol\,m^{-3}$)
d	diameter of droplet particle (m)
D	diffusion coefficient ($m^2\,s^{-1}$)
f	vapor fraction
G_k	generation of turbulence kinetic energy ($kg\,m^{-1}\,s^{-3}$)
J	species diffusion flux ($kg\,m^{-2}\,s^{-1}$)
L	Monin–Obukhov length (m)
$\dot{m}$	release rate ($kg\,s^{-1}$)
N	molar flux of vapor ($mol\,m^{-2}\,s^{-1}$)
Nu	Nusselt number
P	static pressure (Pa)
Pr	Prandtl number
Re	Reynolds number
Sc_t	Schmidt turbulent number
T	temperature (K)
u	local velocity ($m\,s^{-1}$)
u_{10}	average wind velocity at 10 m ($m\,s^{-1}$)
v_p	droplet velocity ($m\,s^{-1}$)
w	release velocity ($m\,s^{-1}$)
Y	species mass fraction
$\Delta_v h$	latent heat ($J\,g^{-1}$)
λ	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
ρ	density ($kg\,m^{-3}$)
μ	viscosity (Pa s)

nia is highly soluble in water and has toxic and corrosive effects caused by its alkalinity. Liquid ammonia is corrosive and evaporation of ammonia may cause extreme cooling when spilled on the skin or eyes; cold burns may result. When inhaled, ammonia dissolves in upper airways and small amounts also in the lower respiratory tract; damage to upper airways is therefore more severe (Meulenbelt, 2007).

Ammonia is usually stored in highly pressurized vessels in liquefied state at ambient temperature or in cryogenic tanks.

There are different possible types of accidental ammonia releases:

1. Ammonia gas jet from a pressurized vessel (release from gaseous phase).
2. Two-phase ammonia jet from a pressurized vessel (release from liquid phase).
3. Evaporation of a pool of liquid ammonia in which the temperature is lower than or equal to its boiling point—the temperature can drop to near −70 °C.
4. Leakage of liquid ammonia from a cryogenic tank (liquid ammonia at a temperature below the boiling point and at atmospheric pressure).

It is clear that ammonia dispersion depends on the type of release.

In the present work, the key issue was to develop a software tool for more realistic prediction of dispersion of the second type of ammonia release, based on the CFD approach using the commercial software package Fluent 6.3.

The software tool for ammonia dispersion was modeled 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 vapor was modeled by the Eulerian approach. The liquid phase consisting of particle droplets with different diameters was modeled by the Lagrangian approach.

However, in order to be able to reach realistic simulation, it must be validated against relevant experimental data to ensure that the vapor dispersion predictions are sufficiently accurate. Therefore, in this paper, the data obtained by mathematical simulation were compared with the experimental data from the FLADIS field experiment (Nielsen et al., 1997). The FLADIS experiment was also chosen in this paper because of its perfectly organized data and the free access to them on the webpage. This allowed using time series of meteorological conditions as wind speed, wind direction and source strength as the inflow boundary conditions. For more realistic simulation, input flow to the computational domain for the relevant atmospheric stability and the side periodic boundary conditions were used.

2. Governing equations

The Reynolds-averaged conservation equations for mass, momentum, energy (temperature) and concentration were used to simulate the processes of interest. It was assumed that the averaged ideal gas law describes the state of air as well as the state of the released gas:

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

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

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

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

where the turbulent viscosity μ_t, the turbulent thermal conductivity λ_t, and the turbulent dispersion coefficient D_t are turbulence characteristics of particular transport phenomena, i.e., heat transport and mass transport, respectively.

In the work of Schatzmann and Leitl (2002) it is reported that, among turbulence models, the large eddy simulation (LES) approach provides better information than the Reynolds-averaged Navier Stokes (RANS) closure models. Computational demands of the LES approach are still too high to make it viable for routine purposes. For this reason, RANS closure is usually employed and the relatively simple and widely tested k–ε model has been almost universally adopted in the study of dispersion despite its known limitations. The k–ε model typically results into reasonable agreement with experimental data concerning the mean flow and pollutant concentration (Burman, 1998; Gilham et al., 2000; Kim and Baik, 2003; McBride et al., 2001; Schatzmann and Leitl, 2002;