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.

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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 known ‘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-
Ammonia 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 spilt 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 \(-70\degree C\).
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:

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

(1)

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

(2)

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

(3)

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x_j}(u_j(\rho Y_i)) = \frac{\partial}{\partial x_j} \left[ \rho(D_{n,m} + D_i) \frac{\partial Y_i}{\partial x_j} \right] + S_n$$

(4)

where the turbulent viscosity \(\mu_t\), the turbulent thermal conductivity \(\lambda_t\), 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;
Sklavounos and Rigas, 2004; Würtz et al., 1996). The turbulent viscosity $\mu_t$ was calculated using the Prandtl–Kolmogorov equation:

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon}$$  \hspace{1cm} (5)

as a function of turbulent kinetic energy, $k$, and its dissipation rate, $\varepsilon$, by the closure model defined as follows:

$$\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ (\mu + \frac{\mu_t}{\kappa}) \frac{\partial \varepsilon}{\partial x_i} \right] + G_k - \rho \varepsilon$$  \hspace{1cm} (6)

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ (\mu + \frac{\mu_t}{\kappa}) \frac{\partial u_i}{\partial x_j} \right] + c_{1k} \frac{\varepsilon}{k} G_k - c_{2k} \rho \frac{\varepsilon^2}{k}$$  \hspace{1cm} (7)

In Eqs. (5) and (6), the constants are: $C_\mu = 0.09$, $c_{1k} = 1.44$, $c_{2k} = 1.92$, $\sigma = 1.3$, $\kappa = 1.0$; and the default turbulent Schmidt number $S_N = 0.7$ was used.

The liquid phase consisting of particle droplets was modeled by the Lagrangian approach. The discrete phase particle trajectories can be computed by integrating the force balance equation. The fluid phase influences the particles via drag, turbulence and momentum transfer. The particles influence the fluid phase through source terms. Mass, momentum as well as energy transfer between the phases were included. For the discrete phase (small droplets of liquid ammonia), the equation of motion is defined as:

$$\frac{d\vec{v}_p}{dt} = F_D (u - \vec{v}_p) + \frac{\mu}{\rho_p} \frac{d\vec{v}_p}{dt} + \vec{F}$$  \hspace{1cm} (8)

and the enthalpy balance as:

$$m_p \frac{dT_p}{dt} = \alpha A_p (T_a - T_p) + \frac{dm_p}{dt} \Delta_{ho}$$  \hspace{1cm} (9)

where $\alpha$, the convective heat transfer coefficient, is obtained from the Nusselt correlation reported in (Ranz and Marshall, 1952):

$$Nu = \frac{\alpha D_p}{\chi} = 2.0 + 0.6Re_d^{1/2}Pr^{1/3}$$  \hspace{1cm} (10)

and the mass balance is defined as:

$$N_n = k_l (C_{n,k} - C_{n,\infty})$$  \hspace{1cm} (11)

where $k_l$, the mass transfer coefficient, is obtained from the Nusselt correlation (Ranz and Marshall, 1952) by the following equation:

$$Nu_l = \frac{k_l D_p}{D} = 2.0 + 0.6Re_d^{1/2}Sc^{1/3}$$  \hspace{1cm} (12)

### 3. Fladis experiment

Field experiments of the pressure liquefied ammonia dispersion were carried out in the Risø National Laboratory (Nielsen et al., 1997). The source was a flashing jet oriented in the horizontal downwind direction with the strength of 0.25–0.6 kg s\(^{-1}\) and duration in the range of 3–40 min.

Temperature of the storage tank was not controlled and therefore it was close to ambient temperature. The system was pressurized with nitrogen in order to reduce the likelihood of two-phase flow inside the release nozzle and to avoid pool formation in front of the source. Ammonia was extracted from the liquid phase at the bottom of the tank through a siphon pipe, and the pressure was maintained by adding inert nitrogen gas at the top of the tank.

Due to the evaporation heat the flash boiling ammonia jet became much colder and therefore heavier than the surrounding air. The main focus was to study the dispersion in all its stages, i.e., heavy gas dispersion (measured gas concentration in the distance of 20 m) and, further downstream where the flow developed into a plume of neutral buoyancy, the passive gas dispersion (measured gas concentration in the distance of 70 and 235 m). Distribution of concentration sensors is schematically depicted in Fig. 1.

The present paper provides a comparison of the results obtained by CFD modeling with experimental data from the FLADIS 15 trial. In this trial, the source strength was approximately 0.51 kg s\(^{-1}\) and the duration of ammonia release was 185 s. Averaged temperature during the experiment was 16.7 °C and the pressure was 101.9 kPa. The computed Monin–Obukov length was 396 m which corresponds to the D stability class. In this trial, the source was a 6.3 mm diameter nozzle pointing horizontally in the ideal downwind x-direction with an elevation of 1.5 m. Averaged wind speed was 6.1 m s\(^{-1}\) (measured in 10 m). Using the data from wind velocity sensors, the friction velocity was set to the value of 0.51 m s\(^{-1}\).

### 4. Boundary and initial conditions

Analytical solutions of the Navier–Stokes equations exist for only the simplest flows under ideal conditions. For real flows, however, they can be solved numerically using boundary conditions describing the flow properties on the computational domain boundaries. The modeling area used was 350 m × 300 m × 100 m in the x, y, z directions, respectively. Wind velocity and wind direction are probably the most significant parameters in the problem definition procedure since they determine the dilution of the emitted gas by passing volumes of air. The atmospheric stability class is represented by the inflow boundary condition for the velocity turbulent kinetic energy $k$ and the dissipation of turbulent kinetic energy $\varepsilon$ (Han et al., 2000). The $k$–$\varepsilon$ model requires that the wind velocity turbulent kinetic energy $k$ and the dissipation of turbulent kinetic energy $\varepsilon$ are provided. Therefore, the inlet boundary
conditions for the computational domain were specified by the Dirichlet condition (the values of variables on the boundaries are given).

The power law velocity profile was used according to the stability class reported by Barratt (2001), i.e., \( n = 0.1 \) for stability class D.

\[
U = U_10 \left( \frac{z}{z_{10}} \right)^n
\]  \hspace{1cm} (13)

According to the work of Han et al. (2000), the boundary layer may be subdivided into a surface layer, in which stress is nearly constant with height, and an outer layer. A separate set of algorithms can be assigned to each sublayer. In the surface layer, the turbulent kinetic energy and the dissipation of turbulent kinetic energy are given by (Hogstrom, 1996; Rao and Nappo, 1996):

\[
k = 6u_z^2
\]  \hspace{1cm} (14)

\[
\varepsilon = \frac{u_z^3}{Kz} \left( 1.24 + 4.3 \frac{z}{L} \right)
\]  \hspace{1cm} (15)

where \( K = 0.4 \) is the von Karman constant.

The expression for the outer layer can be assigned according to the level of stratification. In the neutral and moderately stable boundary layer can be obtained from (Hogstrom, 1996; Rao and Nappo, 1996):

\[
k = 6u_z^2 \left( 1 - \frac{z}{H} \right)^{1.75}
\]  \hspace{1cm} (16)

\[
\varepsilon = \frac{u_z^3}{Kz} \left( 1.24 + 4.3 \frac{z}{L} \right) \left( 1 - 0.85 \frac{z}{H} \right)^{1.5}
\]  \hspace{1cm} (17)

The bottom boundary condition was specified by a no-slip condition. The velocity components equaled zero and the other variables were set accordingly to the wall functions. This approach avoids the need of resolving the turbulent boundary layer near the wall.

The outlet boundary of the computational domain was defined by specifying zero normal gradients for all variables. This approach assumes that the flow is fully developed and the variables do not change in the flow direction therefore it is typically used for external flows. It is important to point out that the outlet boundary must be far enough from the ammonia source, otherwise, significant errors can propagate throughout the domain.

The side boundaries (left and right boundaries parallel to the average wind direction) are very frequently model using symmetry boundary condition. However, this approach is quite inapplicable for dynamic simulations, where the wind direction meanders. The symmetry assumes that no flow crosses the boundary and that there is no scalar flux across the boundary. Thus, the normal component of velocity is set to zero and all other variables have boundary values set to equal the flow values. This type of boundary condition does not allow air to escape through the boundary. As a consequence, the flow direction in the domain aligns parallel to the side boundaries and therefore air exits perpendicularly through the outlet boundary. However, the goal of the presented work was to model atmospheric dispersion in “real” environment in which the wind velocity and especially wind direction are changing. One possibility was to set the velocity inlet boundary condition on both left and right side boundaries and to set the flow direction and the wind speed identically to the inlet to the domain. The results obtained by this approach are much better than in case of a symmetry boundary condition, but the movement of air in the domain is not completely “realistic” due to step changes of the flow direction in the domain.

Much better description can be achieved using a periodic boundary condition. In general, periodic boundary conditions are used when the physical geometry of interest and the expected pattern of the flow/thermal solution have a periodically repeating nature. They are used when the flows across two opposite planes in the computational model are identical (Fluent, 2005). The transitional periodic boundary condition allows air to escape through the side boundaries; moreover, an identical amount of air enters from the opposite periodic plane at the same time. Using this type of side boundary condition, it is possible to generate a very realistic environment for the atmospheric dispersion. It is very important to use a wide enough computation grid when using the periodic boundary condition. Otherwise the ammonia escaped from one side of the domain will enter the domain from the opposite side. In the presented case study, 99% of ammonia escaped from the domain through the outlet.

Comparison of different types of side boundary conditions is depicted in Fig. 2 which compares the averaged computed and measured crosswind concentration profiles 235 m far from the release point. From this figure it is clear that the steady state simulation results mostly overpredict the maximal concentration. The steady states approach (independent on time) gives higher concentration because it is calculated at constant release rate (with infinite duration), wind direction and wind velocities are independent on time.

The concentrations for transient behavior with symmetry and periodic boundaries were calculated with averaging time equal to the time interval when constant (“quasi steady state”) ammonia rate was reached—see Fig. 5. The reason for choosing this averaging time was to compare the averaged concentration for the “quasi steady state” with the concentrations calculated for the correct steady state conditions.

It is evident that the steady state approach is not very correct for the calculation of concentration by CFD when the release duration is very short.

On the other hand, relatively good agreement can be found in case of the symmetry boundary condition. However, the position of the maximal concentration does not correspond with the experimental data. The best results can be obtained using the periodic side boundary conditions (solid blue line).
It is clear that the calculated average concentration profiles are shifted to the same direction as the experimental average concentration.

The flow rate and total mass of liquefied ammonia introduced were consistent with the experimental data from the FLADIS experiment. For the liquid phase, the initial temperature was set to 239 K (boiling temperature) and the initial speed was also set to the value corresponding with the velocity of the liquefied ammonia flow through the orifice. The source of ammonia release was modeled as a source in the balance equations without exactly modeling the release from pipe. The Rosin–Rammler distribution for droplets diameter distribution of the ammonia liquid phase was applied (Johnson and Woodward, 1999) as the mass fraction of droplets with diameter greater than diameter $D$:

$$R = \exp\left(\frac{D}{D_m}\right)^n$$

where $D_m = 50 \mu m$, $n = 2.5$, the maximal allowed diameter was set as $D_{max} = 100 \mu m$ and the minimal as $D_{min} = 10 \mu m$.

5. Mesh

One of the most important steps in the process of CFD simulation preparation is the geometry construction. In the discretization process, the domain was divided into a number of discrete volume elements. In the presented work, the computational grid consisted of approximately 500,000 hexahedral volume elements. Hexahedral meshes are much more computationally efficient than tetrahedral meshes. Typically, a hexahedral mesh requires half the resolution in each of the three directions which represents a reduction by almost an order of magnitude in the number of elements.

Several tests on the influence of computational domain and grid size were performed to ensure the independence of the solution from the domain and the grid size. The mesh was periodically refined by approximately 25% and the computation was repeated until the variation in results was acceptable. It was found that the sufficient number of grid points is approximately 200,000.

6. Solution

The dispersion of ammonia 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 using the Eulerian approach. The liquid phase consisting of particle droplets with different diameters was modeled using the Lagrangian approach to the discrete phase. Fluent 6.3 was used to solve 3D RANS. To obtain more accurate results and to avoid numerical fluctuations, the second order discretization scheme was used. The convergence criterion was set to residuals equal or less than $10^{-5}$ for the continuity equation.

The analysis presented in this paper focuses on the simulation of the FLADIS 15 trial in dynamic mode. Therefore, it was necessary to develop a special code able to dynamically generate inlet boundary conditions from the measured atmospheric data from the FLADIS 15 trial. As detailed data of the experimental inlet wind velocity, wind direction and ammonia source strength were available, they were introduced to the CFD code by a user defined function (UDF). Time evolution of the wind speed (measured in 10 meters) is depicted in Fig. 3. The wind speed was measured 7.5 m prior to the ammonia source and 0.5 m right from the ideal centerline. This roughly corresponds with the position of the ammonia source in respect to the domain inlet boundary. Therefore, this data were used in each solution step to generate the corresponding vertical wind velocity profile which was used in the inlet boundary condition.

Another important parameter strongly affecting the ammonia cloud behavior is the wind direction. Wind direction was also measured in the position corresponding to the inlet boundary position. Next figure (Fig. 4) describes the measured wind direction data from the FLADIS 15 trial. The flow direction vector on the inflow boundary was adjusted according to the data measured at each simulation time. The wind meandering in the computation domain allows generating quite realistic conditions for the gas dispersion.

As the goal of this work was to describe the conditions of the FLADIS 15 trial in more detail, it was necessary to ensure that the release rate and the total mass of released ammonia is consistent with the experiment. Therefore, the mass flow of the liquid phase was adjusted according to the experimental data depicted in Fig. 5.

7. Results

As it was already mentioned, the power law was used to generate the initial velocity profile in each integration step of the
Fig. 5 – Experimentally measured release rate of ammonia form FLADIS 15 trial.

Fig. 6 – Calculated velocity profile for neutral (D) atmospheric boundary layer and measured data from the FLADIS 15 trial.

Fig. 7 – Calculated vs. measured air temperatures on the centerline in the height of 1 m. The results show that the model predictions describe general behavior of the air temperature with some discrepancies. It is evident that the closest thermocouple (1 m above the terrain and 5 m from the release point) measured temperature significantly below the boiling point. It was due to the impact of the ammonia jet consisting of fine droplets on the thermocouple results in the formation of a very cold liquid ammonia film (Nielsen et al., 1997). The film of liquid ammonia was evaporated and the temperature was lower (near −70 °C) than its boiling point.

Fig. 8 – Calculated vs. measured vertical air temperature profiles 8 m far from the release point in the center of the sensor field (y = 0 m).

Fig. 9 – Comparison of calculated vs. measured concentration evolution at the point x = 25 m, y = 0 m, and z = 1.5 m.

Fig. 10 – Comparison of calculated vs. measured concentration evolution at the point x = 70 m, y = 0 m, and z = 2.0 m.
Fig. 11 – Comparison of calculated vs. measured concentration evolution at the point $x = 235$ m, $y = 0$ m, and $z = 2.0$ m.

Fig. 12 – Concentration crosswind profiles 25 m far from the source.

Fig. 13 – Concentration crosswind profile 70 m far from the source.

It means that the measured temperature did not represent the surrounding gas-phase temperature while the thermocouple was wet. Fig. 8 shows a comparison of the calculated and experimentally measured vertical temperature profiles 8 m far.

Fig. 14 – Concentration crosswind profiles 235 m far from the source.

Fig. 15 – Comparison of calculated vs. measured crosswind profiles 25 m far from the source.

Fig. 16 – Comparison of calculated vs. measured crosswind profiles 235 m far from the source.

<table>
<thead>
<tr>
<th>Trial</th>
<th>$m$ [kg s$^{-1}$]</th>
<th>$f$</th>
<th>$w$ [m s$^{-1}$]</th>
<th>$L$ [m]</th>
<th>$u_{10}$ [m s$^{-1}$]</th>
<th>Stability</th>
</tr>
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<td>Fladis 19</td>
<td>0.27</td>
<td>0.185</td>
<td>18</td>
<td>59</td>
<td>3.7</td>
<td>E</td>
</tr>
<tr>
<td>Fladis 24</td>
<td>0.46</td>
<td>0.186</td>
<td>22</td>
<td>$-76.9$</td>
<td>5.03</td>
<td>C</td>
</tr>
<tr>
<td>Fladis 26</td>
<td>0.21</td>
<td>0.199</td>
<td>11.5</td>
<td>$-16$</td>
<td>3.0</td>
<td>B</td>
</tr>
</tbody>
</table>
from the source. The plot shows a better agreement between the predicted and measured temperatures than in the previous case (centerline temperature profile; Fig. 7).

Gas concentration is ultimately the parameter of most interest. Here too, it is desirable to compare model calculations with data for various downwind distances. As an example, next series of figures (Figs. 9–11) shows a comparison of the FLADIS 15 trial gas concentration data measured 25, 75 and 235 m far from the source. The measured data are marked with dashed red lines and the data obtained using CFD simulations are represented by blue solid lines. First figure (Fig. 9) represents the ammonia concentration evolution in the center of the sensor field ($y=0$) in the height of 1.5 and 25 m far from the release point. There is a relatively good agreement with the experimental results. On the other hand, the maximal disagreement occurred at the time of 190 s when the measured

![Fig. 17 – CFD prediction of horizontal ammonia mole fraction profile at the height of 1.5 m for time: (a) 50 s; (b) 100 s; (c) 150 s; (d) 200 s; (e) 250 s; (f) 300; (g) 350 s; (h) 400 s.](image)
concentration was about two times higher than the computed one. Next figure (Fig. 10) describes the concentration evolution on the neutral sensor field (75 m far from the release point). In this case, difference between the measured and the predicted maximal concentration was less significant than in the previous case. From this point of view, the last figure from this series (Fig. 11) represents probably the best agreement as the difference at the maximal concentration was lower than 10%. However, it is important to point out that the predicted concentration evolution shows a very significant time advance. This may be caused by the small difference between the inlet and outlet velocity profiles (Fig. 6).

The time evolution of concentration provides very important information on the quality of model prediction. However, such a validation is quite strict. For many practical applications it is much more important to estimate the averaged concentration at the desired location. In case of toxic gases, the toxic dose is often defined as follows:

$$\text{toxic dose} = \int_{t_0}^{t} c \, dt \quad (19)$$

The toxic dose is used to determine the possible health consequences of a toxic release incident outcome. It is clear that the results provided by the dynamic simulation using the CFD approach can be relatively directly used to establish the toxicological criteria to assess the probability of an adverse outcome.

In Figs. 12–14, the averaged computed and measured crosswind concentration profiles are compared. The averaged concentrations were calculated from Eq. (19), where the toxic dose is divided by the time interval \((t - t_0)\). The comparison depicted in Fig. 12 shows that the predicted profile is wider than the measured one. On the other hand, the maximal predicted concentration is by approximately 20% lower than that measured. Validation of the model prediction on the neutral sensor field, Fig. 13 (70 m from source), represents a very good agreement with the experimental data. Similarly, in case of the far sensor field (Fig. 14), the qualitative and quantitative agreement between the predicted gas concentration profile and the data points obtained from the Fladis 15 trial is very good.

Furthermore from the results follows that the calculated average concentration profiles are shifted to the same direction as the experimental average concentration. This is caused by the application of the side periodic boundary condition which allows simulating more realistic atmospheric condition in the computational domain. It should be noted that this shift were not observed when the side symmetry boundary conditions were applied. To validate this approach, another three FLADIS trials were chosen to be compared with the simulation results. The selected trials are characterized with different atmospheric stability class, source strength, wind speed and direction. The main characteristics of the selected trials are presented in Table 1.

The next series of figures compares the averaged concentration profiles 25 m (Fig. 15) and 225 m (Fig. 16) far from the release point.

For illustration, the next series of pictures (Fig. 17a–h) describes the model predictions of the ammonia mole fraction at the height of 1.5 m. From these pictures it is clear that the model gives relevant responses to the basic atmospheric inputs (wind velocity, Fig. 3, and wind direction, Fig. 4) and to the release rate of ammonia (Fig. 5).

8. Conclusion

In this paper, the CFD dynamic approach was successfully applied in the simulation of the FLADIS experimental data. The dynamical approach means that time series of meteorological conditions as wind speed, wind direction and source strength were applied as the inflow boundary conditions. Furthermore, for more realistic simulation of the input flow of air, for the relevant atmospheric stability, to the computational domain, the side periodic boundary conditions were used.

Concerning the two-phase flow nature of the release, the equilibrium thermodynamic simplification and the Raoult’s law of phase change provide reasonable results in terms of temperature and concentration predictions. It was shown that model predictions qualitatively describe general behavior of air temperature near the source. In the next step, the ammonia concentration fields were compared. The simulation predicted, with a reasonably good agreement, the gas concentration history as well as the cross-wind concentration distributions in the dispersion field. But although the CFD models are able to model complex geometries, they are limited by the application of the turbulence closure models.
Finally, the key stones of the presented methodology are summarized into a few recommendations:

- In order to limit the CPU time, a non-uniform grid is preferred, with minimum grid size applied close to the ground, obstacles and source of the release. The grid can be expanded with an expansion ration not higher than 1.2. In the case of a flat terrain (no obstacles presented in the domain) the sufficient number of grid points is approximately 200,000.
- It is strongly recommended to use realistic (experimental) data for the wind velocity and wind direction and introduce them into the domain via inlet boundary conditions. To obtain realistic environment for ammonia dispersion it is recommended to use the transitional periodic boundary condition on the side boundaries.
- One or two equations turbulence models can be used to produce reasonable results. It is important that the selected model considers the local stability effects in a multiphase medium as well as the non-isotropic effects of eddy diffusivity.

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