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Numerical Modeling of Dispersion Process for Different Density of Gas Mixtures – 2d and 3d Numerical Approach

Abstract

The dispersion of the toxic gases due to the natural/industrial accidents can have the tragic consequences. To prevent the effects of these disasters different approaches have been introduced in the literature. In this paper we aimed to prepare the Computational Fluid Dynamics (CFD) the model of emergency escape of toxic gases of different density, e.g. the chlorine and the ammonia.

The Aloha and Ansys-Fluent software for multiphase transport description was applied. For 2d simulation the Degadis model was used, while for the 3d approach the multiphase Volume of Fluid model (VOD) was applied. For the reconstruction of atmospheric conditions different air velocity (flowing in one direction) was included according to the Pasquil Stability Class. Moreover, different wind conditions were compared with the windless conditions.

The comparison of the dispersion process for two gases with different density, for the same mathematical domain, indicated the different volume concentration in function of the height and the wind velocity. The implications of the spreading pattern from the risk assessment and risk mitigation point of view were discussed. With the increase of height and wind velocity, a decrease of gas concentration for both gases was observed. Moreover, for the ammonia for the windless case, the volume fraction profile was irregular, while for the chlorine the circular profile was observed. With the increase of the wind value, the shape of the ammonia and the chlorine profile became narrower. Similar, as it was for the two-dimensional model wider cloud for the ammonia compared to the chlorine was observed.

Keywords: Ammonia dispersion, chlorine dispersion, emergency gas release, 2d dispersion, 3d dispersion, CFD

Numeryczne modelowanie dyspersji gazów o różnej gęstości w ujęciu dwuwymiarowym i trójwymiarowym

Abstrakt

Dyspersja toksycznych gazów w wyniku awarii przemysłowych lub naturalnych katastrof może prowadzić do tragicznych konsekwencji. W celu zapobiegania tego typu zdarzeniom w literaturze fachowej proponowane są różne rozwiązania. Celem niniejszego artykułu było opracowanie matematycznego modelu dla procesu awaryjnego uwolnienia gazów toksycznych, tj. chlor i amoniak.

W badaniach analizowano dwa podejścia, tj. dwuwymiarowy i trójwymiarowy opis zjawiska dyspersji gazu. W tym celu zastosowano oprogramowanie Aloha i Ansys-Fluent. Do dwuwymiarowego opisu zjawiska dyspersji gazu wykorzystano model Degadisa, a dla trójwymiarowego opisu zjawiska dyspersji model VOF. W celu rekonstrukcji rzeczywistych warunków atmosferycznych zastosowano różne prędkości przepływu powietrza, zgodnie z klasami stabilności Pasquila. Co więcej, w badaniach uwzględniono również przypadek bez przepływu wiatru.

Porównanie procesu dyspersji dwóch gazów o różnej gęstości dla takiej samej domeny obliczeniowej wskazuje na różny układ stężeń analizowanych gazów w funkcji wysokości, a także prędkości wiatru. Zaobserwowano, iż wraz ze wzrostem wysokości i prędkości wiatru malało stężenie obu analizowanych gazów. Co więcej, dla amoniaku w bezwietrznym przypadku profil stężenia miał kształt nieregularny. Wraz ze wzrostem prędkości wiatru kształt profilu stężenia amoniaku i chloru stawał się coraz węższy. Zarówno dla modelu dwuwymiarowego, jak i dla modelu trójwymiarowego zaobserwowano, iż profil stężenia amoniaku był szerszy w porównaniu z profilem stężenia chloru.

Słowa kluczowe: dyspersja amoniaku, dyspersja chloru, uwolnienie awaryjne gazu, dyspersja 2d, dyspersja 3d, CFD

1. Introduction

Dense clouds tend to persist at the ground level or the human breathing level which may lead to the magnification of their harmful potential (Siddiqui et al., 2012). The presence of the high population gases in such areas multiplies the magnitude of the consequences (Pontiggia et al., 2010). Dispersion of toxic gases due to the natural or the industrial accidents can have tragic consequences. To prevent the effects of these disasters different approaches have been introduced in the literature (Lovreglio et al., 2016). To assist in the emergency response decisions and planning in case of dangerous gases release, the computational models are applied (Steven R. Hannaa et al., 2009). Different numerical tools may account details of the flow and dispersion much better than the standard widely-used simple dense gas models (Biao Sun et al., 2013; Tsenga et al., 2012). The most commonly used numerical tools for the simulation of dense gas dispersion are as follows: PHAST (Wang et al., 2017), ALOHA (Thoman et al., 2006a), ANSYS (Polanczyk et al., 2013; Salamonowicz et al., 2015). However, the crucial rule is to achieve the real character of multiphase transport for the particular case (Daskirana et al., 2017). The turbulent dispersed multiphase flows are common in many engineering and environmental applications (Balachandar and Eaton, 2010; Fox, 2014). However, reliable numerical model indicates the calculation of gas transport not only in the horizontal plain (Thoman et al., 2006b) but also including the three-dimensional movement (Labovský and Jelemenský, 2010). Therefore, in this paper we aimed to prepare three-dimensional computational model of gas mixtures with different densities.

2. Material and Methods

In this study the influence of the gas density on the dispersion process was analyzed. Therefore, numerical description of dispersion during emergency release for two gases with different density was prepared. Physical properties of the analyzed materials were as follows: air (ρ = 1.23 kg/m^3, η = 1.79 10^{-5} kg/(m s)), ammonia (ρ = 0,69 kg/m^3, η = 1.02 10^{-5} kg/(m s)), chlorine (ρ = 2.95 kg/m^3, η = 1.33 10^{-5} kg/(m s)) (Steven R. Hanna et al., 2009; Tan et al., 2017). The following assumptions were made: constant environmental conditions (T = 25 °C and P = 101325 Pa), constant air humidity (φ = 50 %), free escape of gas into open space with small buildings, area of investigation was equal to 0.1 km^2, the total amount of escaped gases was 180 kg and 1.8 kg for the ammonia and the chlorine, respectively.

Two strategies were considered: the two-dimensional dispersion (Aloha software) and the three-dimensional dispersion (Ansys-Fluent). First, for the horizontal description of gas concentration (eq.1)the Aloha software was applied (Biao Sun et al., 2013; Tsenga et al., 2012).

$$C = \frac{M}{(2\pi)^{3/2}\sigma_x,\sigma_y,\sigma_z}\left[exp\left(-\frac{(x-ut0^2}{2\sigma_x^2}-\frac{y^2}{2\sigma_y^2}\right)\right]\left[exp\frac{-(z-H)^2}{2\sigma_z^2}+exp\frac{-(z+H)^2}{2\sigma_z^2}\right] \quad (1)$$

where:
x,y,z – distance from dispersion source, m;
C – concentration, kg/m^3;
G – speed of emission, kg/s;
H – height of dispersion source, m;
σ_y, σ_z – dispersion coefficient, m;
u – wind speed, m/s;
M – amount of ejected substance, kg;
t – time until ejection, s.

The mathematical domain was composed of rectangular (length = 2000 m, width = 600 m) with point leakage (diameter: 0.1 and 0.3 for chlorine and ammonia, respectively), in 100 m from shorter side (wind inlet), in longitudinal position. Following the boundary conditions the *velocity inlet* (shorter side, closer to the gas leakage)and the *free outlet* (remaining sides) were applied. According, to the Pasquil Stability Classes six values of wind velocity were analyzed (Krügera and Rohinton, 2013).

In the next step, to analyze dispersion not only in the horizontal plane, the three-dimensional model was considered. Gas transport phenomena was described with the use of the Navier Stokes equations (eq.2 – eq.4) (Ganta et al., 2014).

$$\rho\left(\frac{\partial v_x}{\partial t}+v_x\frac{\partial v_x}{\partial x}+v_y\frac{\partial v_x}{\partial y}+v_z\frac{\partial v_x}{\partial z}\right)=\rho g_x-\frac{\partial p}{\partial x}+$$

$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(2\frac{\partial v_x}{\partial x})\right)+\frac{\partial}{\partial y}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial y}+\frac{\partial v_y}{\partial x})\right)+\frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_x}{\partial z}+\frac{\partial v_z}{\partial x})\right) \quad (2)$$

$$\rho\left(\frac{\partial v_y}{\partial t}+v_x\frac{\partial v_y}{\partial x}+v_y\frac{\partial v_y}{\partial y}+v_z\frac{\partial v_y}{\partial z}\right)=\rho g_y-\frac{\partial p}{\partial y}+$$

$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(\frac{\partial v_y}{\partial x}+\frac{\partial v_x}{\partial y})\right)+\frac{\partial}{\partial y}\left((\mu+\mu_t)(2\frac{\partial v_y}{\partial y})\right)+\frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_y}{\partial z}+\frac{\partial v_z}{\partial y})\right) \quad (3)$$

$$\rho\left(\frac{\partial v_z}{\partial t}+v_x\frac{\partial v_z}{\partial x}+v_y\frac{\partial v_{zy}}{\partial y}+v_z\frac{\partial v_z}{\partial z}\right)=\rho g_z-\frac{\partial p}{\partial z}+$$

$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial x}+\frac{\partial v_x}{\partial z})\right)+\frac{\partial}{\partial y}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial y}+\frac{\partial v_y}{\partial z})\right)+\frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial z})\right) \quad (4)$$

where:
vx,vy,vz – velocity components for x, y, z directions, m/s;
t – time, s;
g – acceleration in x, y, z direction, m^2/s;
μ – fluid viscosity, Pa s;
ρ – fluid density, kg/m^3;
μt – turbulent viscosity, Pa s.

At the beginning, with the use of the SpaceClaim–Ansys software (ANSYS, USA) the three-dimensional numerical geometry was created (Fig. 1a). Six surfaces created a closed volume (length = 2000 m, width = 600 m, height = 200 m). 0.3m above the ground a cylindrical hole, representing a gas leakage, was placed (diameter: 0.3 m and 0.1 m for ammonia and chlorine, respectively). After the discretization process (ICEM-Ansys software (ANSYS, USA)) the three-dimensional numerical mesh composed of tetrahedrons with boundary layer was prepared (Fig. 1b). After the mesh independent tests, the number of numerical grid elements was established at approximately 2 000 000. Moreover, in order to reconstruct irregularities of the urban area, a boundary layer composed of 10 layers was included.

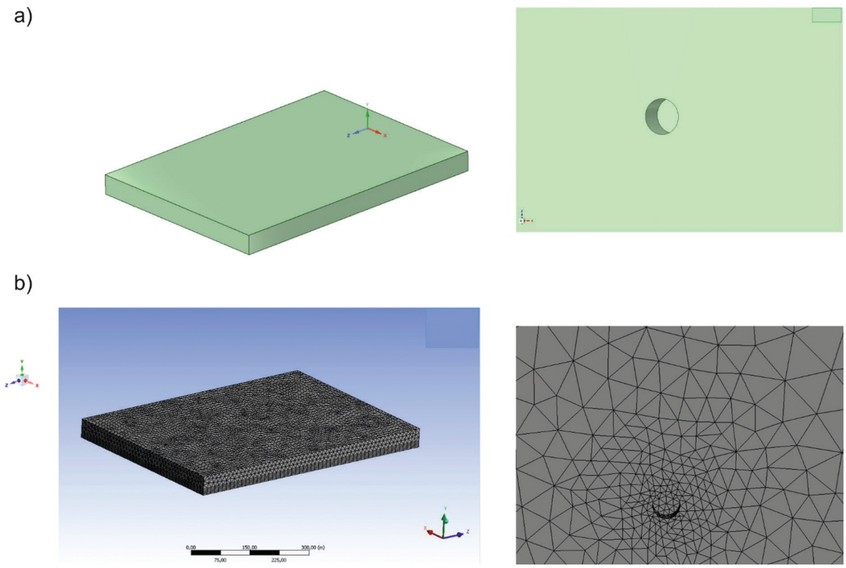

Fig. 1. Three-dimensional geometry of analyzed object: a) three-dimensional numerical domain, b) three-dimensional numerical mesh.

With the use of the Ansys-Fluent processor the gas dispersion was simulated. The multiphase Volume of Fluid model (VOD) for gas mixture transport was applied (Biao He et al., 2017). Depending on the analyzed case, each time air was defined as the first phase and the second phase was defined as the ammonia orthe chlorine. The following boundary conditions were used: *mass flow inlet* (for gas leakage), *wall* (bottom – as a ground), *velocity inlet* (one surface), and *pressure outlet* (remaining surfaces). With the use of the *velocity inlet* boundary air inlet to the analyzed domain was defined. The velocity profile was experimentally set (Table 1) and configured as a function of height *u(h)* (eq.5) including the existence of obstacles (urban and rural area). For each of analyzed cases different air velocity was set, according to the Pasquil Stability Classes (Table 1) (Krügera and Rohinton, 2013). In addition, the influence of wind was investigated. Therefore, the gas mixture escape for the windless day was also considered.

$$u(h) = u_{10}\left(\frac{h}{10}\right)^{p} \quad (5)$$

where:
$u(h)$ – air velocity, m/s;
u_{10} – air velocity at the level of 10m, m/s;
h – height, m;
p – wind correlation coefficient for urban and rural area, – .

Table 1. Maximal air velocity for different Pasquil Stability Class at the 10m height

Stability classes	Air velocity at the height 10m [m/s]	P [-]
A	2	0.109
B	3	0.112
C	4	0.120
D	5	0.142

continued Table 1.

Stability classes	Air velocity at the height 10m [m/s]	P [-]
E	3	0.203
F	2	0.253

Source: authors

Gas escape was described with the use of the *mass flow inlet* boundary. Mass fractions for two considered phases were as follows: y_{O2}=0 and y_{NH3}=1 or y_{Cl2}=1 for air and the ammonia/chlorine, respectively. The mass fractions at the inlet of air were set as y_{O2}=1 and y_{NH3}=0 or y_{Cl2}=0 for air and the ammonia/chlorine, respectively. For the free flow outside the domain, without reduction of the velocity to 0 m/s, at the outlets *pressure outlet* boundary was set. For the bottom *wall* boundary with surface roughness (pretending the different size of the buildings) was applied. Transient conditions (1 hour of dispersion) were assumed. The assumption was made according to the Reynolds number turbulent flow, described with the *k*-*ε* mode.

3. Results

There were analyzed the two – and three-dimensional dispersion of two different gases (ammonia and chlorine) with different density the ammonia (ρ = 0,69 kg/m^3) and the chlorine (ρ = 2.95 kg/m^3)). Each time the gas escape into open space was considered.

3.1. Two-dimensional dispersion

In the first step with the use of the Aloha software, the ammonia and the chlorine dispersion was investigated. For the first stability class (A) cloud of dispersed gas, for both analyzed substances, had similar shape and distance. Moreover, for the ammonia about 10 times higher range was observed between A and F class, while for the chlorine 4 times higher distance for F class compared to A class was noticed. Furthermore, comparison of both gases indicated wider cloud for ammonia compared to the chlorine. For the same value of wind velocity much longer distance of cloud for the ammonia compared to the chlorine was observed. For B class difference between the ammonia and the chlorine was about 25 %, while for F class the ammonia cloud was about 3.6-fold longer compare to the chlorine gas.

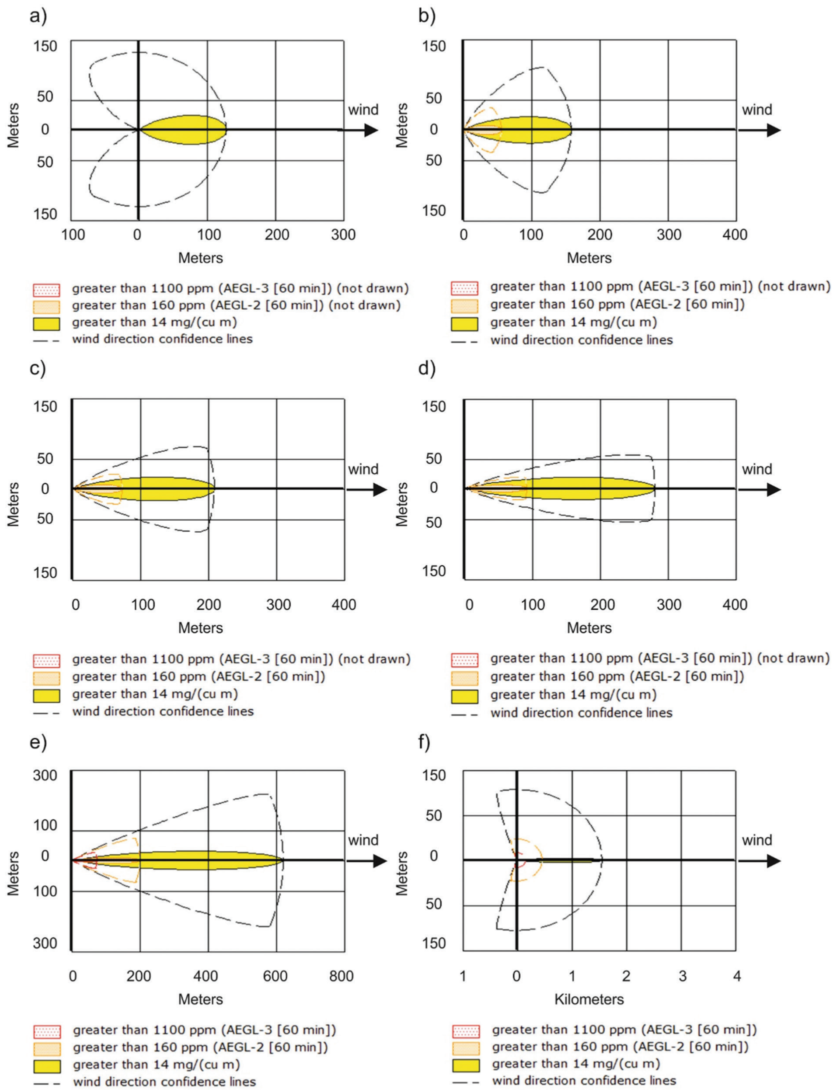

Fig. 2. The ammonia distribution for: a) wind velocity 2 m/s (A Class), b) wind velocity 3 m/s (B Class), c) wind velocity 4 m/s (C Class), d) wind velocity 5 m/s (D Class), e) wind velocity 3 m/s (E Class), f) wind velocity 2 m/s (F Class)
Source: authors

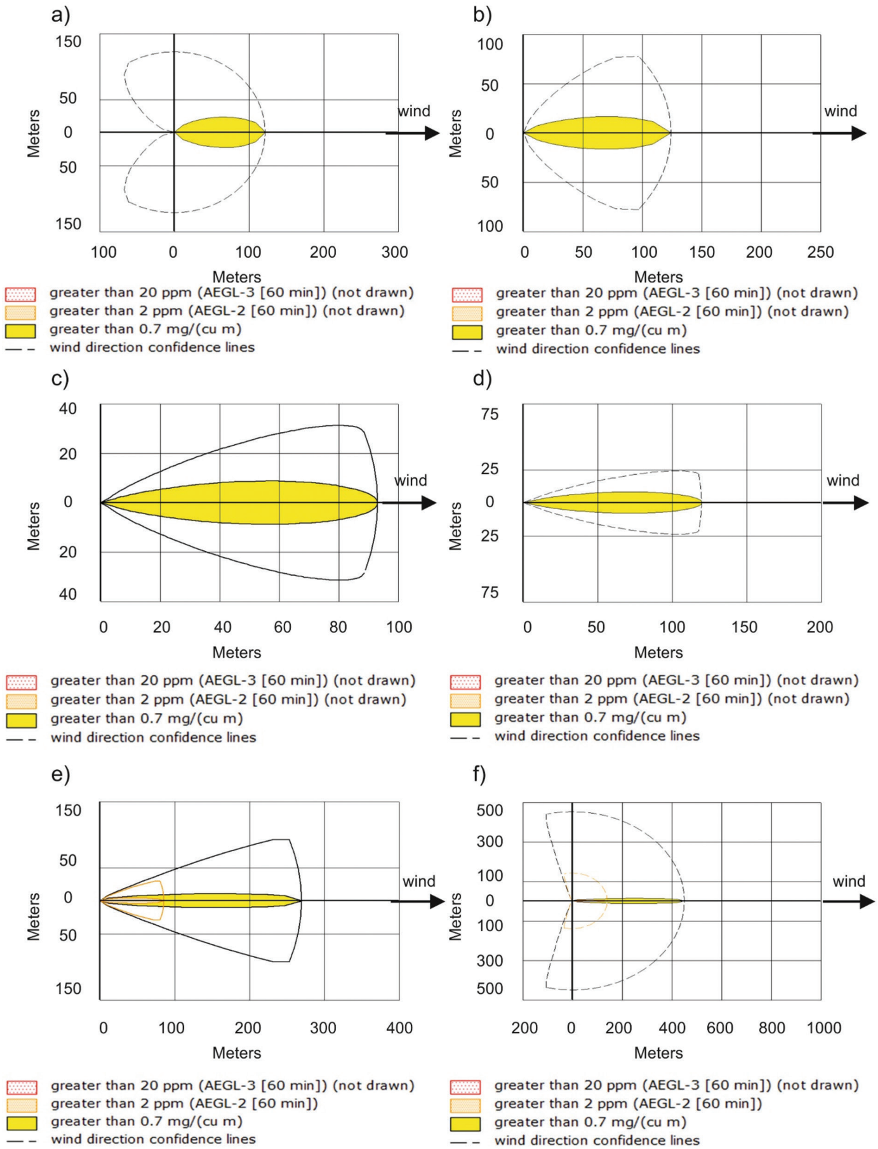

Fig. 3. The chlorine distribution for: a) wind velocity 2 m/s (A Class), b) wind velocity 3 m/s (B Class), c) wind velocity 4 m/s (C Class), d) wind velocity 5 m/s (D Class), e) wind velocity 3 m/s (E Class), f) wind velocity 2 m/s (F Class)

Source: authors

3.2. Three-dimensional dispersion

In the next step, with the use of the Ansys-Fluent software, three-dimensional gas mixture transport was analyzed. At the beginning the windless case was investigated. The ammonia indicated irregular shape of the concentration profile (Fig. 4a), while the chlorine cloud had the circular profile (Fig. 4b).

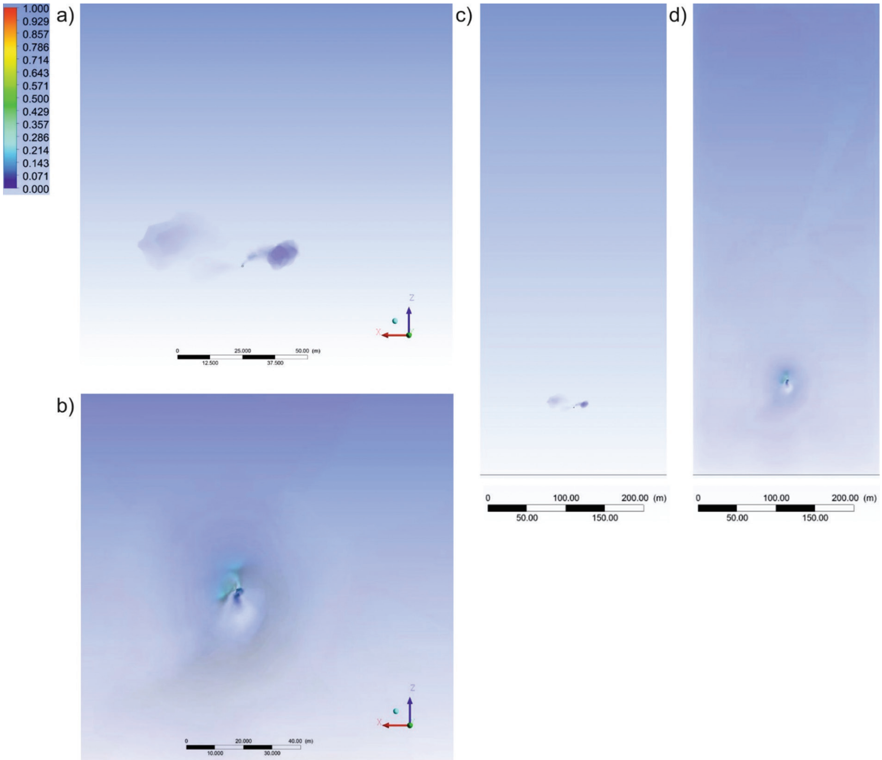

Fig. 4. Windless condition for: the ammonia distribution (a,c), the chlorine distribution (b,d)
Source: authors

The analysis of gas concentration 0.5 m above the source of leakage indicated higher amount of the chlorine gas compared to the ammonia (Fig. 5a). Moreover, the relocation of maximal value for the ammonia (about 40m from a source of gas leakage) was observed, while for the chlorine it was approximately in the center of the gas leakage (Fig. 5b). At the level of 10.5 m the volume fraction of the ammonia gas was equal to 0.000016 (Fig. 5b). The increase of height with 0.5 m did not indicate any change of the ammonia volume fraction (Fig. 5b). While, for the chlorine, at the level of 10.5m,the volume fraction was equal to 0.036 (Fig. 5).The increase of height with 0.5 m indicated approximately 47 % the decrease of the chlorine volume fraction (0.017) (Fig. 5a).

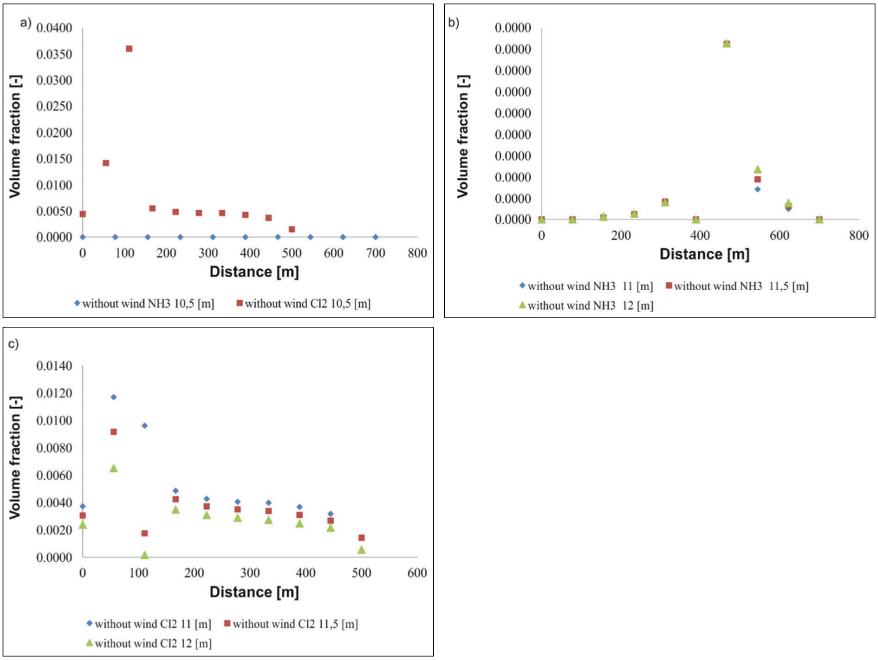

Fig. 5. Gas dispersion without wind in function of height for: a) 10.5 m above the source of dispersion in the center for the ammonia and the chlorine, b) 11 m, 11.5 m and 12 m above source of dispersion in the center for the ammonia, c) 11 m, 11.5 m and 12 m above the source of dispersion in the center for the chlorine

Source: authors

In the next step, the influence of wind was analyzed. For both gases (the ammonia and the chlorine)the implementation of wind indicated the cloud relocation ahead of the source of leakage. With the increase of wind value, the shape of the ammonia and the chlorine cloud became narrower (Fig. 6). Similar, as it was for two-dimensional model, wider cloud for the ammonia compared to the chlorine was observed. The increase of wind velocity induced narrowing of the gas concentration profile for both substances (Fig. 6a, b, 6e, f). Moreover, for the wind velocity equal to 2 m/s the higher ammonia concentration compared to the chlorine was observed. Increase of wind velocity induced a decrease of the level of the ammonia and the chlorine.

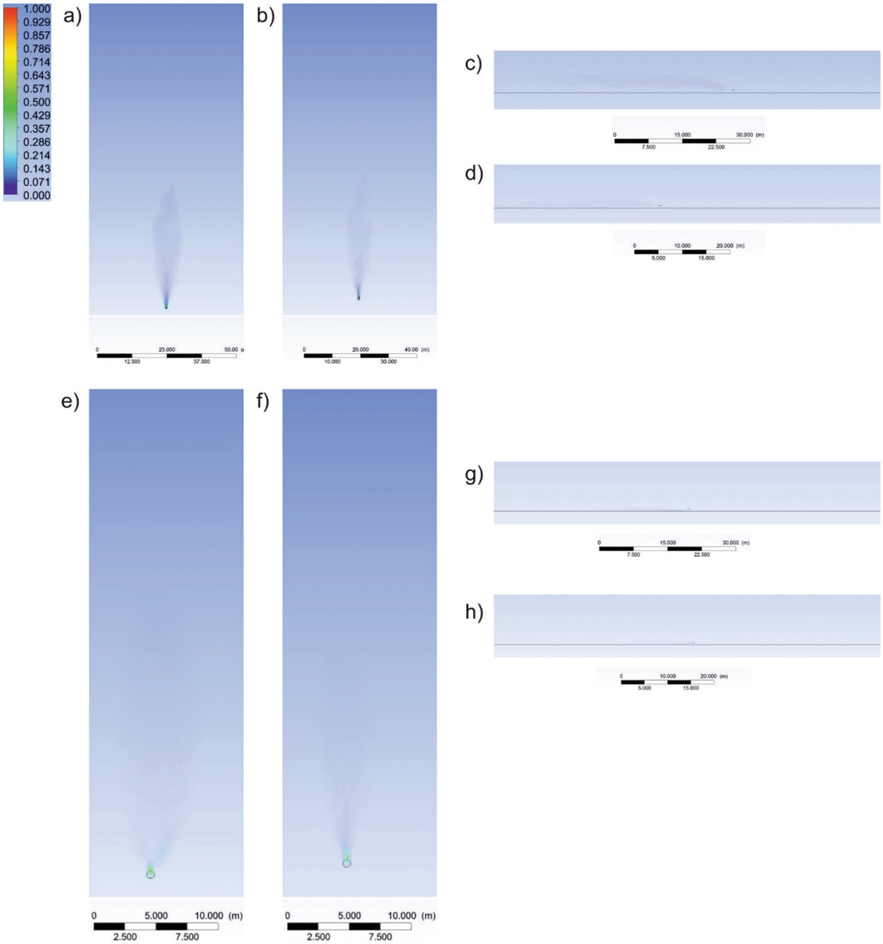

Fig. 6. Gas dispersion for: a) ammonia (wind velocity 2 m/s) – view from above, b) chlorine (wind velocity 2 m/s) – view from above, c) ammonia (wind velocity 2 m/s) – side view, d) chlorine (wind velocity 2 m/s) – side view

Source: authors

The analysis of the gas concentration in function of the height indicated the highest ammonia concentration for 10.5 m (0.00106 and 0.0011 for A class (2 m/s) and B class (5 m/s), respectively) (Fig. 7a). While, for the chlorine for

10.5 m height it was 0.0025 and 0.0012 for A class (2m/s) and B class (5 m/s), respectively (Fig. 7c). Moreover, for the height 11m volume, the fraction of the ammonia was equal to 0.0012 and 0.0008 for 2 m/s and 5 m/s, respectively. While, for the chlorine at the same level volume, the fraction was equal to 0.0007 and 0.0002 for 2 m/s and 5 m/s respectively. The comparison of constant and dynamic cases (windless case and wind velocity equal to 2 m/s) for the ammonia indicated the increase of volume fraction, while, for the chlorine the decrease was observed. Moreover, the comparison of the ammonia and the chlorine at 10m for 2 m/s indicated 2.5-fold increase of the chlorine concentration. While, for 5 m/s similar concentration was observed for both gases, 0.0011 and 0.0012 for the ammonia and the chlorine, respectively (Fig. 7b). Furthermore, for 11 m height about 1.7-fold higher volume concentration for the ammonia compared to the chlorine was observed (2 m/s). While, for 5m/s, there was about 4.6-fold decrease of the chlorine concentration compared to the ammonia (Fig. 7d).

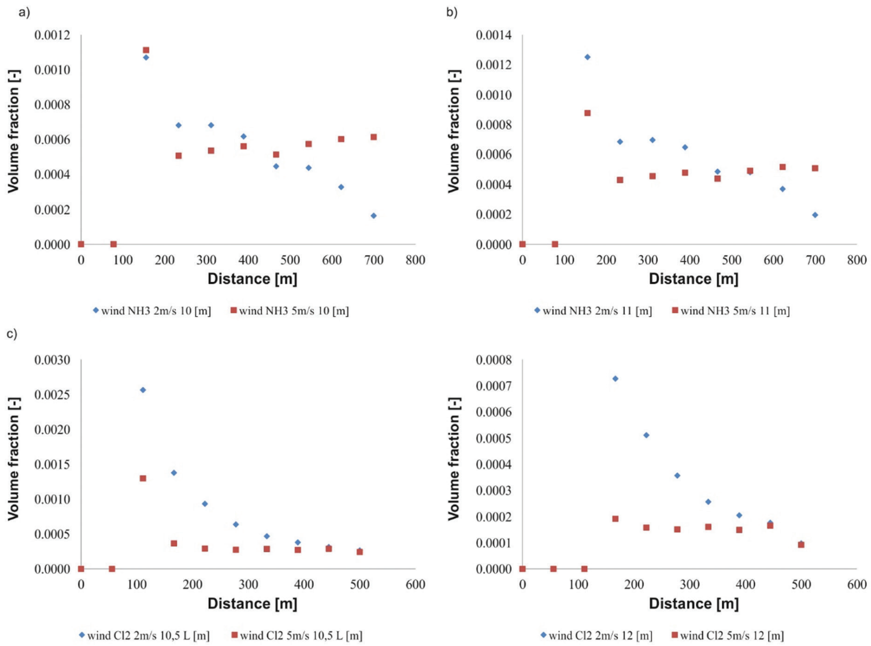

Fig. 7. Gas dispersion in function of the wind velocity: a) the ammonia (wind velocity 2 m/s), b) the ammonia (wind velocity 5 m/s), c) the chlorine (wind velocity 2 m/s), d) the chlorine (wind velocity 5 m/s)

Source: authors

4. Conclusions

In conclusion, two different approaches to gas mixture dispersion (two-, three-dimensional) were discussed. The main difference was the absence of height in two-dimensional simulations. However, the results from 2d solver allowed to predict the range of polluted cloud in the horizontal direction. While, 3d approach with the use of Ansys-Fluent allowed deeper analysis including both the horizontal and the vertical distribution of the chlorine. With the increase of wind value, the shape of the ammonia and the chlorine profile became narrower. Similar, as it was for the two-dimensional model.

Moreover, comparison of the windless and the wind conditions indicated high impact of the wind velocity on clouds shape. For the windless case irregular shape of the ammonia concentration profile was observed, while for the wind application the main ammonia concentration moved ahead the source of dispersion. Furthermore, the chlorine in the windless case had the circular profile around the source of gas escape. While, for the wind application the main chlorine concentration moved ahead the source of dispersion, as it was for the ammonia.

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