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3D Simulation of Chlorine Dispersion in Rrural Area

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1. Introduction

Prediction of dispersion of hazardous substances resulting from accidental leakage in environment is essential for analysis of risk and emergency response (Dong et al. 2017, Piecuch & Piecuch 2013). After release into the atmosphere, chlorine cloud may cause serious injury to human health (Li et al. 2015). Dense gases tend to accumulate at ground level or human breath level (Scargiali et al. 2011, Siddiqui et al. 2012). The presence of hazardous gases in such areas multiplies the negative effects (Pontiggia et al. 2010).

So far, different approaches are applied to prevent the effects chlorine cloud dispersion (Lovreglio et al. 2016). To assist decisions and planning of emergency response in case of release of dangerous gases computational techniques are applied (Hannaa et al. 2009). Reliable numerical description of multiphase processes, i.e. dispersion still represents one of the most challenging applications (Markiewicz 2012). It is often an iterative process that requires a multiple modeling to understand different aspects of analyzed problems (He et al. 2017). There are different approaches such as 2D or 3D numerical description of dispersion processes (Andreinia et al. 2016, Ganta et al. 2014). However, reliable numerical model includes calculation of gas transport not only in horizontal plain (Thoman et al. 2006) but it also includes 3D movement (Labovský & Jelemenský 2010). Moreover, as different character of flow is considered in dispersion process, different turbulence models are applied (Hongna et al. 2015, Ming-Liang et al. 2010, Tominaga & Stathopoulos 2009).

Various numerical tools are applied for description of dispersion process i.e. PHAST software (Wang et al. 2017), ALOHA software (Thoman et al. 2006), ANSYS software (Polanczyk et al. 2013, Salamonowicz et al. 2015). Development of numerical algorithms has enabled the computational fluid dynamics (CFD) models to be used extensively in indoor dispersion studies (Dong et al. 2017). Numerical methods based on computational fluid dynamics (CFD) may facilitate the precise investigation of the hazardous substances dispersion (Meroney 2012). Therefore, the aim of the study was to prepare a transient CFD model describing the phenomena of chlorine dispersion in a dynamic setup including different environmental factors.

2. Materials and methods

Emergency chlorine ejection into atmosphere was prepared using the following boundary conditions: free ejection of chlorine into open space (T = 25°C and P = 101325 Pa); the total amount of ejected chlorine was equal to 1.8 kg. The properties of analyzed gases were as follow: air (ρ = 1.23 kg/m^3, η = 1.79 10^{-5} kg/(m s)), chlorine (ρ = 2.95 kg/m^3, η = 1.33 10^{-5} kg/(m s)) (Steven R. Hannaa et al. 2009).

Two approaches of chlorine concentration estimation were analyzed: first – horizontal (2D) simulation (eq.1) (Aloha software) (Sun et al. 2013, Thoman et al. 2005, Tsenga et al. 2012) and the second – horizontal and vertical (3D) simultaneous simulation (ANSYS software) (Polanczyk et al. 2013, Wawrzyniak et al. 2012a, Wawrzyniak et al. 2012b).

2.1. 2D approach of dispersion

2D approach was analyzed with the use of Aloha software. Mathematical domain was described with rectangle (length = 500 m, width = 200 m) (Fig. 1a). Chlorine ejection was described with the circular hole (diameter = 0.1 m) placed 100 m from wind inlet to the domain. Following boundary conditions were applied: velocity inlet (circular surface), outlet (remaining lines). Reconstruction of dispersion in real conditions required usage of Pasquill stability classes (Krügera & Emmanuel 2013). Each time constant humidity (φ = 50%) was considered.

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

$$X(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z u} exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)\right]\right\} \tag{1}$$

where:
X(x,y,z) – atmospheric concentration for chemical releases, [mg/m^3],
Q – source term release rate for chemical releases, [mg/s],
x – downwind distance (relative to source location), [m],
y – crosswind distance (relative to plume centerline), [m],
z – vertical axis distance (relative to ground), [m],
H – effective release height (relative to ground), [m],
y – crosswind distance (relative to plume centerline), [m],
σ_y, – horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction, [m],
σ_z – vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction, [m],
u – average wind speed, [m/s].

2.2. 3D approach of dispersion

In the second step 3D dispersion of gas mixture (including height) was prepared with the use of Ansys-Fluent 18 software. For 3d simulation Reynolds Averaged Navier-Stokes equations (eq. 2-4) were applied (Ganta et al. 2014, Zieminska-Stolarska et al. 2015).

$$\rho\left(\frac{\partial v_x}{\partial t}+v_x\frac{\partial v_x}{\partial x}+v_y\frac{\partial v_x}{\partial y}+v_z\frac{\partial v_x}{\partial z}\right)=\rho g_x-\frac{\partial p}{\partial x}+$$
$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(2\frac{\partial v_x}{\partial x})\right)+\frac{\partial}{\partial y}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial y}+\frac{\partial v_y}{\partial x})\right)+\frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_x}{\partial z}+\frac{\partial v_z}{\partial x})\right) \tag{2}$$

$$\rho\left(\frac{\partial v_y}{\partial t}+v_x\frac{\partial v_y}{\partial x}+v_y\frac{\partial v_y}{\partial y}+v_z\frac{\partial v_y}{\partial z}\right)=\rho g_y-\frac{\partial p}{\partial y}+$$
$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(\frac{\partial v_y}{\partial x}+\frac{\partial v_x}{\partial y})\right)+\frac{\partial}{\partial y}\left((\mu+\mu_t)(2\frac{\partial v_y}{\partial y})\right)+\frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_y}{\partial z}+\frac{\partial v_z}{\partial y})\right) \tag{3}$$

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

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

where:
v_x,v_y,v_z – 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],
μ_t – turbulent viscosity, [Pa s].

First, 3D geometry of prism was prepared with the use of a pre-processor (length = 500 m, width = 200 m, height = 50 m) (Fig. 1b). In the lower part of analyzed domain, cylindrical geometry representing chlorine ejection was located (0.3 m above the ground with diameter = 0.1 m). Next, digital grid composed of tetrahedrons with boundary layer was created. After mesh independent tests the number of numerical grid elements was established at approximately 900 000, with boundary layer composed of 10 layers. To simulate chlorine ejection into atmosphere a multiphase approach was considered. As previously described the volume of Fluid model (VOF) in Ansys-Fluent was applied (He et al. 2017).

Flow of two phases, air and chlorine, was assumed. The following boundary conditions were used: mass flow inlet (one surface), wall (one surface – as a ground), pressure outlet (three surfaces) and velocity inlet (one surface). At the inlet do the geometry, near the source of chlorine ejection, velocity inlet boundary representing flowing air was applied. Velocity profile was experimentally set (Table 1) and configured as a function of height u(h) (eq. 5).

Chlorine was applied with the use of mass flow inlet boundary equal to 1.8 kg/h. At the outlets pressure outlet boundary condition was applied. Finally ground was described with wall boundary with roughness, pretended appearance of buildings. Moreover, 1 hour of dispersion was assumed. According to the Reynolds number turbulent flow, described with the *k*-*ε* model, was established.

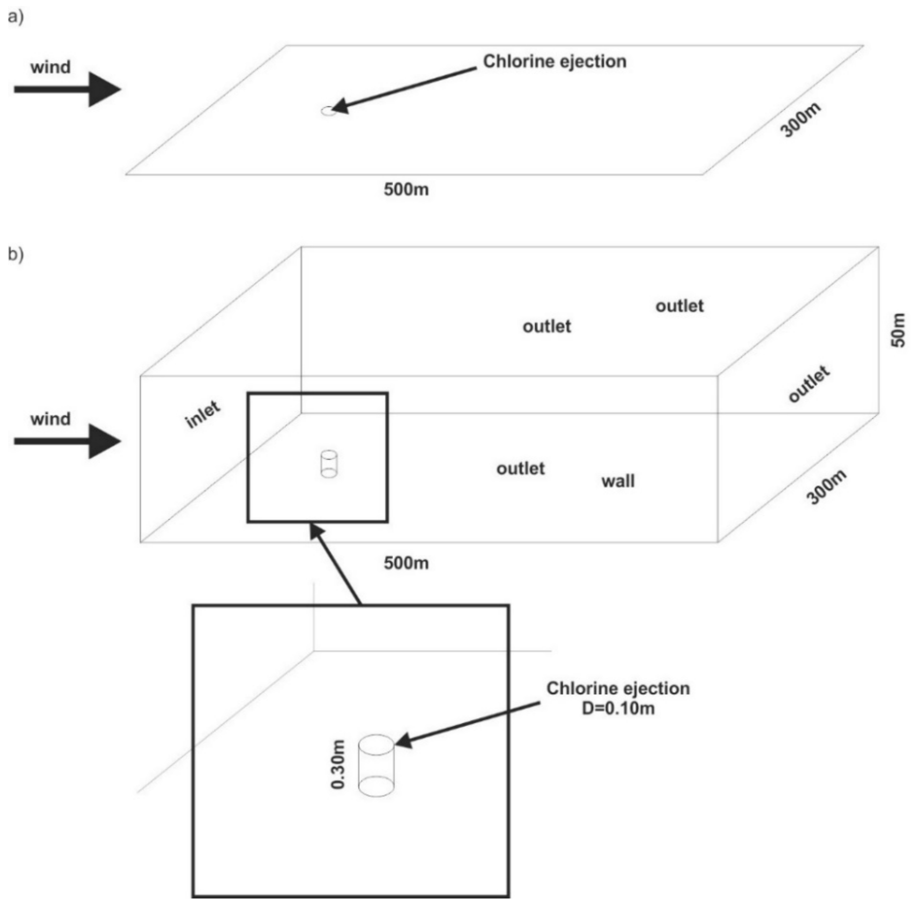

Fig. 1. Mathematical domain for: a) 2D dispersion, b) 3D dispersion.
Rys. 1. Matematyczna domena obliczeniowa dla: a) dwuwymiarowej dyspersji, b) trójwymiarowej dyspersji.

Table 1. Maximal air velocity for different stability class at the 10 m height.
Tabela 1. Maksymalne wartości prędkości wiatru dla różnych klas stabilności na wysokości 10 m.

Stability classes [-]	Air velocity at the height 10 m [m/s]	P [-]
A	2	0.109
B	3	0.112
C	4	0.120
D	5	0.142
E	3	0.203
F	2	0.253

3. Results

Two approaches for chlorine dispersion process were analyzed. It was observed that for horizontal chlorine distribution increasing wind velocity lead to longer and narrower chlorine cloud (Fig. 2). For the case when wind velocity was increased from 2-3 m/s (A-B stability classes) width of chlorine cloud was about 50 m and cloud length was increased from 120 m (2 m/s) to 150 m (3 m/s). Meanwhile, when velocity was decreasing from 3-2 m/s (E-F stability class), cloud became longer and narrower to about 25-20 m, and the length of chloride cloud was increased from 610 m (3 m/s) to 1300 m (2 m/s).

To include height parameter for chlorine distribution 3D model was analyzed. As the default values for turbulent model *k-ε* of flow was applied and two stability classes (A and B) (Fig. 3c and Fig. 3d) were simulated. Additionally, chlorine dispersion without wind was analyzed (Fig. 3a and Fig. 3b).

Analysis of chlorine distribution indicated that the highest concentration was in the axis of chlorine ejection. Moreover, when wind was neglected circular profile of chlorine was observed (Fig. 3a and Fig. 3b). Quantitative analysis of chlorine distribution indicated a decrease in volume fraction in function of height (from approximately 0.033 for 10.5 m to 0.0005 for 13.5 m). While with wind condition the model presented changes of chlorine profile shape which had the same direction as wind (Fig. 3c and Fig. 3d). Similarly to the case without wind a decrease in chlorine concentration in the function of height was observed. For the velocity 2 m/s (A stability class) the range of chlorine volume fraction was 0.025-0.0001, while for the velocity 3 m/s (B stability class) the range of chlorine volume fraction was 0.019-0.0005.

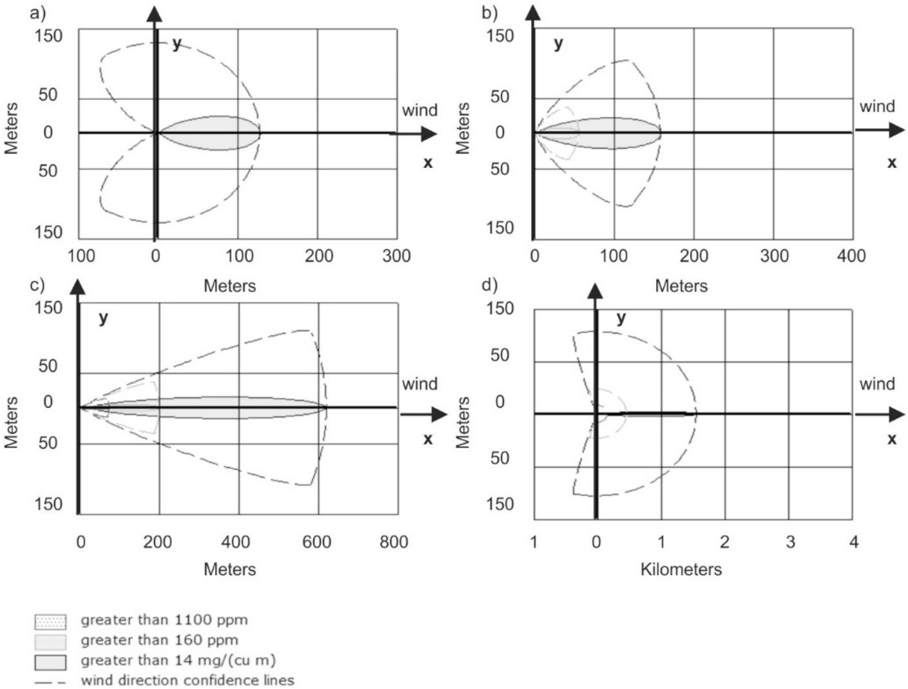

Fig. 2. An example of horizontal distribution of chlorine for: a) wind velocity 2 m/s (A class), b) wind velocity 3 m/s (B class), c) wind velocity 3 m/s (E class), d) wind velocity 2 m/s (F class).
Fig. 2. Przykład poziomej dystrybucji chloru dla: a) prędkości wiatru 2 m/s (klasa stabilności A), b) prędkości wiatru 3 m/s (klasa stabilności B), c) prędkości wiatru 3 m/s (klasa stabilności E), d) prędkości wiatru 2 m/s (klasa stabilności F).

Comparison of windless approach with velocity equal to 2 m/s indicated approximately 25% decrease of chlorine volume fraction for wind case. While, comparison of both cases at the level of 11 m indicated approximately 5% difference. Finally, for the height 13.5 m about 95% decrease of chlorine fraction (0.0001) compare to 10.5 m height was observed. Furthermore, for all analyzed cases maximal chlorine concentration was noticed in a distance of about 20-50 m from the source of chlorine dispersion in direction of wind movement.

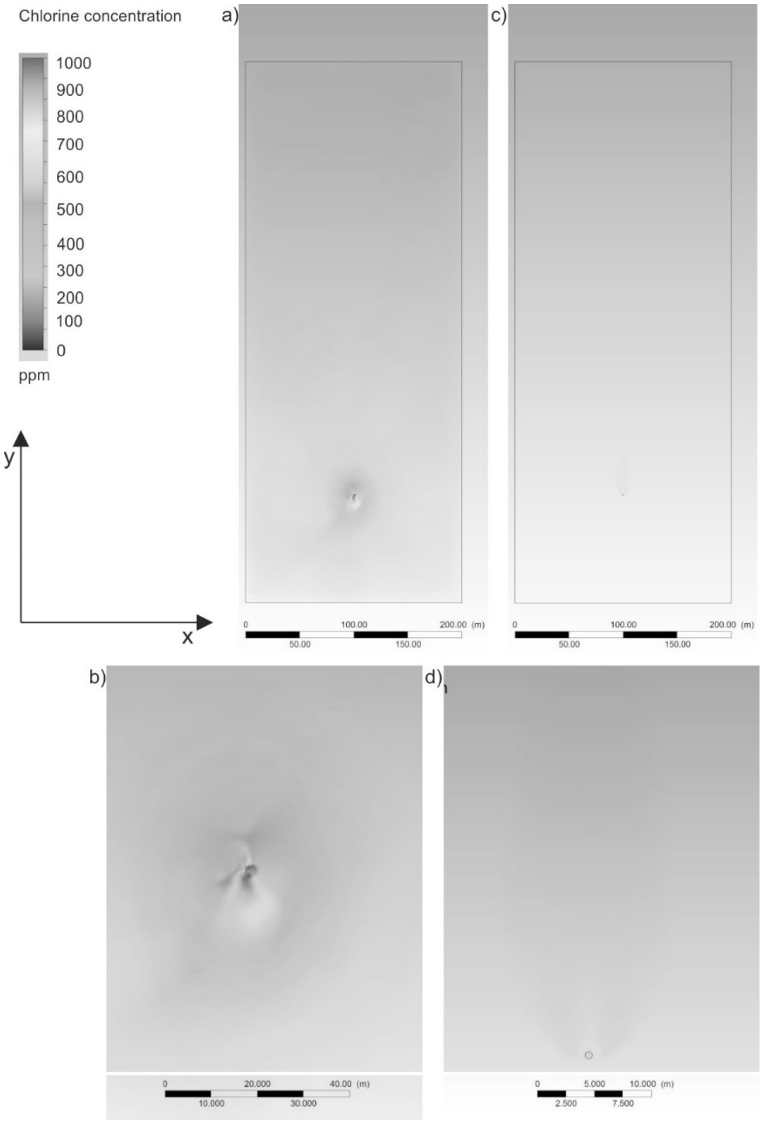

Fig. 3. An example of chlorine distribution for: a-b) chlorine dispersion without wind (a – top view, b – zoomed top view); c-d) chlorine dispersion including wind (2 m/s) (c – top view, d – zoomed top view)

Rys. 3. Przykład dystrybucji chloru dla: a-b) rozprzestrzeniania chloru bez uwzględnienia wiatru (a – widok z góry, b – powiększenie widoku z góry), c-d) rozprzestrzeniania chloru z uwzględnieniem wiatru (a – widok z góry, b – powiększenie widoku z góry)

4. Discussion

In this research, the effects of the environmental situations, like different wind intensity, with the release and spread of chlorine in the indoor space were presented. The numerical analysis of dispersion produced both horizontal and vertical distribution of chlorine in analyzed mathematical domain. Similar to our study, Labovsky et al. investigated CFD model of chlorine dispersion however in urban environments. They found that the CFD approach determines the variation of properties, velocity, and concentration along the flow streamlines, which enhances the effectivity of this approach in the presence of obstructions, and in handling a complex terrain (Labovsky & Jelemensky 2013).

In our study we assumed turbulent character of flow, therefore, standard k-ε model was applied to describe its properties. It was in line with Xing et al. who observed that the results from the standard *k-ε* model were in acceptable agreement with the experimental data for the gas dispersion process (Xing et al. 2013). Contrary to this Sklavounos et al. found that the standard *k–ε* model overestimate maximal concentration of heavy gas (Sklavounos & Rigas 2004). Nevertheless, our study indicated that this turbulent model may be used in simulation of chlorine dispersion.

To reconstruct a realistic conditions of wind appearance, a velocity profile at the inlet to the mathematical domain was applied. It was in line with Mack et al. who investigated CO_2 dispersion where experimentally measured inlet profile of wind was applied (Mack & Spruijt 2014). Moreover, it was observed that wind indicated chlorine cloud movement. Similarly, Safakar et al. who investigated chlorine dispersion, observed the effect of various temperatures and wind on spreading the dense gases. Moreover, they noticed that above the ground level the chlorine concentration increased slowly (Safakar et al. 2016). While, Hanna et al. reported that near the source, the obstacles tend to slow down the dense gas cloud and may constrain it causing an increase in concentration (Hanna et al. 2009).

5. Conclusions

2D model allowed prediction of polluted cloud in horizontal direction, while 3D model allowed description of horizontal and vertical distribution of chlorine. It was observed that with increase of Pasquill stability class the area of chlorine dispersion had similar character for horizontal model as well as for 3D model.

Comparison of constant and dynamic setup indicated high impact of wind. For the windless case circular profile of chlorine concentration around dispersion source was observed. While, for the wind application the main chlorine concentration moved ahead the source of dispersion. Analysis of chlorine concentration in function of height resulted in decrease of chlorine appearance in upper level of mathematical domain. While, analysis of chlorine concentration in function of wind intensity indicated extension of chlorine cloud with decrease of concentration.

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Symulacja 3D dyspersji chloru w terenie wiejskim

Abstract

Prediction of hazardous substances dispersion resulting from accidental leakage in environment is essential for risk analysis and emergency response. Different numerical tools are applied for description of dispersion process. Development of numerical algorithms has enabled the computational fluid dynamics (CFD) models to be used extensively in indoor dispersion studies. Numerical methods based on computational fluid dynamics (CFD) may facilitate the precise investigation of the hazardous substances dispersion. Therefore, the aim of the study was to prepare a transient CFD model describing the phenomena of chlorine dispersion in a dynamic setup including different environmental factors. Reliable computational description of dispersion process still represents one of the most challenging applications. Therefore, we aimed to prepare a transient 2D and 3D numerical models of chlorine dispersion from a ground source in a dynamic setup. For 2D simulation a Degadis model was used, while for 3D approach a multiphase Volume of Fluid model (VOF) was applied. For both analyzed cases area of investigation was equal to 0.1 km^2. Furthermore, for 3D simulations height was equal to 50 m. For the reconstruction of atmospheric conditions Pasquill stability classes and one-direction wind were applied. Analysis of chlorine concentration in function of wind intensity indicated extension of chlorine cloud with decrease of concentration. Moreover, comparison of constant and dynamic setup indicated high impact of wind. In case of windless conditions circular profile of chlorine concentration around dispersion source was noticed. Wind directed the chloride cloud which dispersed accordingly to the wind direction. As expected chloride concentration decreased with altitude. 2D model allowed prediction of polluted cloud in horizontal direction, while 3D model allowed description of horizontal and vertical distribution of chlorine. It was observed that with increase of Pasquill stability class the area of chlorine dispersion had similar character for horizontal model as well as for horizontal and vertical model (3D). For the windless case circular profile of chlorine concentration around dispersion source was observed. Additionally, for the wind application the main chlorine concentration moved ahead the source of dispersion. Analysis of chlorine concentration in function of height resulted in decrease of chlorine appearance in upper level of mathematical domain.

Streszczenie

Predykcja dyspersji substancji niebezpiecznych z przypadkowych wycieków jest niezbędna w analizie ryzyka. W tym celu do opisu procesu dyspersji stosowane są różne numeryczne narzędzia. Rozwój matematycznych algorytmów umożliwia stosowanie m.in. techniki CFD na szeroką skalę. Tym samym celem niniejszej pracy było opracowanie dwuwymiarowego i trójwymiarowego modelu opisującego zjawisko dyspersji chloru z naziemnego źródła. Dla dwuwymiarowego podejścia zastosowano model Degadisa. Natomiast dla trójwymiarowego podejścia wielofazowy model VOF. Dla obu przypadków powierzchnia analizowanego obszaru wynosiła 0.1 km^2. Co więcej, dla trójwymiarowego podejścia wysokość analizowanej domeny obliczeniowej wynosiła

50 m. W celu rekonstrukcji parametrów atmosferycznych uwzględniono klasy stabilności Pasquilla oraz wpływ wiatru. Dwuwymiarowy model umożliwiał analizę procesu dyspersji w płaszczyźnie poziomej, podczas gdy model trójwymiarowy umożliwiał analizę zarówno w płaszczyźnie poziomej jak i pionowej. Analiza obu modeli wskazuje, iż wzrost intensywności wiatru wydłuża zasięg chmury chloru, z jednoczesnym spadkiem jego stężenia. Co więcej, w przypadku nieuwzględnienia przepływu wiatru obserwowano kołowy profil stężenia chloru dookoła źródła dyspersji. Natomiast przepływający wiatr powodował zmniejszenie koncentracji chloru wraz z wysokością. Również zaobserwowano, iż uwzględnienie klas stabilności Pasquilla miało porównywalny efekt w przypadku podejścia dwuwymiarowego i trójwymiarowego. Uwzględnienie wiatru powodowało przemieszczenie maksymalnej wartości stężenia chloru znad źródła dyspersji. Co więcej, analiza stężenia chloru w funkcji wysokości wskazuje na zmniejszenie zawartości chloru w górnej części domeny matematycznej.

Słowa kluczowe:
dyspersja chloru, CFD, model dyspersji gazu ciężkiego, przepływ turbulentny, model awaryjnej odpowiedzi

Keywords:
chlorine dispersion, CFD, dense gas dispersion models, turbulent flow, emergency response model