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Computational modeling of gas mixture dispersion in a dynamic setup – 2d and 3d numerical approach

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Abstract. The aim of the study was to prepare a mathematical model of gas mixture dispersion with the use of Computational Fluid Dynamic (CFD) technique. Three dimensional chlorine dispersion in a dynamic setup with the use of Volume of Fluid model (VOD) model was applied. The area of investigation was equal to 0.1km^2 and the high of the mathematical domain was equal to 50m. Atmosphere was considered in two stages: as one direction of wind flow and no wind. Comparison of constant and dynamic conditions 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.

1 Introduction

There are different techniques to estimate the risk of uncontrolled ejection of chemical substances storied in dedicated tanks. Moreover, the European Seveso II Directive requires operators of major hazard facilities to prepare safety reports including evaluation of the effects of dangerous substances release to the environment [1]. Numerical methods are commonly used techniques for the description of dispersion process [2]. Reliable computational description of multiphase processes, i.e. dispersion still represents one of the most challenging applications [3]. It is often an iterative process requiring multiple modeling frameworks to understand different aspects of the flow problem [4, 5]. Different commercial codes for 2d and 3d numerical description of dispersion process are used, however steady state conditions are considered. Moreover, referring to the character of multiphase flow in dispersion process different turbulence models are applied [6, 7]. Therefore, in this paper we aimed to prepare a transient numerical model describing the phenomena of chlorine dispersion in a dynamic setup including different environmental factors.

2 Material and Methods

In this study a mathematical description of an emergency chlorine ejection into the atmosphere with the flowing air was prepared. The following assumptions were made: (1)

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free ejection of chlorine into the open space (T = 25°C and P = 101325Pa); (2) the total amount of ejected chlorine was equal to 1.8 kg. Physical properties of the analyzed materials were as follow: air (density – ρ = 1.23 kg/m^3, viscosity – η = 1.79 10^{-5} kg/(m s)), chlorine (density – ρ = 2.95 kg/m^3, viscosity – η = 1.33 10^{-5} kg/(m s)) [8].

First, for the horizontal estimation of chlorine concentration (eq.1) Aloha software was applied [9, 10].

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

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].

2d geometry was composed of four lines creating a closed surface (Length = 500m, Width = 200m). Boundary conditions were as follow: velocity inlet (one line), free outlet (remaining lines). Moreover, chlorine ejection was described with the circular hole (Diameter = 0.1m) placed 100m from wind inlet to the domain. Six cases with different air velocity, according to the Pasquil Stability Classes [11], at the inlet to the domain were analyzed. Each time constant humidity (φ = 50%) was considered.

Next, 3d dispersion of gas mixture (including height) with the use of Fluent-Ansys 17.2 software (license to the University) was prepared. For 3d multiphase transport Navier-Stokes equations (eg.2 - 4) were applied [5].

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

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

$$\rho\left(\frac{\partial v_z}{\partial t}+v_x\frac{\partial v_z}{\partial x}+v_y\frac{\partial v_{zy}}{\partial y}+v_z\frac{\partial v_z}{\partial z}\right)=\rho g_z-\frac{\partial p}{\partial z}+$$
$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial x}+\frac{\partial v_x}{\partial z})\right)+\frac{\partial}{\partial y}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial y}+\frac{\partial v_y}{\partial z})\right)+\frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial z})\right) \tag{4}$$

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, with the use of a preprocessor SpaceClaim–Ansys software (ANSYS, USA) 3d mathematical domain was prepared (Fig.1a). 3d geometry was composed of six surfaces creating a closed volume (Length = 500m, Width = 200m, Height = 50m). In the lower part of the analyzed domain, 0.3m above the ground, cylindrical geometry (Diameter = 0.1m) representing a place of chlorine ejection was located. Next, with the use of mesh generator ICEM-Ansys software (ANSYS, USA) numerical grid composed of tetrahedrons with boundary layer was prepared (Fig.1b). After mesh independent tests the number of numerical grid elements was established at approximately 1 000 000. Moreover, in order to reconstruct irregularities of the real ground a boundary layer composed of 10 layers, next to the surface representing ground, was included.

a) b)

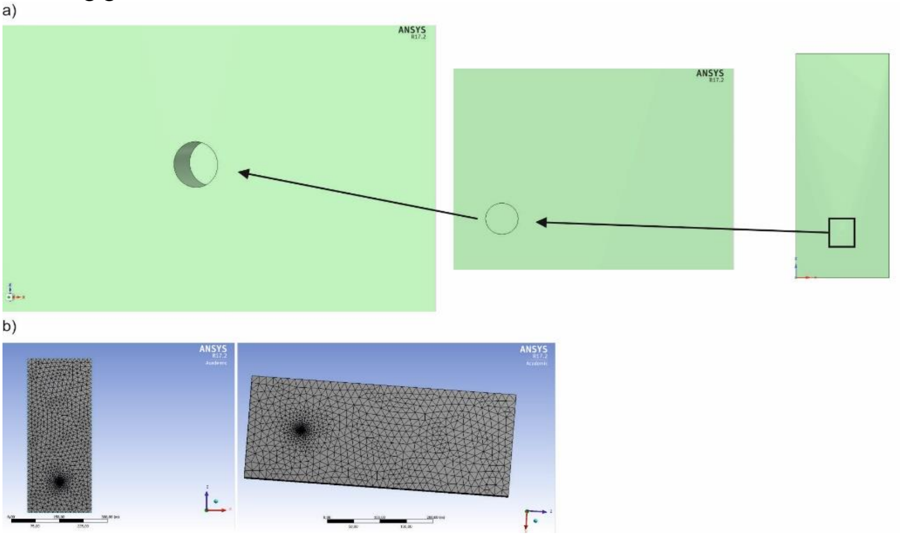

Fig. 1. 3d mathematical model of analyzed object: a) 3d numerical domain, b) 3d numerical grid.

In order to simulate 3d chlorine transport in a dynamic setup (flow of air) a processor Ansys-Fluent software (ANSYS, USA) with multiphase Volume of Fluid model (VOD) was applied [12]. Flow of two phases, i.e. air and chlorine was assumed. At the inlet do the domain, 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).

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

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, [-].

For each of six analyzed cases different maximal velocity of air depending on the Pasquil Stability Classes [11] was applied. Moreover, to analyze the influence of wind on chlorine transport no wind case was added.

Source of chlorine ejection was described with the use of mass flow inlet boundary. For the free flow outside the domain, without reduction of velocity to 0m/s, at the outlets pressure outlet boundary was set. Finally, between fluid and solid, to describe the ground of analyzed domain, wall boundary was assigned. Additionally, surface roughness on the bottom (pretended different size of buildings) was applied. Transient conditions for calculations (1 hour of dispersion) were assumed. According to the Reynolds number turbulent flow, described with the k-ε model, was established.

Table 1. Maximal air velocity for different 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
E	3	0.203
F	2	0.253

3 Results

In this study 2d and 3d computer simulations of chlorine dispersion were performed. In the first step, with the use of Aloha software the range of chlorine cloud in horizontal configuration in function of wind velocity was analyzed. It was observed that for different Pasquil Stability Classes the area of chlorine dispersion became longer and narrower (Fig.2a–Fig.2f). Moreover, there was 4 times higher range of chlorine dispersion for the F stability class compare to the A class.

In the next step, chlorine dispersion was analyzed in a function of height with the use of Ansys-Fluent solver. According to the default parameters of k-ε model application, simulation procedure was narrowed up to four Pasquil Stability Classes (from A to D). At the beginning dispersion of chlorine for the windless day was analyzed (Fig. 3).

The highest chlorine concentration was observed in the axis of chlorine dispersion source. Absence of wind resulted in circular profile of chlorine spreading. Moreover, with increase of height a decrease of chlorine concentration was observed. At the level of 10.5m volume fraction of chlorine gas was equal to 0.036 (Fig4a and Fig.4c). While, increase of height with 0.5m indicated approximately 47% decrease of chlorine volume fraction into 0.017 (Fig.4b). Finally, for the height 13.5m 96% decrease of chlorine fraction (0.0005) compare to 10.5m height was observed (Fig.4b).

In the next step, the influence of wind was analyzed. Consideration of wind in dispersion process indicated change of chlorine profile shape. Wind factor induced chlorine only ahead of dispersion source. Therefore, contrary to the windless case, chlorine concentration between source of wind and source of dispersion was equal to 0. With the increase of wind value the shape of chlorine profile became narrower, as it was presented in 2d approach. Similar, to the windless case, increase of height indicated decrease of chlorine concentration (Fig.5).

The highest chlorine concentration for A class (v=2m/s) was equal to 0.026 (Fig.6a–6b). Comparison of constant and dynamic cases (windless case and wind velocity equal to 2m/s) indicated approximately 28% decrease of chlorine volume fraction for wind velocity equal to 2m/s. Increase of height with 0.5m indicated approximately 62% decrease of chlorine volume fraction (0.016) (Fig.6c). While, comparison with windless case about 6% difference was observed. Finally, for the height 13.5m about 99% decrease of chlorine fraction (0.00009) (Fig.6h) compare to 10.5m height was observed. For D class (v=5m/s) the highest chlorine volume fraction was equal to 0.013 (Fig.6b). There was about 50% decrease of volume fraction between D and A class, for 5m/s. Moreover, analysis of chlorine volume fraction in function of height indicated about 72% and 82% decrease of volume fraction for A class and windless case, respectively (Fig.6a–6d). Furthermore, for all analyzed cases maximal chlorine concentration was observed in distance about 20-50m from the source of chlorine dispersion in direction of wind movement.

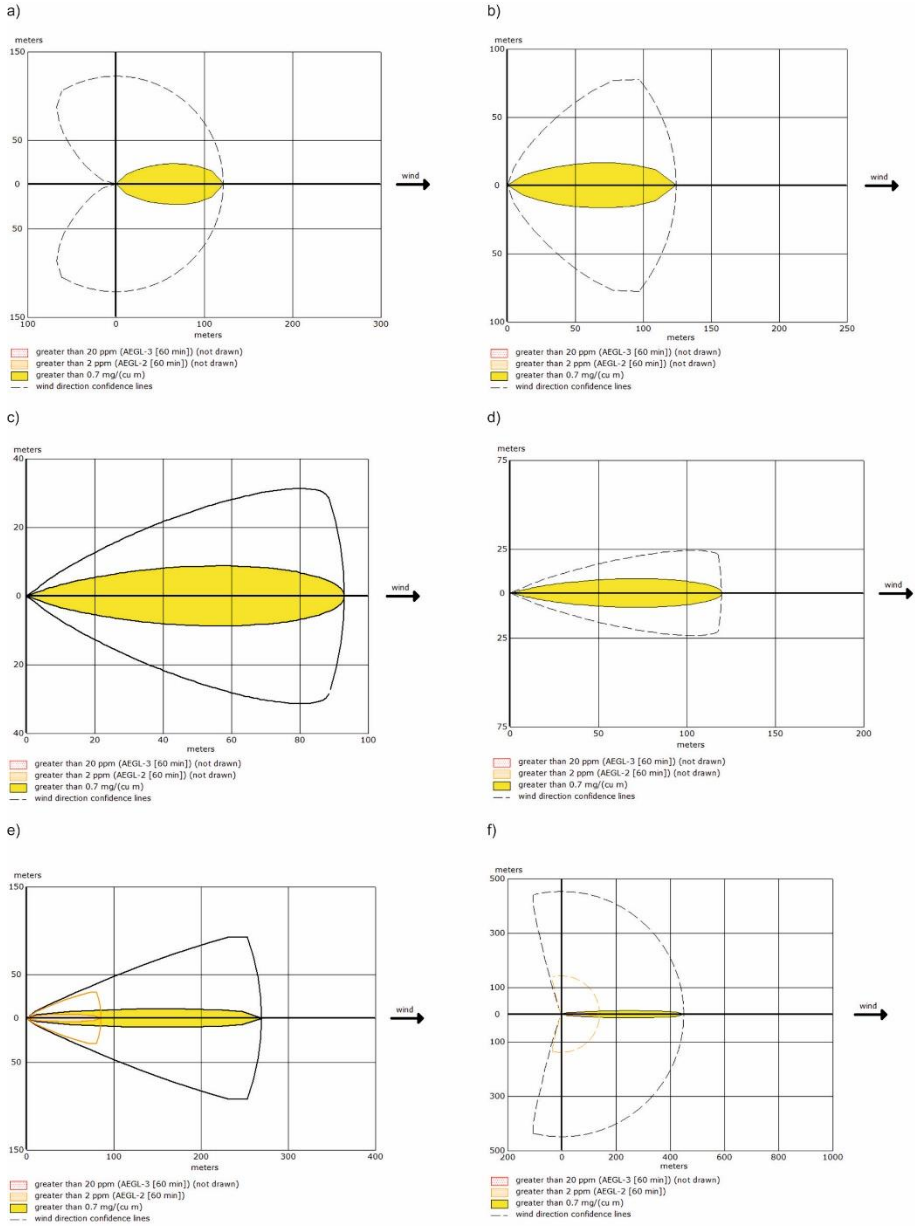

Fig. 2. An example of chlorine dispersion for: a) wind velocity 2m/s (Pasquil Stability Class - A); b) wind velocity 3m/s (Pasquil Stability Class - B); c) wind velocity 4m/s (Pasquil Stability Class - C); d) wind velocity 5m/s (Pasquil Stability Class - D) e) wind velocity 3m/s (Pasquil Stability Class - E); f) wind velocity 2m/s (Pasquil Stability Class - F).

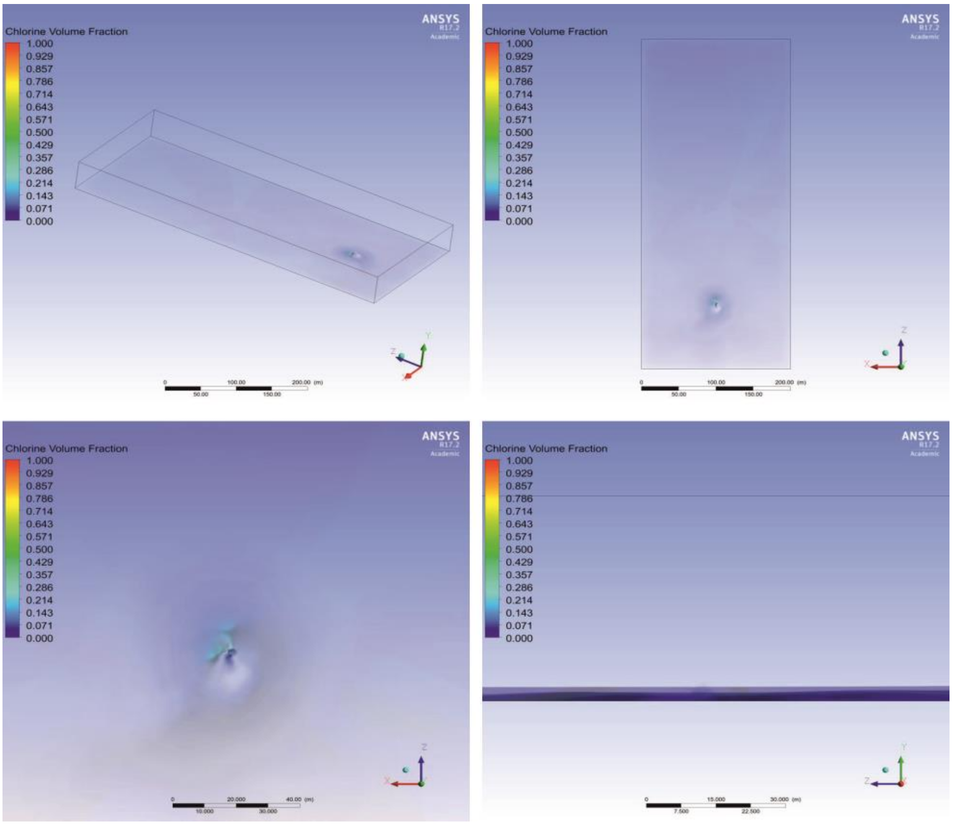

Fig. 3. Chlorine dispersion without wind.

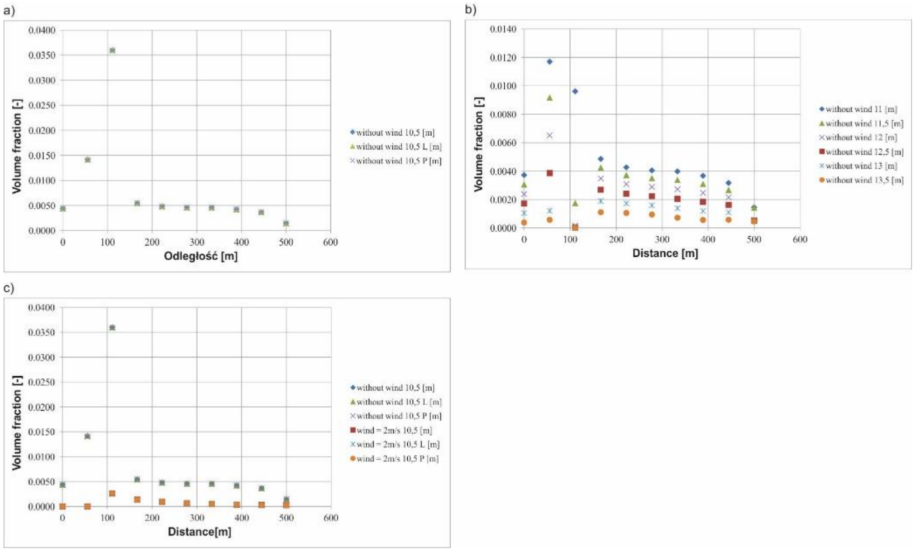

Fig. 4. Chlorine dispersion without wind in function of height for: a) 10.5m above the source of dispersion in center, 0.5m on the left and 0.5m on the right; b) from 11m up to 13.5m with 0.5m step.

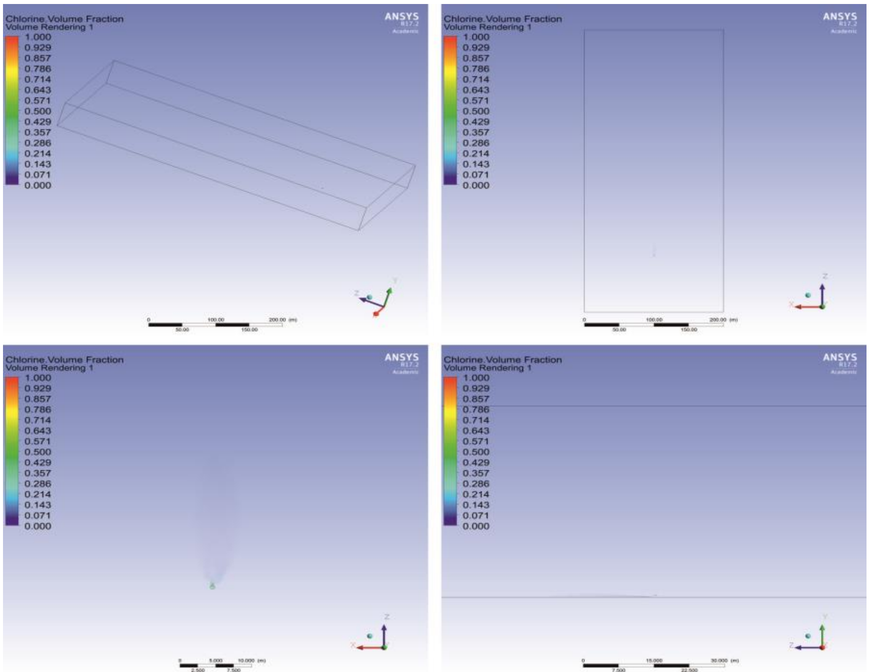

Fig. 5. Chlorine dispersion regarding wind influence (2m/s).

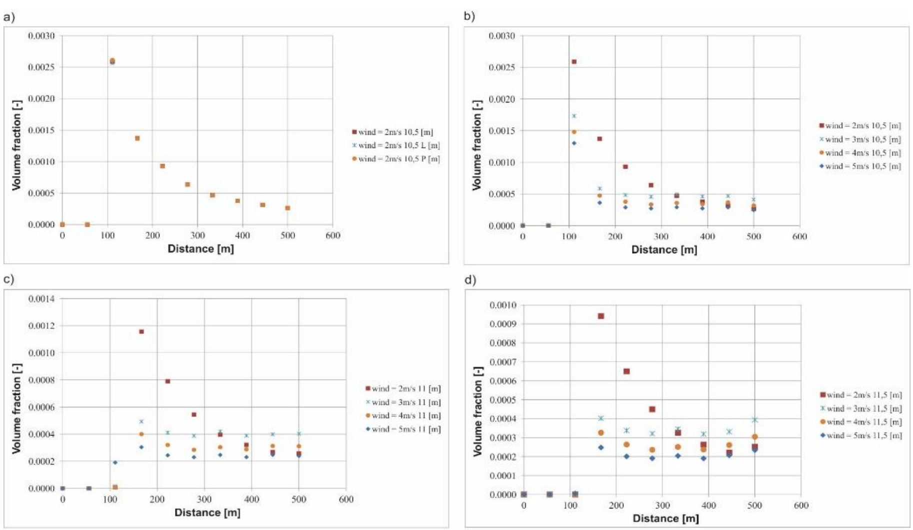

Fig. 6. Chlorine dispersion including wind in function of height for: a) 10.5m above the source of dispersion in center, 0.5m on the left and 0.5m on the right; b) 10.5m for wind velocity 2-5m/s; c) 11m for wind velocity 2-5m/s; d) 11.5m for wind velocity 2-5m/s.

4 Conclusions

In summary, the presented study discussed two different approaches (2d and 3d models) for computer simulation of dispersion process. Absence of height in 2d simulations was the main technical difference. Results from 2d solver allowed to predict the range of polluted cloud in horizontal direction. While, 3d approach with the use of Ansys-Fluent allowed deeper analysis including both horizontal and vertical distribution of chlorine.

It was observed that for 2d and 3d simulations with increase of Pasquil Stability Class (increase of wind velocity) the area of chlorine dispersion had similar character (for both approaches it became longer and narrower). Moreover, there was 4 times higher range of chlorine dispersion for the F stability class compare to the A class.

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 wind velocity indicated extension of chlorine cloud with decrease of the volume fraction. Moreover, analysis of chlorine concentration in function of height resulted in volume fraction profile flatten with decrease of value in upper level of analyzed domain.

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