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Numerical Simulation of Emergency Release of Liquid Petroleum Gas on a Car Gas Station

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Abstract: LPG storage tanks may be seriously threatened by a fire coming from nearby fuels or by leakage appearance. The aim of the study was to prepare a three-dimensional model of LPG release on a car gas station under different environmental conditions. CFD simulations of liquid and gas phase release from a tank localized on a car gas station was performed. First, ALOHA software was applied to determine mass flow rate, while Ansys software was used to determine the shape and size of hazardous zone. To reflect real condition atmospheric stability classes were applied. It was observed that for classes A-D the hazardous zone was decreasing. While, for E and F class the range was increased. It was noticed that the location of the leakage affects the extent of the danger zone. For the leaking below the liquid surface analyzed LPG has liquid form. While, for the leaking above the liquid surface analyzed LPG has gas form. Furthermore, for liquid leakage the largest hazard zone of release was observed.

Keywords: gas emergency release, liquid petroleum gas, CFD simulation, atmospheric stability class

1. Introduction

The large population density increases probability of any hazardous material release (Pontiggia et al. 2011, Piecuch et al. 2015, Polanczyk et al. 2019, Majder-Lopatka et al. 2020). Dispersion of storage gases due to the natural or the industrial accidents may lead to tragic consequences (Polanczyk et al. 2018, Polanczyk et al. 2020). Moreover, transportation of liquefied flammable products is affected by severe accidents (D'Aulisa et al. 2014, Polanczyk et al. 2018). To prevent the effects of these disasters different approaches have been introduced in the literature (Lovreglio et al. 2016, Polanczyk et al. 2018). Past accident data analysis shows that about 33% of accidents occurred during road or rail LPG transportation resulted in boiling liquid expanding vapor explosions (D'Aulisa et al. 2014, Polanczyk et al. 2020). When exposed to severe distant source radiation induced by fire, LPG tanks may be subjected to severe heat-up and consequent pressurization, which may lead to the catastrophic rupture of the tank (Scarponi et al. 2017). LPG storage tanks may be seriously threatened by a fire, particularly in those cases where negligence or regulatory gaps allow a very close exposure of these tanks to flames coming from nearby fuels or by leakage appearance (EmrysScarponi et al. 2020). Furthermore, fragments resulting from the destruction of the tank shell can be projected to the surrounding, potentially worsening the consequences of the explosion (Tugnoli et al. 2013). The lack of an effective safety distance between the LPG tank and the surrounding fuels caused the opening of the safety relief valves and intense jet fires (EmrysScarponi et al. 2020).

To assist decisions and planning in case of hazardous gases numerical techniques are applied (Hannaa et al. 2009, Polanczyk & Salamonowicz 2018). Moreover, in industrial processes numerical tools are present (Wawrzyniak et al. 2012, Wawrzyniak et al. 2012, Czapczuk et al. 2017). In recent years, more detailed models for the simulation of LPG vessels exposed to fire were developed, based on computational fluid dynamics (CFD) Various computational 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) and FDS (Salamonowicz et al. 2021). However, the simulation set up considered only full engulfment conditions, and the possible transient evolution of fire scenario was not systematically considered. Therefore, the aim of the study was to prepare a three-dimensional model of LPG release on a car gas station under different environmental conditions.

2. Materials and methods

2.1. Case study

Analyzed case was composed of the area included one gas tank, three gas distributors, one building and one carport. During a regular day the side surface of Liquid Petroleum Gas (LPG) tank on a car gas station was unsealed. The emergency release was provoked by the lack of proper maintenance, inspection and damage on detachable flange connections. Two different approaches of unsealed tank were considered: 1) in the lower part of the tank (0.3 m measuring from the ground), where liquid phase is localized, liquid phase of LPG leak appeared; 2) in the upper part of the tank (0.7 m measuring from the ground), where gas phase is localized, gas phase of LPG leak appeared.

According to the first approach the phenomenon was directed into the leak appearance above the liquid level and release of gas vapors. The LPG released in this way is further dispersed. While, propane-butane is heavier then air, the released gas slowly settle on the ground and flood the depressions, e.g. sewage wells. The dispersed gas creates an explosive atmosphere which together with ignition source may explode. Moreover, gas remaining in depressions of the land may remain there for a long time.

According to the second approach the phenomenon was directed into the leak appearance in the part of the tank with liquid LPG. As a result a boiling pool of propane-butane is formed on the ground (boilling temperature -41.2°C). Combustible vapors arising from boiling pool are mixing with air and creating an explosive atmosphere.

2.2. Model description

The fluid dynamic response of the LPG tank exposed on different environmental conditions was modeled by two- and three-dimensional simulations. The following boundary conditions for numerical simulation of LPG release on a car gas station were assumed: free ejection of LPG into open space (T = 25°C and P = 101325 Pa, air ($\rho = 1.23$ kg/m^3, $\eta = 1.79\ 10^{-5}$ kg/(m s)). The properties of analyzed LPG were approximated as for the following composition: propane - mass fraction 0.595, n-butane – mass fraction 0.405, temperature 25°C.

In the first step, with the use of Ansys SpaceClaim software (ANSYS, Canonsburg, PA USA) and technical documentation a three-dimensional model (length = 200 m, width = 100 m, heigh = 20 m) of a gas station was reconstructed (Fig. 1). In the analyzed domain 6 objects were localized (one gas tank, three distributors, one building and one carport) (Table 1).

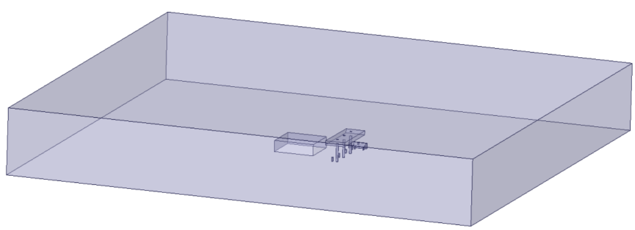


Fig. 1. Three-dimensional model of a gas station

The following boundary conditions were used: mass flow outlet from the unsealed tank, wall (for all obstacles). Moreover, at the inlet to the geometry, velocity inlet boundary representing flowing air was applied.

Table 1. Dimensions of objects on the car gas station

Object	Length [m]	Width [m]	Height [m]
Gas tank	4	1	1
Distributor	0.5	0.5	1.5
Building	20	10	4
Carport	10	5	7

Next, digital grid with the use of Ansys Meshing software (ANSYS, Canonsburg, PA USA) composed of tetrahedrons with boundary layer was created. After mesh independent tests the number of numerical grid elements was established at approximately 5 000 000, with boundary layer for whole analyzed domain composed of 10 layers (Fig. 2).

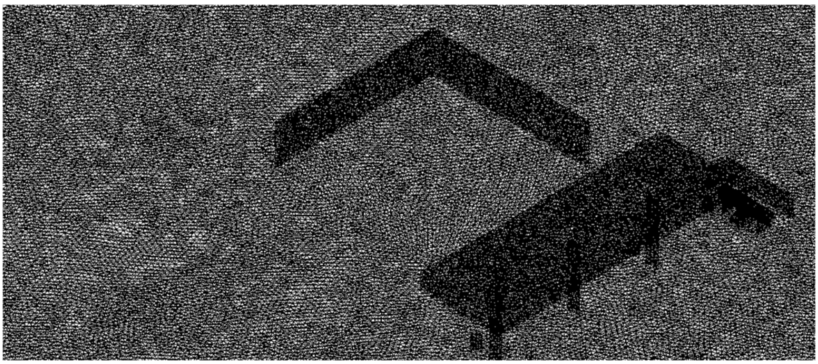


Fig. 2. Three-dimensional mesh model of gas station.

Moreover, for the calculation of mass flow rate (eq. 1) Aloha software was used (Thoman et al. 2005, Tsenga et al. 2012, Sun et al. 2013). Mathematical domain was limited to the cylindrical tank (diameter = 4 m, high = 1 m, length = 1 m). However, there were no obstacles. For the gas phase upwards emission at 1.5 m level was observed. While, for the liquid phase downwards emission was observed at 0.5 m level was observed. Moreover, gas phase leak was analyzed at constant temperature equal to 25°C. While, for the liquid phase, the gas temperature was lowered due to the immediately phase transition from liquid to gas after it escaped into the atmosphere through the leaks. Therefore, gas phase was observed closer to the ground after release from the tank, while it is heavier than air and is colder than air. Convergence level was set at 1 e^{-5}.

Next, three-dimensional LPG release with the use of Ansys Fluent 19 software (ANSYS, Canonsburg, PA USA) was analyzed. Reynolds Averaged Navier-Stokes equations (eq.1-3) were applied (Ganta et al. 2014, Zieminska-Stolarska et al. 2015).

$$\left(\frac{\partial v_x}{\partial t} + v_x\frac{\partial v_x}{\partial x} + v_y\frac{\partial v_x}{\partial y} + v_z\frac{\partial v_x}{\partial z}\right) = \rho g_x - \frac{\partial p}{\partial x} +$$
$$\frac{\partial}{\partial x}\left((\mu+\mu_t)(2\frac{\partial v_x}{\partial x})\right) + \frac{\partial}{\partial y}\left((\mu+\mu_t)(\frac{\partial v_z}{\partial y} + \frac{\partial v_y}{\partial x})\right) + \frac{\partial}{\partial z}\left((\mu+\mu_t)(\frac{\partial v_x}{\partial z} + \frac{\partial v_z}{\partial x})\right) \tag{1}$$

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

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

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],
μt – turbulent viscosity, [Pa s].

In this work, the k–ε model was used to represent the effects of turbulence (Pontiggiaa et al. 2010). Moreover, as a wind speed is a crucial parameter, reconstruction of dispersion in real conditions required usage of Pasquill stability class. While, it required reflection of the wind profile along the height depending on the atmospheric stability Pasquill stability class (Table 2) (Eduardo Krügera and Emmanuel 2013).

Table 2. Velocity profile in function of atmospheric stability class

Stability class	Coefficient [-]	Wind speed [m/s]	Equation
A	0.109	1	$v = (y/10)^{0.109}$
B	0.112	3	$v = (y/10)^{0.112}$
C	0.12	5	$v = (y/10)^{0.12}$
D	0.142	7	$v = (y/10)^{0.142}$
E	0.203	3	$v = (y/10)^{0.203}$
F	0.253	2	$v = (y/10)^{0.253}$

3. Results

The methodology presented in this work provides a numerical tool to assess whether the exposure of a LPG tank to a given atmospheric scenario can be deemed safe (Scarponi et al. 2020). The influence of environmental parameters as well as released phase on the size of hazardous zone was analyzed. The methodology presented in this study provided a numerical tool to assess whether the exposure of an LPG tank to a given environmental scenario can be deemed safe on a car gas station. To reconstruct a realistic conditions of wind appearance, an atmospheric stability classes were applied. It was in line with Mack et al. who investigated CO_2 dispersion where experimentally measured inlet profile of wind was simulated (Mack & Spruijt 2014). Moreover, in our study we assumed turbulent character of flow, therefore, standard k-ε model was used 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). However, 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 LPG release.

In the first step, ALOHA software was applied to estimate the range of emergency zone. While, the leak was not limited by any obstacles, equal emergency range was observed for both analyzed phases (Table 3). Increasing of atmospheric stability class from A to F resulted in hazardous zone range equal to 11 m for gas phase and liquid phase.

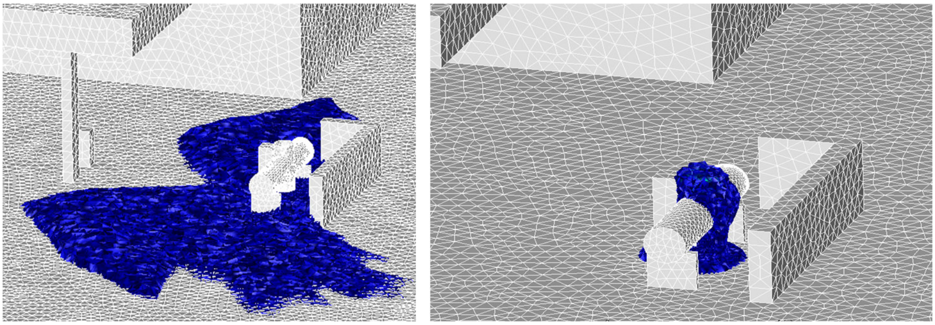
In the next step the three-dimensional car gas station was analyzed. It was observed that wind direction and atmospheric stability class as well as retaining wall and anti-burst wall had impact on the explosive range for both phases (Table 4). For the same atmospheric stability classes higher range of zone for gas phase compare to the liquid phase was observed. Fig. 3 presents a leak of LPG for both phases, the iso-surfaces are presented for a concentration of 2%, which corresponds to the lower explosive limit (LEL). Liquid phase was spread on the ground, while gas phase surrounded LPG tank. When B atmospheric stability class was applied liquid was longitudinally concentrated, while gas phase was mostly concentrated under a tank (Fig. 4). For C atmospheric stability class, the range of liquid phase zone was about 5 times shorter compare to the gas phase (Fig. 5). Moreover, comparison of C and D atmospheric stability class indicated further decrease of hazard zone range (Fig. 6). While, for E and F atmospheric stability class increase of hazardous zone was observed. For E class the range of hazardous zone was equal to 4.5 m and 37.5 m for gas and liquid, respectively. While, for F class the range of hazardous zone was equal to 45 m and 19.6 m for gas and liquid, respectively.

Table 3. The range of explosive zone calculated with ALOHA software

Phase	Atmospheric stability class	Range of zone [m]
Gas	A	11
	B	11
	C	11
	D	11
	E	11
	F	11
Liquid	A	11
	B	11
	C	11
	D	11
	E	11
	F	11

Table 4. The range of explosive zone calculated with Ansys software

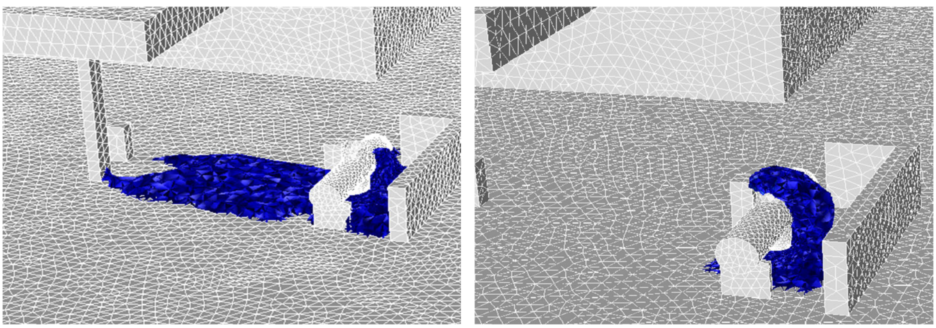
Phase	Atmospheric stability class	Range of zone [m]
Gas	A	3.5
	B	1.9
	C	1,0
	D	0.8
	E	4.5
	F	5,0
Liquid	A	17.5
	B	11,0
	C	5.5
	D	2.3
	E	37.5
	F	19.6



(**a**) (**b**)

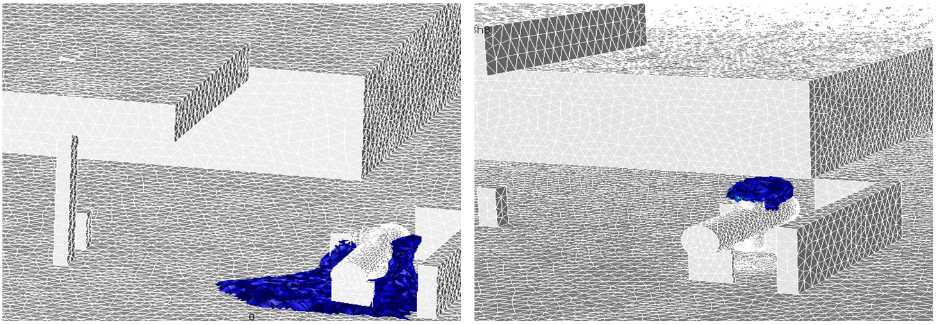
Fig. 3. Graphical representation of LPG leak for the atmospheric stability class A: (**a**) gas phase of propane, (**b**) liquid phase of propane. Color bar presents mole fractions of propane

Each time released LPG was not presented behind anti-burst wall. Which corresponds to the real situation on a car gas station. Moreover, hazardous zone only for F stability class for gas phase was presented in the area of distributors. Furthermore, for A stability class for gas phase hazardous zone was observed close to the building.



(**a**) (**b**)

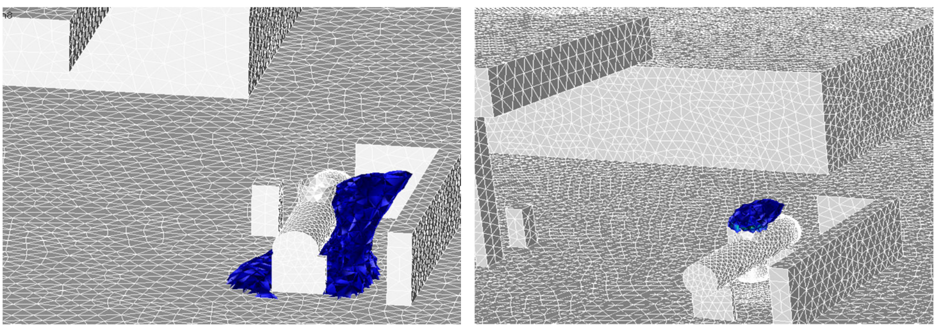
Fig. 4. Graphical representation of LPG leak for the atmospheric stability class B: (**a**) gas phase of propane, (**b**) liquid phase of propane. Color bar presents mole fractions of propane



(a) (b)

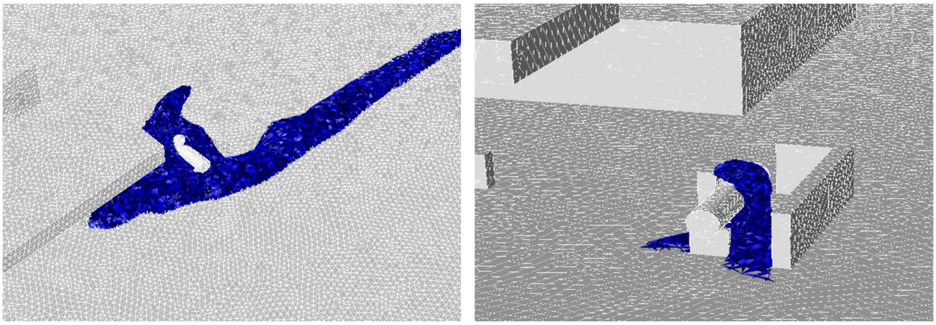
Fig. 5. Graphical representation of LPG leak for the atmospheric stability class C: (**a**) gas phase of propane, (**b**) liquid phase of propane. Color bar presents mole fractions of propane

Moreover, it was noticed that not only a character of wind (different atmospheric stability class) but also the direction of wind had impact on the range and size of hazardous zone (Fig. 9). When wind was directed from the left side of the mathematical domain, longitudinal range of hazardous zone was equal to 11 m (Fig. 9a), while wind directed from the right side affected extend of the hazardous zone to 15 m. Which was caused by appearance of retaining wall as well as anti-burst wall.



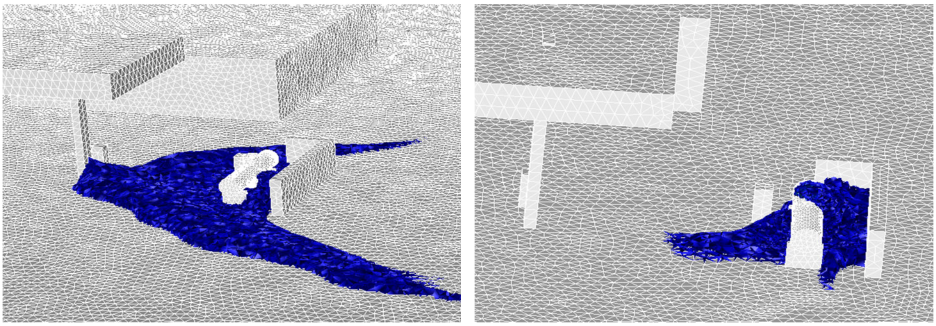
(a) (b)

Fig. 6. Graphical representation of LPG leak for the atmospheric stability class D: (**a**) gas phase of propane, (**b**) liquid phase of propane. Color bar presents mole fractions of propane



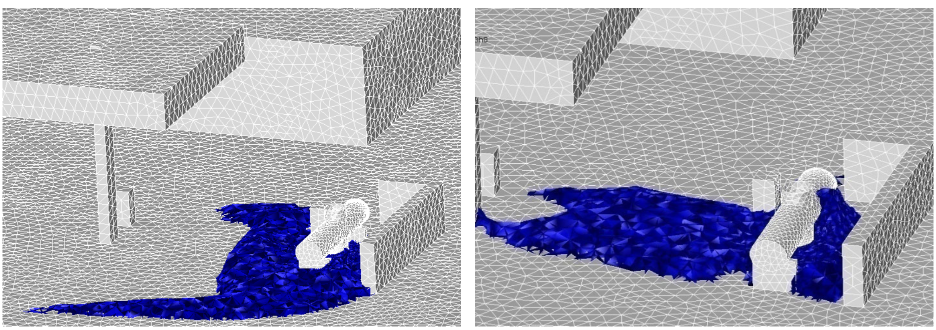
(**a**) (**b**)

Fig. 7. Graphical representation of LPG leak for the atmospheric stability class E: (**a**) gas phase of propane, (**b**) liquid phase of propane. Color bar presents mole fractions of propane



(**a**) (**b**)

Fig. 8. Graphical representation of LPG leak for the atmospheric stability class F: (**a**) gas phase of propane, (**b**) liquid phase of propane. Color bar presents mole fractions of propane



(**a**) (**b**)

Fig. 9. Comparison of liquid phase release for different wind direction for the atmospheric stability class B: (**a**) for the left side of the analyzed domain, (**b**) from the right side of the analyzed domain

3.1. Limitation to the study

Presented model was analyzed within one car gas station. In the future we would like to analyze different spatial configurations of gas car stations. Moreover, we analyzed the process under constant temperature. In the future we would like to include different environmental temperatures which may reflect different seasons.

4. Conclusions

The proposed CFD model enabled analysis of LPG emergency release from a tank at the car gas station. It was observed that urban obstacles have a significant effect on gas propagation. All analyzed cases indicated that the explosive zone was located several dozen centimeters above ground. Moreover, the range of the explosion hazard zone is strongly dependent on the weather conditions. Considering the obtained results, it can be observed that the lower the wind speed, the greater the explosion hazard zone. The leakage of the gas and liquid phase was the largest for the low wind speed (wind speed class: A, E, F). Furthermore, LPG tanks should be located in an open area which enables freely diluting of released gases.

Moreover, it was observed that the location of the leakage affects the extent of the danger zone. For the leaking below the liquid surface analyzed LPG has liquid form. While, for the leaking above the liquid surface analyzed LPG has gas form. Furthermore, for liquid leakage the largest hazard zone of release was observed.

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