

Simulation of the LPG Leakage and Dispersion Process to the Factory Environment using Computational Fluid Dynamics (CFD)

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Liquefied Petroleum Gas (LPG) is a hydrocarbon gas that exists in liquefied form as an energy-saving, clean, convenient fuel, it has been widely used in civil and industrial applications such as oil fields, gas and oil industry. This present work considers the flammable gas release and dispersion safety evaluation caused by the LPG (50 % propane, 50 % n-butane) leakage and diffusion from an accidentally punctured pipe (with the diameters varies from 1-3 mm) during the operation of a 33 m³ LPG tank. Process equipment during a puncture can swiftly release hazardous compounds in sufficient quantities to distribute throughout a working and local area in clouds. LPG leakage diffusion model is created using the computational fluid dynamics (CFD) method, and the characteristics of LPG dispersion and the various of LPG release rate - dispersed by natural wind in an open area, with wind speeds range of 1.0 – 10.0 m/s corresponding to different atmospheric stability classes from A to F are computed and simulated. The result shows that wind speeds have a considerable impact on the spread of LPG from the release site to different distances in the domain. The maximum LPG concentration distribution is 101.71 ppm at 1 m/s wind velocity, while the minimum is 3.12 ppm at 10 m/s wind velocity. This suggests that the dispersion of LPG in the environment is minimal, accounting for roughly 0.01% of its total volume, which implies that LPG stations are not at significant risk in the event of a small puncture ranging from 1 to 3 mm in diameter. In the simulation work, the realizable k- ϵ model is utilised for the turbulence model. This study can provide guidance to authorities to comply with fire protection regulations, firefighting and prevention, and emergency response measures, which can ensure the safety of the factory operating in particular and neighbouring factories in the industrial area in general.

1. Introduction

Liquefied Petroleum Gas (LPG) mainly composed of propane and other relatively – short hydrocarbon (Sarker et al., 2022) undoubtedly plays a pivotal role in the national industry, primarily due to its significant economic benefits, including its cleanliness, energy efficiency, and its classification as a new type of fuel (Lyu et al., 2022). However, it is imperative to recognize that alongside these advantages, the potential dangers associated with the storage, transportation, and leakage of LPG must be given serious consideration (Li et al., 2019). LPG tanker is easily affected by many factors such as environmental storage, personnel leading to tanker failure, leakage and explosion accidents. LPG storage is consequently crucial for studying the effects of LPG leakage and planning for disaster investigations using CFD. The consequence of LPG leakage accidents happens quickly and violently in the process industry, leading to experimental investigation still many limits and extremely complex due to the large – size location and large – scale equipment (Balisampang et al., 2017). In order to address the accidental leakage, researchers utilize mathematical modelling and simulation software as references to predict the potential consequences of LPG.

Numerous studies have focused on tank failures and the effects of storage tanks at various levels. Wang et al. (2020) investigated the fireball characteristics of an LPG tanker after explosion by using FDS software. This research indicated that a fuel mass of 10,000 kg resulted in the maximum peak radiation flux of the fireball. Yu

et al. (2016) investigated that the explosion accident of LPG tank which simulated by using ALOBA and a Cartesian matrix. Besides studying explosion and flame properties, these studies use simulations to investigate the impact of factors such as wind speed, leakage direction, and diffusion, which play important roles in the occurrence and effects of leakage accidents (Wan et al., 2021). Utilizing computational fluid dynamics (CFD), the detection of harmful gases involves modelling the dispersion of H_2S , evaluating gas leakage, and analysing the impact of factors such as wind direction and equipment configuration on the release (Gu et al., 2018).

This paper aims to bridge the gap in exploring CFD-based simulation for LPG tank leakage, which simulates the effects and assess the safety of the factory. In this study, the influence of wind speed and LPG concentration is simulated by CFD simulation. The three-dimensional (3D) simulation will provide a visualization of the impact of wind direction and speed on the concentration and diffusion range of the leaked LPG. The study investigates different leak diameters and wind speeds on multiple levels. The simulation results consider the Pasquill-Gifford atmospheric stability classes, which take into account dispersed wind speeds and the concentration distribution in the direction of the wind to make specific predictions about the incidents and extent of diffusion.

2. Methodology

2.1 Research data

The LPG supply station used in this study consists of two base standings for the LPG tank and is located Binh Duong province of Vietnam ($11^{\circ}06'30.4''N$ $106^{\circ}33'33.9''E$), which indicated in Figure 1a. The station was 21 m long, 5.9 m wide, and 4 m high, and the wind was naturally blown from the left to right side of the station as shown in Figure 1b and all measurements in the LPG tank drawing are expressed in mm.

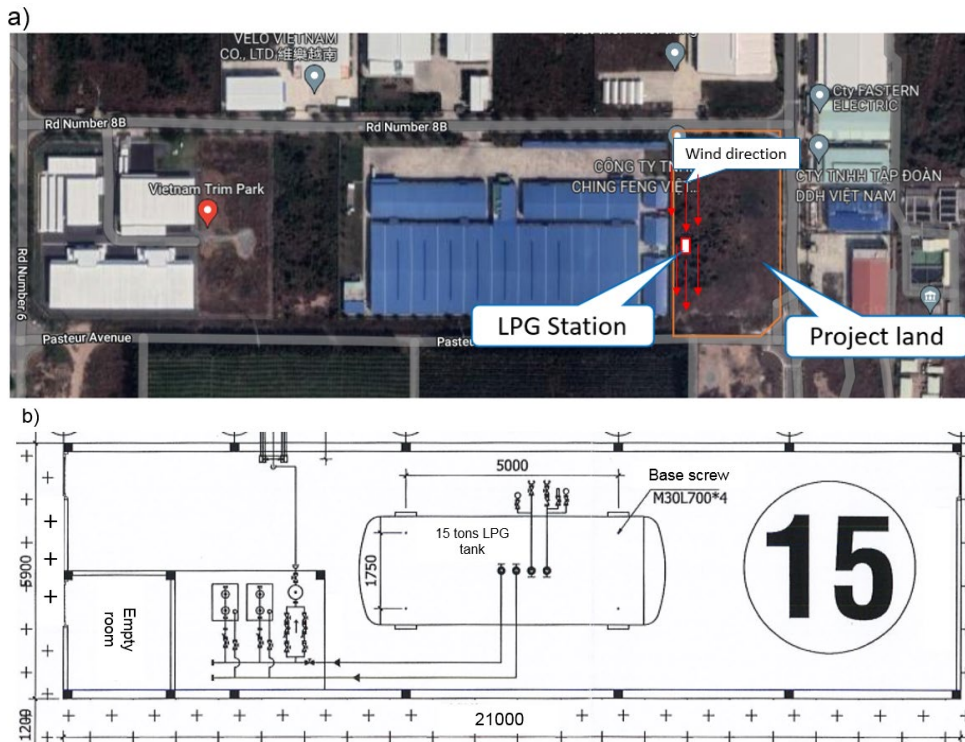


Figure 1: (a) LPG station on satellite map and (b) the top view of the LPG tank

2.2 Mathematical representations

2.2.1 Physical model

Figure 2 illustrates the geometric and grid model of the computational domain, which is 21 meters long and 5.9 meters wide. It is assumed that there is a puncture in the pipe, 1 mm to 3 mm in diameter, which serves as the emission source. The poly-hexcore meshing method is employed to achieve exceptional results. In order to ensure accurate simulation results, this study utilizes high-performance computational resources with cell counts ranging from 164,822 to 191,751.

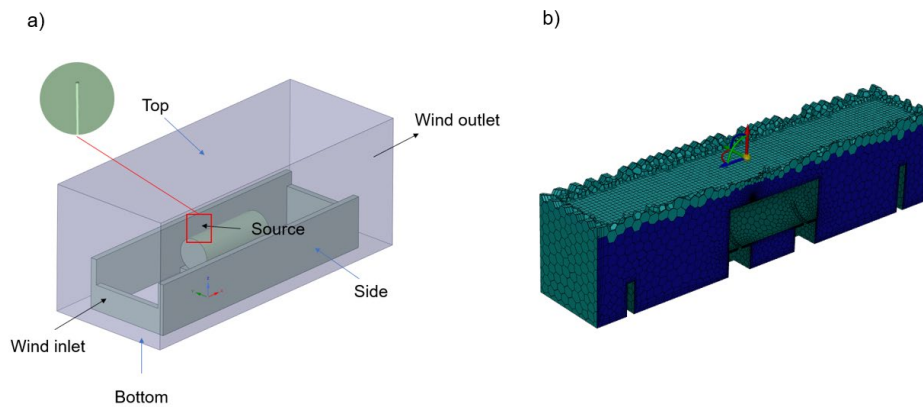


Figure 2: (a) Geometry and (b) mesh generation of the LPG tank

2.2.2 Turbulence model

The flow in an LPG tank leakage can be turbulent, depending on the specific conditions of the leak and the surrounding flow. LPG is stored in tanks under high pressure, and if a leak occurs, the gas will rapidly expand and flow out of the tank. Turbulence can cause the heavy gas to mix more quickly with the surrounding air, which can increase the size and extent of the gas cloud. This phenomenon can be primarily attributed to the high rates of emission and the complex interactions. The κ - ϵ turbulence model (Han et al., 2018) is a realizable model that is based on the transport equations for turbulent kinetic energy (κ) and its dissipation rate (ϵ).

2.2.3 Species transport

The species transport can be used to predict the concentration and distribution of LPG in the air over time and space. The equations can also be used to optimize the design and operation of LPG storage and transportation systems, to minimize the risk of leakage and dispersion. This model represents a mixture of propane (LPG) and air. Species transport modelling facilitates the analysis of moisture transfer within objects. By choosing to preserve the equation for chemical components, the software can predict the local mass fraction of each substance (Y_i). This is achieved by solving the convective diffusion equation for the i^{th} substance in the mixture. The general form of this conservation equation is described in Han et al. (2018).

2.2.4 Boundary conditions

A problem's numerical solution depends on the values supplied at the boundary conditions at streams, which must be defined in order to have a numerical solution. Table 1 contains the parameters for the model's boundary conditions while Table 2 shows the boundary conditions of the problem.

Table 1: Operating conditions

The operating conditions	Governing Equations
Solver	3D simulation Implicit formulation Pressure-based (coupled) Steady state analysis
Energy equation	Activated
Viscous model	Realisable k- ϵ model
Species	Diffusion Energy Source

Table 2: Boundary conditions

Boundary conditions	Materials	Parameters	Value
Release source	Propane (C_3H_8)	Mass flow rate [kg/s]	0.0025;
	Butane (C_4H_{10})		0.0101;
			0.0227
Inlet	Air	Temperature [$^{\circ}C$]	30
		Velocity [m/s]	1;3;5;10
Outlet	Air	Temperature [$^{\circ}C$]	30
		Pressure gauge [Pa]	0.0

3. Result analysis and discussion

3.1 The effect of natural wind (W) speed on the dispersion behaviour

Figure 3 illustrated the wind velocity results at the plane of symmetry for three case studies involving leak diameters of 1 mm, 2 mm, and 3 mm, denoted as cases 1, 2, and 3, respectively. Each case is examined under increasing wind velocities of 1 m/s, 3 m/s, 5 m/s, and 10 m/s. The results indicate that higher wind speeds promote faster dispersion and wider dissemination of pollutants. Conversely, lower wind speeds can lead to the accumulation and concentration of pollutants in specific areas.

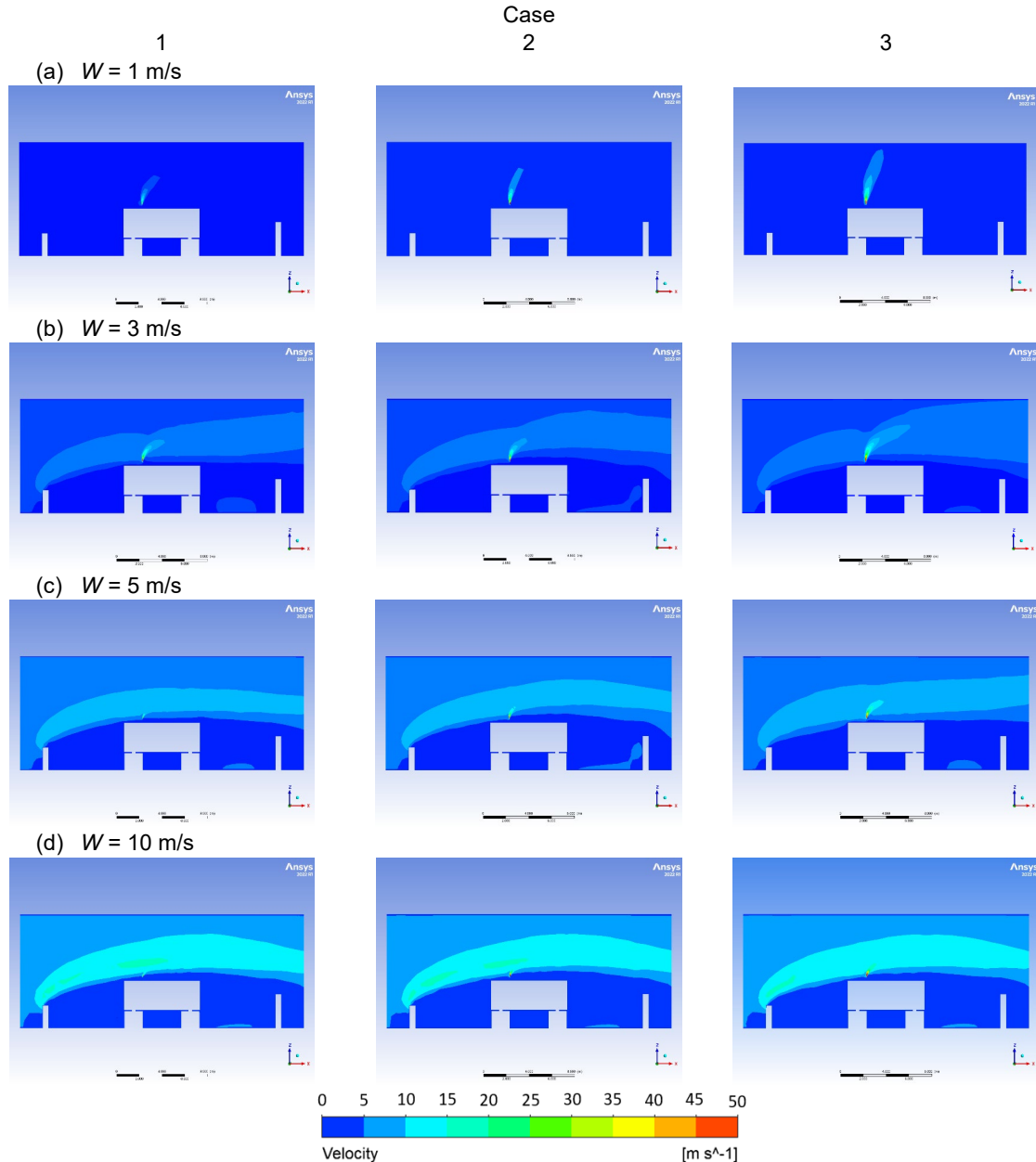


Figure 3: Velocity cloud image in the axis symmetry plane

The presence of the front wall has a significant influence on the wind field, impacting the diffusion of LPG emissions. Initially, the wind begins with velocities of 1 m/s, 3 m/s, 5 m/s, and 10 m/s, subsequently reaching measured speeds of 3 m/s, 6 m/s, 10 m/s, or even 15-20 m/s after passing the front wall. As the wind encounters the leak site, it combines with the discharged LPG source and generates an upward trend in the region. The blocking effect of objects intensifies ambient air turbulence, accelerating wind flow speed and enhancing LPG dilution behind the front wall, while the rear wall has minimal influence on the wind field and exhaust gas

dispersion. It is important to acknowledge that higher wind speeds play a crucial role in facilitating the dispersion process, leading to reduced overall concentration levels that are confined to the immediate vicinity of the station.

3.2 Concentration distribution in the LPG station

Figure 4 presents the results of the volume ratio of LPG for each case study, considering leak diameters of 1 mm, 2 mm, and 3 mm (cases 1, 2, and 3), along with varying wind speeds of 1 m/s, 3 m/s, 5 m/s, and 10 m/s. When LPG gas is mixed with air at a volume ratio of 1.8 %, it does not cause an explosion or fire upon contact with a lighter flame. Serious fire and explosion hazards can arise when the gas content ranges from 1.8 % to 10 %, in the absence of a fire source or static electricity (Ilahi et al., 2018). This study consequently considered the volumetric range of LPG from 0 % to 1.8 %, corresponding to the Lower Flammability Limit (LFL) of LPG, to ensure that no fire occurs in the event of a leakage source. There is 10 % LPG gas mixture will only ignite due to the characteristics of the mixture. Figure 4 illustrates the leakage spread throughout the room in three cases, considering different stability layers at the plane of symmetry. The LPG volume fraction measured in the study can be converted into ppm volume by multiplying to 10^6 . In all three cases, the highest average LPG ppm concentration occurs at a wind speed of 1 m/s, with recorded values of 10.14 ppm, 39.54 ppm, and 101.71 ppm. These concentrations will gradually decrease to the minimum concentrations of 3.12, 7.39, 12.45 ppm with the highest wind speed of 10 m/s for all 3 of cases. This is evident due to the difference in emission flow through different leak points, the larger the leak diameter, the higher the emission flow rate.

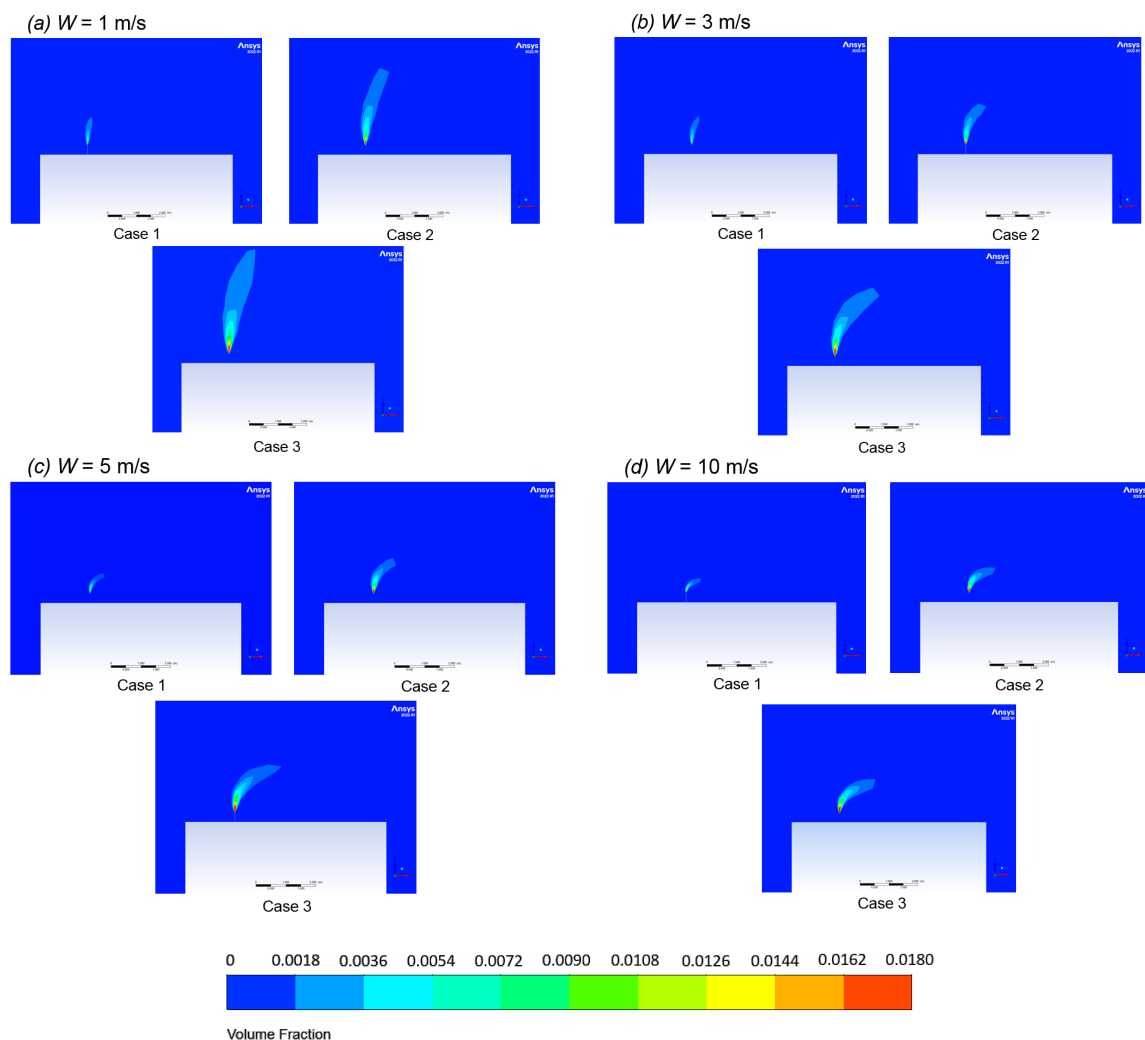


Figure 4: LPG volume fraction for cases with different wind speeds

The influence of wind on the diffusion of LPG leakage, as well as its transport and dilution effects are obvious. At the LPG measurement point with a value of 0.001, it is observed that the recorded emission height tends to

decrease as the wind speed increases. This phenomenon occurs because higher wind speeds result in stronger air-gas mixing, accelerating the dilution of the leak source and gradually reducing the concentration of the LPG volume fraction. In case 3, where the wind field is at its lowest with a speed of 1 m/s, the highest elevation of 4.198 m (measured from the emission source) is recorded. Subsequently, this elevation gradually decreases to values of 2.34 m, 1.52 m, and 1.15 m in the subsequent wind cases due to the higher wind speeds.

4. Conclusions

This study involved the creation of a three-dimensional model to simulate LPG leakage. The dimensions of the model were based on factory drawings, and the simulation was conducted on a symmetrical half to minimize pressure and calculation time. The simulation was run under steady-state conditions and yielded several conclusions. The average concentration of LPG in parts per million in the room remained below the lower flammability limit (LFL) percentage in all cases. The highest recorded concentration was just 100 ppm, which equates to around 0.01 %, in case 3 with the wind speed of 1 m/s. While the LPG concentration was lowest in case 1 with wind speed of 10 m/s - only 3.12 ppm dispersed in the area compared to 10.14 ppm when there was only 1 m/s diffuse wind. This means that the higher the wind speed, the higher the concentration of LPG diffused in air. Immediate and resolution of LPG leaks is crucial for preventing serious accidents, although stations with 1-3 mm diameter leaks pose relatively low risk due to low average concentration and varying diffusion wind velocities. These findings suggest that CFD simulation is an effective and potential approach to predict the consequences of LPG leak dispersion in open plant spaces. This method can effectively predict the impact of LPG dispersions quickly and raise public safety concerns.

Acknowledgments

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References

- Baalisampang, T., Abbassi, R., Garaniya, V., Khan, F., Dadashzadeh, M., 2017, Fire impact assessment in FLNG processing facilities using Computational Fluid Dynamics (CFD), *Fire Safety Journal*, 92, 42–52.
- Gu W., 2018, Risk Level Analysis of Petrochemical Hazardous Gas Leakage Based on Odour Recognition and CFD Simulation Technology, *Chemical Engineering Transactions*, 68, 337-342.
- Han, U., Oh, J., Lee, H., 2018, Safety investigation of hydrogen charging platform package with CFD simulation. *International Journal of Hydrogen Energy*, 43(29), pp.13687-13699.
- Ilahi, N. I., Baco, S., Achmad, A. S., Umriah, E., 2018, Early leakage protection system of LPG (liquefied petroleum gas) based on ATMega 16 microcontroller. *IOP Conference Series: Materials Science and Engineering*, 336(1), 12021.
- Li, Y.-L., Yang, Q., Chin, K.-S., 2019, A decision support model for risk management of hazardous materials road transportation based on quality function deployment. *Transportation Research Part D: Transport and Environment*, 74, 154–173.
- Lyu, S., Zhang, S., Huang, X., Peng, S., Li, J., 2022, Investigation and modeling of the LPG tank truck accident in Wenling, China. *Process Safety and Environmental Protection*, 157, 493–508.
- Sarker, T. R., Nanda, S., Meda, V., Dalai, A. K., 2022, Process optimization and investigating the effects of torrefaction and pelletization on steam gasification of canola residue. *Fuel*, 323, 124239.
- Wan, C., Wanli, D., Ye, P., Yuxian, D., 2021, A potential value mining method for flight departure time based on LDA model. *2021 IEEE 3rd International Conference on Civil Aviation Safety and Information Technology (ICCSIT)*, 98–102.
- Wang, Y., Gu, X., Xia, L., Pan, Y., Ni, Y., Wang, S., Zhou, W., 2020, Hazard analysis on LPG fireball of road tanker BLEVE based on CFD simulation. *Journal of Loss Prevention in the Process Industries*, 68, 104319.
- Yu, E. H. Y., Tran, D. H. D., Lam, S. W., Irwin, M. G., 2016, Remifentanyl tolerance and hyperalgesia: short-term gain, long-term pain? *Anaesthesia*, 71(11), 1347–1362.