CHEMICAL ENGINEERING TRANSACTIONS
VOL. 111, 2024

A publication of
AIDIC
The Italian Association
of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Valerio Cozzani, Bruno Fabiano, Genserik Reniers

ISBN 979-12-81206-11-3; **ISSN** 2283-9216

DOI: 10.3303/CET24111053

CFD Modelling of LPG Dispersion in a Road Environment

Fabio Lozano[a,*], Morgan Johansson[a], Joosef Leppänen[a], Mario Plos[b]

[a]Chalmers University of Technology, Gothenburg, SE-41296, Sweden
[b]Swedish Transport Administration, Gothenburg, SE-41104, Sweden
fabio.lozano@chalmers.se

Inland transportation of Liquified Petroleum Gas (LPG) is often carried out using road tankers. An accident during road transport may lead to an unintended discharge of LPG on the road, which could mix with the surrounding air to form a flammable fuel-air cloud. This cloud is normally characterized by an irregular shape and non-uniform concentration, depending on factors such as geometrical and meteorological conditions and the properties of the leakage. Furthermore, the presence of vehicles on the road may significantly affect the dispersion and concentration of the cloud and may cause partial confinement or obstruction of the cloud, which could potentially become a source of dangerous gas explosions on the road. This paper presents a numerical study of dispersion of LPG in a road environment following an unintended leakage from a road tanker. The work was conducted using the computational fluid dynamics (CFD) code FLACS-CFD. The purpose was to quantify the extension of the gas cloud within the flammability limits for different leak properties, wind conditions, and traffic layout. For each case, an equivalent gas cloud with a regular shape and stoichiometric concentration was determined using the Q9 cloud model. Based on the results, recommendations for the choice of equivalent gas volume for different standard scenarios are presented.

1. Introduction

Liquified Petroleum Gas (LPG) is a hydrocarbon fuel commonly used both for domestic and industrial purposes around the world. LPG normally consists of a mix of either mostly propane, mostly butane, or mixes including both propane and butane. LPG will be in gaseous state at ambient conditions but can be liquefied at relatively low pressure. Due to this property, LPG is typically transported in liquid form in pressurized vessels at temperatures above the normal boiling point of the gas. Inland transportation of LPG is often carried out using road tankers, although transport by rail tank wagons or pipes is also used in some countries.

LPG is highly flammable. An accidental release of LPG during transport may result in catastrophic events such as fires, vapor cloud explosions (VCEs), or BLEVEs (Boiling Liquid Expanding Vapor Explosions). Among these events, VCEs are often considered the most likely (Bubbico et al., 2000). A VCE may be the result of ignition of a fuel-air cloud (also known simply as a gas cloud) formed by mixing of the released fuel with the surrounding air. The severity of the explosion depends, among other aspects, on the geometrical conditions of the site.

A risk analysis is usually conducted to estimate the consequences of a VCE on a road. An essential part within this process is the estimation of the extension of the gas cloud within the flammability limits. The dispersed gas cloud normally exhibits an irregular shape and non-uniform concentration, which depends on factors such as geometrical and meteorological conditions and the properties of the leakage. On a road, the presence of vehicles in the surrounding area may significantly affect the dispersion and concentration of the cloud. The calculation of the cloud size can be achieved with the help of tools based on computational fluid dynamics (CFD) (Shen et al., 2020) or analytical dispersion models (Nielsen, 1998). Alternatively, in a significantly simplified but conservative approach, the entire gas inventory contained within the reservoir under consideration could be assumed to contribute to the formation of a flammable cloud at a stoichiometric state.

Dispersion analysis allows identification of critical areas where powerful explosions could be initiated (i.e., blast sources). These are regions within the cloud that are (partially) confined or obstructed. On an open road, an example of such regions is the space underneath closely located vehicles. It is today widely accepted that only

Paper Received: 15 March 2024; Revised: 21 June 2024; Accepted: 27 June 2024
Please cite this article as: Lozano F., Johansson M., Leppänen J., Plos M., 2024, CFD Modelling of LPG Dispersion in a Road Environment, Chemical Engineering Transactions, 111, 313-318 DOI:10.3303/CET24111053

the combustion energy of the portion of the cloud in such regions contributes to strong blast generation (Committee, 2005). The combustion energy in turn is a function of the volume of the blast source.

After identification of the blast sources within the flammable cloud, estimation of the explosion overpressure is conducted. In normal practice, simplified methods such as the TNO-MEM (van den Berg, 1985) or the TNT-equivalency method are used. A common assumption when calculating the explosion overpressure is that the fuel-air mixture has a stoichiometric concentration at the blast source (which yields the highest explosion pressure). However, in the real irregular and non-uniform gas cloud, the mixture is normally rich in the vicinity of the leakage and lean towards the edge of the cloud. Consequently, when faced with scenarios in which the volume of the potential blast sources (i.e., the confined or obstructed regions where a powerful explosion can be initiated) is similar to the volume of the dispersed gas cloud, it may be overly conservative to assume stoichiometric concentration for the entire confined or obstructed regions. This situation may arise on congested roads in which the size of the group of vehicles present on the road is similar or exceeds the size of the gas cloud. For such cases, it may be more appropriate to consider a reduced volume of a stoichiometric mixture. That is, not all vehicles within the cloud would form a blast source simultaneously. Alternatively, the volume of the entire obstructed region may be used for estimation of the combustion energy, but with a non-stoichiometric concentration. The first approach is more appealing, as it can be implemented by adopting the concept of Equivalent Stoichiometric Cloud (ESC), which is today commonly used in probabilistic explosion assessments (Tam et al., 2021). This approach was used in this study. It consists in transforming the real dispersed flammable cloud into a regular cloud with a cuboid shape and uniform concentration, normally at stoichiometric state.

The aim of this study was to determine the maximum equivalent stoichiometric clouds for different LPG release scenarios on a road based on CFD calculations to evaluate the appropriate volume of the blast source for overpressure calculation. In other words, the goal was to estimate the number of vehicles that together form the blast source for different standard scenarios. Furthermore, the influence of different factors, such as the number of vehicles, distance to the release, and wind speed on the resulting ESC was investigated.

Several models for estimation of the ESC can be found in the literature (Tam et al., 2021). In this study, the Q9 model, implemented in the software FLACS-CFD (Gexcon AS, 2022), was adopted. The Q9 model considers both the flame speed and the expansion ratio, as given by Eq(1), in which V_{Q9} is the equivalent stoichiometric volume, V_i is the unobstructed volume in the i-th control volume, V_e is the volume expansion ratio at constant pressure, and ER is the equivalence ratio (ER = 1 corresponds to a stoichiometric concentration). The factor ER_{fac} varies between 0 and 1 depending on the equivalence ratio according to Eq(2), in which S_L is the laminar burning velocity, and ER_{LFL} and ER_{UFL} are the equivalence ratio at the lower flammability limit (LFL) and upper flammability limit (UFL). Moreover, the Q7 model, which gives the gas volume restricted by the UFL and LML, was calculated for comparison purposes.

$$V_{Q9} = \frac{\sum_{i=1}^{n}\left[V_i \cdot [V_e(ER_i) - 1] \cdot ER_{fac}(ER_i)\right]}{\max\left\{[V_e(ER) - 1] \cdot ER_{fac}(ER) : ER_{LFL} \leq ER \leq ER_{UFL}\right\}} \tag{1}$$

$$ER_{fac}(ER) = \frac{S_L(ER_i)}{\max\{S_L(ER) : ER_{LFL} \leq ER \leq ER_{UFL}\}} \tag{2}$$

2. Case study

The common setting for the studied scenarios was a hypothetical accidental release of LPG (100% propane assumed) during transport by road. Transport was carried out in a road tanker with properties as described in Table 1. The road consisted of two carriageways with two lanes each. The release was assumed to occur at the center of one of the carriageways at a distance L_{leak} from the closest vehicle, as shown in Figure 1. All vehicles had the same simplified geometry shown in Figure 1, which is meant to represent a typical personal car. The meteorological conditions at release were taken as 20 °C, stability class D (neutral) and wind speed of 2.0 m/s at a reference height of 10 m. In total, 20 different dispersion scenarios were created by varying the properties of the leak, the distance L_{leak}, and the number of vehicles.

The hypothetical release of LPG from the high-pressure tank was assumed to be a stationary jet release whose main axis is parallel with the road, see Figure 1. Besides the thermodynamic state in the tank (e.g., pressure, temperature), the properties of the jet release depend on the location of the orifice on the surface of the tank and the area and shape of the puncture. Depending on the location of the orifice, LPG may be released in the form of vapor, liquid, or two-phase flow. In this study, only the first two cases were included. First, the orifice was placed above the liquid level (3.2 m above ground). For this case, the released fuel will be in gaseous phase. Secondly, the orifice was located below the liquid level (1.8 m above ground), meaning that the released fuel will be liquid. In Sweden, it is common practice to consider three release scenarios, representing a large, medium, and small release. Hence, orifices with diameter 100 mm, 50 mm, and 20 mm were used in this study. The discharge coefficient was taken as 0.85 for all cases. Table 2 gives the leak properties and mass outflow rate. The duration of the leak was set to 60 s.

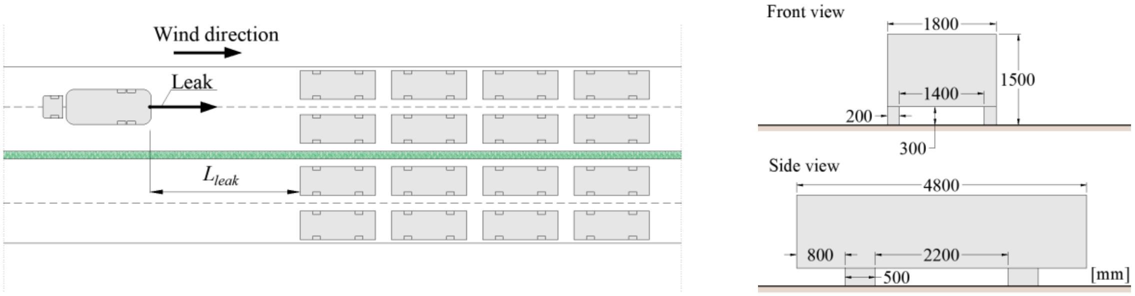
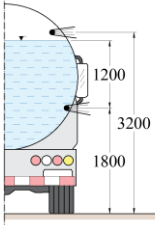


Figure 1: General setup and geometry of the case study.

Table 1: Asumed technical data of the LPG tank.

Properties	Value	Unit
Diameter of the tank	2.55	m
Nominal capacity	28	m^3
Maximum working (absolute) pressure	1,920	kPa
Filling degree	80	%
Storage (absolute) pressure	840	kPa
LPG load (100% propane)	12,000	kg
Ambient temperature	20	°C

Table 2: Leak properties.

Release	Phase	Leak diameter [m]	Leak height [m]	Liquid height [m]	Mass flow [kg/s]	
G-100	Gas	0.10	3.2	---	15.1	
G-50	Gas	0.05	3.2	---	3.8	
G-20	Gas	0.02	3.2	---	0.6	
L-100	Liquid	0.10	1.8	1.2	195	
L-50	Liquid	0.05	1.8	1.2	48.7	
L-20	Liquid	0.02	1.8	1.2	7.8	

3. CFD Modelling

3.1 General

The dispersion calculations were performed with the finite volume software FLACS-CFD (Gexcon AS, 2022), which solves the compressive Navier-Stokes equations on a structured cartesian grid. The calculation domain was divided into a core domain and a stretched domain (which lies between the core domain and the model boundaries). Cubic cells with size 0.3 m were used in the core domain. In the stretched domain, the cells were gradually stretched with a factor of 1.2. However, the cell size was limited to a maximum value of 4.0 m. Where relevant, the cell size was refined around the leak according to the guidelines specified by the user's manual. Grid sensitivity analysis within the core domain was carried out for some selected cases. Cell sizes of 1.0 m, 0.5 m and 0.3 m were tested. The maximum error in calculated V_{Q9} between consecutive cell sizes was 9%, which was considered satisfactory for this study. Based on this, the smallest evaluated cell size was used.

The mock-up vehicles were modelled entirely inside the core domain. The leak was placed at the center of the core domain (in the plane of the orifice). The wind speed was set to 2.0 m/s in the $x+$ direction at a reference height of 10 m. NOZZLE boundary condition was used at the non-wind boundaries, WIND boundary condition was used otherwise.

The total calculation domain was defined by x = [-20 m, 150 m], y = [-50 m, 50 m] and z = [0 m, 20 m]. The leak was placed at x = -5.0 m. The number of cells varied between 5×10^5 and 1.2×10^6 depending on the local refinement around the leak. Calculations were carried out in parallel with 4 CPUs. Average calculation time per scenario was around 5 hours.

3.2 Modelling of the release source

A release of LPG in gaseous phase begins as sonic flow at the orifice, followed by supersonic expansion. At some distance from the puncture, the jet achieves pressure equilibrium with the ambient fluid. Numerical modeling of this process is complicated and is outside the capabilities of the used CFD software. Instead, the conditions at the position where the jet pressure is equal to the atmospheric pressure were calculated analytically and used as input data for the CFD calculations. That is, the gaseous release was represented in the CFD model as a pseudo-source after expansion of the jet. At the pseudo-source, the jet consists of pure propane (i.e., $ER = \infty$). The single planar shock model implemented in the utility program JET2 (Gexcon AS, 2022) was used to calculate the properties of the pseudo-source, presented in Table 3.

When the LPG is released as a liquid, part of or all the liquid will evaporate quickly in a process called flashing. After flashing, a two-phase jet develops downstream. Some of the liquified gas stays in the jet in the form of droplets, while the rest may rain out and form an evaporating pool on the ground (Committee, 2005). The droplets in the jet will gradually evaporate due to air entrainment until the liquified gas has completely evaporated. From this point on, the process can be described as a single-phase vapor jet. Thus, this type of release was introduced in the CFD model as a single-phase jet. The properties of the jet after complete evaporation, presented in Table 3, were calculated using the utility program FLASH2 (Gexcon AS, 2022). After evaporation, the jet consists of a rich mixture of propane and air (ER = 5.9). The mass fraction of liquefied gas that rains out and forms a pool was found to be negligible in all cases, hence modelling of evaporation and subsequent dispersion of the pool was not necessary for the studied scenarios.

Steady-state conditions were assumed for all leaks, since no time-dependent calculations are possible for liquid releases in the CFD software used. The steady-state assumption is reasonable for situations in which the mass outflow rate is small relative to the total inventory in the tank. This is the case for most scenarios in this study, apart from release L-100. Therefore, for this release, the results are not expected to be fully accurate, but they are still shown for the sake of comparison.

Table 3: Input data concerning the release source for CFD modelling.

Release	Area* [m^2]	Mass flow rate* [kg/s]	Velocity [m/s]	ER [-]	Released fuel** [kg]
G-100	6.2×10^{-2}	15.1	131	∞	903
G-50	1.6×10^{-2}	3.8	131	∞	226
G-20	2.5×10^{-3}	0.6	131	∞	36
L-100	26.5	711	13.8	5.9	11700
L-50	6.6	178	13.8	5.9	2925
L-20	1.1	28.4	13.8	5.9	468

*At the position after expansion (for gas release) or evaporation (for liquid release).
**For a release duration of 60 s.

4. Results

The setup and results for the 20 studied dispersion scenarios are summarized in Table 4. The vertical profile of the dispersed cloud, expressed in terms of ER, is shown in Figure 2 for eight selected scenarios. Among the gaseous releases, the greatest ESC calculated with the Q9 model has a volume of 634 m^3. This volume was obtained for Scenario 6 (leak diameter of 100 mm and 4×4 vehicles). For the same scenario, V_{Q7} is equal to 1,872 m^3. That is, V_{Q9} is about 34 % of the total volume within the flammability limit. If the total released gas (during 60 s) were used to estimate the cloud size at stoichiometric state for this scenario, it would result on a volume of around 12,000 m^3, which is considerable larger than V_{Q9}. This shows that simplifications regarding the concentration of the gas cloud may lead to overly conservative predictions. Assuming 1.5 m between vehicles and a cloud height of 3.0 m, the calculated ESCs indicate that, for a leak size of 100 mm in the gaseous state, a reasonable number of vehicles to be considered as the blast source would be 4×3 (three vehicles on four lanes lane) or 2×5 (five vehicles on two consecutive lanes). For smaller diameters, the calculated ESCs were shown to be significantly smaller and to only constitute an explosion hazard in the immediate vicinity of the leakage, see Figure 2.

In general, liquid releases resulted in much greater ESCs compared to gaseous releases. The risk associated with release L-20 appears to be similar to that of release G-100, although scenarios with L-20 were found to be more sensitive to the presence of vehicles. Based on the results for L-20, a reasonable number of vehicles to be considered as blast source would be 4×4 (four vehicles on all four lanes lane) or 2×8 (eight vehicles on two consecutive lanes). For L-50 and L-100, the risk zone extended beyond the calculation domain (150 m); therefore, V_{Q9} and V_{Q7} for these scenarios are likely to be larger than those presented in Table 3. However, the results suggest that for these two release scenarios, the volume of the blast source could be limited by the geometrical conditions, rather than by the concentration of the gas cloud. That is, for these scenarios, the number of vehicles used as the blast source would depend on the traffic conditions.

It is also relevant to perform simulations of explosion of the dispersed clouds and the calculated ESCs (with volume V_{Q9}) to verify the accuracy of the transformation method in terms of overpressure and specific impulse. This was done for a few cases (not shown in this paper). The maximum overpressure at the blast source as well as peak overpressure and peak specific impulse at different monitor points were compared. In general terms, simulations with ESCs provided similar results (±25% error) compared to the corresponding dispersed cases. However, a more detailed evaluation is required to confirm these results.

Table 4: Calculated V_{Q9} and V_{Q7} for the studied scenarios.

Scenario	Leak	Vehicles	L_{leak} [m]	V_{Q9} [m^3]	V_{Q7} [m^3]
1	G-100	---	---	443	1,757
2	G-100	2x4	5	576	1,804
3	G-100	2x4	15	564	1,710
4	G-100	2x4	25	523	1,773
5	G-100	4x4	5	577	1,832
6	G-100	4x4	15	634	1,872
7	G-100	4x4	25	594	1,973
8	G-50	---	---	32	113
9	G-50	2x4	15	39	206
10	G-50	4x4	15	40	207
11	G-20	---	---	3	10
12	G-20	2x4	15	3	10
13	G-20	4x4	15	3	10
14	L-100	---	---	>17,000	>40,000
15	L-50	---	---	>8,313	>21,910
16	L-50	2x4	15	>9,928	>22,085
17	L-50	4x4	15	>11,215	>24,917
18	L-20	---	---	406	1,720
19	L-20	2x4	15	1,100	2,900
20	L-20	4x4	15	1,179	3,135

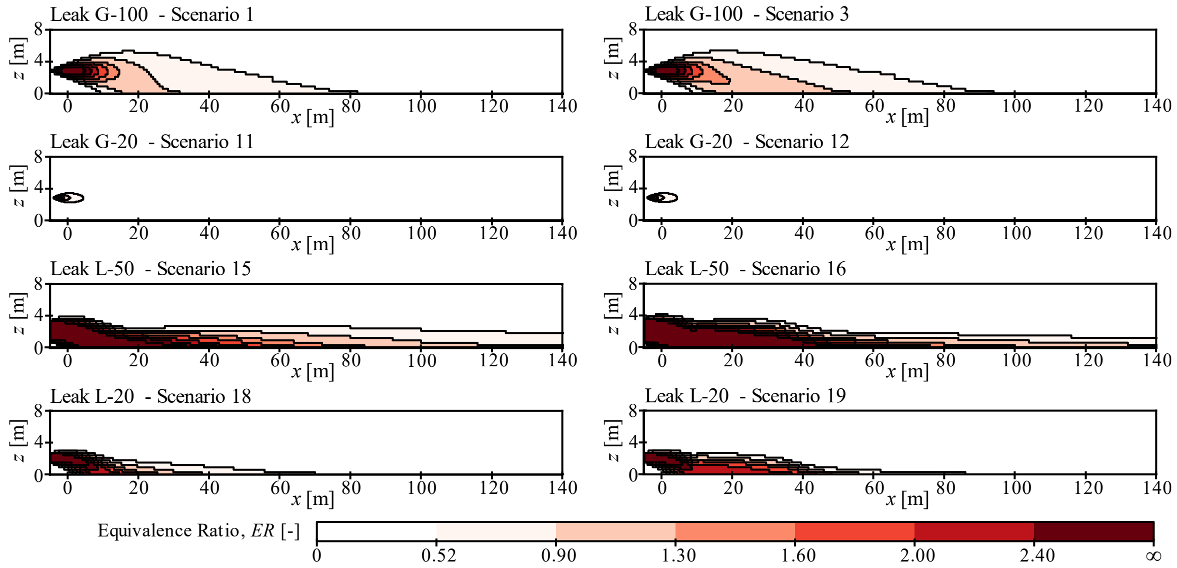


Figure 2: Vertical profile of the dispersed cloud (plotted at the y-coordinate of the leak) for some selected scenarios. ER = 0.52 and ER = 2.40 correspond to LFL and UFL in a propane-air mixture.

The influence of different parameters (besides the leak properties) was studied for a few selected scenarios. Figure 3 a) shows average V_{Q9} for different leak types and number of vehicles, normalized based on V_{Q9} for the respective scenarios without vehicles. For all studied cases, introducing vehicles in the scenario resulted in an increase of the volume of the ESC. This effect was particularly strong for leak L-20. However, this enhancing effect was not as significant for L-50, possibly because the vehicles were largely located within the rich region of the mixture in the L-50 scenarios. In Figure 3 b), the influence of the wind speed on Scenario 3 was evaluated. The results showed that lower wind speeds allowed for more optimal mixing of propane and air resulting in greater ESC. Finally, the influence of a noise barrier (length 100 m and height 4 m) parallel to the road was investigated for Scenario 3. The noise barrier was placed at two different distances from the vehicles. The results suggest that a barrier close to the vehicles may lead to a significant increase of the ESC, though this effect diminishes for barriers located further away.

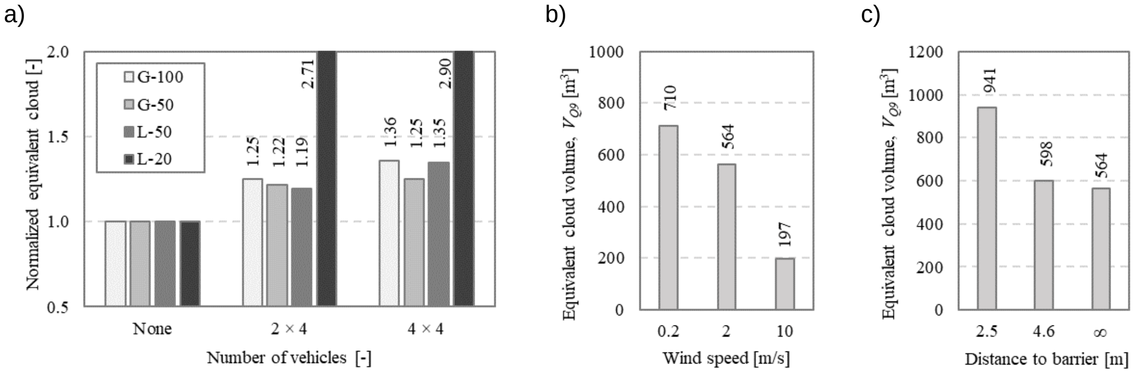


Figure 3: Influence of different parameters on the ESC. a) number of vehicles, b) wind speed (for Scenario 3), c) presence of noise barrier (for Scenario 3).

5. Conclusions

This study conducted a numerical study of LPG dispersion on a road for different standard release scenarios, with particular focus on the transformation of the dispersed cloud into an equivalent stoichiometric cloud that yields similar explosion characteristics in a domain of about 150 m from the release. For a purely gaseous release (diameter ≤ 100 mm) and for small liquid releases (diameter ≤ 20 mm), the results showed that it may be overly conservative to assume that all vehicles within the flammable dispersed cloud form the blast source if a stoichiometric concentration is assumed for the blast source for the evaluation of the explosion. Instead, the study informs on appropriate maximum equivalent gas cloud volumes that can be used as a source of blast, which could be translated to a maximum number of vehicles that should be considered as the blast source, even if more vehicles are present within the flammable region. For medium or large liquid release (diameter ≥ 50 mm), it was found appropriate to determine the blast source based on the traffic conditions within the flammable region of the cloud.

Acknowledgments

This work was financed by the Swedish Transport Administration, Swedish Fortifications Agency, and Swedish Civil Contingencies Agency. The calculations were performed on the high-performance computing cluster *Vera*, provided by Chalmers e-Commons at Chalmers.

References

Bubbico R., Ferrari C., Mazzarotta B., 2000, Risk analysis of LPG transport by road and rail, Journal of Loss Prevention in the Process Industries, 13(1), 27–31.

Committee for the Prevention of Disasters, 2005, Methods for the calculation of physical effects (’Yellow book’).

Gexcon AS., 2022, FLACS-CFD v22.1 User’s Manual.

Nielsen M., 1998, Dense gas dispersion in the atmosphere, Risø National Laboratory.

Shen R., Jiao Z., Parker T., Sun Y., Wang Q., 2020, Recent application of Computational Fluid Dynamics (CFD) in process safety and loss prevention: A review, Journal of Loss Prevention in the Process Industries, 67, 104252.

Tam V. H. Y., Tan F., Savvides C., 2021, A critical review of the Equivalent Stoichiometric Cloud model Q9 in gas explosion modelling, Eng., 2(2), 156-180.

van den Berg A. C., 1985, The multi-energy method: A framework for vapour cloud explosion blast prediction, Journal of Hazardous Materials, 12(1), Article 1.