

# Computational Fluid Dynamics Modeling of Liquid Hydrogen Release and Dispersion in Gas Refuelling Stations

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The hydrogen consumption is expected to grow in the near future, and a forecasted energy transition after the COVID-19 pandemic may increment such growth. For this reason, there is the need for a solution to increase the hydrogen density for both storage and transportation purposes. The release of hydrogen from its handling equipment is a scenario that must be assessed to define the technology feasibility. Both confined and unconfined hydrogen releases have been broadly studied in the scientific literature. However, the focus has been placed mainly on the release and dispersion of compressed gaseous hydrogen. Hydrogen distribution to the future gas refuelling stations in liquid (cryogenic) phase rather than compressed gas is one of the options to increase the truck payload. For this reason, potential liquid hydrogen (LH<sub>2</sub>) release with a consequent pool formation and gas dispersion is one of the scenarios to consider by the associated risk assessment.

The aim of this study is to comprehend the hydrogen behaviour after a liquid release in a refuelling station, which represents a semi-confined space, by means of a commercial computational fluid dynamics (CFD) tool: the FLame ACceleration Simulator (FLACS). The LH<sub>2</sub> pool formation as well as the dispersion of the hydrogen gas cloud in the surrounding were investigated. Different parameters such as the variation in density of the extremely cold gas and the lower flammability limit (LFL) of the gas cloud were measured. As expected, the wind speed and direction significantly affect the position and dilution of the flammable gas cloud within and outside the facility. Few solutions to prevent further consequences from the LH<sub>2</sub> releases such as a vapour cloud explosion were proposed to spark the interest on future studies on safety barriers for this type of accident scenario.

## 1. Introduction

After the COVID-19 pandemic, the energy transition from fossil fuels toward renewables and sustainable fuels is expected to accelerate (DNV-GL, 2020a). For this reason, the hydrogen consumption might grow rapidly in the near future since it may be a renewable and zero-emission fuel, able to store the surplus energy produced by the renewables such as wind and solar energies. If large amounts of hydrogen are handled, it could be convenient to increase its density and hence its storage capacity by means of a liquefaction process. Liquid hydrogen (LH<sub>2</sub>) has a density of 70.85 kg m<sup>-3</sup> at boiling point (20.3 K) at atmospheric pressure (NIST, 2019). If it is released on the ground, it easily evaporates due to the large difference in temperature with the environment. The density of its gaseous phase close to the boiling point at atmospheric pressure is 1.33 kg m<sup>-3</sup>, thus it behaves as a cold dense gas when released (Hansen, 2020). Moreover, hydrogen is an extremely flammable gas and its dispersion might lead to a fire or even a vapour cloud explosion (VCE) due to its very low minimum ignition energy (0.017 mJ (Ono et al., 2007)). Despite these safety drawbacks, hydrogen is currently employed in a large number of applications, and thanks to its high gravimetric energy density (120 MJ kg<sup>-1</sup>) it is suitable to power several types of vehicles, including cars and buses, trains, ships, aircrafts and spaceships (Ustolin et al., 2020). Worldwide, the number of hydrogen refuelling stations for cars and buses is increasing, especially in Japan, Germany and California (Isenstadt and Lutsey, 2017). These refuelling

stations may be considered as an emerging technology due to the low number of existing facilities, and their implementation in urban areas requires a very high level of attention in terms of safety. For this reason, different aspects such as the separation distances suggested by different regulations might be overestimated by the safety codes. For instance, Hecht et al. (2019) employed different risk assessment techniques to propose the footprint reduction of the hydrogen stations and therefore update the NFPA 2 (National Fire Protection Association) regulation currently employed in the USA.

The idea of this study is to evaluate the consequences of a loss of containment of an LH<sub>2</sub> road tanker in a hydrogen fuelling station during the transferring operation. The FLACS software was employed to conduct a CFD analysis of the release. The aim of this study is to provide useful results to aid the further development of the safety codes related to hydrogen stations. Furthermore, a brief literature review of both experiments and numerical simulations of LH<sub>2</sub> releases is presented to provide a broad overview of the topic.

## 2. Liquid hydrogen releases: experiments and numerical simulations

In the past, different types of hydrogen releases were studied, either in gaseous or liquid phase, outdoor or in enclosure. However, few LH<sub>2</sub> experiments releases were carried out in the last 40 years. One of the first LH<sub>2</sub> release experiment was conducted by NASA in 1981 at the NASA's White Sands Test Facility in New Mexico (Witcofski, 1981). In particular, different large-scale releases of LH<sub>2</sub> with a duration of approx. 35 s were carried out from a 5.7 m<sup>3</sup> Dewar pressurised with gaseous helium up to 690 kPa (Witcofski & Chirivella, 1984). The LH<sub>2</sub> flowed in a 30 m foam-insulated pipe with an internal diameter of 152 mm before being spilled downward through a diffuser on a 1.2 by 1.2 m steel plate installed at the centre of a 9.1 m diameter spill pond made of compacted sand at the bottom. In 1994, LH<sub>2</sub> release experiments were carried out by the Federal Institute for Materials Research and Testing (BAM) and the Research Center Juelich in Drachhausen, Brandenburg, Germany as part of the Euro-Québec Hydro-Hydrogen Pilot Project to study the behaviour of the dispersed cloud between buildings (Schmidtchen et al., 1994). In these experiments, the dispersion and the pool formation were studied separately. In the first case, the LH<sub>2</sub> was released for 60 s with a flowrate of 0.8 kg s<sup>-1</sup>, from a 50 mm diameter nozzle placed 0.5 m above a 0.5 m<sup>2</sup> aluminium plate which was installed 1 m above the ground (Schmidtchen et al., 1994). A diffuser was added at the end of the line to study the pool formation. In this case, the LH<sub>2</sub> was collected in an open cylindrical tank with a 40 cm diameter installed at the diffuser exit. The surface below this catching pot was either solid (aluminium plate) or liquid (swimming pool filled with water) (Verfondern & Dienhart, 1997). This was one of the first analysis of LH<sub>2</sub> spill onto water. In 2012, the Health and Safety Laboratory (HSL) conducted a series of experiments of both unignited and ignited releases of LH<sub>2</sub> at the HSL facility in Buxton, UK (Royle & Willoughby, 2014) (Hall, 2014). The LH<sub>2</sub> was released through a 25.4 mm diameter nozzle orientated either vertically downward or horizontally at different heights from a tank with a pressure of 1 bar<sub>g</sub> at a constant flowrate of 60 l min<sup>-1</sup>. The nominal pressure at the outlet of the pipe was 0.2 bar<sub>g</sub>. The spills duration varied from 215 to 561 s (Royle & Willoughby, 2014). Recently, DNV-GL conducted in its Spadeadam facility in UK a series of both outdoor and in enclosure LH<sub>2</sub> release experiments on request of the Norwegian Defence Research Establishment (FFI) (DNV-GL, 2020b) (DNV-GL, 2020c). The LH<sub>2</sub> was spilled from a nozzle with a nominal diameter of 25.4 mm oriented either horizontally or vertically downward, and some of the releases were also ignited at different locations within few seconds after the leakage started. The pressure of the LH<sub>2</sub> tank was varied from 0.8 up to 10 bar<sub>g</sub> which corresponded to a maximum mass flow of 49.9 kg min<sup>-1</sup>, while the release duration varied from 3 up to 15 min. Several authors tried to reproduce most of the abovementioned experiments by means of different CFD codes. For instance, the CHAMPAGNE code was used by Chitose et al. (2002) to simulate large-scale LH<sub>2</sub> spills. The Ansys Fluent fluid simulation software package was adopted by Schmidt et al. (1999) to reproduce the BAM experiments described above and by Liu et al. (2019) for simulating the NASA tests which were replicated as well by Sklavounos and Rigas (2005) by means of the CFX code. The CFD in-house code ADREA-HF was widely employed in different studies where the LH<sub>2</sub> spills were simulated. In particular, this code was used to simulate the BAM experiments (Statharas et al., 2000), the NASA tests (Venetsanos and Bartzis, 2007) and the HSL experiments (Giannissi et al., 2014) (Giannissi and Venetsanos, 2018). Furthermore, the ADREA-HF code was selected to conduct the CFD analysis of an LH<sub>2</sub> release from the hose between a dispenser and a car in a mock-up hydrogen refuelling station (Baraldi et al., 2009). This is the only CFD analysis on LH<sub>2</sub> release focussed on hydrogen refuelling stations. Finally, the FLACS software was adopted by different authors to evaluate the consequences of an LH<sub>2</sub> release from a car in a tunnel (Middha & Hansen, 2009), reproduce the NASA tests (Middha et al., 2011) and the HSL experiments (Ichard et al., 2012) (Hansen, 2020). A detailed literature review of the LH<sub>2</sub> release modelling which considers integral and shallow layer equations models beyond the CFD codes is available in (Batt, 2014).

### 3. Methodology

#### 3.1 Hydrogen refuelling station description

The Iwatani hydrogen station sited in Ariake, Tokyo, Japan was selected for this analysis. This facility was built in 2003 and was the first LH<sub>2</sub> refuelling station in Japan. It has a surface of 3,200 m<sup>2</sup> and a storage capacity of 10 m<sup>3</sup> of LH<sub>2</sub> (Iwatani, 2010). The LH<sub>2</sub> is then compressed up to 350 bar to refuel the vehicles. The layout of the station was retrieved from Google Maps. The facility is enclosed among two urban streets, one of which is quite wide since it has five lanes, walk paths and bike lanes on both sides. The station is oriented from North-West to South-East. In this analysis, it was assumed that the station is aligned with the North-South direction and a continuous leakage occurred during the hydrogen delivery either from the rear of the LH<sub>2</sub> tanker or the hose employed to transfer the LH<sub>2</sub> from the truck to the storage tank of the facility. In Figure 1, the CAD drawing of the hydrogen station used as geometry for the CFD simulations is depicted. The blue terrain represents the border between the facility and the road on the East side. Furthermore, on the rear of the truck the red arrow represents the leak position, in this case oriented vertically upward.

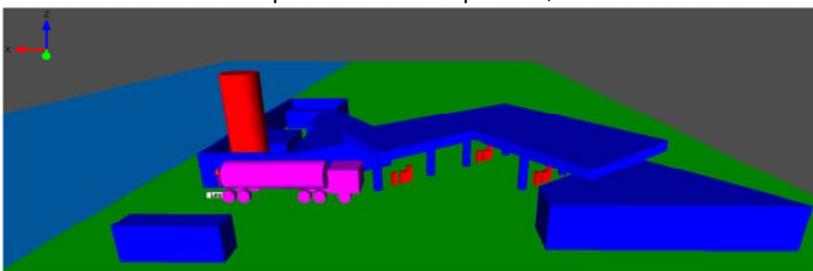


Figure 1: View of the hydrogen refueling station from North (Y direction in the software).

#### 3.2 Source model and CFD approach

The approach selected in this study is similar to the one proposed by Hansen (2020) who simulated the HSL experiments by means of the CFD FLACS code. In particular, a steady-state leakage of cold gaseous hydrogen mixed with air was simulated. It was assumed that prior to the loss of containment the truck tank had a pressure of 5 bar, since it is close to the maximum operating pressure of the LH<sub>2</sub> tank (7 bar (Ustolin et al., 2020)), a filling degree of 80% and both hydrogen liquid and vapour phases contained in the tank were at saturation temperature (27.7 K (NIST, 2019)). An effective hole diameter of 10 mm was selected for the continuous LH<sub>2</sub> release according to the guideline on the loss of containment of a pressurized tank provided in the Purple book (Uijt de Haag and Ale, 2005). The jet parameters were estimated by means of the FLASH utility implemented in the FLACS software because it is not practical to simulate the liquid flashing directly with the CFD code. The user defined substance option was selected to define the hydrogen properties retrieved from (NIST, 2019) since hydrogen is not implemented nor validated in the FLASH utility. For this reason, the same evaluation was conducted with the Fire, Release, Explosion, and Dispersion (FRED) software (Gexcon, 2020b) and the EFFECTS tool (Gexcon, 2020c) in order to compare and verify the results. A good agreement between the three tools was found, thus the FLASH outcomes were used as input for the dispersion and ventilation scenario in the CFD FLACS code. In this case, the equivalence ratio (ER) of the released gas in the entrained jet is a fundamental input for the release simulation in the CFD code. Therefore, ER is used by FLACS also to evaluate if the hydrogen concentration is within the flammability range (Gexcon, 2020a). The hydrogen lower flammability limit (LFL) in air is 4% in volume while the upper flammability limit (UFL) is 75% at ambient temperature, while this range slightly shrinks at cryogenic temperatures (Pio and Salzano, 2019). However, the hydrogen LFL and UFL were kept equal to 4 and 75% to obtain conservative results.

Three different configurations were selected by changing the orientation of the leakage as well as the wind direction and speed. The worst-case scenarios in which the hydrogen concentration reaches the highest values inside the facility, and in which the flammable cloud extends furthest away from the gas station were sought. In the first case, neutral atmospheric stability with stagnant wind conditions and a vertical either downward or upward leak from the transferring hose were considered. In the second case, a wind speed of 2 m s<sup>-1</sup> and a horizontal leakage from the tank in the same direction of the wind were selected. In particular, the wind was blowing from West (X direction) and pushing the dispersed gas toward the road located on the East side of the hydrogen station. In this case, the Pasquill class F was selected. Except for the wind and the Pasquill class, the atmospheric conditions were the same for all the configurations: pressure equal to 101,352 Pa and temperature of 15°C. The leak duration was 120 s since after this time steady-state conditions were reached for the flammable cloud. Moreover, the leak was starting after 2 s for the vertical leaks and 15 s for the horizontal jet in order to achieve a stable velocity field due to the wind. The turbulence is simulated in

FLACS with the k-epsilon model. Furthermore, the heat switch option was activated in FLACS to take into account the heat transfer between the cold gas and the objects. This is an important feature since the hydrogen dispersion depends on its evaporation rate affected by the heat transfer with the surroundings.

In FLACS, the distributed porosity concept is used for representing complex geometry and a structured Cartesian grid is employed to spatially discretise the domain by using a finite volume method (Gexcon, 2020a). In this study, two different domains were created with the following dimensions: 50 x 40 x 26 m for the vertical leaks (Z direction) and 90 x 40 x 11 m for the horizontal leak (X direction). The grid was uniform in the proximity of the leak and then stretched toward the boundaries with a growing ratio of 1.10. Furthermore, the grid was refined around the leak in all directions. For this reason, the Courant-Friedrichs-Lewy (CFL) number was set equal to 100 according to the guidelines provided in the FLACS user manual (Gexcon, 2020a). A sensitivity analysis was conducted to verify the grid independence for each domain. As result, the minimum cell size was equal to 4.8 cm, located at the release point, and the total number of cells for the two domains previously described was 1,983,891 and 2,009,250 for the vertical and horizontal leaks, respectively. Finally, a gas monitor region with the same dimensions of the entire domain was created to estimate the flammable hydrogen mass and cloud volume. A summary of the different configurations selected in the simulations is collected in Table 1.

*Table 1: CFD analysis configurations*

Simulation nr.	Domain dimensions (m)	Leak orientation	Leak duration (s)	Wind speed (m/s)	Wind direction
25	50 x 40 x 26	- Z	120	0	-
33	50 x 40 x 26	+Z	120	0	-
31	90 x 40 x 11	+X	120	2	West

#### 4. Results

The outcomes of the FLASH utility provided the leak characteristics after the complete evaporation of the LH<sub>2</sub>. The LH<sub>2</sub> mass flowrate at the hole was 0.372 kg s<sup>-1</sup>, the velocity 107.2 m s<sup>-1</sup>, while all the LH<sub>2</sub> completely evaporated at 0.45 m from the release source and the entrained jet at this point reached a mass flowrate of 0.893 kg s<sup>-1</sup>, velocity of 44.6 m s<sup>-1</sup>, temperature equal to 20.07 K, density of 2.68 kg m<sup>-3</sup>, and an equivalence ratio of 24.46. FLASH estimated that rainout was not formed. The jet parameters used as input of the CFD analysis in FLACS are reported in Table 2.

*Table 2: entrained jet parameter estimated with FLASH and employed as input in the CFD analysis*

Area (m <sup>2</sup> )	Mass flowrate (kg s <sup>-1</sup> )	Temperature (K)	Density (kg m <sup>-3</sup> )	Velocity (m s <sup>-1</sup> )	Equivalence ratio (-)
0.0075	0.893	20.07	2.68	44.6	24.46

In the case of a dispersion, the hydrogen concentration is one of the most important parameters to evaluate. The CFD analysis provided the flammable H<sub>2</sub> mass and the volume of the flammable cloud composed by the air-hydrogen mixture when the hydrogen concentration is between LFL and UFL. In Table 3, these two parameters together with the maximum horizontal and vertical distance reached by the cloud are collected.

*Table 3: CFD analysis results*

Simulation nr.	Flammable H <sub>2</sub> mass (kg)	Flammable cloud (m <sup>3</sup> )	LFL cloud horizontal distance (m)	LFL cloud vertical distance (m)
25	3.99	520	12.5 (+Y)	25.9
33	6.27	825	18.0 (+X)	15.0
31	2.17	302	60.0 (+X)	2.7

It can be noticed that the largest flammable cloud (825 m<sup>3</sup>) was formed when the leakage was oriented vertically upward (see Figure 2) and the stagnation wind conditions were considered, while the longest horizontal distance was reached by the cloud during the horizontal release. In the latter case, the cloud was free to spread without any obstacles in the simulation. However, according to the satellite images, a truck deposit composed by two-story building can be found approximately 50 m from the assumed release point in the jet direction.

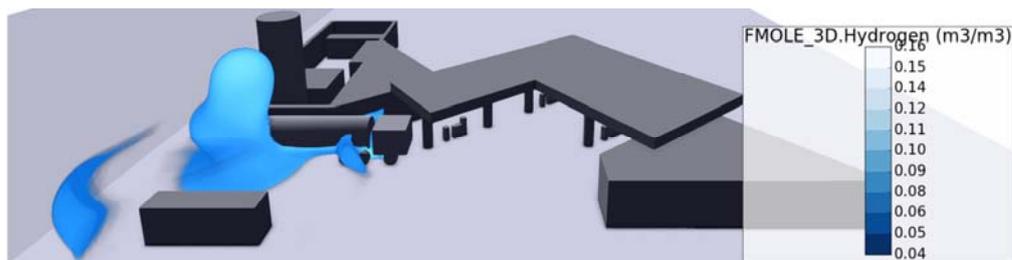


Figure 2: 3D plot of the  $H_2$  flammable cloud at 76 s for the vertical upward release (simulation nr. 33).

## 5. Discussion

The CFD analysis demonstrated that the largest flammable cloud was generated when stagnation wind conditions were present and the leakage was vertical upward. If an ignition source is present within the cloud catastrophic consequences may occur. However, the combustion is affected by several parameters ( $H_2$  mass and concentration, level of confinement, and wind flow field (Baraldi et al., 2009), thus the flammable cloud volume cannot be the only parameter used to evaluate the consequences either of a potential fire or vapour cloud explosion (VCE). Another hazard is represented by the cloud dispersed toward the street and the surrounding buildings. Approximately 50 m East of this refuelling station, a two-story building of a shipping company with a truck terminal is found. This may represent a concern because several ignition sources might be met by the dispersed cloud. It must be mentioned that the accident scenario considered in this study was conservative due to the assumptions. Firstly, the tank was assumed to be almost full (80%) with a pressure (5 bar) close to the maximum operative one. Secondly, a steady-state leak with the maximum flowrate was selected. Thirdly, the liquid temperature inside the tank was assumed to be the saturation one. Therefore, the entire liquid jet immediately evaporated without generating any rain out, while during the HSL experiments (Royle & Willoughby, 2014) a pool was formed even though a smaller mass flowrate release ( $0.07 \text{ kg s}^{-1}$ ) was achieved in that case. Therefore, the leak was simulated as a cold gas already mixed with air. Finally, any mitigation measures were neglected, and each simulation was carried out until the flammable cloud reached steady-state conditions. Generally, a potential loss of containment from hydrogen equipment must be always prevented due to the extremely high flammability of hydrogen. As results of this study, appropriate and effective mitigation measures must be adopted when this fuel is handled and stored in refuelling stations sited in urban areas. One mitigation measure suggested by Baraldi et al. (2009) was the shutdown of the pumping system 5 s after the leak started. The employment of gas detection sensors that work reliably at cryogenic conditions is strictly necessary. Furthermore, physical barriers can be adopted to impede the spread of the flammable cloud toward the street and the surrounding buildings. Finally, ignition sources must be always avoided inside the facility, especially during the refuelling of vehicles or when the  $LH_2$  is supplied to the station by the road tanker. Additional numerical simulation and experimental studies on  $LH_2$  dispersion in refuelling stations are suggested. Moreover, the combustion of the dispersed cloud must be analysed in order to estimate the yield of either a fire or a VCE. A thorough consequence analysis is part of the risk assessment strictly necessary to aid the writing of safety guidelines and regulations for the design and maintenance of hydrogen refuelling stations sited in urban areas.

## 6. Conclusions

The consequences of the  $LH_2$  jet dispersion after the loss of containment from a road tanker during the hydrogen supply in a refuelling station were evaluated by means of the CFD software FLACS. Different scenarios were analysed by changing the leak direction and the wind speed. The prevention and mitigation of the dispersion must be always considered to avoid catastrophic consequences such as fires and explosions. Additional studies on the flammable cloud combustion inside and in the surrounding of the hydrogen station are suggested.

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