Numerical analysis of vapor dispersion from compressed hydrogen (H_2) storage vessels

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Abstract. The rising demand for hydrogen fuel, driven by the emergence of fuel cell electric vehicles, underscores the need to optimize refueling station efficiency and affordability while prioritizing safety and performance. Compressed gas hydrogen storage emerges as a practical solution however safety across production, storage, and distribution is paramount for broader acceptance of hydrogen technologies. Any incidents could undermine public trust, emphasizing the importance of mitigating risks such as hydrogen leakage. This study investigates hydrogen dispersion and conducts consequence analyses for potential hazards, considering stability, ambient temperature, wind speed, and process parameters like vessel temperature, pressure, and leakage diameter. It assesses various scenarios, including high-pressure storage vessels and generic refueling station layouts, by employing integral models of ALOHA, PHAST and HyRAM. Findings showed that process parameters significantly influence hazard severity, with leakage diameter having a notable impact. Common safety vulnerabilities in fuel cell vehicles and refueling stations are highlighted, emphasizing adherence to international regulations and standards for enhanced safety protocols.

1 Introduction

Hydrogen is a promising energy carrier. The primary issue of hydrogen utilization is safety in various scenarios for the coming hydrogen economy, due to its wider flammable range of 4–75 vol.% (in air) and a very low ignition energy of 0.019 mJ [1]. Storing and transporting hydrogen gas in large volumes and over long distances are the biggest challenges in the hydrogen supply chain. In general, hydrogen storage can be divided into two types: physical method and material storage method. The physical method involves compressed gas, cold/cryo-pressed and liquid hydrogen, while the material storage method is based on new materials (i.e. hydrogen carrier) that can alternately absorb and release hydrogen. However, due to its simplicity, compressed hydrogen is still the most widely used H_2 storage method in the world, used in over 80% of the world's H_2 filling stations. Gaseous H_2 is pressurized to 350-700 bar and stored in cylinders, tanks or underground pits. Assuming hydrogen leakage from the storage tank, a series of events were assumed to happen in sequences, such as a gas jet spill, hydrogen dispersion and vapor cloud explosions (VCEs). In that manner, safety issues associated with handling pressurized hydrogen (such as release, fire, and explosion) tend to escalate as when a larger-scale hydrogen production is needed, and more hydrogen fuel-cell vehicles are demanded. This work focuses on hydrogen leakage, which is typically induced by structural failure in refueling stations and transit vehicles, with attention to eliminate public concern and provide references for design, legislation, and standards.

Rodionov et al. evaluated the risk assessment of the hydrogen explosion related to a hydrogen-driven engine car, stated that hydrogen explosion in open and semi-confined environments has a high level of risk with potential injuries to people and damage to cars and area of the hydrogen explosion [2]. For the safe design of retail facilities, through the development of appropriate codes, it is essential to understand all the hazards that could arise following an accidental release of hydrogen and to have data to allow the appropriate standards to be developed. These data can be also used to develop and validate models used in quantitative risk assessment tools and tools based on computational fluid dynamics (CFD) or tool based on integral models e.g. DEGADIS, SLAB, PHAST, HGSYSTEM, and ALOHA [3–5].

The present study was formulated in order to determine the consequences caused by hydrogen dispersion, adopting integral model software of ALOHA, PHAST and HyRAM. Variables such as wind speed and the leak hole diameter were selected as the factors to simulate the consequences of hydrogen storage leakage accidents. The impacts of each variable on accident consequences were analyzed for obtaining the reasonable and effective reference in actual accidents and conducting fire risk assessment.

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2 Research Method

For this study, three models are adopted to evaluate the safety evaluation namely ALOHA, PHAST and HyRAM, which has been built upon the Gaussian dispersion model of continuous, buoyant air pollution flumes that capable to simulate the accidental release of hazardous substances and the dispersion of chemical vapor.

2.1 ALOHA Software

ALOHA is a program designed to model chemical releases for emergency responders and planners. ALOHA allows modeling of many release scenarios: toxic gas clouds, Boiling Liquid Expanding Vapor Explosions (BLEVE), jet fires, vapor cloud explosions and pool fires. Depending on the release scenario, ALOHA evaluates the corresponding type of hazard. ALOHA displays its estimate as a threat zone, which is an area where hazards (such as toxicity, flammability, thermal radiation or damaging overpressure) exceed a user-specified level of concern. It is possible to generate a variety of scenario-specific outputs, including threat zone plots, threats at specific locations and source strength graphs. ALOHA also defines its limitation clearly and state the reason behind. For example, it cannot make predictions further than 10 kilometers downwind from a release point. There are several reasons that imposed this limitation on ALOHA. The primary reason for this cutoff is related to the equations ALOHA uses to predict threat zone length [6].

2.2 PHAST Software

PHAST (Process Hazard Analysis Software Tool) is a comprehensive consequence analysis tool. It examines the process of a potential incident from the initial release to far field dispersion, including modelling of pool vaporisation and evaporation, and flammable and toxic effects. PHAST is able to simulate various release scenarios such as leaks, line ruptures, long pipeline releases and tank roof collapse in pressurised / unpressurised vessels or pipes. An integral-type dispersion model called UDM (Unified Dispersion Model) calculates several consequence results: i) cloud behaviour ii) transition through various stages such as jet phase, heavy phase, transition phase and passive dispersion phase, iii) distance to hazardous concentration of interest and iv) footprint of the cloud at a given time. PHAST release and dispersion models are also available in the form of an Excel interface, called MDE Generic Spreadsheets™. Sensitivity studies can be easily carried out using these Spreadsheets, since they allow direct control of input parameters and output results, easy parameter variation and multiple runs (simultaneous simulation of various scenarios) [7]. PHAST v.6.53 has been used in this work.

2.3 HyRAM Software

HyRAM is a comprehensive methodology and accompanying software toolkit for assessing the safety of hydrogen fueling and storage infrastructure. It can be used to perform Quantitative Risk Assessment (QRA) with integrated consequence analysis and/or run deterministic consequence models in standalone fashion. The HyRAM software toolkit provides a consistent, documented methodology for QRA with integrated reduced-order physical models that have been validated for use in hydrogen systems. HyRAM also contains probabilistic data and models that have been vetted by the hydrogen research community. HyRAM is intended to facilitate evidence-based decision making to support codes and standards development and compliance [8].

Table 1. Initial condition and Potential incidence of release.

Potential release	**Scenario I: Rupture in tank at a refueling station (HRS)**	**Scenario II: Rupture of storage hydrogen tank in a car**
Simulation scenarios	**a) Pipeline** • Diameter = 0.15, 0.20 and 0.30 m • Pipe length = 200 m • Pressure in pipe = 70 bar • Wind speed: 2 and 8 m/s from North • Ambient temperature = 33°C • Humidity = 46 % **b) For storage tank** • Direct source of hydrogen (worst-case scenario) • Leak hole diameter of 15 cm • Volume: 300 litre • Uncongested area of hydrogen refueling station • Vessel pressure = 500 bar	Use Toyota Mirai as model for the simulation: • Moving car – possible being hit at back (25-L hydrogen storage tank) • Possible rupture of all connected storage tanks (Total volume is 141 litre) • Storage pressure = 700 bar • Car moving in semi-confined area, e.g., tunnel • Car parked in a confined area and congested area, e.g., multilevel parking

For this work, hydrogen refueling station (HRS) facilities with storage involving compressed gas hydrogen have been chosen as the subjects of simulation as shown in Fig. 1. Suppose leakage occurred at Pasir Gudang highway, in Malaysia with longitude and latitude of 1.4825ºN, 103.8811ºE. The initial condition of the simulation and for the potential incidence of release, three hypothetical scenarios (I ,II and III) have been created with environmental configurations as shown in Table 1.

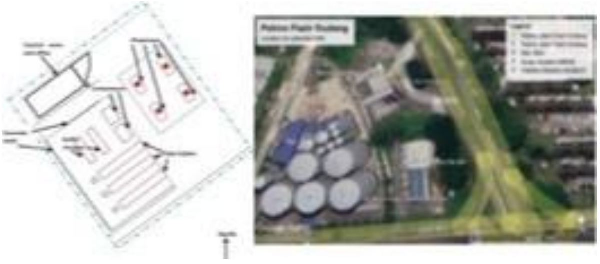

Fig. 1. Schematic generic diagram and layout of the refueling station [9] and location of the HRS.

For the mobile vehicle, Mirai car was adopted as our reference to evaluate the consequences analysis (see Fig. 2).

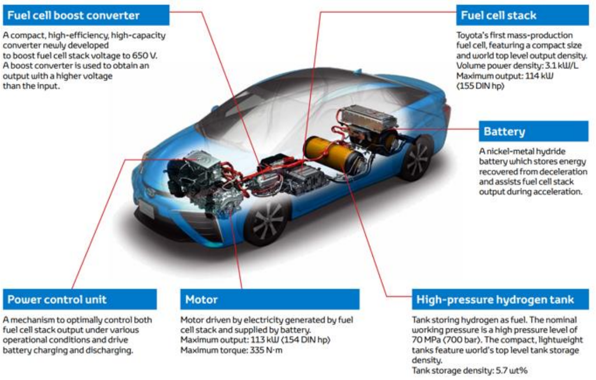

Fig. 2. Toyota Mirai main component [10].

2.4 Possible consequences of hydrogen release

Releases of hydrogen can be either instantaneous or continuous. The "instantaneous release" is a sudden violent burst of equipment such as the burst of high pressurized hydrogen storage vessel. The result is a depressurization of the hydrogen (physical explosion) and subsequent dispersion of the hydrogen cloud. Ignition of the hydrogen cloud will result in a flash fire (vapor cloud fire). A confined vapor cloud explosion (Confined VCE) may occur if the released hydrogen accumulates in a confined area or if there is a considerable amount of pipe work in the cloud envelope. The consequences of continuous release will depend on the time of ignition. Direct ignition results in a jet fire, while delayed ignition results in a flash fire or results in an explosion (when released hydrogen piles up in a confined or semi-confined area). A fireball is not likely to occur for gaseous hydrogen, so it has not been considered into our consequence calculations. To conclude, four typical consequences of gas hydrogen release are considered in modelling: physical explosion, jet fire, flash fire and confined vapor cloud explosion as illustrated in Fig.3.

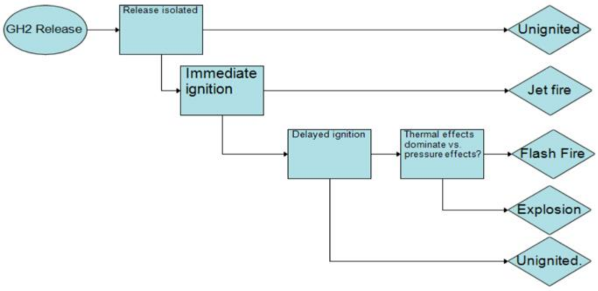

Fig. 3. Event sequence diagram for hydrogen gas releases [8].

3 Results and Discussion

3.1 Results for the worst-case scenario of I and II

The main consequences of hydrogen leakage in this work are jet fire (radiation intensity) , flammable cloud and blast overpressure of vapor cloud explosion. Table 2 summarizes the maximum distance from the maximum jet fire, maximum flammable vapor cloud and blast overpressure when hydrogen leaks at different wind speeds i.e. 2 and 8 m/s when ALOHA simulation is adopted. It can be depicted that the effect of the wind speeds on from the hydrogen leakage sources is minimum at the stable climate condition. However, when the leak hole diameter pipe increases in case of Scenario I, the maximum distance from flammable vapor cloud and maximum radiation level increase with a higher leakage diameter due to an increased release rate and an increased amount of hydrogen. For instance, from 15 to 30 cm leakage in pipe, the maximum distance from flammable vapor cloud and the thermal radiation jet fire increases ~ 2.3 – 2.8 times.

Table 2. Threat zones of hydrogen release computed in the ALOHA simulation at wind speed of 8 m/s

8 m/s wind speed			
Scenario I: Dispensing pipes at the HRS			
Leak hole diameter	**Thermal radiation threat zone**		
	10.0 kW/sq	5.0 kW/sq	2.0 kW/sq
15 cm	47 m	66 m	102 m
20 cm	67 m	93 m	144 m
30 cm	107 m	150 m	233 m
	Flammable threat zone		
	60 % LEL	10% LEL	
15 cm	538 m	1600 m	
20 cm	817 m	2500 m	
30 cm	1500 m	5000 m	
Scenario II: Leaks from the mobile storage tank			
Leak hole diameter	**Thermal radiation threat zone**		
	10.0 kW/sq.	5.0 kW/sq	2.0 kW/sq
15 cm	12 m	16 m	25 m

	Flammable threat zone		
	60 % LEL	10% LEL	
15 cm	N.A	118 m	
Direct	N.A	110 m	

Table 3. Threat zones of hydrogen release computed in the ALOHA simulation at wind speed of 2 m/s

2 m/s wind speed			
Scenario I: Dispensing pipes at the HRS			
Leak hole diameter	**Thermal radiation threat zone**		
	10.0 kW/sq	5.0 kW/sq	2.0 kW/sq
15 cm	47 m	65 m	101 m
20 cm	66 m	92 m	143 m
30 cm	107 m	149 m	231 m
	Flammable threat zone		
	60 % LEL	10% LEL	
15 cm	5000 m	>10 km	
20 cm	8900 m	>10 km	
30 cm	> 10 km	> 10 km	
Scenario II: Leaks from the mobile storage tank			
Leak hole diameter	**Thermal radiation threat zone**		
	10.0 kW/sq.	5.0 kW/sq	2.0 kW/sq
15 cm	11 m	16 m	25 m
	Flammable threat zone		
	60 % LEL	10% LEL	
15 cm	N.A	118 m	
Direct	N.A	110 m	

For Scenario I, when comparative study was done by adopting HyRAM, it was found that ~30 – 40% larger values attained for thermal radiation in HyRAM as compared to that of ALOHA as tabulated in Table 3. However, the values obtained in HyRAM is smaller ~20% as compared to ALOHA when overpressure is determined by both models. It can be said that for thermal radiation in HyRAM, the harm level is a function of both the heat flux intensity and the duration of exposure [8,11–14]. Harm from radiant heat fluxes is often expressed in terms of a thermal dose unit (V) which combines the heat flux intensity and exposure time as V=I^(4/3)t where I is the radiant heat flux in W/m^2 and t is the exposure duration in seconds. HyRAM allows the user to decide between thermal probits [15] and this could contribute to higher values obtained for thermal radiation however, output from HyRAM give a good agreement with actual scenario as studied by Guo et al. [16].

For Scenario II, it can be said that the congested situation gave higher maximum distance of blast overpressure (0.55 bar) and 60% LEL flammable cloud i.e. 24 m and 97 m, respectively as seen in Fig. 4. It can be explained as; the multilevel parking and available cars can represent congestion and if engulfed by a vapour cloud, can lead to significant flame acceleration. The turbulent energy created by the congestion has a greater effect on explosiveness than does the total amount of leakage or premixed volume [17]. Hence the implication is that it is not necessary to release large quantities of hydrogen to obtain high overpressures on ignition. A release of relatively small quantities with rapid ignition may give a severe event.

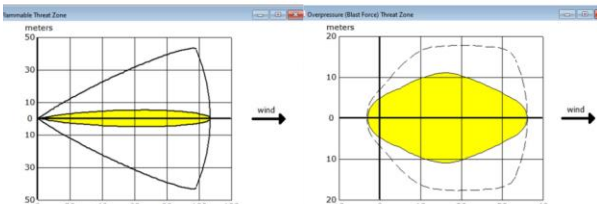

Fig. 4. Threat zones of hydrogen release from the vehicle storage leakage at total rupture for uncongested scenario

Comparison was made using HyRAM model to determine the corresponding thermal radiation heat and overpressure when dispersing from similar condition in Scenario II as illustrated in Fig. 5. From the figures, it implies that HyRAM underpredict the overpressure harm distance yet overpredict the thermal heat radiation harm distance as compared to values obtained from ALOHA. The simpler model used by HyRAM without considering the surrounding condition could contribute to the under and over predicted values. Theoretical correlation involving TNT and BTS should be used for future reference since HyRAM adopts TNT and BTS on the prediction calculation for overpressure.

3.2 Results on separation distances prediction for hydrogen refuelling station storages – Scenario III

Safety distances remain a subject on which different countries have not yet come to a consensus. The subject of safety distances is the object of the ISO draft standard 19880, which is in the process of being elaborated and which is projected to be finalised in the coming years. The standard will be certainly specific for Europe without consensus, which practically have different clearance standard as demonstrated in Table 5. Fig. 6 provides deterministic separation distances/harm distances based on one possible consequence of a hydrogen leakage event for Scenario III: the radiant heat flux from an ignited hydrogen jet on the effect of the leak diameter with operating pressure ranges between 200 to 1040 bar for 300 litres storage tank. The figure shows the separation distances required to limit the exposure of a person to a radiant heat flux of 1.6 kW/m which is generally accepted as a level that will not result in harm to an individual even for long exposures. It can be demonstrated that varying the leak size in the calculation shows that larger leaks produce longer threat distance for thermal radiation as predicted by all models i.e. HyRAM, PHAST and ALOHA. The harm distance calculated in the models gave underpredicted results at all pressures than those calculated by NFPA 55 of about ~11% for HyRAM values and up to almost 50% for PHAST results of thermal radiation of 1.6 kW/m^2 (except for ALOHA) and such differences are surely imputable to the parameters of the simulation code.

Table 4. Comparative study between ALOHA and HyRAM.

Leak hole diameter	**Thermal radiation threat zone**					
	10.0 kW/sq		5.0 kW/sq.		2.0 kW/sq.	
	ALOHA	HyRAM	ALOHA	HyRAM	ALOHA	HyRAM
15 cm	47 m	140 m	66 m	220 m	102 m	320 m
20 cm	67 m	198 m	93 m	300 m	144 m	430 m
30 cm	107 m	250 m	150 m	450 m	233 m	<550 m

Leak hole diameter	**Overpressure threat zone**					
	0.56 bar		0.24 bar		0.07 bar	
	ALOHA	HyRAM	ALOHA	HyRAM	ALOHA	HyRAM
15 cm	373 m	55 m	432 m	72 m	800 m	140 m
20 cm	535 m	70 m	610 m	98 m	1100 m	180 m
30 cm	875 m	110 m	1000 m	140 m	1900 m	260 m

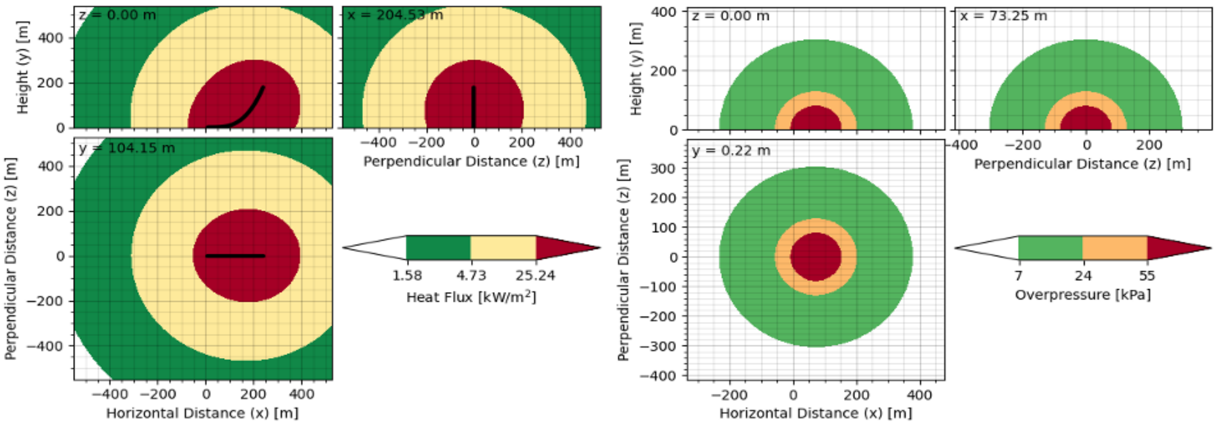

Fig. 5. HyRAM results for Scenario II.

Table 5. Clearance distance adopted by other countries (ISO)

			Canada	China	France	Germany	Italy	Japan	Korea	Sweden	UK	US NFPA2	US
CLEARANCE DISTANCES *The clearance distance is the minimum distance between the potentially hazardous installation /equipment and the vulnerable targets within the fueling station. Here, the hydrogen installation is regarded to be the source, while the surrounding people /objects are considered to be the targets.*	Personnel of the HRS (1st party)	m									-		
	Users of the HRS (clients, 2nd party)	m					10				-		
	Public (Third party)	m									8	4,6	2 (2h fire)
	Other fueling facilities within the fueling station, like delivery facilities.	m								12			
	Gasoline storage	m	3,1 to 7,6 (below ground)	3-8		3	10			25	8	4,6	
	LPG storage	m	7,6 to 15,2 (above ground)			8	20			25	8	4,6	
	CNG hazardous elements	m	7,6 to 15,2	5-12			15	6		12	5	4,6	
	Bulk liquid oxygen storage	m	7,5 to 15			5		10	10 (5 if firewall)	12	5		
	Between H2 dispensing and others fuels (LPG, CNG, gasoline)	m		4			8				-	4,6	
	Buildings inside the plant	m		5-15	8					12	-		
	Building of combustible material	m	15,2							12	8	4,6	5
	Building openings /windows / access doors	m	3,1 to 7,6							Same as for buildings in general	8	10,7	6

The figures also suggest that only leak diameter between 2-4 m gave a good agreement with clearance distance adopted by all countries as illustrated in Table 4. It should be noted that the calculation is solely based on the physic consequences model without consideration on the frequency leak model of the equipment failures since the available hydrogen data is not sufficient for the application of traditional statistical analysis [18]. For future work, it is recommended to adopt Bayesian model for data to combine this limited data with generic estimates of component leakage rates.

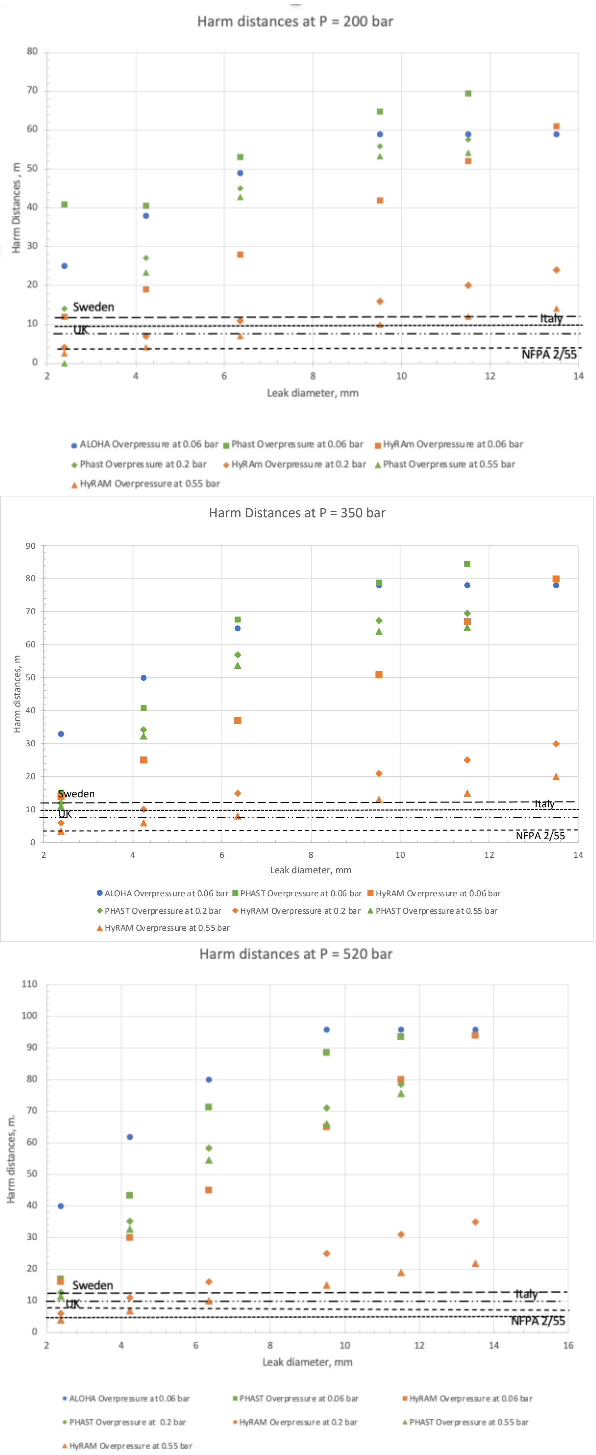

Fig. 6. Harm distances against leak diameter at different operating pressure.

4 Conclusion

The current study evaluates parameters affecting the hydrogen dispersion and ignition using integral models. Hydrogen appears to pose risks of the same order of magnitude as other fuels. From the findings from this paper, several conclusions could be drawn.

(1) It can be said that effect distances are based on the selection of hydrogen leak sizes, following the basis of NFPA 55 separation distance guide
(2) Due to the limitation of the data on frequency leaks of the equipment corresponding on hydrogen usage, Bayesian model approach is suggested to be adopted for comprehensive data collection with generic estimates of component leakage rates.
(3) The integral models adopted in this work shows slight discrepancies between values, however, they gave consistent results by varying the leak size in the calculation shows that larger leaks produce longer threat distance.

Thus, detail and comprehensive numerical simulation of leakage and diffusion in CFD also needs to be further optimized from the aspects of grid, turbulence model and reaction kinetics conditions, an accurate concentration prediction model and a leakage and diffusion model must be developed with the combined action of momentum and buoyancy. Synergy between micro (CFD) and macro (integral model) approach to establish universal mechanism to quantify both causes and consequences of hydrogen leaks for different high-pressure hydrogen storage.

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