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Safety investigation of hydrogen charging platform package with CFD simulation

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ABSTRACT

Hydrogen has been expected as one of the most promising green energy sources, especially in transportation section. Despite its great potential as a new source of energy, it is reluctant to build hydrogen charging stations for the fear of accidents such as hydrogen leakage, fire, and following explosion. To reduce those problems and promote the acceptance of hydrogen charging station, this study focuses on the hydrogen charging platform package (HCPP) which is a new type of the mobile hydrogen station. Hydrogen leakage cases are investigated using CFD (computational fluid dynamics) simulation. The simulation is performed with the whole configuration of the HCPP including main components, storage, compressor, and dispenser. Based on the risk assessment, hydrogen leak scenarios with high possibilities of accidents are simulated. The simulation results show the leak length of hydrogen gas, its dispersion, and the various ranges of volume ratios of leaked hydrogen gas. Based on the simulation results, it is clearly confirmed that the leaked hydrogen gas with high concentration stays inside the HCPP. Therefore, the effects of ventilation to reduce the possibility of the explosion are continuously considered to investigate the safety of the HCPP in the case of the leakage accident.

Introduction

Hydrogen has received a great attention for its high possibilities for the next generation green energy sources. It is the most abundant materials, accounting for almost over 75% of the mass fraction or 90% of the volume fraction of the whole existed materials on the universe. Even though the hydrogen is expected as a fine alternative source of energy with abundant quantities, safety concerns about using hydrogen are still prevalent. It is a highly flammable fuel with its own wide range (4–75% concentration by volume) of burn in the air. Therefore, it is needed to verify its safety first for use in various areas. In particular, hydrogen has been used occasionally as fuel for some fuel cell vehicle. With an increasing interest in reducing the carbon dioxide emissions exhausted from the vehicles, hydrogen fueled car emerges as a promising alternative. Numerous studies on hydrogen have been conducted from several countries for development of hydrogen industry. Especially, lots of experiments such as hydrogen leakage, ignition, fire and explosion have been actively carried out and the computational fluid analysis through the computer simulation has been also largely underway to analyze the several characteristics of hydrogen and prove the stability of hydrogen station. Many hydrogen stations have been built and operated on some countries.

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Nomenclature

$D_{i,m}$	mass diffusion coefficient
D_t	turbulent diffusivity
E	energy
G_k	generation of turbulence kinetic energy due to the mean velocity gradients
G_b	generation of turbulence kinetic energy due to the buoyancy
HCPP	hydrogen charging platform package
J_i	diffusion flux
$J_{T,i}$	thermal (Soret) diffusion coefficient
k_{eff}	effective thermal conductivity
LEL	lower explosive limit
$\dot{m}_{qp}$	mass transfer from phase q to phase p
$\dot{m}_{pq}$	mass transfer from phase p to phase q
M	molar mass
RVR	risk volume ratio
R_i	net rate of production
S_{α_q}	source term
S_i	rate of creation
Sc_t	turbulent Schmidt number
S_h	source term from radiation
T	temperature
UEL	upper explosive limit
VR	volume ratio
Y_i	local mass fraction
Y_M	contribution of the fluctuating dilatation in compressible turbulence
ϕ	diameter
α_q	face value of the q^{th} volume fraction
μ_t	turbulent viscosity
ρ	density
σ	average collision diameter
σ_k	turbulent Prandtl number for k
σ_ε	turbulent Prandtl number for ε
Ω	collision integral

Although their numbers are continuously increasing, there are a lot of difficulties in the construction and operation of the hydrogen station. The hydrogen station takes up a lot of space because it includes a production facility to produce hydrogen. An off-site hydrogen station which stores hydrogen in a tube tank and supplies when needed is in the spotlight. However, related research is not enough and the problem of site selection due to the large space occupation is not solved completely. As an alternative to solve the problems of the existing hydrogen station, the hydrogen charging platform package (HCPP) is proposed. It is a fine supply system for advantage of easy installation with a small volume occupation that its components are close together. Unlike the conventional hydrogen charging stations, the HCPP is completely an off-site charging station that consists of all components for supplying hydrogen in a single container, requiring only small area to be installed and used. Additionally, it has a good mobility that can be carried by a delivery truck with tube trailers. This type of hydrogen charging station is under study for commercialization as a part of the hydrogen industry development in many countries. Even though the HCPP is gradually regarded as capable of solving the problems of the conventional hydrogen station, there is still a lack of research for actual operation. Especially, there is great deal of concern about its safety due to the operation of high pressure gas. Studies of quantitative and qualitative risk assessments [1–6] based on the methods of FTA (Fault Tree Analysis), FMEA (Failure Mode and Effect Analysis) and HAZOP (Hazard and Operability Study) about the existing hydrogen charging station are checked preferentially to know the hydrogen incident and its cause. In addition, the papers analyzing the hydrogen accident using simulation software are examined. Schmidt et al. (1999) simulated the hydrogen leakage from the tanks and pipes according to the release rate, time, and amount to analyze the behavior of the hydrogen/air mixture clouds [7]. Houf and Schefer (2008) also performed the hydrogen leakage simulations to compute the trajectory of the buoyant jet and the hydrogen concentration [8]. Olvera and Choudhuri (2006) investigated the hydrogen buoyant characteristic by comparing the diffusion pattern of methane and hydrogen. It could be clear that hydrogen is very light and is dispersed rapidly into the air [9]. Schefer et al. (2008) modeled the turbulent jet flow of the hydrogen gas from the circular leak geometry to analyze the buoyant regime and its effect [10]. Kikukawa (2008) carried out the simulation of the hydrogen leakage toward the barrier, analyzing its effect through the leakage from various angles [11]. Middha and Hansen (2009) conducted the hydrogen leakage simulation from the hydrogen vehicle with various stored inventories [12]. Chernyavsky et al. (2011) selected the complex eddy simulation method to present the subsonic turbulent jet into the atmosphere [13]. Kim et al. (2013) simulated the hydrogen leakage and explosion, analyzing the safety distance from the incident using CFD software [14]. Swain et al. (2003) and He et al. (2016) compared the dispersion of hydrogen and helium gas, predicting the safety in an enclosure [15,16]. In addition to the studies about the risk assessments of the released gas, the studies on the accident of fire and explosion of the leaked gas by the ignition source [17–21] are reviewed for reference. From the literature review, it was found out that there are extremely limited safety studies on the mobile hydrogen charging station, the HCCP. Therefore, this paper presents the computational fluid analysis of the HCCP to discuss its safety in the event of hydrogen gas leakage incident, developing the CFD model and diagnosing the safety. The external leakage and internal leakage simulation are mainly conducted to analyze the leak length, dispersed length, and volume fraction of hydrogen gas in the air. Because hydrogen has a wide flammable range of 4–75% in air, it is important to analyze the volume of hydrogen in the hazardous range to prevent the risk of fire or explosion. Thus, the risk volume ratio of released hydrogen gas is mainly analyzed. As numerous studies emphasize the importance of the effect of ventilation [22–29] as a way to reduce the risk of increasing concentration of the leaked gas, the ventilation system is also considered to prove its effect to reduce the hydrogen concentration. Finally, calculating the diffusion coefficient of fuels, the comparison between hydrogen and other fuels is done for ensuring the safety of hydrogen.

Risk assessment

The preliminary investigations about the conventional charging station are conducted before developing the simulation model and interpreting the computational results. After identifying numerous papers related to the risk assessments and computational fluid analysis about the hydrogen charging station, the flow chart of main accident scenario that caused by the hydrogen leakage based on the information from risk assessments is decided and drawn in Fig. 1. Accidents that are possibly and frequently occurred in hydrogen station are usually caused by hydrogen leakage and gradually proceed to next stage.

The incident of hydrogen leakage can be started for various reasons. The causes of the accident by hydrogen gas leakage inside the platform package are listed in Table 1. Actual operating conditions for each process are listed along with frequent accident causes and ongoing safety plans. The arranged events are very similar to the accidents of existing hydrogen charging stations but more frequently occur in the compact and complicated charging systems like the HCPP.

Simulation model development

Geometry modeling

In the simulation models, two geometries each for external leakage and internal leakage are designed and described in Fig. 2. The HCPP with dispenser hose and tube trailer vessels surrounded by protective walls are laid out together for external leakage and the interior shapes of the HCPP are modeled with some main components of the hydrogen filling station including pressure vessels, compressor, and dispenser unit for the case of internal leakage. Those models are designed in the simple shape with computational domain 19 m(W) × 35 m(L) × 3 m(H) for external leakage and 2.4 m(W) × 6.1 m(L) × 2.6 m(H) for internal leakage. The specific dimensions of the components are shown in Fig. 2.

In the process of developing the HCPP model, technical specifications of the hydrogen charging station operated in actual are reviewed and the specification suitable for a small charging station such as HCPP is considered and listed in Table 2.

Numerical method

As a computational fluid analysis software, FLUENT, which can analyze the entire range of flow from subsonic (incompressible) to supersonic (compressible), even hypersonic, is used. In the CFD simulation, the four main calculation models, Species, Multiphase, Energy, Viscous [30,31] are adopted to solve the continuity, momentum, volume fraction, and turbulent flow equations respectively. Specifically, the method of Species Transport model accompanied with Volume of Fraction is used to depict the hydrogen leakage and dispersion with $k-\varepsilon$ turbulence model.

Species transport equation

To figure out the mass and volume fraction of the hydrogen molecules diffused in the atmosphere, a conservation equation for specific species is solved with the solution of a convection-diffusion equation. The conservation equation has the following form of Eqn. (1).

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla\cdot(\rho \vec{v} Y_i) = -\nabla\cdot\vec{j_i} + R_i + S_i \tag{1}$$

For species i from Eqn. (1), R is the net rate of production of species and S is the rate of creation by addition from the dispersed species. $\vec{J}$ is the diffusion flux which is changed its form depending on whether it is a laminar flow or turbulent flow. Hydrogen gas is dispersed into turbulent flows in our computational model, so the form of the diffusion flux is going to be Eqn. (2).

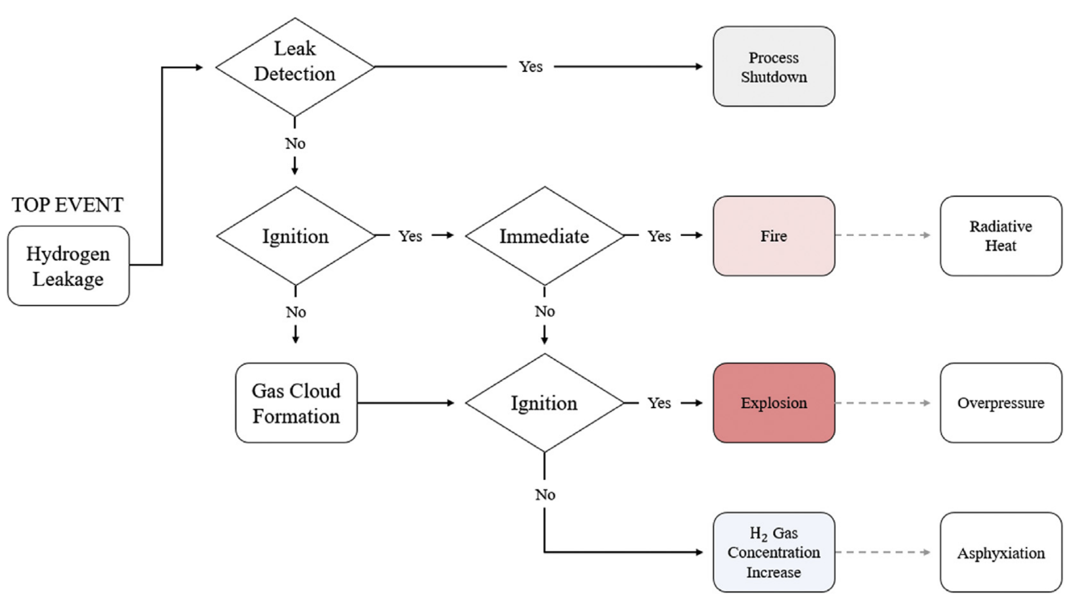

Fig. 1 – Flow chart of accident scenario by hydrogen leakage.

Table 1 – Causes of hydrogen leak accident.

Process facility	Operating pressure [MPa]	Operating temperature [°C]	Cause of accident	Safety plan
Compressor	20 ~ 85	20 ~ 85	- Valve-connection problem - Packing wear of components	- Hydrogen gas sensor - Fire sensor
Storage	15 ~ 85	20 ~ 85	- Leak in connection pipes - Wear in ball of control valve	- Emergency shutdown valve (ESV) - Process shutdown
Dispenser unit	35	−20 ~ −60	- Poor assembly of components - Direct leak via the dispenser hose due to malfunction	- Ventilation system - Periodic check
	70	−40 ~ −60	- Poor connection between the dispenser and vehicle	- Operation procedure education
Tube trailer	10 ~ 20	−60 ~ 25	- External impact	- Safety education

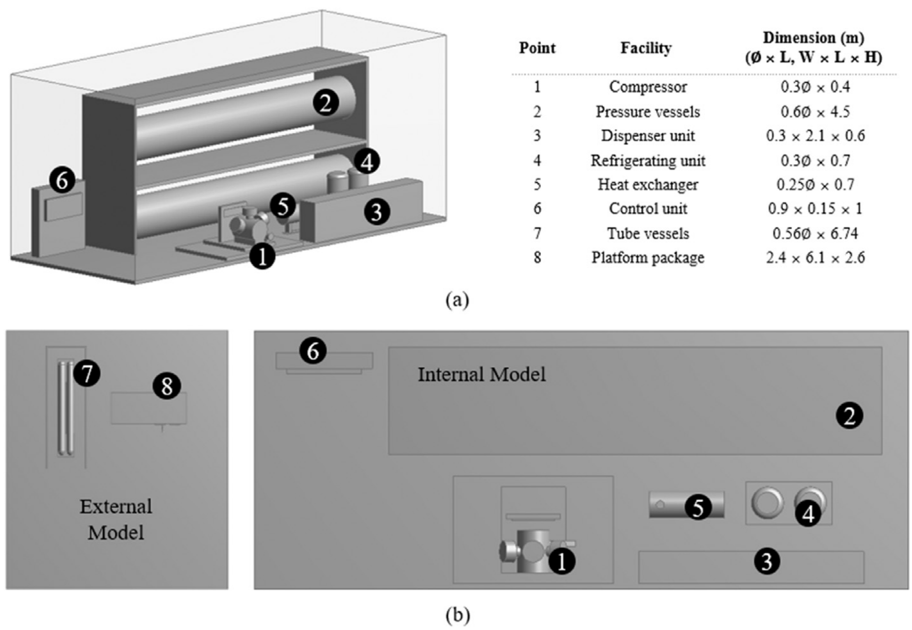

Fig. 2 – Overview of HCPP (a) and top views of CFD model (b).

Table 2 – Technical specification of hydrogen charging platform package.

Supply rate ($Nm^3 \cdot h^{-1}$)	100–200		
Vehicles charged per day	40–100		
Vehicle charging	Type	Filling pressure	Charging time
	Passenger car	35 MPa	3–5 min
	Bus	70 MPa	3–5 min
Main components	Equipment	Remark	Operating conditions
	Gas compressor	2 Stage diaphragm/Hydro-Booster	35–90 MPa/20–85 °C
	Pressure vessel	Protective vessel	–
	Storage vessel	Type 4250 L × 3 = Total 30 Kg	20–90 MPa/20–85 °C
	Dispenser unit	Single or dual	35, 70 MPa/-60 ~ −20 °C
	Dispenser hose	30 mm diameter nozzle	–
	Refrigeration unit	Gas cooler	−60 ~ −20 °C
	Heat exchanger	Shell and tube HX	–
	Control unit	Operation control	–
	Tube trailer	Temporary storage	20 MPa

$$\vec{j_i} = -\left(\rho D_{i,m} + \frac{\mu_t}{Sc_t}\right)\nabla Y_i - D_{T,i}\frac{\nabla T}{T} \tag{2}$$

In above equation presenting mass diffusion, μ_t, D_t and Sc_t are turbulent viscosity, turbulent diffusivity, and turbulent Schmidt number respectively.

Multiphase model

Multiphase model is employed to search the volume fraction of hydrogen gas from that of the air. The method of Volume of Fluid (VOF) is used to realize two phases of materials. Air is selected as the first phase and hydrogen is selected as the second phase in the model. The volume fraction of two gas is determined by solving a momentum equation for the domain of calculation model. For the qth phase, the equation is represented as Eqn. (3).

$$\frac{1}{\rho_q}\left[\frac{\partial}{\partial t}\left(\alpha_q\rho_q\right) + \nabla\cdot\left(\alpha_q\rho_q\vec{v}_q\right) = S_{\alpha_q} + \sum_{p=1}^{n}\left(\dot{m}_{pq} - \dot{m}_{qp}\right)\right] \tag{3}$$

where $\dot{m}_{pq}$ is the mass transfer between phase q and phase p. With the assumption of the value of zero for the source terms in above governing equation, the primary-phase volume fraction is solved with the following constraint of Eqn. (4).

$$\sum_{q=1}^{n}\alpha_q = 1 \tag{4}$$

Volume fraction equation in this study is solved with an implicit scheme for transient calculation.

Energy equation

To predict the hydrogen gas temperature, mass, and velocity, energy equation along with continuity and momentum equations, FLUENT computes the energy equation related VOF model with the following form of Eqn. (5).

$$\frac{\partial}{\partial t}(\rho E) + \nabla\cdot\left(\vec{v}(\rho E + \rho)\right) = \nabla\cdot\left(K_{eff}\nabla T\right) + S_h \tag{5}$$

From the energy equation, K_{eff} is the effective thermal conductivity shared by the hydrogen and the air. Additionally, in the VOF model energy is treated as Eqn. (6).

$$E = \frac{\sum_{q=1}^{n}\alpha_q\rho_q E_q}{\sum_{q=1}^{n}\alpha_q\rho_q} \tag{6}$$

Turbulence model

The leakage process of hydrogen is progressed as a transient model. In this study, the realizable $k-\varepsilon$ turbulence model is employed to simulate the gas diffusion. $k-\varepsilon$ turbulence model is the most commonly used turbulence model to simulate turbulent flow conditions in computational fluid dynamics (CFD). Realizable $k-\varepsilon$ turbulence model is a more improved equation to describe more complicated flow than the standard $k-\varepsilon$ turbulence model. It is composed of two transport equations each for turbulent viscosity k and for the dissipation rate ε. The transport equations are described as Eqn. (7) and Eqn. (8).

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho c u_j) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + P_k + P_b - \rho\varepsilon - Y_M + S_k \tag{7}$$

and

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_j}(\rho\varepsilon u_j) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu}{\sigma_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right] + \rho C_1 S_\varepsilon - \rho C_2\frac{\varepsilon^2}{k + \sqrt{\upsilon\varepsilon}} + C_{1_\varepsilon}\frac{\varepsilon}{k}C_{3_\varepsilon}P_b + S_\varepsilon \tag{8}$$

where $C_1 = max\left[0.43, \frac{\eta}{\eta+5}\right]$, $\eta = S\frac{k}{\varepsilon}$, $S = \sqrt{2S_{ij}S_{ij}}$

P_k, P_b in Eqn. (7) each represents the generation of turbulence kinetic energy due to the mean velocity gradients and due to the buoyancy.

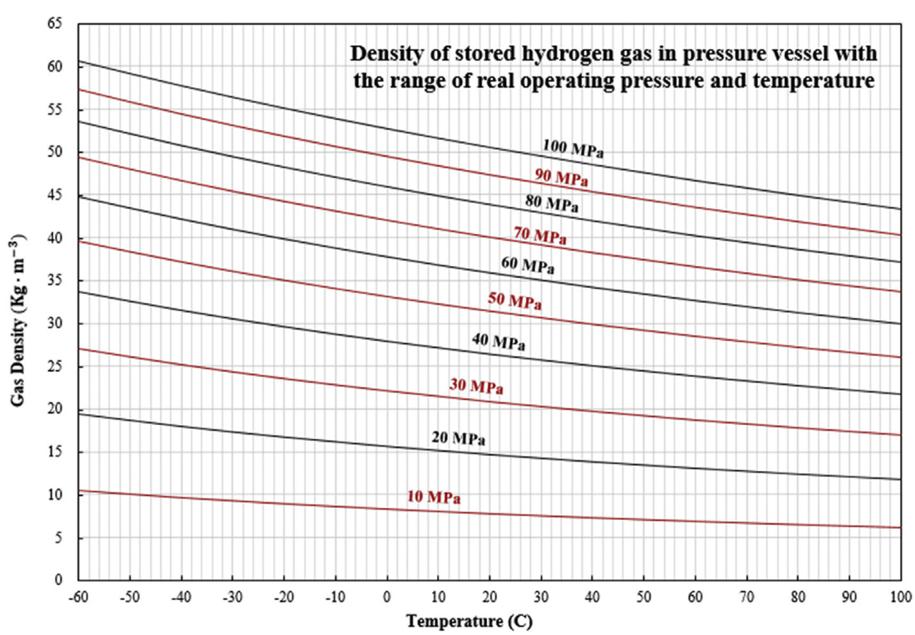

Fig. 3 – Stored hydrogen gas density.

Thermal property of hydrogen

The density of the gas is generally dependent on the operating pressure and temperature. Hydrogen gas, which is compressed through the compressor, is stored in a pressure vessel at various pressure stages. The stored hydrogen gas densities at various stage of pressure and temperature are shown in Fig. 3. The graph below is produced using software HyRAM (Hydrogen risk assessment model) [32] developed by Sandia National Laboratories in the United States. The density values are compared referring to the chart of the ILK Dresden [33], the research institute in Germany. As a result of the comparison, it is clear that there is no significant difference and the boundary conditions of software model are calculated with reference to Fig. 3.

Model validation

The validation model is designed with one leakage hole, 2 walls, and atmosphere region. The side view of the validation model with mesh generated is shown in Fig. 4. The method of Multizone is used to generate the mesh to be hexa dominant in mesh software. The dense meshes are generated around the leak hole and gradually becomes less dense. To prove that our calculation model is valid, comparisons of our simulation result with others are done. The validation data refer to the papers [34,35], and compare with experimental data and CFD model data simulated previously. Those data are listed in Table 3. As also mentioned in previous papers [35], there is still an instability of hydrogen concentration value for the reason of strong buoyancy characteristic of hydrogen gas. The higher the altitude, the higher the instability of hydrogen concentration value is. This instability is considered to have been applied at point 6, which is located at the highest point of validation model. Except for point 6, the values of the remaining five points are within 10% of the average values obtained from the existing experimental and computational fluid analysis. The contour of leaked hydrogen is also described in Fig. 4 with the range of concentration between 0 and 10% in the atmosphere. The error graph analyzing the hydrogen concentration at specific points is also shown in Fig. 5.

Simulation matrix

To run the numerous gas leakage cases, the simulation matrix is created by analyzing the causes of the accident through the risk assessment and development of the CFD model. Various simulation cases to be analyzed in next chapter are summarized in Table 4. The actual operating conditions are listed with accident location. Various cases with different leak hole diameters are progressed and the presence or absence of the vent hole is indicated together in each simulation.

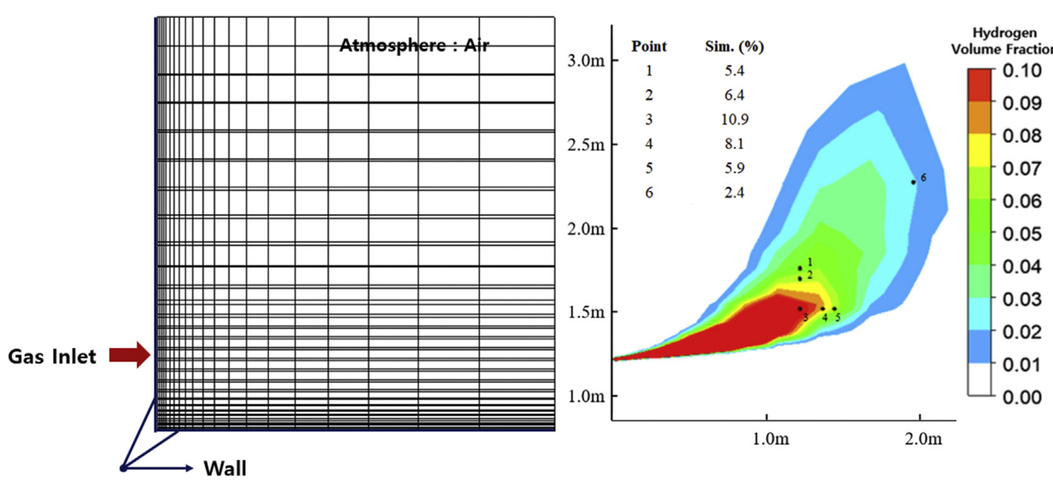

Fig. 4 – Mesh figure for validation model (left) and contour of leaked hydrogen for 45s (right).

Table 3 – Validation of leakage model.

Point	Experimental data hydrogen (%)	Ref [22] CFD model 45s hydrogen (%)	Ref [23] CFD model 45s hydrogen (%)	Simulation 45s hydrogen (%)	Ref [22] CFD Model 60s hydrogen (%)	Simulation 60s hydrogen (%)
Point 1	5.0 ~ 5.9	6	5.9	5.4	5.6	5.4
Point 2	5.6 ~ 7.0	7.2	6.8	6.4	6.8	6.3
Point 3	9.4 ~ 10.8	10.4	9.3	10.9	10.2	10.7
Point 4	8.1 ~ 9.4	7.8	7.1	8.1	7.7	7.7
Point 5	5.6 ~ 6.6	5.6	5.5	5.9	5.5	5.6
Point 6	3.5 ~ 4.6	3.7	4.2	2.4	4.3	2.4

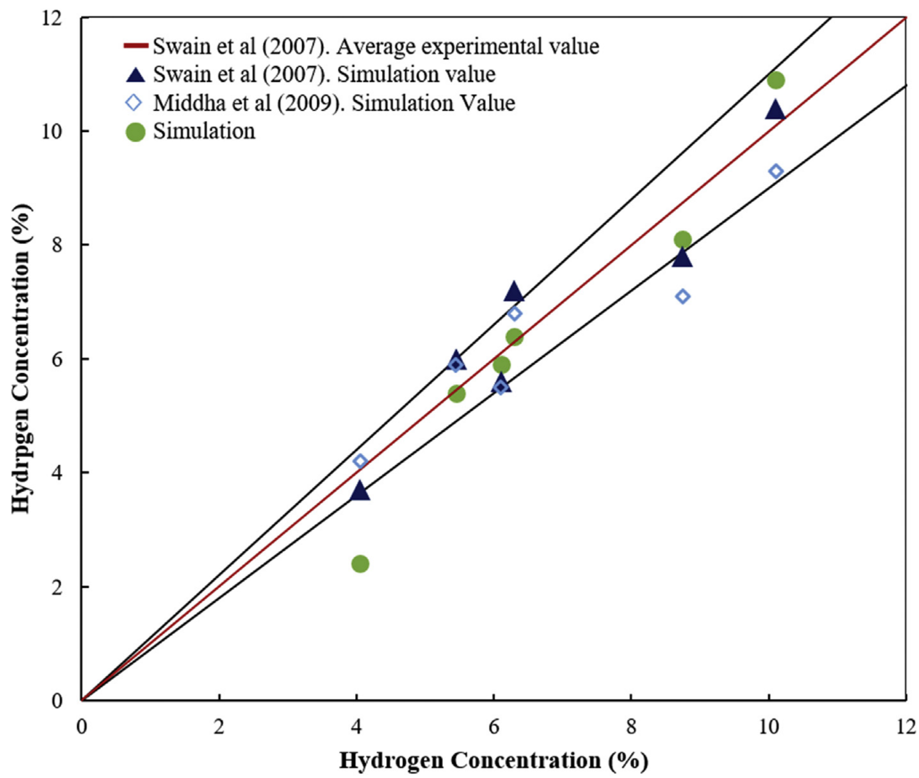

Fig. 5 – Comparison with other experimental and simulation data.

Table 4 – Simulation matrix.

Leak type	Accident location	Pressure [MPa]	Temperature [°C]	Leak hole diameter [mm]	Ventilation
External Leakage	Dispenser Hose	1, 5, 10 to 70 with 10 increment	−40	30 (Nozzle Diameter)	X
Internal Leakage	Compressor	50	50	2, 3, 5, 10, 20, 50	X
	Compressor	50	50	2, 3, 5, 10, 20, 50	X
	Pressure Vessel	90	85	2, 3, 5, 10, 20, 50	X
	Pressure Vessel	90	85	10, 20, 50	O
	Dispenser Unit	70	−40	10, 20, 50	O
	Dispenser Unit	70	−40	10, 20, 50	O

Simulation results

External leakage

In the case of external leakage, the accident scenario is that the hydrogen gas leaks at a very high velocity due to malfunction of the dispensing hose during the charging process. The hydrogen gas leakage through the dispenser hose directly under the operating temperature −40C is simulated. From the nozzle size of 30 mm diameter, the hydrogen gas is released rapidly into the atmosphere. Pressure ranges which can be operated during the filling process in the HCPP dispenser are divided and simulated in turn. Even though the hydrogen leaks are subsonic flow due to high sound speed, the actual leak velocity from the high pressurized vessel is extremely fast. Under the assumption that the shutoff-valve is operated in 10 s after the hydrogen gas leak, the leak length for the continuous gas leak during 10 s and dispersed distance of the leaked gas for 10 s after the leak are analyzed and listed in Table 5. It is identified clearly that the leak length and the dispersed distance are gradually increased with the augmentation of the operating pressure.

Table 5 – External gas leak for 10 s from dispenser hose nozzle.

Pressure [MPa]	Leak velocity [$m \cdot s^{-1}$]	Leak Length [m]	Dispersed Distance after 10 s [m]
1	13	0.84	0.84
5	65	1.44	1.44
10	126	3.95	3.95
20	241	7.23	9.94
30	346	7.25	12.95
40	442	9.71	13.94
50	530	9.78	15.70
60	612	10.25	16.56
70	689	10.79	17.38

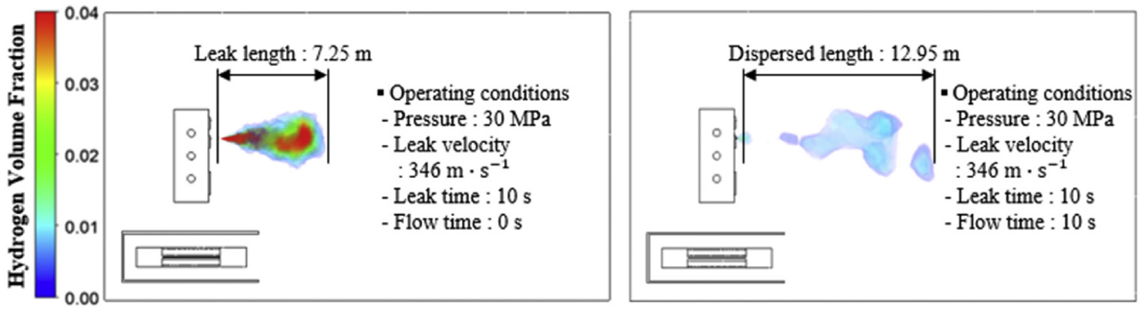

Fig. 6 – Leak length (left) and dispersed distance 10 s (right) after the leak at 30 MPa pressure.

The simulation results post-processed by CFD-POST are represented in Fig. 6. The leak length in the case of 30 MPa operating pressure is shown at the first left picture. The hydrogen gas contour being diffused for 5 s and 10 s after the leak stopped by the operation of shutoff-valve are continuously shown respectively in the remaining images. The increasing tendency of leak length and dispersed distance referring to Table 5 is shown in Fig. 7. CFD simulation results are specifically analyzed like that the leak length tends to increase gradually up to a pressure of 20 MPa, but there is no significant change at the high pressure above 20 MPa.

From Figs. 6 and 8, the simulation results are showed that it is difficult to reach the lower limit of 4% for being burned and also hard to form a vapor cloud in the air as the leaked hydrogen gas are spread in a short time. Consequently, it can be seen that the external leakage is much safer than the internal leakage mentioned below. Hydrogen has a property of being rapidly diffused when leaking into the atmosphere because of lower density than the air. The leaked hydrogen gas is dispersed very quickly into the atmosphere, so the height of computational domain is limited to 3 m under the assumption that there is no ignition source above its height. All results of external leakage are analyzed under this same condition.

Internal leakage

As mentioned above, the external leakage has a low possibility of explosion because it is hard to reach the lower explosive limit (LEL), 4%, in the air as time goes. Before verifying the safety of hydrogen leakage in earnest, leakage simulation without the ventilation system except the door is conducted preferentially to understand the spreading behavior of the leaked hydrogen gas and the hazard is evaluated. In this paper, the whole volume of the leaked gas per volume of station, which is 34.5 m^2 for our HCPP model, is regarded as 'Volume Ratio (VR)' and showed as Eqn (9).

$$\text{Volume Ratio} = \frac{\textit{Volume of leaked hydrogen gas}(m^3)}{\textit{Inside volume of hydrogen station}(m^3)} \tag{9}$$

and then the volume of hydrogen gas included in the flammable range (4–75% in air) per volume of the station is also defined as 'Risk Volume Ratio (RVR)' and treated as Eqn (10).

$$\text{Risk Volume Ratio} = \frac{\textit{Volume of leaked hydrogen gas within the range of flammable}(m^3)}{\textit{Inside volume of hydrogen station}(m^3)} \tag{10}$$

VR is used to analyze the trend of the total gas ratio accumulated in the ceiling due to the buoyant diffusion of leaked hydrogen. RVR represents the ratio of dangerous gas, which actually contains the risk of fire and explosion. Both two terms are defined to analyze the simulation results, but RVR, which represents the dangerous gas ratio that can lead to fire and explosion accidents by ignition, is mainly used for the analysis of the effect of the ventilation system used to ensure the safety of the hydrogen station. Thus, the change of RVR per time according to the ventilation system is figured out. The change of VR and RVR per time are shown similar for all leakage cases and this trend is shown clearly in Fig. 9. The leakage diameters are classified into 2, 3, 5, 10, 20, and 50 mm, selected based on the actual leakage cases. The 50 mm is selected for analysis under extreme situations.

Leakage simulation without ventilation system

Gas leaks are started from the compressor, pressure vessel, and dispenser unit, the principal components of hydrogen station. Assuming that the safety valve is normally operated as in the case of external leakage, the total leak time is equal to 10 s, and each leak velocity is determined on the operating conditions of each device. The specific information is shown in Fig. 9 along with the graphs of the risk analysis. It is the group of graphs expressing the RVR and VR analysis according to leak hole size. The results of the analysis of the leak from the compressor are shown in the top graphs (Fig. 9a), the pressure vessel in the center (Fig. 9b), and the lower part in the dispenser unit in the bottom (Fig. 9c). The same tendency that the RVR and VR increase as the leak diameter size increases are displayed for all three cases. However, in the case of 50 mm, the RVR becomes lower than the 10 mm as time goes. This is due to the considerable amount of leaked hydrogen gas from the large hole, resulting in a rapid accumulation of

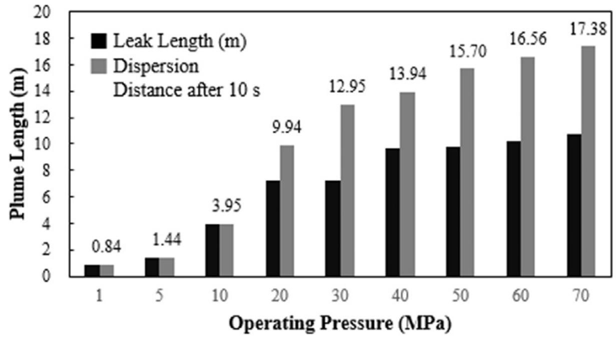

Fig. 7 – Leak distance according to pressure.

hydrogen gas in the HCPP ceiling. The concentration of hydrogen gas is increased sharply by the fast accumulation, exceeding the flammable range of 4–75%, reducing the RVR. This result is similar to the VR analysis. The VR increases gradually as the leak diameter increases, but the volume of hydrogen gas in the case of 50 mm could be rather reduced due to the rapid aggregation. This tendency is found in the results of leakage cases of the pressure vessel and the dispenser unit excluding the compressor.

Ventilation effect

In order to lower the volume of leaked hydrogen gas, the ventilation system shall be fully installed. The ventilation system is generally divided into two categories, natural methods such as windows, doors, ceiling ducts. and mechanical methods such as fans or blowers. In this paper, the effect with natural ventilation system of circular holes with the diameter of 0.5 m designed on the ceiling is considered by analyzing the risk volume ratio of leaked hydrogen gas. The ventilation effect when the hydrogen gas is leaked from the compressor with the variation of leak hole size volume is described in Fig. 10.

For all cases, the ventilation effect is confirmed clearly. For the leak diameter size of 10 mm and 20 mm, the effect of the ventilation system is very apparent, and furthermore, almost all of risk volume of released hydrogen gas disappears within 60 s. However, for the extreme case of 50 mm leak hole diameter, the ventilation effect seems not to be sufficient enough that the rate of RVR reduction becomes significantly lower after 60 s of the gas leakage. This effects are also shown when the gas is leaked from the other components, pressure vessel and dispenser unit, describing in Figs. 11 and 12 respectively.

The effect is shown to be the lowest for the case of gas leakage from the pressure vessel with the fastest leak velocity. It is dependent on the leakage position and the various peripheral shapes in addition to the leakage rate. The relatively small amount of the hydrogen gas leakage from 10 mm to 20 mm small leak hole diameter are diffused rapidly via the vent holes over time, lowering the risk of explosion. However, for the extreme case of 50 mm leak hole diameter, the ambiguous phenomenon is occurred which concentration of leaked gas remains between the lower explosive limit (LEL) and the upper explosive limit (UEL) as it is accumulated and is not sufficiently ventilated. Therefore, the additional safeguard, such as process shutdown, is needed to be considered for the case of extreme circumstances.

Discussion

The diffusion coefficients for some gaseous fuels are calculated to confirm that the hydrogen gas is much safer than the other fuel gases when leaked to the atmosphere. The various fuels used in the transportation sector are shown in Table 6. The gaseous fuels, including hydrogen and natural gas, along with their formulas and the remaining four liquid fuels are listed. Additionally, the representative properties of each fuel are represented in each row. Diffusing rapidly into the atmosphere for low density, hydrogen is very difficult to accumulate in the open space and similarly hard to reach the LEL. Comparing the LEL, hydrogen has the highest value which means more gas is needed than other gases to be ignited. The auto-ignition temperature of hydrogen is also higher than other fuels and it is very unlikely to be self-ignited when

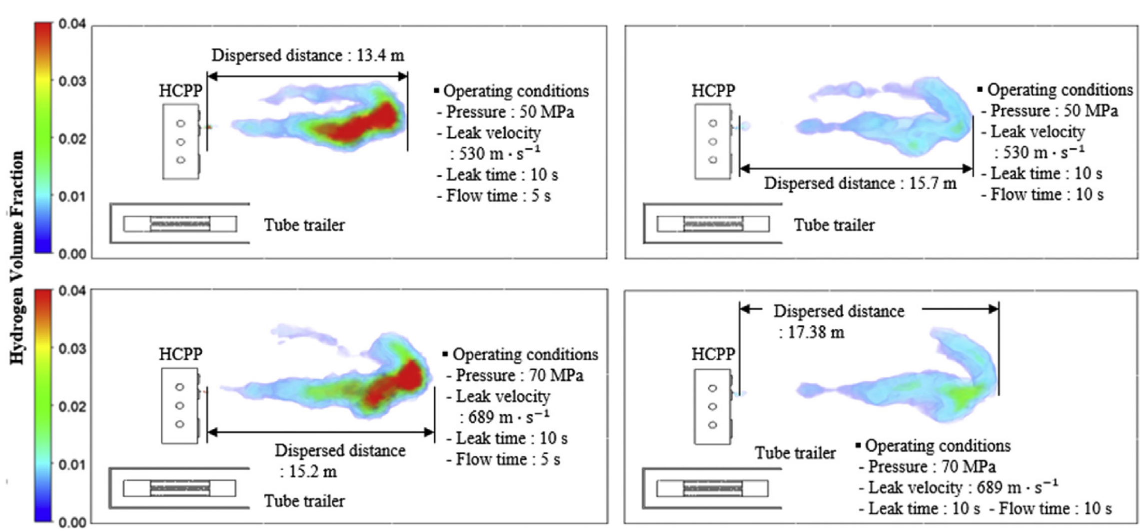

Fig. 8 – Dispersed distance after 5 s (left) and 10 s (right) after the leak at 50 MPa and 70 MPa pressure.

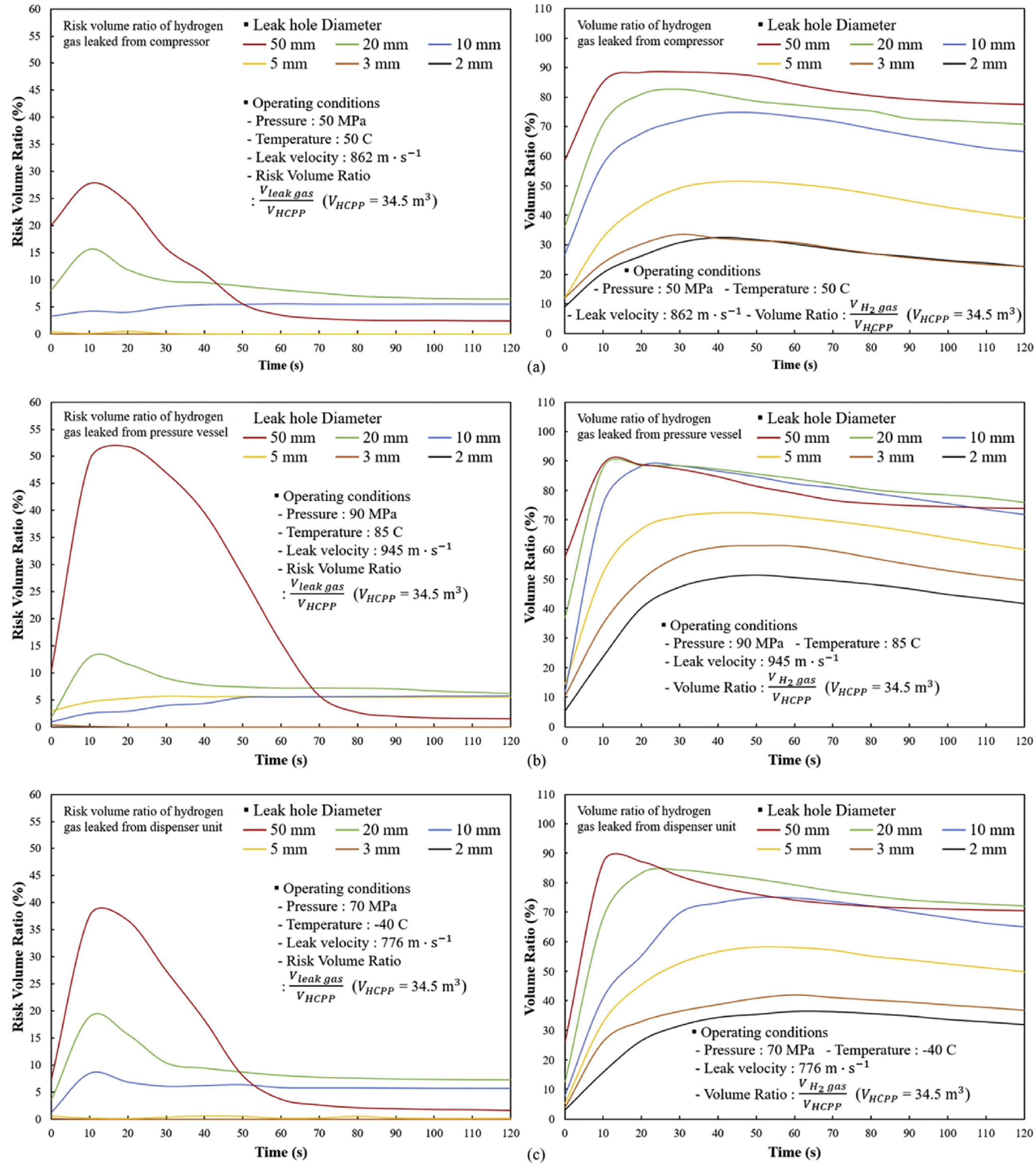

Fig. 9 – Risk volume ratio and volume ratio over time.

released to the atmosphere or even during high pressure processes.

In order to compare the degree of diffusion of gaseous fuels in the atmosphere, Chapman-Enskog theory [36–38] to calculate the diffusion coefficient D ($cm^2 \cdot s^{-1}$) for a gaseous mixture is used, resulting in the following equation:

$$D = \frac{(1.858 \times 10^{-3}) \cdot T^{3/2} \cdot \sqrt{1/M_{air} + 1/M_{fuel}}}{P \cdot \sigma^2 \cdot \Omega} \tag{11}$$

where T and P are the ambient temperature (K) and pressure (atm), M is the molar mass ($g \cdot mol^{-1}$), σ is the average collision diameter (Å) of a gas mixture, lastly Ω is the collision integral.

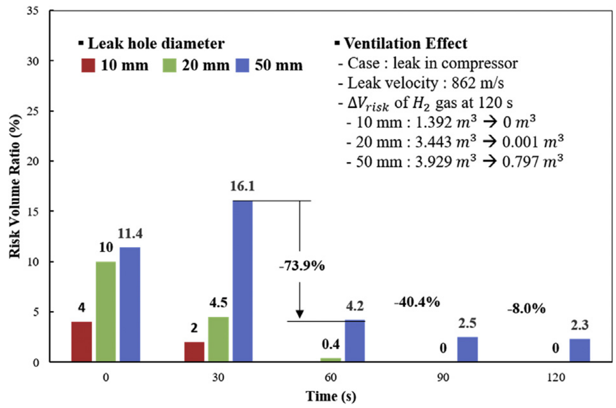

Fig. 10 – Ventilation effect in the case of leakage from the compressor.

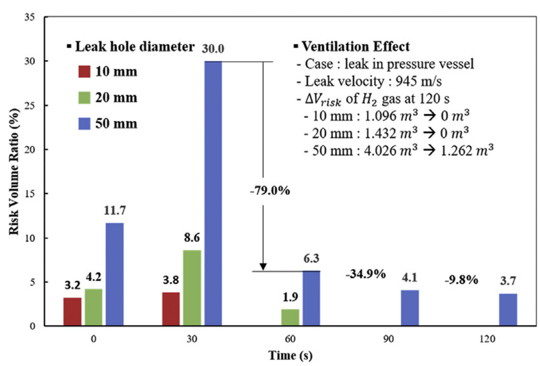

Fig. 11 – Ventilation effect in the case of leakage from the pressure vessel.

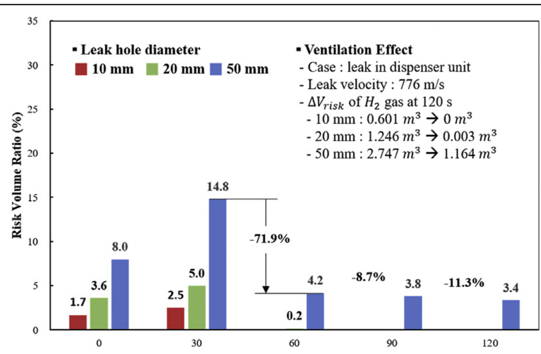

Fig. 12 – Ventilation effect in the case of leakage from the dispenser unit.

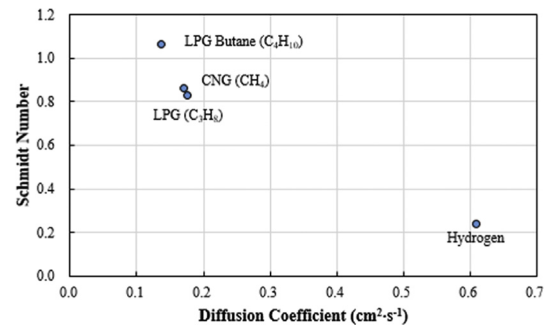

Fig. 13 – Gaseous fuel comparison.

With calculated diffusion coefficient, the Schmidt number defined as the ratio of momentum diffusivity and mass diffusivity is analyzed for some fuels which are mostly used for the transportation. Liquid fuels such as gasoline, diesel, and kerosene are excluded from the comparison because they are generally slower to diffuse into the atmosphere than gas fuels. Comparisons are made only for representative fuels used mostly in the industry. As a result of the comparison, it can be seen that hydrogen with low Schmidt number has a higher diffusion capacity in the atmosphere compared to the other gaseous fuels, and these results are shown in Fig. 13. Through this comparison, hydrogen gas is seemed less dangerous than other gaseous fuels and also could be showed its potential as an alternative energy by reducing the safety concern.

Conclusions

In this study, CFD simulation of hydrogen leakage has been mainly performed for safety diagnosis of the new mobile hydrogen station, HCPP. First of all, the causes of accident related to the hydrogen leakage are analyzed. Then, the CFD model is developed and validated with experimental data. The simulations are largely divided into external and internal leakage cases. The leak length and diffusion distance according to the operating pressure are analyzed for the external leakage, and this will be used as a reference for installation of the protective wall or safety distance. In the case of internal leakage, the volume ratio and the risk volume ratio according to the leak hole diameter are analyzed. In addition, the ventilation effects are analyzed for the cases of leakage from

Table 6 – Comparison of fuels mainly used in transportation.

Fuel	Chemical formula	LEL [%]	Auto ignition temperature [°C]	Density [$g \cdot L^{-1}$]	Diffusion coefficient [$cm^2 \cdot s^{-1}$]	Schmidt number
Hydrogen	H_2	4.0	500–571	0.08	0.61	0.24
LPG (Propane)	C_3H_8	2.1	480	1.91	0.18	0.83
CNG (Methane)	CH_4	5.0	580	0.67	0.17	0.86
LPG (Butane)	C_4H_{10}	1.6	240–500	2.46	0.14	1.06
Gasoline	C_8H_{18} (l)	1.4	246–280	720	–	–
Diesel	$C_{10}H_{22}$ (l)	0.6	210	730	–	–
Kerosene	$C_{12}H_{23}$ (l)	0.6	210	780	–	–
Heavy oil	$C_{19}H_{30}$ (l)	0.7	210–262	960	–	–

the compressor, pressure vessel, and dispenser unit by installing the vent holes above the ceiling for CFD models with leak hole diameter of 10 mm, 20 mm, and 50 mm. The remarkable contents are summarized as follows:

- Validation of the CFD model for hydrogen gas leakage is conducted. The hydrogen gas concentration is compared with experimental data and other CFD data. The errors for the concentration are within 10% except for one point which value is fluctuated due to strong buoyant characteristics of hydrogen.
- External leakage simulation is performed and the leak length and its dispersion distance over time are analyzed. Both values are increased as operating pressure are increased. However, it could be considered to be relatively safe compared to internal leakage because it is difficult to reach the risk concentration beyond 4%.
- Volume ratio and risk volume ratio are analyzed for internal leakage simulation. The simulations are operated depending on whether the presence of ventilation system. Specifically, the simulations with ventilation system are done for CFD models with 10 mm, 20 mm and 50 mm leak hole diameter. In general cases of 10 mm and 20 mm, most risk volume of hydrogen gas is disappeared within 60 s. However, the ventilation effect to reduce the risk volume could not be seen sufficient in extreme case of 50 mm leak diameter.
- Fuels according to the diffusion coefficient and Schmidt number are compared. As a result of comparing two values, it can be seen that hydrogen gas is relatively safe as compared with other gaseous fuels when leaking into the atmosphere.

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