A NUMERICAL SIMULATION OF HYDROGEN DIFFUSION FOR THE HYDROGEN LEAKAGE FROM A FUEL CELL VEHICLE IN AN UNDERGROUND PARKING GARAGE

Choi, J.[1], Kang, S.[1], Hur, N.[1*], Lee, E.D.[2], Lee, K.B.[2]
[1] Department of Mechanical Engineering, Sogang University, Seoul, 121-742, Korea
[2] Department of Advanced Vehicle Safety Research, KATRI, Hwaseong-si, 445-871, Korea
***nhur@sogang.ac.kr**

ABSTRACT

In the present study, the diffusion process of hydrogen leaking from a FCV (Fuel Cell Vehicle) in an underground parking garage is analyzed by numerical simulations in order to assess the risk of a leakage accident. The temporal and spatial evolution of the hydrogen concentration as well as the flammable region in the parking garage was predicted numerically. The effects of the leakage flow rate and an additional ventilation fan were investigated to evaluate the ventilation performance to relieve the accumulation of the hydrogen gas. The volume of the flammable region shows a non-linear growth in time and rapidly increases eventually. The present numerical analysis can provide a physical insight and quantitative data for safety of various hydrogen applications.

1. INTRODUCTION

Recently, there has been a lot of interest in using hydrogen fuel for automobiles such as a fuel cell vehicle (FCV). This is due to several advantages of hydrogen such as its regenerative feature, no production of carbon dioxide, and possible increase of the thermodynamic efficiency. Meanwhile, there have been many concerns on the safety of hydrogen as an automotive fuel. Hydrogen is a light gas with a relatively large flammable region and a fast flame speed [1]. Hydrogen has a flammable range of 4~74% and a detonation range of 18~59% in the volume fraction. These imply that a hydrogen explosion accident can incur more serious medical and economic loss compared to conventional fuels. These features raise several safety issues in production, transportation and storage of the hydrogen gas.

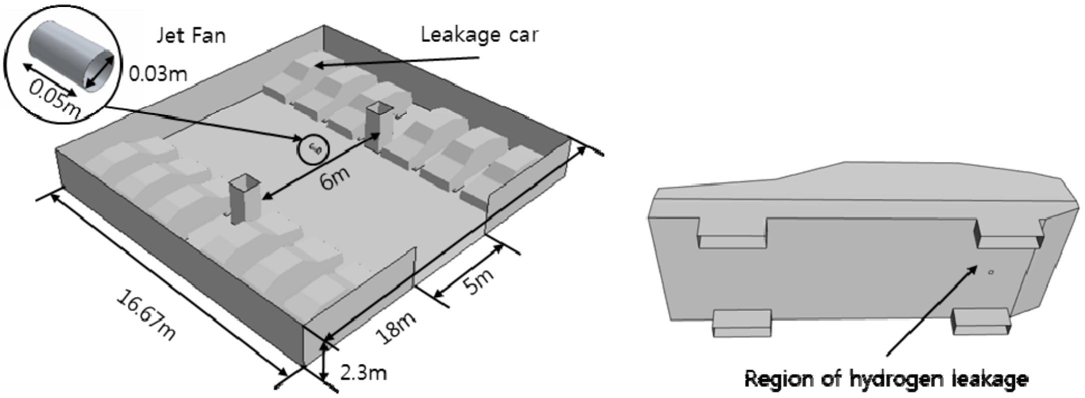
Thus, it is very important to assess the safety of hydrogen fuel for automobiles in various situations. One of the most dangerous situations is a leakage of hydrogen from a FCV in an underground parking garage. Theoretically, it is straightforward to do an experiment of a hydrogen leakage accident and measure the diffusion characteristics. However, an experiment of hydrogen leakage has a high risk in safety because of the possibility of hydrogen explosion. In order to avoid the high risk of a hydrogen experiment, a numerical simulation has become a very important tool as an alternative. A simulation using computational fluid dynamics (CFD) techniques can provide detailed data such as the concentration of hydrogen, the flammable region, the diffusion characteristics, etc.

In the literature, there are several previous studies on hydrogen leakage phenomena [2-6]. Takeno et al. [7] performed an experimental study on hydrogen diffusion in case of leakage from a pressurized vessel. Liu et al. [8] proposed a numerical model for the diffusion process of hydrogen which produced results consistent with the data of Takeno et al. Vudumu & Koylu [9] did a numerical study of the mixing process of hydrogen from a modeled accident and assessed the flammability. They performed simulations for different geometries such as closed, partially closed and open areas and predicted the change of the flammable regions in time. Mukai et al. [10] investigated the diffusion phenomena of hydrogen from a FCV inside a tunnel, underground parking garage. For each case, they investigated the diffusion characteristics and the safety risk. Although several studies have been done for hydrogen leakage, most of studies have focused on the diffusion characteristics of hydrogen, and there are only few studies that focused on the temporal change of the flammable region in a closed area such as an underground parking garage. The change of the flammable region can be affected significantly by the flow rate of hydrogen. Besides, there are only few studies which performed a quantitative analysis of the change of the flammable region by a ventilation fan.

In the present study, we investigated the diffusion phenomena of hydrogen for a model parking garage that meets the official Korean regulations. The objectives are to make a quantitative analysis based on detailed simulations of hydrogen diffusion and to evaluate safety for a few situations of hydrogen leakage in a parking garage. We performed a parametric study by changing the flow rate of hydrogen leaking from a model vehicle and analysed the diffusion phenomena based on the temporal change of the flammable region. We also investigated the effect of ventilation fans with different discharge rates on the change of the flammable region.

2. DESCRIPTION OF PROBLEM AND CASES

In the present study, we considered an underground parking garage and used a model that satisfies the official Korean regulations. Fig. 1 shows the configuration and dimension of our model. It is assumed that the parking garage has 12 slots and hydrogen leaks from a FCV parked at one of the corners away from the entrance. The location of the FCV with leakage is selected for the most dangerous situation in the given condition. The size of a slot is chosen as the smallest one allowed by the law based on the assumption that a smaller parking garage tends to be more dangerous than a larger one for a given hydrogen leakage rate. The width of each slot is 2.3m. As shown in Fig. 1 (b), a FCV is modelled as a typical shape of a car and hydrogen is assumed to leak from a pipe near the hydrogen tank in the rear. The leakage area is assumed as a square of 5cm in length and the leakage velocity is set to satisfy the assumed volume flow rate of leaking hydrogen. The atmospheric pressure is assumed at the entrance



(a) The model parking garage and cars with hydrogen leakage (b) Position of hydrogen leakage

Figure 1. Geometry of underground parking garage and position of hydrogen leakage for numerical simulations.

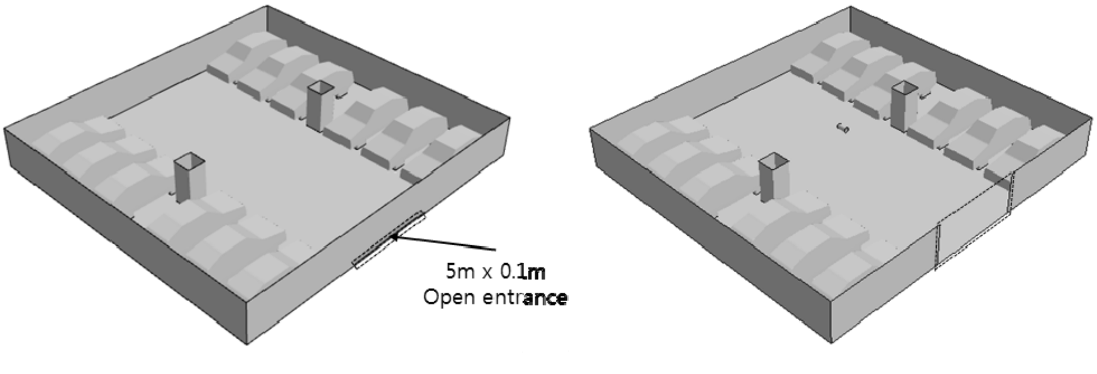


Figure 2. Domain and boundary conditions considering a closed entrance with a small opening (left) and open entrance (right).

of the parking garage and the no-slip condition is used at walls.

As shown in Fig. 2, two different configurations were considered based on the shape of the entrance and the existence of an indoor ventilation fan. In the first configuration, the size of the entrance is 5m in width and 0.1m in height (closed with a small opening) and there is no ventilation fan. We assumed this case as the worst scenario for this model parking garage. In the second configuration, the size of the entrance is 5m in width and 2.3m in height (open) and there is an indoor ventilation fan running constantly. The effect of the ventilation fan is simulated by an additional source term to the momentum equation. The size and discharge rate of the ventilation fan is set based on the specification of several fans commercially available. The cases considered in the present study are described in Table 1. We considered several different leakage rates of hydrogen as the primary parameter. The unit of the leakage rate Q is the mass rate of hydrogen with the energy equivalent to a gasoline leakage regulated by U.S. FMVSS 301 [12]. This unit has been conventionally used in several previous studies for hydrogen and other explosive gases and is equivalent to 131 L/min in the present study. For the case with the open entrance and ventilation fan, three different air volumes of the fan are considered.

Table 1. Conditions of different cases.

No.	Garage door	Leakage Rate	Air volume of ventilation fan
1	Closed with a small opening	1Q	-
2		2Q	-
3		3Q	-
4		4Q	-
5		5Q	-
6		10Q	-
7	Open	5Q	-
8			20 m^3/min
9			40 m^3/min
10			60 m^3/min
11		10Q	-
12			20 m^3/min
13			40 m^3/min
14			60 m^3/min

The flammable region at a given time is identified by the flammable condition of hydrogen. From Cengel & Boles [11], the flammable range is 4~74% in the volume fraction of hydrogen.

3. COMPUTATIONAL SETUP

For simulating flows with hydrogen diffusion and identifying the flammable region, three basic conservation equations of continuity, momentum and scalar were used. The equations for mass and momentum conservation in Cartesian coordinates are:

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0 \qquad (1)$$

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho u_j u_i-\tau_{ij}\right)=-\frac{\partial p}{\partial x_i}+g_i\left(\rho-\rho_0\right) \qquad (2)$$

where ρ is the density, t is the time, x_i is the Cartesian coordinates, u_i is the velocity components, τ_{ij} is the stress tensor components, and p is the pressure. The last term in the momentum equation is the buoyancy force term where g_i is the gravitational acceleration vector and ρ_0 is the reference density. The conservation equation of hydrogen species is:

$$\frac{\partial(\rho y_m)}{\partial t}+\frac{\partial}{\partial x_j}\left(\rho u_j y_m+F_{m,j}\right)=S_m \tag{3}$$

where y_m is the mass fraction of hydrogen gas and $F_{m,j}$ is the diffusion flux in the direction x_j. The scalar source S_m was used to model the hydrogen gas inflow under the car. For the turbulent flow, transport equations for the turbulence kinetic energy and dissipation rate were solved by using the realizable $k-\varepsilon$ model:

$$\frac{d}{dt}\int_V \rho k dV+\int_A \rho k\mathbf{v}\cdot d\mathbf{a}=\int_A\left(\mu+\frac{\mu_t}{\sigma_k}\right)\nabla k\cdot d\mathbf{a}+\int_V\left[G_k-\rho\left(\left(\varepsilon-\varepsilon_0\right)+\Upsilon_M\right)+S_k\right]dV \tag{4}$$

$$\frac{d}{dt}\int_V \rho\varepsilon dV+\int_A \rho\varepsilon\mathbf{v}\cdot d\mathbf{a}=\int_A\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\nabla\varepsilon\cdot d\mathbf{a}+\int_V\left[C_{\varepsilon 1}+S\varepsilon+\frac{\varepsilon}{k}(C_{\varepsilon 1}C_{\varepsilon 3}G_b)-\frac{\varepsilon}{k+\sqrt{\nu\varepsilon}}C_{\varepsilon 2}\rho(\varepsilon-\varepsilon_0)+S_\varepsilon\right]dV \tag{5}$$

where S_k and S_ε are the user-specified source term, and ε_0 is the ambient turbulence value in the source terms that counteract the turbulence decay. k is the turbulence kinetic energy, μ is the viscosity, $\mu_t=\rho C_u k^2/\varepsilon$ is the turbulent viscosity, σ is the turbulent Prandtl number, ε is the mean strain tensor. The turbulent coefficients are set as $C_{\varepsilon 1}$ $\left(=\max(0.43,\eta/(\eta+5))\ where\ \eta=Sk/\varepsilon\right)$, $C_{\varepsilon 2}$ (=1.9), σ_k (=1.0) and σ_ε (=1.2) in this model. G_k is the turbulence production term. G_k is written as:

$$G_k=\mu_t S^2-\frac{2}{3}\rho k\nabla\cdot\mathbf{v}-\frac{2}{3}\mu_t\left(\nabla\cdot\mathbf{v}\right)^2 \tag{6}$$

where S is the modulus of the mean strain rate tensor. In the present study, the density is assumed to be constant; therefore, the equations of mass and momentum conservation are simplified as:

$$\frac{\partial u_i}{\partial x_i}=0 \tag{7}$$

$$\frac{\partial u_i}{\partial t}+\frac{\partial u_j u_i}{\partial x_j}=-\frac{\partial(p/\rho)}{\partial x_i}+\frac{\partial(\tau_{ij}/\rho)}{\partial x_j}+g_i\left(1-\frac{\rho_0}{\rho}\right) \tag{8}$$

The density is updated from the mass fraction of hydrogen computed from Eq. (3)

In order to solve the above equations, we used a commercial CFD software STAR-CCM+ V5.06. In order to simplify the coupling of the continuity equation and the buoyancy term in the momentum equation, we ignored the compressibility of the flow in our simulation. The numerical study by Ahn et al. [13] showed that there is virtually no compressibility effect in case of a relatively small leakage rate of hydrogen. Polyhedral elements are used for the computational grids. The total number of the computational mesh points is approximately 2 million for the case without a ventilation fan and 3 million for the case with a fan.

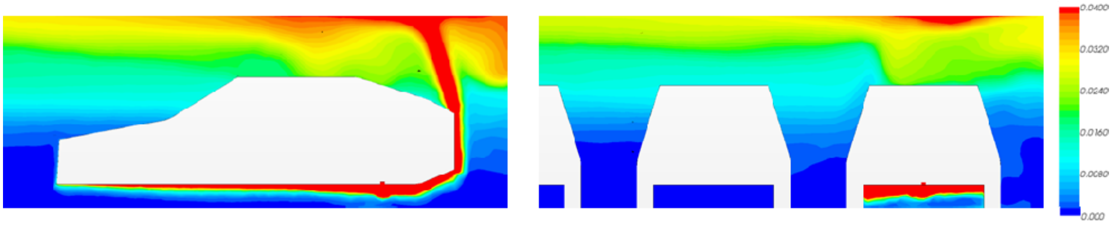


Figure 3. Contours of the volume fraction of hydrogen: the side view (left); the rear view (right) of the cars (leakage flow rate : 5Q, leakage time : 10min)

4. RESULTS AND DISCUSSION

Fig. 3 shows contours of the volume fraction of hydrogen and shows a typical pattern of the diffusion process. Hydrogen leaking from the bottom of the car flows in two directions – parallel to the bottom of the car and to the ceiling of the parking garage. Because of the light molecular weight of hydrogen, the majority of the gas moves up and flows parallel to the ceiling, as shown in the figure. Considering that the pure red color denotes the flammable regions, they are located near the car bottom and locally develop near the top of the ceiling. For the cases without a ventilation fan, the volume of the flammable region clearly increases in time. The volumetric ratio of the flammable region is defined as:

$$\eta = \frac{\text{Volume of the flammable region (volume fraction of H}_2\text{=4~74\%)}}{\text{Total volume of the domain}}$$

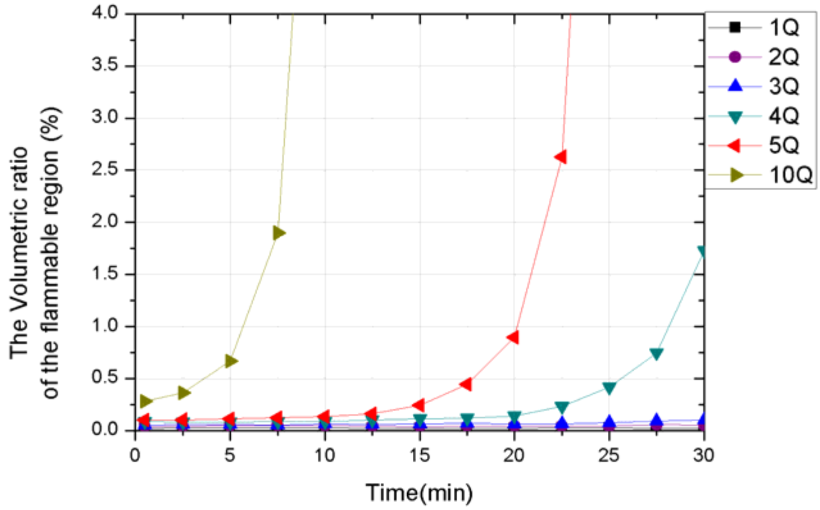
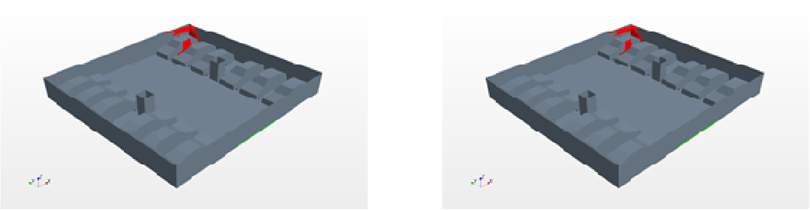
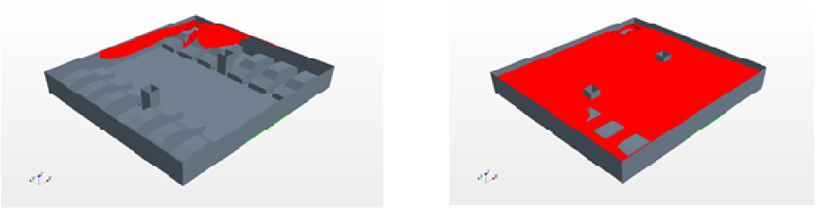


Figure 4. Time history of the volumetric ratio of the flammable region for different leakage flow rates.

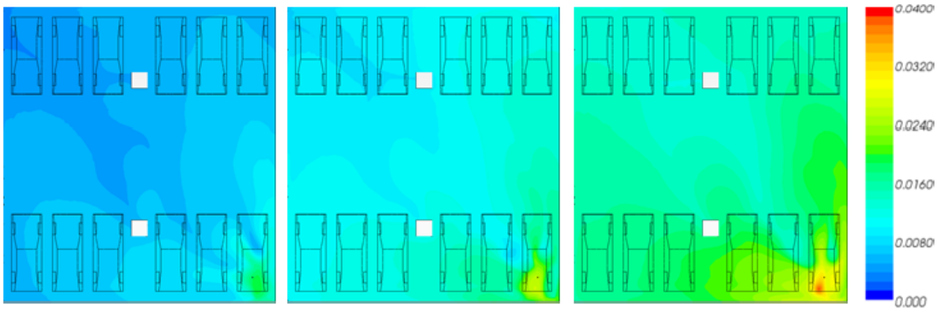


(a) 4Q, after 20 min. (b) 5Q, after 20 min.

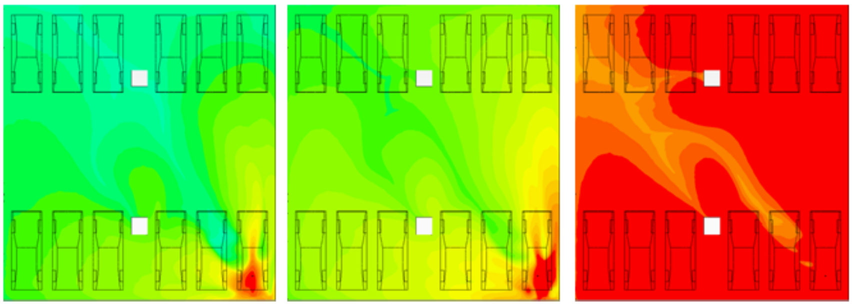


(a) 4Q, after 30 min. (b) 5Q, after 30 min.

Figure 5. Iso-surfaces of the flammable region for different leakage flow rates and times.



(a) 1Q (b) 2Q (c) 3Q



(d) 4Q (e) 5Q (f) 10Q

Figure 6. Contours of the volume fraction of hydrogen at the ceiling of the parking garage for different leakage flow rates (when the computation time is 10 minute)

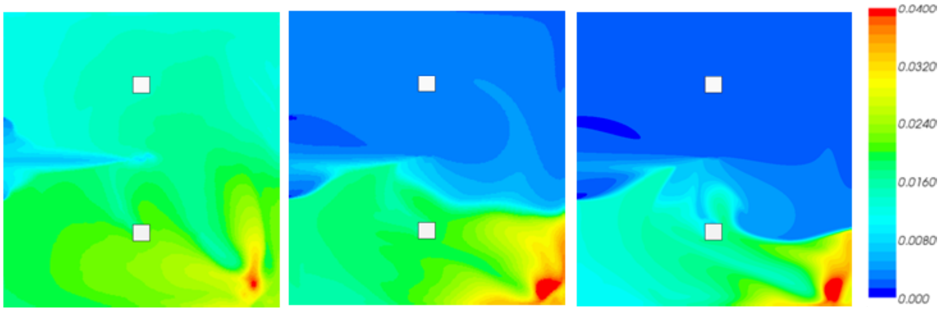
Fig. 4 shows the time history of the volumetric ratio of the flammable region for different leakage flow rates. As shown in the figure, there is a time after which the volumetric ratio increases very rapidly. The time when the rapid change begins is delayed as the leakage flow rate decreases. As shown later, 1the reason of the rapid increase of the flammable region is related to the fast diffusion velocity of hydrogen and accumulation near the ceiling. Because of the fast diffusion process, the hydrogen concentration near the ceiling is relatively uniform in space. The hydrogen concentration tends to increase uniformly near the ceiling, as the light hydrogen gas is accumulated. Later, as the volume fraction of hydrogen becomes close to the flammable limit (4%), the volume of the flammable region suddenly increases, which is observed in Fig. 4.

Fig. 5 shows a comparison of the flammable regions for two different leakage flow rates equal to 4Q and 5Q. Between two cases, the difference in the leakage flow rate is relatively small and the iso-surfaces look similar up to 20 minutes from the start. However, two cases shows very different flammable regions after 30 minutes from the start, which is related to the observation from Fig. 4.

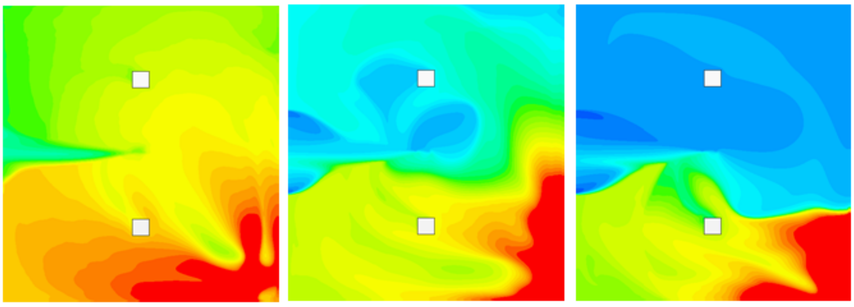
Fig. 6 shows contours of the volume fraction of hydrogen at the ceiling of the parking garage for different leakage flow rates after 10 minutes from the start. As shown in Fig. 3, most of the diffusion process occurs near the ceiling and the hydrogen concentration in this region is important to understand the diffusion characteristics. In order to use the concept of the diffusion velocity, the equation of the species conservation is written as:

$$\frac{\partial \rho y}{\partial t} + \nabla \cdot \left(\rho \vec{u} y \right) = -\nabla \cdot \left(\rho \vec{V} y \right) \tag{9}$$

where $\vec{u}$ is the advective velocity, $\vec{V}$ is the diffusion velocity, and y is the mass fraction of hydrogen. This equation can be rewritten as a pure advection equation:



(a) 20m^3/min (b) 40m^3/min (c) 60m^3/min



(d) 20m^3/min (e) 40m^3/min (f) 60m^3/min

Figure 7. Contours of the volume fraction of hydrogen at the ceiling for different ventilation air volumes. Leakage flow rate is 5Q for (a), (b), (c) and 10Q for (d), (e), (f).

$$\frac{\partial \rho y}{\partial t} + \nabla \cdot \left\{ \rho \left(\vec{u} + \vec{V} \right) y \right\} = 0 \tag{10}$$

where $\vec{u} + \vec{V}$ is the total advective velocity. Using the Fick's law, the diffusion velocity is written as:

$$\vec{V} = -\alpha \frac{\nabla y}{y} \tag{11}$$

where α is the diffusivity. As shown in Eq. (9), the diffusion velocity is inversely proportional to the mass fraction of hydrogen. Thus, at the initial stage of leakage, a small value of the mass fraction leads to a relatively fast diffusion velocity and total advective velocity. This can result in a relatively uniform distribution of the mass fraction near the ceiling, which suppresses a linear increase of the flammable region. As hydrogen keeps leaking, it is accumulated near the ceiling due to its light molecular weight.

Fig. 7 shows contours of the volume fraction of hydrogen at the ceiling in the cases with a ventilation fan with different air volumes. It is observed that the flammable region decreases as the air volume of the fan increases. The effect of the fan is also visible from the area of low hydrogen concentration in the opposite side of the leakage spot in the parking garage.

Fig. 8 shows the time history of the volumetric ratio of the flammable region for different leakage flow rates in the cases with a ventilation fan. The time history is compared with the case without a ventilation fan with the same leakage flow rate. It is observed that the volume of the flammable region becomes constant due to the ventilation fan. Notably, the volumetric ratios of the flammable region are not very different for different air volumes of the fan. We anticipate that the cases with different air volumes will show a large difference eventually as the time goes but did not perform a further study on this. We will investigate this topic in the subsequent study.

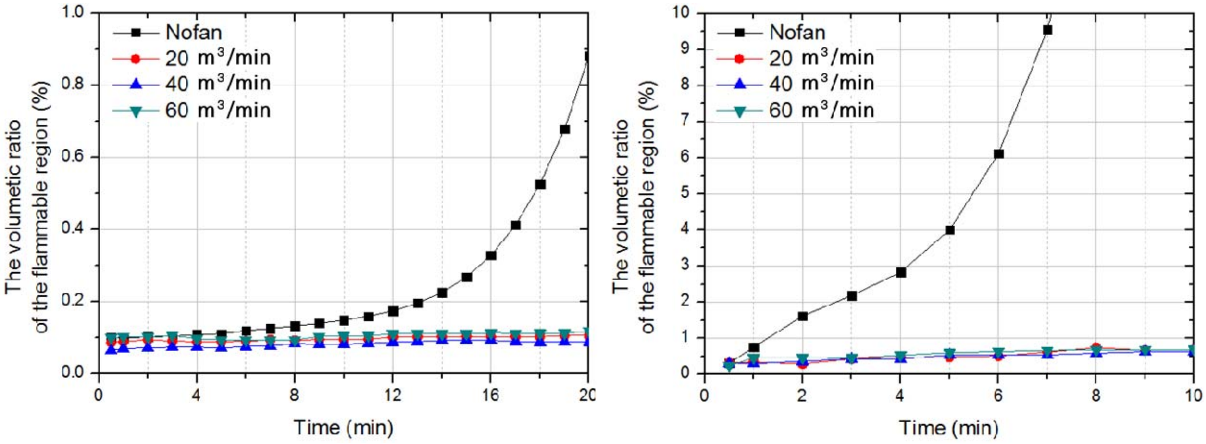


Figure 8. Time history of the volumetric ratio of the flammable region for the leakage flow rate 5Q (left) and 10Q (right)

CONCLUSIONS

The objective of the present study is to analyse safety issues of a fuel cell vehicle in an underground parking garage when hydrogen leaks from the vehicle. In order to provide quantitative data to evaluate the safety, a parametric study was performed by changing the hydrogen flow rate and the air volume of a ventilation fan. From this data, the time evolution of the flammable region was investigated. For cases without a ventilation fan, it is observed that the volume of the flammable region does not increase linearly in the initial stage but rapidly increases afterwards. The time of the rapid change is delayed as the leakage flow rate decreases. This feature is found to be related to the fast diffusion velocity of hydrogen. For cases with a ventilation fan, it is observed that the flammable region decreases as the air volume of the fan increases. The effect of the fan is visible in the area of low hydrogen concentration in the opposite side of the leaking spot in the parking garage. For the conditions and temporal range considered in the present study, the volumetric ratios of the flammable region are not very different for different air volumes of the fan.

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