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# A CFD simulation of hydrogen dispersion for the hydrogen leakage from a fuel cell vehicle in an underground parking garage<sup>☆</sup>

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## ABSTRACT

In the present study, the dispersion process of hydrogen leaking from an FCV (Fuel Cell Vehicle) in an underground parking garage is analyzed with numerical simulations in order to assess hazards and associated risks 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 volume of the flammable region shows a non-linear growth in time with a latency period. The effects of the leakage flow rate and an additional ventilation fan were investigated to evaluate the ventilation performance to relieve accumulation of the hydrogen gas. It is found that expansion of the flammable region is delayed by the fan via enhanced mixing near the boundary of the flammable region. The present numerical results can be useful to analyze safety issues in automotive applications of hydrogen.

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## 1. Introduction

Recently, there has been a lot of interest in using hydrogen 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 a possible increase of the thermodynamic efficiency. Meanwhile, there have been many concerns on the safety of hydrogen in automotive applications. Hydrogen is a light gas with a relatively large flammable region and a fast flame speed [1]. Hydrogen

has the flammable range of 4–74% and the detonation range [2] of 11–59% by volume. These imply that a hydrogen deflagration 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 for automobiles in various situations. One of the most dangerous situations is a leakage of hydrogen from an FCV in an underground parking garage. Theoretically, it is

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straightforward to do an experiment of a hydrogen leakage accident and measure the dispersion characteristics. However, an experiment of hydrogen leakage has a high risk because of the possibility of hydrogen deflagration. In order to avoid the high risk of a hydrogen experiment, a numerical simulation has become a very important alternative [3]. A simulation using computational fluid dynamics (CFD) techniques can provide detailed data such as the concentration of hydrogen, the flammable region, the spatial dispersion, etc.

There are several previous studies on hydrogen leakage phenomena in various situations [4–8]. Takeno et al. [9] performed an experimental study on hydrogen dispersion in case of leakage from a pressurized vessel. Liu et al. [10] proposed a numerical model for the dispersion process of hydrogen which produced results consistent with the data of Takeno et al. Vudumu and Koylu [11] carried out 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 confined, partially closed and open areas and predicted the evolution of the flammable regions in time. Mukai et al. [12] investigated the dispersion phenomena of hydrogen from an FCV inside a tunnel and underground parking garage. For each case, they investigated the dispersion characteristics and the safety risk. Although several studies have been done for hydrogen leakage, most of studies have focused on the dispersion 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 evolution of the flammable region can strongly depend on the flow rate of hydrogen. Besides, there are only few studies which performed a quantitative analysis of the effect of a ventilation fan on flammable envelop size.

In the present study, we investigated the dispersion of hydrogen for a model parking garage that meets the official Korean regulations. There are two objectives: (1) to make a quantitative analysis based on detailed simulations of hydrogen dispersion and (2) 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 analyzed the dispersion phenomena based on the temporal evolution of the flammable region. We investigated the effect of ventilation fans with different discharge rates on the change of the flammable region.

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## 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(a) shows the configuration and dimension of computational domain. It is assumed that the parking garage has 12 slots and hydrogen leaks from an FCV parked at one of the corners away from the entrance. We assume that the location of the FCV with leakage is selected for the most dangerous situation in the given condition. The size of a parking slot is chosen as the smallest one allowed by the regulation based on the assumption that a smaller parking garage tends to be more dangerous than a larger one for the same hydrogen leakage rate; thus, the width of each parking

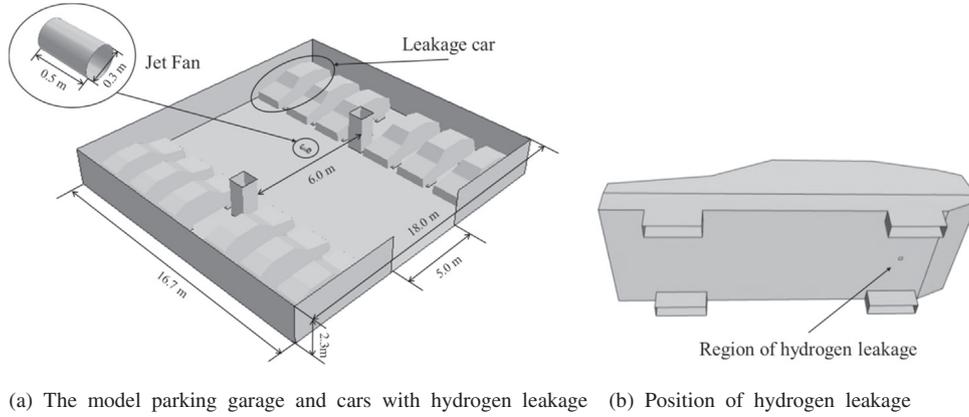
slot is determined as 2.3 m. As shown in Fig. 1(b), an FCV is modeled as a typical shape of a small passenger car and hydrogen is assumed to leak from a pipe near the hydrogen tank in the rear. The leakage area is assumed as a square of 5 cm in length and the leakage velocity is set to satisfy the assumed volume flow rate of leaking hydrogen. Notably, the leakage velocity from a high pressure tank is typically sonic or supersonic and much larger than the leakage velocity we used, because of the relatively large leakage area considered in the present study. In practice, there is a high possibility of a blockage effect by the ground and the other parts located near the bottom of a vehicle. It is expected that the high initial momentum of the gas from the vessel is gradually diffused and damped up to the point where the gas leaves the bottom region of the vehicle. Thus, it is assumed for simplicity that the leakage flow rate rather than the velocity has the major effect on the long term evolution of the flammable region that is the main topic of the present study. Under an assumption that the buoyancy force is important in the present problem, the mass flow rate should be an important factor because it can significantly affect the local and global fraction of hydrogen in the garage at a specific time. The atmospheric pressure is assumed at the entrance of the parking garage and the no-slip condition is used at walls. The pressure value at the entrance is typically higher than the external atmospheric pressure. Since the accurate pressure value depends on the specific configuration of the vent, we conveniently assumed a relatively wide entrance door and vent to ignore the pressure drop and used the atmospheric pressure at the door in our model.

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 5 m in width and 0.1 m in height (closed with a small opening) and there is no ventilation fan. We assumed this case as the worst case scenario for this model parking garage. In the second configuration, the size of the entrance is 5 m in width and 2.3 m 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 [13]. This unit has been conventionally used in several previous studies for hydrogen and other explosive gases and is equivalent to  $Q = 131$  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. The flammable region at a given time is identified by the flammable condition of hydrogen. From Cengel and Boles [14], the flammable range is 4–74% by volume of hydrogen.

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## 3. Computational setup

For simulating flows with hydrogen dispersion and identifying the flammable region, three basic conservation equations of



**Fig. 1 – Geometry of underground parking garage and position of hydrogen leakage for numerical simulations.**

continuity, momentum and scalar were used. The equations for mass and momentum conservation in Cartesian coordinates are:

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

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

where  $\rho$  is the density,  $t$  is the time,  $x_i$  is the Cartesian coordinates,  $u_i$  is the velocity components,  $\tau_{ij}$  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  $\rho_0$  is the reference density which is constant in time and space. The conservation equation of hydrogen species is:

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

where  $y_m$  is the mass fraction of hydrogen gas and  $F_{m,j}$  is the diffusion flux in the direction  $x_j$  defined as:

$$F_{m,j} = -\rho(\alpha_m + \alpha_t) \frac{\partial y}{\partial x_j} \quad (4)$$

where  $\alpha_m$  is the molecular diffusivity and  $\alpha_t$  is the turbulent diffusivity from a turbulence model described below. The scalar source  $S_m$  was used to model the hydrogen gas inflow under the car. For the turbulent flow, transport equations for the turbulent kinetic energy and dissipation rate were solved by using the realizable  $k-\epsilon$  model:

$$\begin{aligned} \frac{d}{dt} \int_V \rho k dV + \int_A \rho k v \cdot dA &= \int_A \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla \epsilon \cdot dA \\ &+ \int_V [G_k + G_b - \rho((\epsilon - \epsilon_0) + Y_M) + S_k] dV \end{aligned} \quad (5)$$

$$\begin{aligned} \frac{d}{dt} \int_V \rho \epsilon dV + \int_A \rho \epsilon v \cdot dA &= \int_A \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \epsilon \cdot dA \\ &+ \int_V \left[ C_{\epsilon 1} + S_\epsilon + \frac{\epsilon}{k} (C_{\epsilon 1} C_{\epsilon 3} G_b) \right. \\ &\left. - \frac{\epsilon}{k + \sqrt{v \epsilon}} C_{\epsilon 2} \rho (\epsilon - \epsilon_0) + S_\epsilon \right] dV \end{aligned} \quad (6)$$

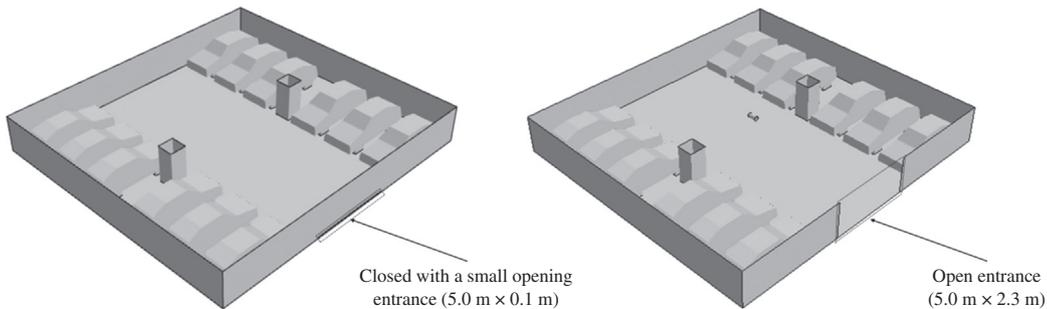
where  $S_k$  and  $S_\epsilon$  are the user-specified source term, and  $\epsilon_0$  is the ambient turbulence value in the source terms that counteract the turbulence decay.  $k$  is the turbulent kinetic energy,  $\epsilon$  is the turbulent dissipation rate,  $\mu$  is the viscosity,  $\mu_t = \rho C_u k^2 / \epsilon$  is the turbulent viscosity, and  $S$  is the modulus of the mean strain rate tensor. The turbulent coefficients are set as  $C_{\epsilon 1} (= \max(0.43, \eta / (\eta + 5)))$  where  $\eta = Sk/\epsilon$ ,  $C_{\epsilon 2} (=1.9)$ ,  $\sigma_k (=1.0)$  and  $\sigma_\epsilon (=1.2)$  in this model.  $G_k$  is the turbulence production term.  $G_k$  is written as:

$$G_k = \mu_t S^2 - \frac{2}{3} \rho k \nabla \cdot \mathbf{v} - \frac{2}{3} \mu_t (\nabla \cdot \mathbf{v})^2 \quad (7)$$

$G_b$  is the buoyancy production term written as:

$$G_b = \beta \frac{\mu_t}{Pr_t} (\nabla T \cdot \mathbf{g}) \quad (8)$$

where  $\beta$  is the coefficient of thermal expansion,  $\nabla T$  is the temperature gradient vector and  $Pr_t$  is the turbulent Prandtl



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

**Table 1 – Conditions of different cases.**

No.	Garage door	Leakage rate	Air volume of ventilation fan
1	Closed with a small opening	1Q (131 L/min)	–
2		2Q (262 L/min)	–
3		3Q (393 L/min)	–
4		4Q (524 L/min)	–
5		5Q (655 L/min)	–
6	Open	10Q (1310 L/min)	–
7		5Q (655 L/min)	–
8		–	20 m <sup>3</sup> /min
9		–	40 m <sup>3</sup> /min
10		–	60 m <sup>3</sup> /min
11	–	10Q (1310 L/min)	–
12	–	–	20 m <sup>3</sup> /min
13	–	–	40 m <sup>3</sup> /min
14	–	–	60 m <sup>3</sup> /min

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

number set to 0.9. The turbulent mass diffusivity  $\alpha_t$  is defined as  $\alpha_t = C_u k^2 / Pr_t \epsilon$ . This formulation is based on the turbulent Lewis number set to unity. While a different choice of  $\alpha_t$  can affect the dispersion process significantly, there have been only few studies on its effect [15]. In most previous studies, the turbulent diffusivity is set as the same value as the turbulent thermal diffusivity that is equivalent to the assumption of the unity turbulent Lewis number. In order to simplify the coupling between the continuity equation and the buoyancy term in the momentum equation, we ignored the compressibility effect in our simulation. Specifically, the density is updated from the mass fraction of hydrogen computed from Eq. (3), not affected by the pressure change. The density of the air–hydrogen mixture is calculated using

$$\rho = \varphi_{H_2} \rho_{H_2} + (1 - \varphi_{H_2}) \rho_{air} \quad (9)$$

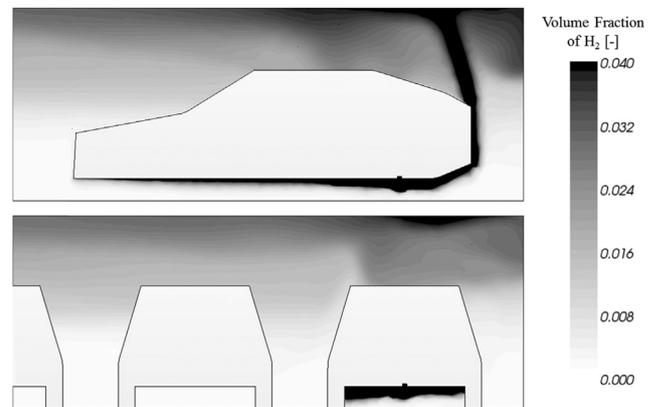
where  $\varphi$  denotes the volume fraction computed from the mass fraction. The values of the density of hydrogen and air ( $\rho_{H_2}, \rho_{air}$ ) are assumed as constants at the standard condition. The numerical study by Ahn et al. [16] for hydrogen dispersion in a tunnel showed that the compressibility effect is minor for a small leakage rate, which implies that the present approach is valid to investigate the temporal evolution of the flammable region.

In order to solve the above equations, we used a commercial CFD software STAR-CCM + V5.06 [17]. 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. The simulations were performed using 16 CPUs in a Linux cluster with Intel Xeon Quad-Core 2.4 GHz 64-bit processor. It takes about 3 days for the case without a ventilation fan and 5 days for the case with a fan.

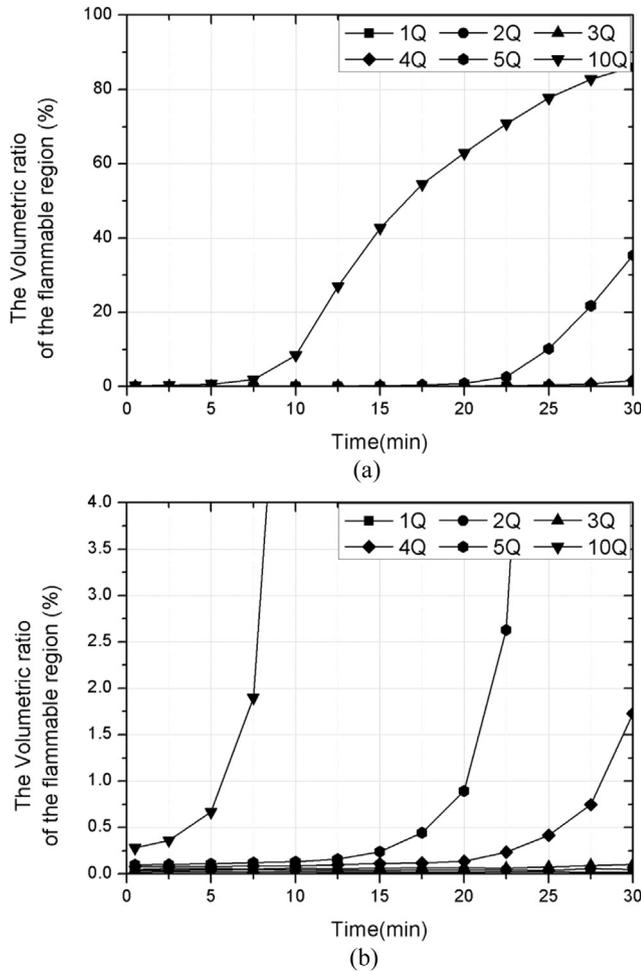
## 4. Results and discussion

Fig. 3 shows contours of the volume fraction of hydrogen and shows a typical pattern of the dispersion 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 black 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:

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, a 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 dispersion 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 lower flammable limit (4%), the volume of the flammable region suddenly increases, as shown in Fig. 4.

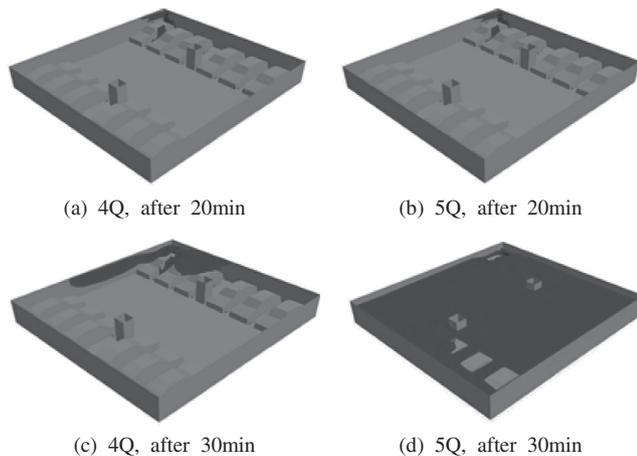


**Fig. 3 – Contours of the volume fraction of hydrogen: The side view (top); the rear view (down) of the cars (leakage flow rate: 5Q, leakage time: 10 min).**



**Fig. 4 – Time history of the volumetric ratio of the flammable region for different leakage flow rates.**

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 min from the start.



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

However, two cases show a very different trend in the flammable region after 30 min from the start. The ratio of the flammable region suddenly increases between 20 and 30 min only for the case of 5Q. This observation is consistent with the rapid expansion of the flammable region as observed in 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 min from the start. As shown in Fig. 3, most of the dispersion process occurs near the ceiling and the hydrogen concentration in this region is important to understand the dispersion characteristics. In order to use the concept of the diffusion velocity, the equation of the species conservation is written as:

$$\frac{\partial \rho y}{\partial t} + \nabla \cdot (\rho \vec{u} y) = -\nabla \cdot (\rho \vec{V} y) \quad (10)$$

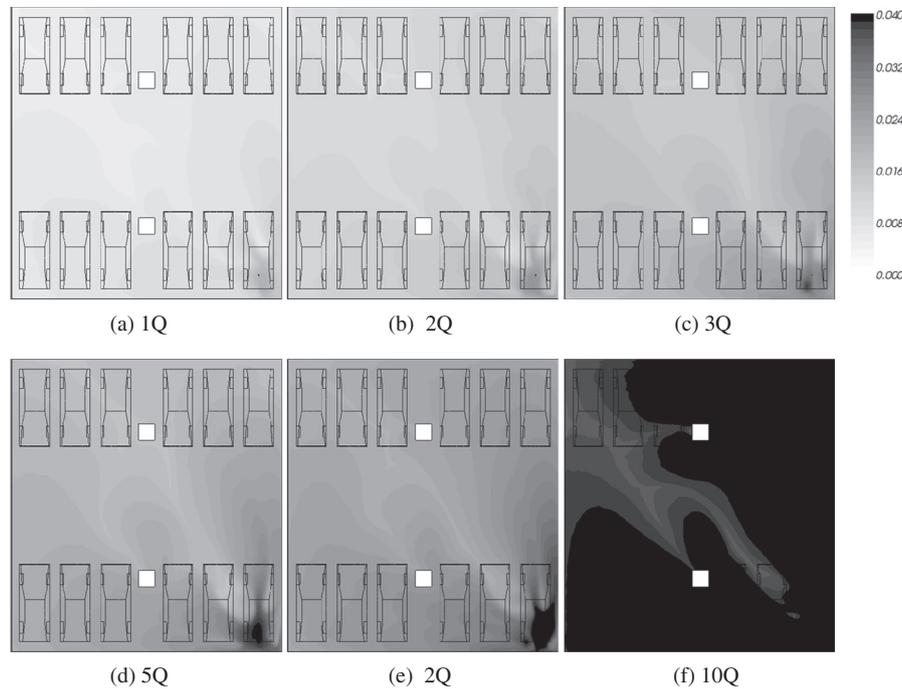
where  $\vec{u}$  is the advective velocity,  $\vec{V}$  is the diffusion velocity, and  $y$  is the mass fraction of hydrogen. This equation can be rewritten as a pure advection equation:

$$\frac{\partial \rho y}{\partial t} + \nabla \cdot \{ \rho (\vec{u} + \vec{V}) y \} = 0 \quad (11)$$

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

$$\vec{V} = -\alpha \frac{\nabla y}{y} \quad (12)$$

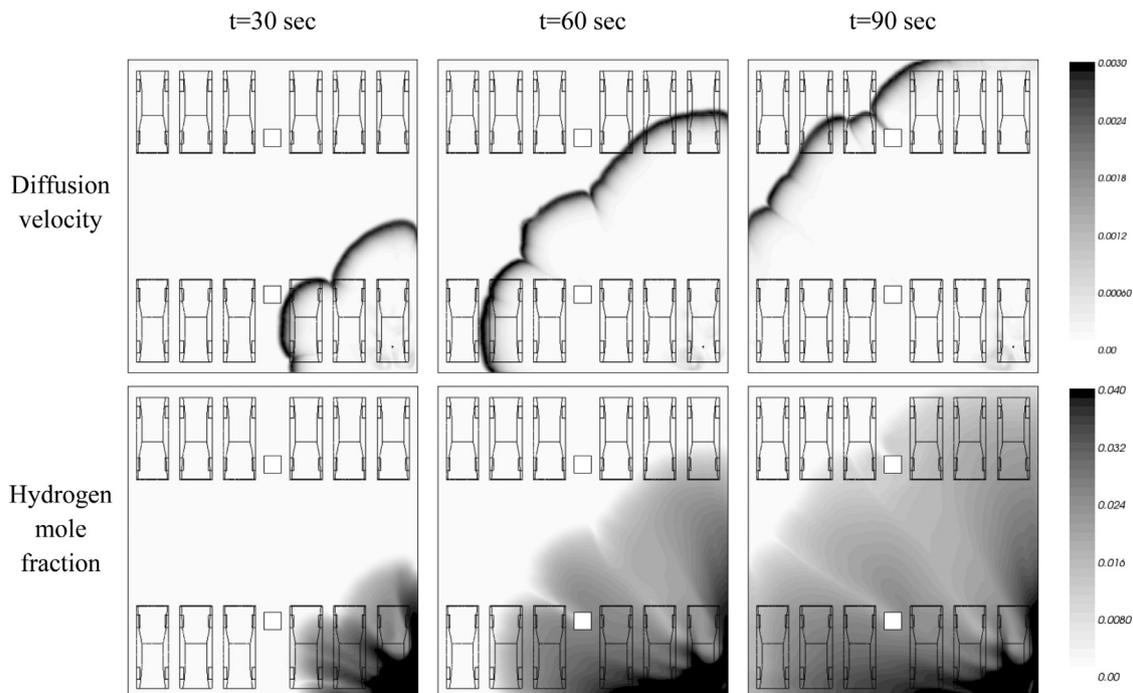
where  $\alpha$  is the total diffusivity that is the sum of the molecular and turbulent diffusivities. In Eq. (12), the diffusion velocity is inversely proportional to the mass fraction of hydrogen. Thus, at the initial stage of leakage, a small value of the mass fraction and relatively large size of the gradient may lead to a relatively fast diffusion velocity and total advective velocity. It is notable that using the total diffusivity as  $\alpha$  in Eq. (12) implies that the corresponding diffusion velocity in Eq. (10) reflects the combined effects of the molecular diffusion and modeled turbulent advection from the velocity fluctuations smaller than the grid scale (i.e. sub-grid scale), while the advection term in Eq. (10) reflects the effect of the advection from the resolved scales. From the flow fields, it was observed that the molecular diffusivity is several times larger than the turbulent diffusivity in the most regions at least 3 m away from the leakage source, which shows that the effect of the molecular diffusion is much larger compared to the modeled (sub-grid) turbulent advection in these regions and the diffusion velocity in Eq. (12) primarily reflects the effect of the molecular diffusion. Fig. 7 shows the contours of the diffusion velocity in Eq. (12) and the mole fraction of hydrogen near the ceiling at different times for the case with the leakage rate equal to 10Q. It is shown that the region with increased diffusion velocity is localized in a narrow band and very similar to the region of 0.5–1.5% in hydrogen mole fraction. The region gradually moves away from the leakage source in time. The maximum size of the diffusion velocity in 0.1–10 cm away from the ceiling ranges 20–100% of the size of the advective velocity, which shows that the molecular diffusion has a significant effect on total dispersion and can increase the total advective velocity in this banded region. Note that the advective transport is dominant in the total dispersion process in the entire



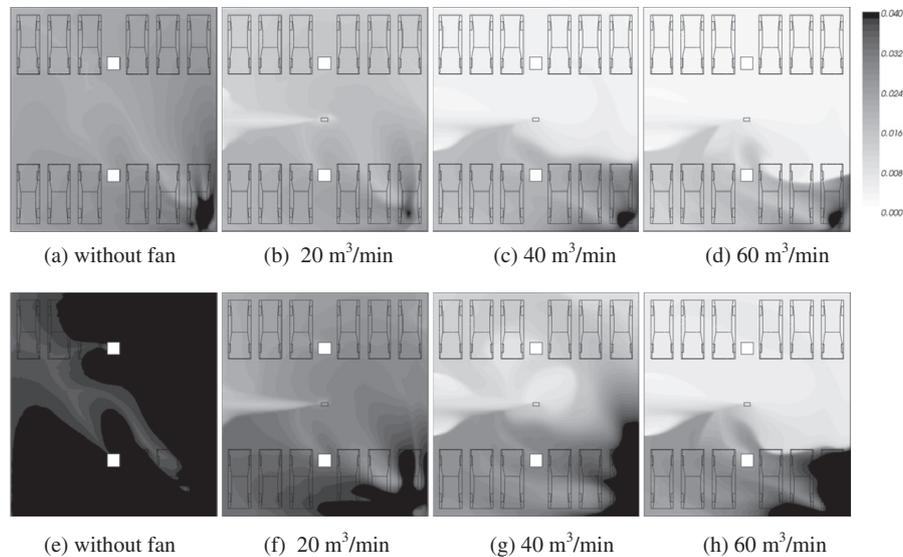
**Fig. 6 – Contours of the volume fraction of hydrogen at the ceiling of the parking garage for different leakage flow rates (when the computation time is 10 min).**

region of the present problem. While the size of the advective velocity tends to decrease monotonously as the distance from the leakage source increases, the increased diffusion velocity in the localized region can result in a non-smooth spatial change of the total advective velocity. Behind the banded region of the increased diffusion velocity, the area with the

hydrogen mole fraction around 2% becomes larger gradually in time, which implies that the relatively fast diffusion velocity at the initial stage of leakage accelerates the dispersion process in this region. This can result in a relatively uniform distribution of the mass fraction near the ceiling, which suppresses a linear increase of the flammable region. The banded



**Fig. 7 – Contours of the diffusion velocity and the mole fraction of hydrogen near the ceiling at different times from the start of the leakage.**



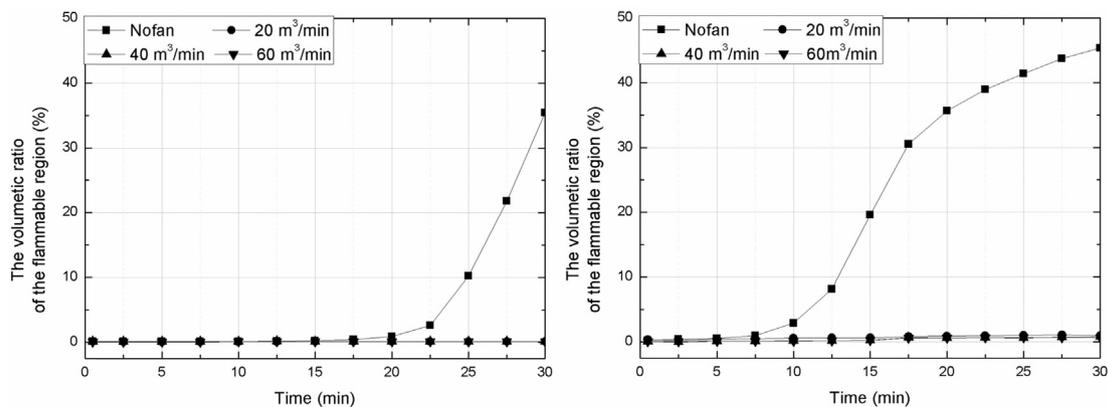
**Fig. 8 – Contours of the volume fraction of hydrogen at the ceiling for different ventilation air volumes. Leakage flow rate is 5Q for (a)–(d) and 10Q for (e)–(h) (when the computation time is 10 min).**

region with an increased diffusion velocity is observed similarly at locations further away from the ceiling below 10 cm but the role of the advection becomes more dominant in this region because the advective velocity increases as the distance from the ceiling. The effect of the advection is closely related to the buoyancy force. As hydrogen leaking continues, it is accumulated near the ceiling due to its lighter molecular weight. The buoyancy force pushes up the light hydrogen gas and the added momentum improves dispersion of the gas away from the leakage source via the advective transport. The effect of the buoyancy force will be decreased as the hydrogen concentration increases from the source. Compared to the molecular diffusion, the advection effect should be still dominant as the concentration gradient also tends to decrease as the gases are mixed further.

Fig. 8 shows contours of the volume fraction of hydrogen at the ceiling for the cases with different air volumes by a ventilation fan compared to the case without a fan. 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 a low hydrogen concentration in the opposite side of the leakage spot in the parking garage. Notably, it is found that the gradient of the volume fraction near the boundary of the flammable region becomes larger as the air volume of the fan increases. Considering that a larger gradient of the volume fraction implies a stronger dispersion process, it is deduced that an important effect of the ventilation fan is to enhance mixing near the flammable region, which delays expansion of the flammable region.

Fig. 9 shows the time history of the volumetric ratio of the flammable region with different leakage rates for the cases with and without a ventilation fan. It is observed that the volume of the flammable region becomes constant due to the ventilation fan, which shows that the accumulation of hydrogen is significantly reduced by the fan. Notably, the volumetric ratios of the flammable region are not very different for different air volumes of the fan. This seems to be related to the fact that the considered values of the air volume of the fan are much larger than the leakage rate of hydrogen which is about 0.655–1.31 m<sup>3</sup>/min.



**Fig. 9 – Time history of the volumetric ratio of the flammable region for the leakage flow rate 5Q (left) and 10Q (right).**

## 5. Conclusions

The objective of the present study is to analyze safety issues in an underground parking garage when hydrogen leaks from of a fuel cell vehicle. In order to produce 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 temporal evolution of the flammable region was investigated using the volumetric ratio of the flammable region. 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 after a latency period. The latency period becomes shorter as the leakage flow rate increases. 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 entire region as the reduced values of the hydrogen concentration. As the air volume of the fan increases, the gradient of the volume fraction near the boundary of the flammable region becomes larger. This shows that an important effect of the fan is to enhance mixing near the flammable region, which delays expansion of the flammable region. 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. These results show the effectiveness of a ventilation fan to avoid a hazardous situation from hydrogen leaking in an underground parking garage.

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