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A study of effective mitigation system for accidental hydrogen fluoride releases

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Hydrogen fluoride (HF) is a strong, pervious gas that is a stimulus on the body, respiratory system, and skin. HF is widely used in electronics manufacturing as a polisher and disinfectant. Interest in HF increased after the HF release accident in Gumi, S. Korea (2012), emphasizing the special attention and management needs with respect to this gas.

In this study, ANSYS FLUENT, a Computational Fluid Dynamics (CFD) program, is used to identify the effect of a physical barrier as a mitigation system against HF and Chlorine leaked from industrial facilities. In a typical industrial facility, there is a barrier that distinguishes the inside and outside of a workplace, but it is not sufficient to prevent hazardous substances from being released outside. However, we assumed various physical barrier heights (3 m, 6 m and 9 m) for mitigating toxic release and used simulations to analyze them to determine how effectively they decreased concentrations offsite. Goldfish experimental data from 1986 were compared to verify the results for HF and Jack Rabbit I test data in 2010 for Chlorine. The results show that HF and Chlorine concentrations can be further decreased with higher barrier heights and their mitigation effectiveness factors were derived. Thus, we can reduce the possibility of offsite exposure to toxic gas release using the mitigation system and make the better and more effective emergency plan with proper mitigation systems .

Key words: mitigation, HF, chlorine, CFD, physical barrier, water curtain

Ⅰ. Introduction

Due to the development of high-tech industries such as the semiconductor, LCD, and solar cell industries, currently, the amount of toxic gases used in South Korea has been showing increasing trends with an annual average increase rate of 39%. In addition, following the Gumi Hube Global hydrogen fluoride release accident in 2012, people's attention to concern about toxic gases increased sharply. Furthermore toxic gas accidents account for high ratios of high pressure gas accidents to the extent that toxic gas accidents account for approximately 25% of 84 high pressure gas accidents that occurred over the last six years and damage caused by those toxic gas accidents have been known to be very large. Therefore, the necessity of systems to mitigate the impact of toxic gas release accidents has come to the fore.

In addition, many models are currently utilized to predict toxic gas releases from tanks, containers, or pipes in which toxic gases are stored at high pressure. However, those models are approaches relying on simple calculation formulas without considering surrounding topography, situations, or barriers and have shortcomings of showing too large resultant values in the case of long distances while showing too small values in the case of short distances. [1],[2]

As such, there are many restrictive conditions against considering even surrounding environments and situations in accident impact evaluation and more precise accident prediction models are required for risk evaluation. In particular, since the impacts of toxic gas releases reach very long distances and are greatly affected by various variables such as surrounding topography, temperatures, and the effects of winds, CFD (Computational Fluid Dynamics) analysis methods that can consider such situations were reviewed.

Examples of studies on actual gas diffusion, various diffusion modeling applied with CFD, and the effects of mitigation systems are as follows. Filippo Gavelli et al. studied the effects of the formation of LNG pools according to ground situations through the CFD code Fluent by comparing and analyzing the effects of LNG when released on ground surfaces and when released on the surface of water and verified that LNG evaporation rates were higher when LNG was released on the surface of water.[3] A. Mack et al. analyzed the behavior of heavy gases using OpenFoam and verified the results through wind tunnel experiments and Fluent, which is a commercial code.[4] In addition, P. Gousseau et al. compared and analyzed the performances of the RANS and LES models, which are turbulence models, in predicting pollutant dispersion around buildings to find that whereas the RANS model calculated faster compared to the LES model, the LES model was more accurate thereby helping the selection of dispersion prediction models through a CFD code thereafter.[5] Steven Hanna et al. simulated and studied data from Jack Rabbit field tests, which are chlorine release experiments, through the SLAB model.[6] In particular, Robert N. Meroney experimented various heavy gas diffusion mitigation systems to find out factors that affect diffusion organized formulas for prediction of the results of diffusion.[7]

In the present study, the behaviors of hydrogen fluoride and chlorine when released were simulated, analyzed, experimented, and verified through Fluent, which is a commercial CFD code, and the effects of physical barriers on the behaviors according to the heights of the barriers were analyzed.

Ⅱ. CFD Simulation

2.1. Simulation Tool

Recently, in foreign countries, the frequency of use of CFD Simulations has been increasing for more precise analyses of accidental releases of inflammable gases or toxic gases from industrial facilities, equipment, and devices used to handle those gases. CFD programs can analyze the possibility of accidents over time as well as in relation to surrounding topography so that the results of analysis can be closer to reality. Currently, the FLACS (Flame Acceleration Simulator) of GexCon and the FLUENT of ANSYS are representative programs suitable for accident impact evaluation. In the present study, the latter one, FLUENT 13.0 of ANSYS Co. was used.

The FLUENT is a representative fluid flow analysis program dedicated to flow analyses that can analyze the entire area of flows including not only incompressible flows but also compressible flows and transonic flows. In addition, it can analyze diverse physical and chemical phenomena such as laminar flows, turbulence, heat transfer issues, chemical reaction issues, multiphase flow issues. Therefore, it is used in all sectors of flow analyses such as process design, product design, etc. and this program is highly reliable. In addition, GAMBIT 2.4.6, a dedicated grid generation program, was used in the modeling of surrounding topography. [8]

2.2 Actual experiment used in verification (Field test)

2.2.1 Hydrogen fluoride release experiment (Goldfish test)

The experiments modeled after the Goldfish test, which is a large scaled hydrogen fluoride release experiment conducted in Frenchman, Nevada in 1986 by Amoco Oil Company and Lawrence Livermore National Laboratory. In the experiments pressurized liquid HF was released at a height of 1 m from the ground and hydrogen fluoride was released three times under different conditions. The conditions used in individual experiments are as shown in Table 1 below. The experiments were conducted without any surrounding topography other than the experimental apparatuses with a scenario to release a 4-inch diameter line from a 5000 gallon tank. The concentrations of the released gases were measured using concentration sensing sensors at points 300 m, 1000 m, and 3000 m away from the release hole in the direction of release[9][10].

Table 1. Condition values of Goldfish test

Test	Spill Rate, gal/min	HF Tank Temp., ℃	HF Tank Pressure, psig	Duration, Sec.	Wind, m/s at 2 m	Centerline Concentration, ppm, at		
						300 m	1000 m	3000 m
1	469.2	40	111	125	56	25473	3098	411
2	175.1	38	115	360	4.2	19396	2392	-
3	171.6	39	117	360	5.4	18596	2492	224

2.2.2 Chlorine release experiment (Jack rabbit test)

The chlorine release experiment was conducted in Dugway Proving Ground in Utah in 2010 with support by the Department of Homeland Security Transportation Security Administration and is called Jack Rabbit Test. The release space was an approximately 2 m deep and 50 m diameter dug area and experimental substances were released at a height of 2 m from the ground toward the ground. In Jack rabbit test, not only chlorine but also many other substances such as ammonia were released and sensors were arranged in circles at various distances (25, 50, 100, 30 0, and 500 m etc.) to measure the concentrations of the substances. In the test, 1 or 2 tons of chlorine was released at each of diverse wind speeds ranging from 1.6 m/s to 6.2 m/s as shown in Table 2 below.[11][12]

Table 2. Condition values of Jack rabbit test

Test number	Total mass released (kg)	Total released duration (s)	Q (kg/s)	Wind speed at 2 m (m/s)	x (m)	Max concentration (ppm)
5	2000	240	8.33	1.6	25	58600
					50	27800
					100	13500
					300	3410
					500	2030
6	2000	57	35.09	6.2	25	55600
					100	9780
					300	1100
					500	330

2.3 Numerical analysis model

2.3.1 Governing equation

The governing equations of CFD simulations are as shown by equation (1) and equation (2) and the conditions are 3D steady state incompressible turbulence flows.

$$\frac{\partial U_i}{\partial x_i} = 0 \quad \text{-------------------------------- (1)}$$

$$\frac{\partial U_i}{\partial t} + U_j \frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu \frac{\partial^2 U_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}\left(\overline{u_i' u_j'}\right) \quad \text{--- (2)}$$

The term $\overline{u_i' u_i'}$ in the above equation of motion is defined as follows.

$$-\overline{u_i' u_j'} = \frac{\mu_t}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij} K \quad \text{----------------- (3)}$$

μ_t in equation (3) is a turbulence viscosity coefficient that can be inferred through dimensionless analysis of high Reynold's number flows. When the turbulence energy generation rate and dissipation rate are assumed to be almost in equilibrium, μ_t is expressed as follows.

$$\mu_t = f_\mu C_\mu \rho \frac{K^2}{\varepsilon} \text{ -------------------------- (4)}$$

f_μ in the above equation is a coefficient determined by the turbulence model and K and ε are turbulent kinetic energy and turbulent energy dissipation respectively determined by the K-ε model. The standard k-epsilon model that is the most commonly used was used for the simulation and the SIMPLE algorithm was used as a scheme for coupling of speed and pressure. [13]

2.3.2 Grid

The grids necessary for the simulations were generated using the dedicated grid generation program GAMBIT 2.4.6 and the Mesh Volume was formed by generating polygonal cells using the Tet/Hybrid tab. The subject fluid was simulated as a mixture of air and toxic gases. In the first simulation that simulated Goldfish test, the total area of a space sized 3500 * 250 * 500 m^3 was analyzed by modeling a half of the total area and using symmetric conditions for the symmetric plane because the left and right of the release point are symmetric. A 0.5 m thick barrier was installed vertically at a distance of 100m in the x direction from the release hole. In addition, the sizes of grids closer to the release hole were made smaller. The total number of grids slightly varied with the height of the barrier. In the case of 9 m barrier, 3,835,599 grids were used.

In the second simulation that simulated Jack rabbit test, the entire size of the space was set to 2500 * 500 * 500 m^3. The location and size of the barrier were set to be the same as the first simulation and the sizes of grids closer to the release hole were made smaller as with the first simulation. The total number of grid used in the case of 9 m barrier was 5,779,184. Figure 1 below shows the Goldfish test simulation grids.

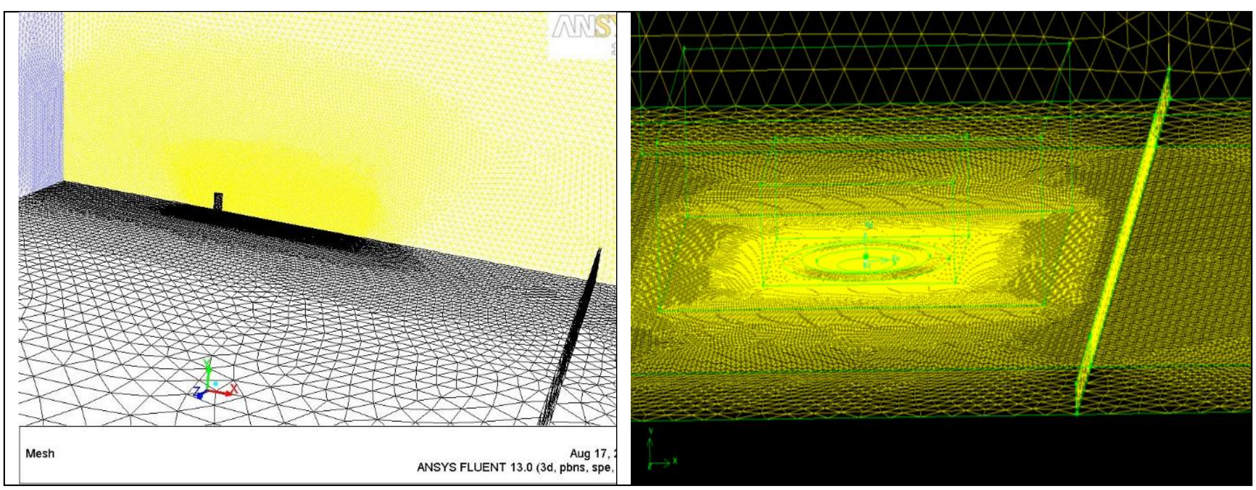

Figure 1. The topography and grids of the Goldfish test simulation (left, FLUENT), the topography and grids of the Jack rabbit test simulation (right, GAMBIT)

Ⅲ. Result and discussion

3.1 Comparison with the experiments and verification

3.1.1 Comparison between values obtained through Goldfish test and the simulation and the effect of the mitigation barrier

The values obtained through the simulation were compared with actual experimental values to secure the reliability of the FLUENT simulation. The experimental values from test 1 already shown in Table 1 above were used for the comparison. Through the comparison, the results as shown in Figure 2 could be obtained. Table 3 shows direct numerical comparison. The experimental values and the values from the FLUENT simulation showed relatively large differences at the first point but the error rates were found to be within 50% at points farther than 1000m from the release hole. Therefore, it can be seen that the simulation result values and the experiment values had similar tendencies.

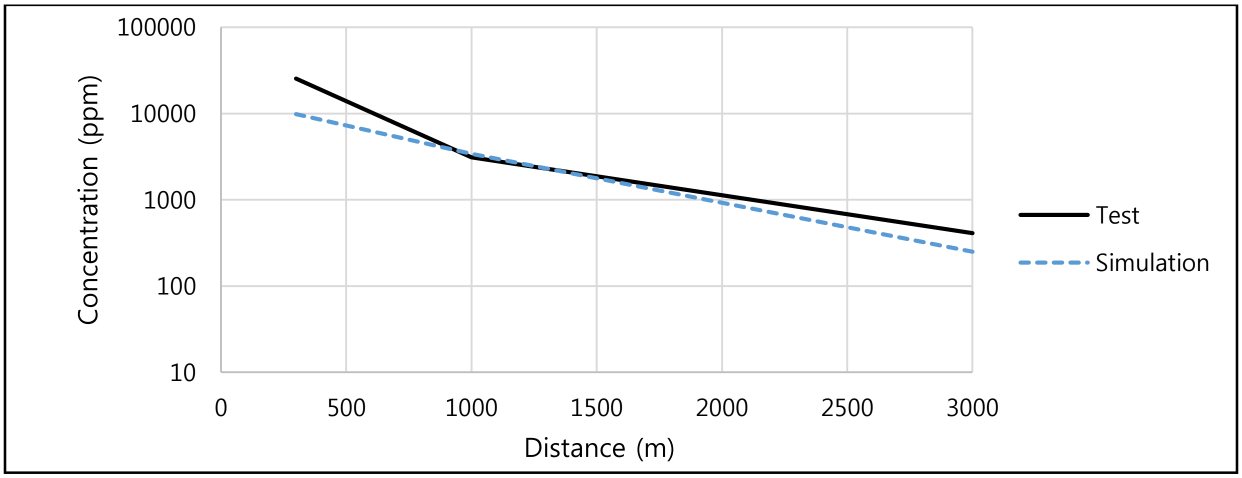

Figure 2. Comparison between values measured in Goldfish test and in the simulation

Table 3. Comparison of Hydrogen Fluoride concentration at 300, 500 and 3000 m (The shaded column contains a value with an error rate not within the range of 50% ~ 200%.)

		Concentration (ppm)	
		Test value	Simulation value
Distance (m)	300	25473	9849
	1000	3098	3427
	3000	411	251

After securing the reliability of the FLUENT simulation, condition change simulations were conducted to see the relationship between barrier heights and mitigation effects according to distances. In the simulations, 3 m, 6 m, and 9 m barriers were installed one at a time at a point 100m away from the release point in the x direction. Figure 3 is a graph that shows concentrations in relation to distances and barrier heights not only indicating that the barrier has mitigating effects but also indicating that the effects increased as the barrier height increased. Table 4 below shows the values of the concentrations of hydrogen fluoride and mitigation rates according to the heights of the mitigation barrier at certain points shown in the graph in Figure 3.

The mitigation effectiveness define by equation (5).

$$Mitigation\ \ effectiveness\ \ (\%) = \frac{C_{No,x} - C_{y,x}}{C_{No,x}} \times 100 \quad \text{--- (5)}$$

* $C_{No,x}$ is concentration without barrier at x meter

* $C_{y,x}$ is concentration of y meter barrier at x meter

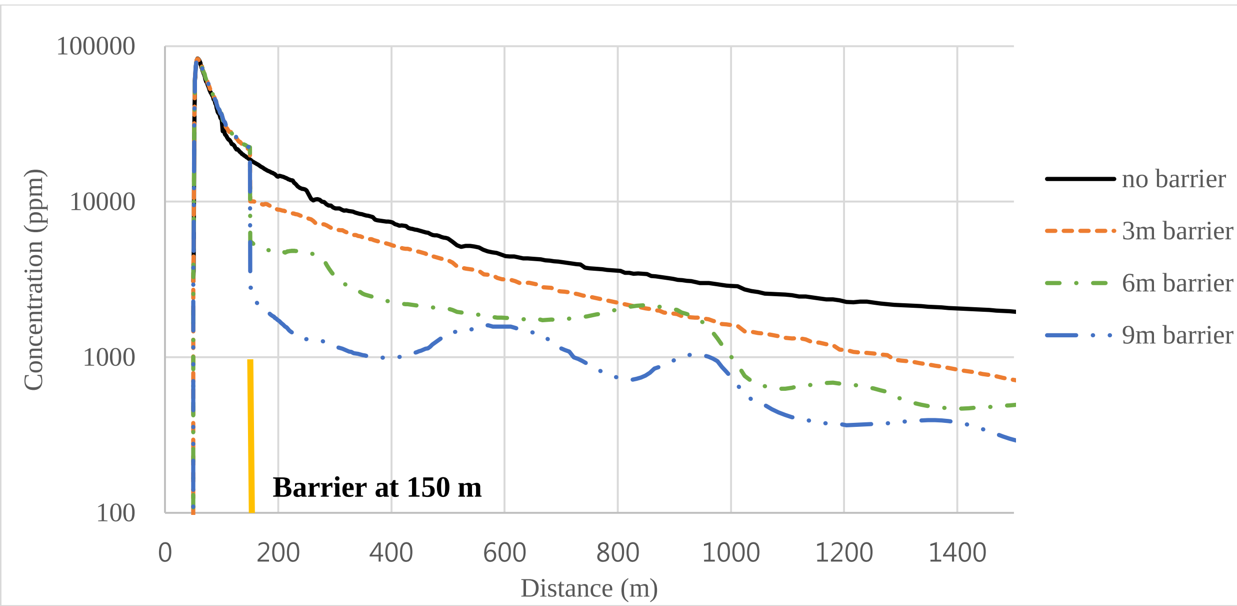

Figure 3. Concentration distribution according to barrier height about Goldfish test

Table 4. Values of the concentrations (upper) of hydrogen fluoride and mitigation rates (lower) according to barrier heights at certain distances in Goldfish test

`	Concentration (ppm)		
	at 100 m from the barrier	at 500 m from the barrier	at 1000 m from the barrier
No barrier	11800	4303	2394
3 m barrier	7880	2967	1241
6 m barrier	4738	1778	679
9 m barrier	1308	1437	379

	Mitigation effectiveness (%)			
	at 100 m from the barrier	at 500 m from the barrier	at 1000 m from the barrier	Average
3 m barrier	33.22	31.05	48.16	37.48
6 m barrier	59.85	58.68	71.64	63.39
9 m barrier	88.92	66.60	84.17	79.90

3.1.2 Comparison between values from Jack rabbit test and the simulation and the effects of the mitigation barrier

As with the Goldfish test simulation, the reliability of the Jack rabbit test simulation was secured through comparison with experimental values. The experimental values from JR 1 test 5, 6 shown in Table 2 presented above were used for the comparison. Since wind speeds have large effects on toxic gas concentration values according to distances, the data from the two tests conducted at different wind speeds were simulated with a view to securing higher reliability. However, Jack rabbit test was simulated not by releasing the gas at the experimental release point but by setting a model in which the entire recessed ground were used as a release hole where chlorine gas would evaporate referring to the paper published by Hanna et al.[x]

The results are presented in Figure 4 below as graphs and in Table 5 as numerical values. The test 5 simulation generally shows similar results with a small difference at the 500 m point. Unlike test 5 simulation, test 6 simulation showed smaller values than experimental values at points close to the release hole and larger than experimental values at points far from the release hole.

Table 5. Comparison of Chlorine concentration at 25, 50, 100, 300 and 500 m (The shaded columns contain

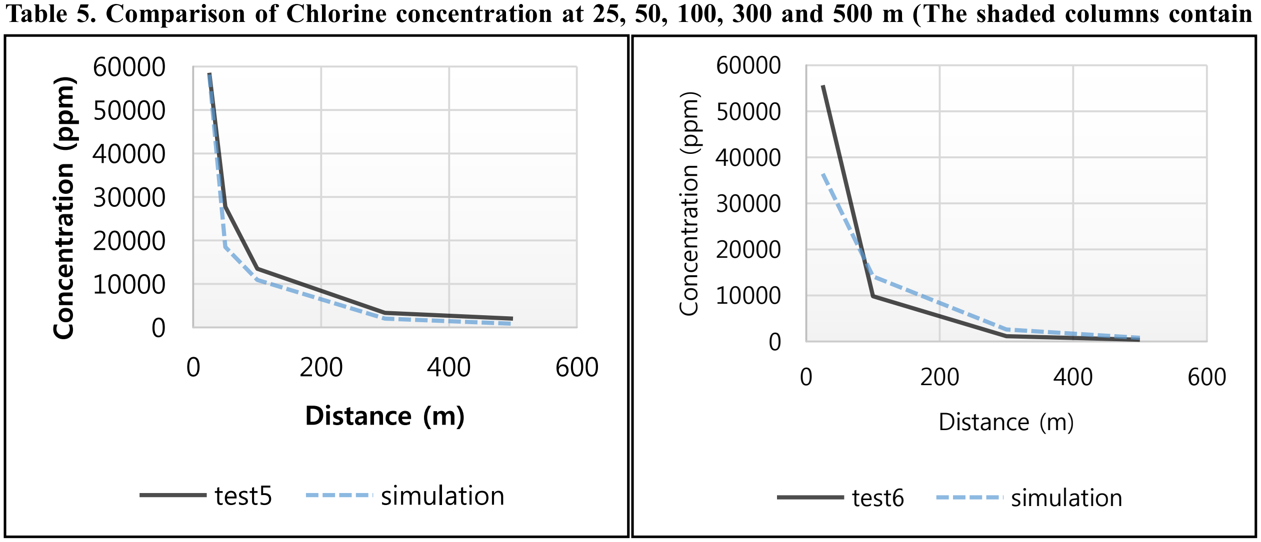

Figure 4. Comparison between values measured in Jack rabbit tests and values measured in the simulation

values with error rates not within the range of 50% ~ 200%.)

		Concentration (ppm)			
		Actual test #5	Simulation for test 5	Actual test #6	Simulation for test 6
Distance (m)	25	58600	58118	55600	36431
	50	27800	18495		
	100	13500	10926	9780	14098
	300	3410	2075	1100	2590
	500	2030	856	330	755

As with the Goldfish test simulation, condition change simulations were conducted to see the relationship between barrier heights and mitigation effects according to distances. In the simulations, 3 m, 6 m, and 9 m barriers were installed one at a time at a point 100m away from the release point in the x direction as with the Goldfish test simulation. Figure 5 shows concentrations in relation to distances and barrier heights with a graph. Table 6 below shows the values of the concentrations of chlorine and mitigation rates according to the heights of the mitigation barrier at certain points shown in the graph in Figure 5.

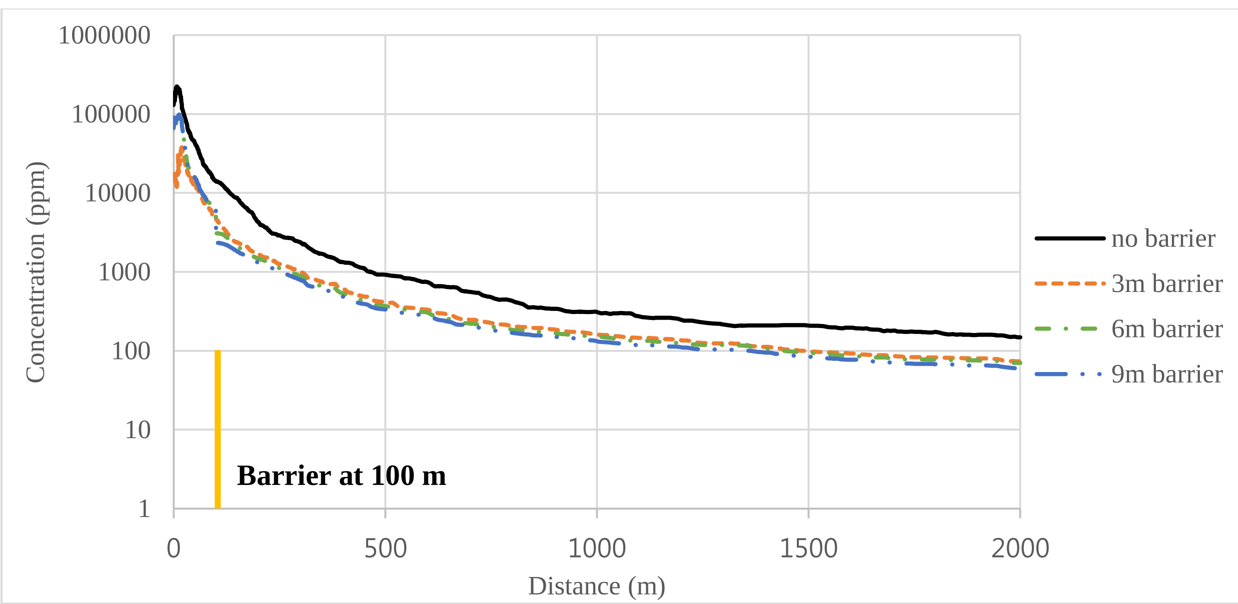

Figure 5. Concentration distribution according to barrier height about Jack rabbit test

Table 6. Values of the concentrations (upper) of chlorine and mitigation rates (lower) according to barrier heights at certain distances in Jack rabbit test

	Concentration (ppm)		
	at 100 m from the barrier	at 500 m from the barrier	at 1000 m from the barrier
No barrier	2916	645	262
3 m barrier	1261	282	142
6 m barrier	1115	250	130
9 m barrier	995	229	116

	Mitigation rate (%)			
	at 100 m from the barrier	at 500 m from the barrier	at 1000 m from the barrier	Average
3 m barrier	56.76	56.28	45.80	52.95
6 m barrier	61.76	61.24	50.38	57.79
9 m barrier	65.88	64.50	55.73	62.03

3.2 Changes in flows over time at the barrier

After identifying that the barrier has mitigating effects according to its heights, toxic gas diffusion flows over time were examined for a 9 m barrier, which is the highest in the simulation. Hydrogen fluoride diffusion flows were examined at 0.1, 0.5, 1.0, 2.0, 5.0, and 10 s and the results are as shown in Figure 6. Chlorine diffusion flows at 10, 30, 60, 180, 300, 600 s are shown in Figure 7. Through the figures, it can be seen that when toxic gases being diffused ran into the barrier, the flows began to move laterally instead of moving forward thereby diffusing the toxic gas faster leading general reduction in the concentration of the toxic gas. Consequently, the range of ERPG-2 concentrations will relatively decrease when a toxic gas accident has occurred and the range of occurrence of damage will also decrease. When an accident has occurred, along with reduction in the range of occurrence of damage, securing the time to evacuate is also an important issue. When there is a barrier, the forward diffusion flow speed will decrease when the diffusion flows have run into the barrier so that the time to evacuate can be secured.

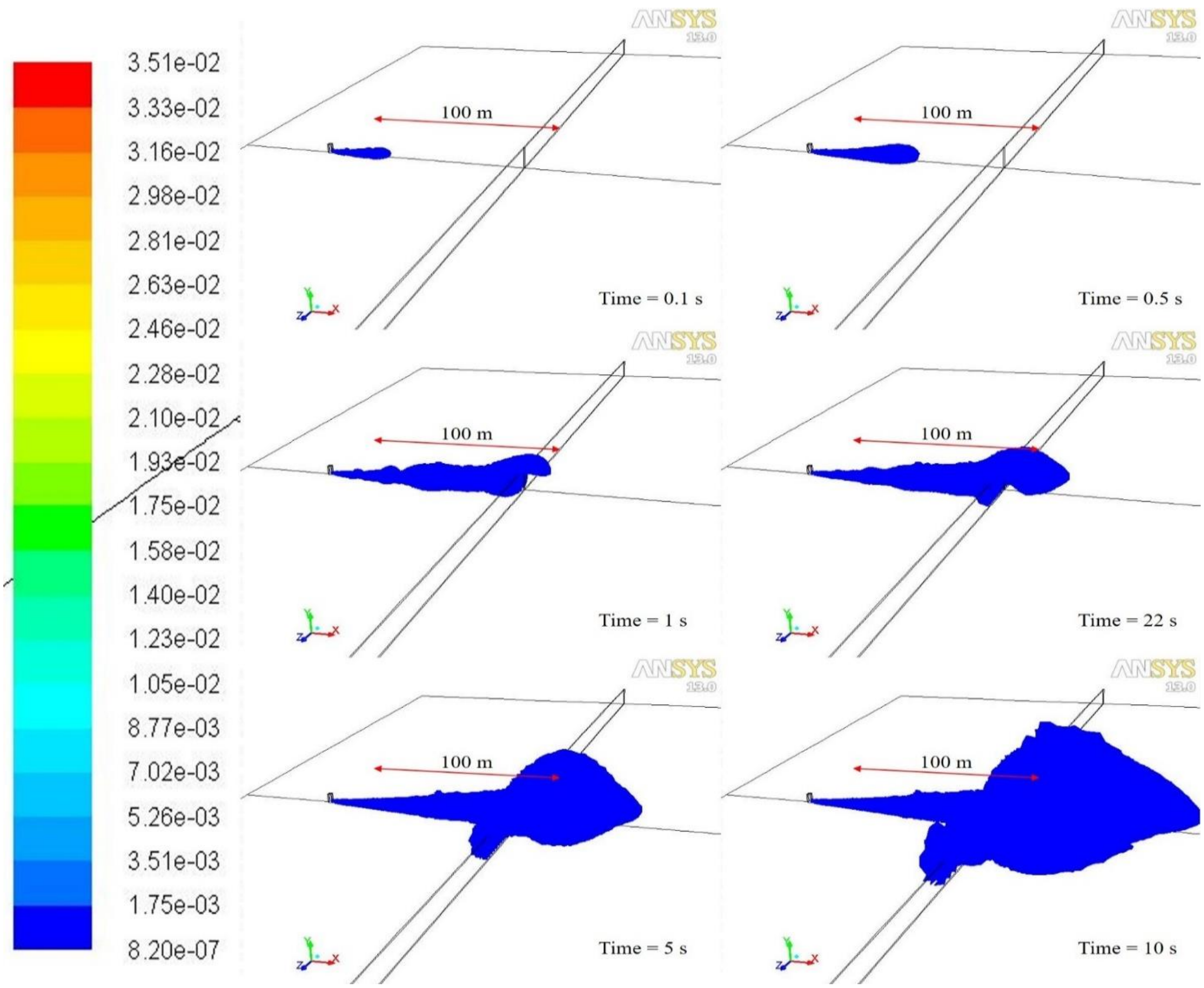

Figure 6. Distribution of the concentrations of ERPG - 2 in hydrogen fluoride over time (0.1, 0.5, 1.0, 2.0, 5.0 and 10 s) at the 9 m barrier

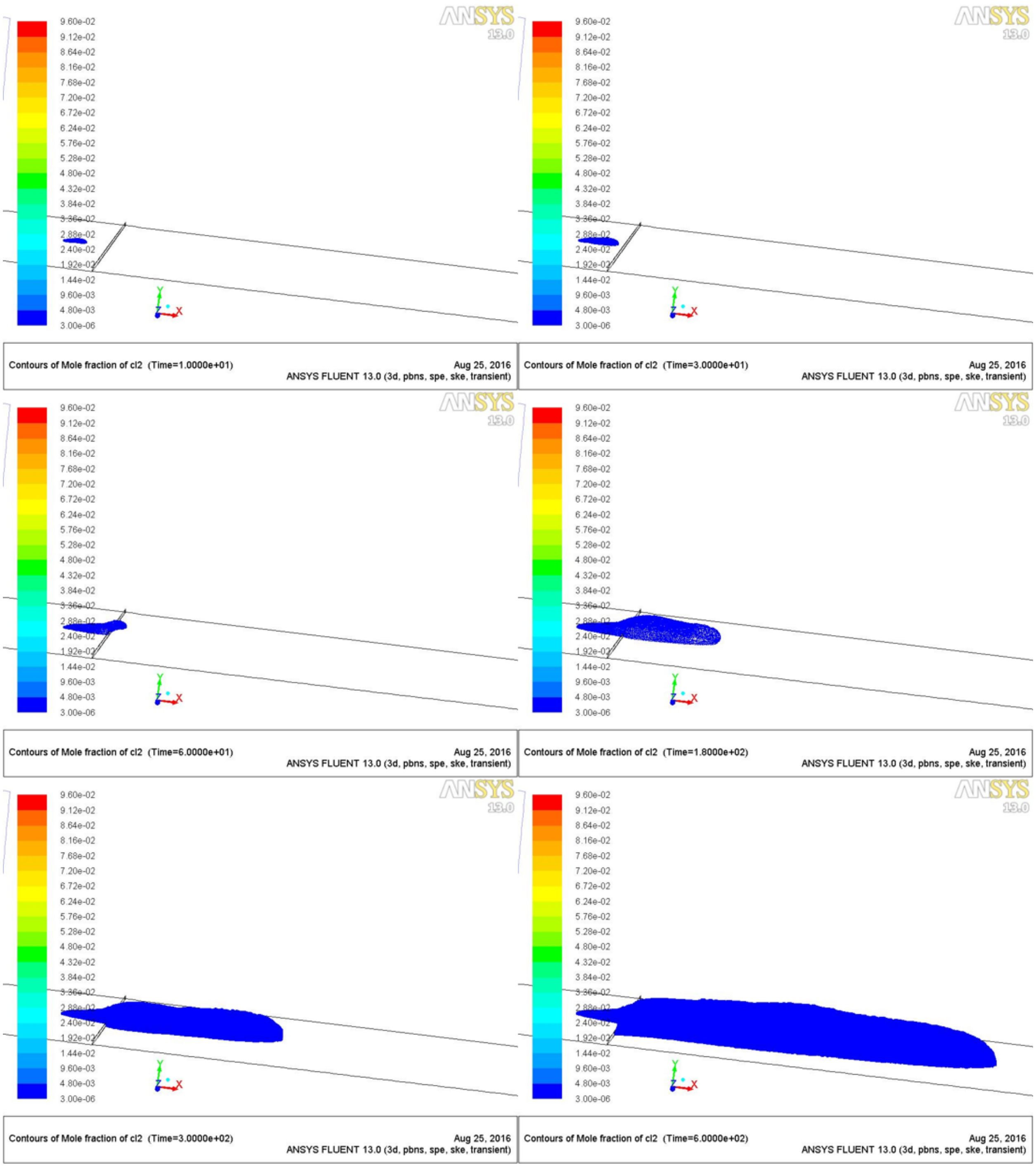

Figure 7. Distribution of the concentrations of ERPG - 2 in chlorine over time (10, 30, 60, 180, 300 and 600 s) at the 9 m barrier

Ⅳ. Discussion

Through the present study, it could be seen that higher physical barriers exert larger effects. In the case of hydrogen fluoride, 3 m, 6 m, and 9 m barriers showed mitigation effects of approximately 37%, 63%, and 80% respectively and in the case of chlorine, 3 m, 6 m, and 9 m barriers showed mitigation effects of approximately 53%, 58%, and 62% respectively. Therefore, the mitigation effects increased considerably along with increases in barrier heights in the case of hydrogen fluoride but did not increase very much along with increases in barrier heights in the case of chlorine although barrier per se had mitigation effects. This is considered attributable to differences in the specific gravity of the two substances, wind speeds, or in release modeling between the two simulations as hydrogen fluoride was horizontally released in the form of jet while chloride was vertically evaporated from the puddle. In the present study, many constraint conditions were assumed. First, in the tests, the toxic substances were released in two phases; liquid phase and gas phase. In both tests, the ratios of liquid substances were quite high as the ratio of liquid phase substances was approximately 80% while the ratio of liquid phase substances was approximately 20%. However, in the simulations, the entire substances were implemented as gas phase substances so that the toxic gases were released with very large momentum at the release point. Therefore, larger turbulence should have been formed and the results should have been affected. Furthermore, solar radiation and humidity were not considered. Therefore, the reactions of hydrogen fluoride with high reactivity with water were not considered and this is considered to have affected the results substantially. In addition, although analyses conducted through multiple experiments can improve reliability, in the present study, only one experiment was conducted. Therefore, the effects of mitigation systems will be verified with diverse substances and experiments and various mitigation systems currently in use or being studied will be examined later with a view to helping the construction of guidelines for effective facility layouts and design.

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