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Accident analysis of the Gumi hydrogen fluoride gas leak using CFD and comparison with post-accidental environmental impacts

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A B S T R A C T

This work uses computational fluid dynamics (CFD) to model the disastrous Gumi hydrogen fluoride gas leak of 2012. To ensure the model's validity, an anhydrous hydrogen fluoride leak field test was validated using a single-phase and two-phase dispersion model, and then compared with other dispersion models. When combined with the anhydrous ammonia leak test, the overall mean relative bias is 0.135 and mean relative square error is 0.068, which is within the valid range for dispersion simulation. The Gumi hydrogen fluoride gas leak disaster is then simulated and compared with the actual impacts. Human fatality occurred only in the plant and probability of death via toxic exposure shows a similar result. Toxic dose measurement by post-accidental vegetation fluoride concentration shows a similar range with CFD results for the downwind side.

1. Introduction

Toxic chemical leaks can cause severe damage to human beings and be disastrous for the environment. Studying past incidents is essential for understanding potential risks associated with toxic chemical leaks. This study uses computational fluid dynamics (CFD) to simulate the disastrous Gumi hydrogen fluoride gas leak of 2012 to compare simulated results with the actual damage it caused.

This 2012 hydrogen fluoride gas leak brought forward the need for a national awareness around chemical safety to make systematic changes in laws, regulations, business cultures and accident responses of organizations on a national level for chemical safety management. (Lee et al., 2016) The 'Chemicals Control Act' passed legislation by the Korean Ministry of Environment and entered into force on January 1, 2015. With this new act, any person who intends to install and operate a hazardous chemical handling facility is required to prepare an evaluation in advance on how a chemical accident caused by hazardous substances would affect the environment external to the place of business. This, therefore, evaluates the impact of a chemical accident on people and the environment. (Chemical Controls Act, Section 2, Article 23).

The purpose of this paper is to simulate the accident in Gumi and to compare it with the post-accidental data. To create realistic simulation settings, an anhydrous hydrogen fluoride dispersion field test named Goldfish was tested before running CFD as a real case to define practical parameter sets.

2. Anhydrous hydrogen fluoride dispersion field test validation

2.1. CFD validation outline

The CFD engine used in this study is a Flare Acceleration Simulator (FLACS) version 10.4. The FLACS has been validated against liquefied natural gas (LNG) dispersion field tests (Hansen et al., 2010), and various other gases (Hanna et al., 2004). Furthermore, an anhydrous ammonia field test was validated with Desert Tortoise data (Ichard, 2012). However, the Goldfish test, an anhydrous hydrogen fluoride field test has not yet been reported.

For validation purposes, statistical performance measures were used based on the LNG vapor dispersion model evaluation protocol (Ivings et al., 2013). The validation target was obtained using the maximum time-averaged concentration across an arc at a specified radius.

Mean Relative Bias (MRB):

$$MRB = \left\langle \frac{C_m - C_p}{\frac{1}{2}(C_m + C_p)} \right\rangle$$

Mean Relative Square Error (MRSE):

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$$\mathrm{MRSE} = \left\langle \frac{(C_m - C_p)^2}{\frac{1}{4}(C_m + C_p)^2} \right\rangle$$

where, C_m is Measured Concentration, C_p is Predicted concentration, and < … > represents the average over all measured pairs of concentrations.

2.2. Goldfish test discharge setting

In the Goldfish test report, GF3 test discharge rate by the time is shown. (Blewitt et al., 1987) This test was conducted under the constant pressure.

$$\dot{m}(t) = C_d A \sqrt{2\rho_f (p - p_a)}$$

Where, $\dot{m}(t)$: mass flow rate $\left(10.18\,\frac{\mathrm{kg}}{\mathrm{s}}\right)$

C_d : coefficient (0.62)

A : leak area $\left(4.60 \times 10^{-4} m^2\right)$

ρ_f : density of fluid $\left(956.503\,\frac{\mathrm{kg}}{m^3}\right)$

$p - p_a$: gauge pressure of the tank $\left(6.67 \times 10^5 \mathrm{Pa}\right)$

Fig. 1 shows this Bernoulli based method tested over the GF3 hydrogen tank weight, and showed that 168.8 gal/min and the measured value was 176.6 gal/min. The discrepancy is only 1.7%, making this a valid method.

2.3. Goldfish test validation simulation settings

The purpose of this field test validation is to find appropriate settings that can be applied to actual accidental cases and eventually to universal CFD calculations for any hypothetical scenario. Thus, high computational loads should be avoided; instead light, still valid model parameters are essential. A relatively rough grid of 10 m × 10 m × 3 m was used for a single-phase approach.

There are 3 sets of field tests for validation, namely GF1, GF2, and GF3. Data from GF4-6 was tested with a water curtain and it is not of interest for the purposes of this study. The result can be found in the field test report (Blewitt et al., 1987). Table 1 shows basic test input information.

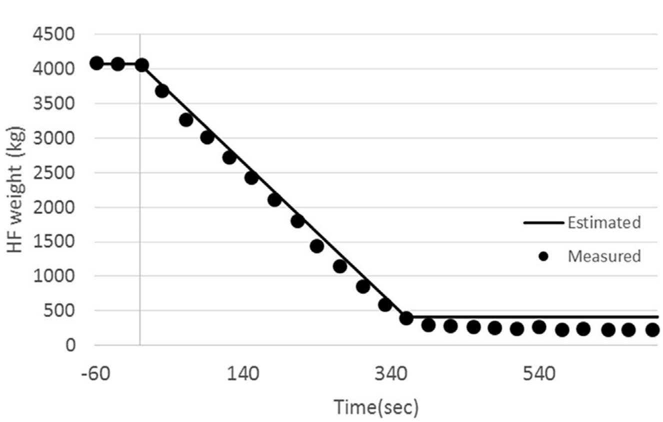

Fig. 1. Measured result and estimated result of GF3 test HF time vs. remaining weight.

Table 1
Goldfish anhydrous hydrogen fluoride gas leak experiment test information.

	UNIT	GF1	GF2	GF3
DATE		01-Aug-86	14-Aug-86	20-Aug-86
SPILL RATE	m^3/min	1.78	0.66	0.65
SPILL DURATION	min	125	360	360
WIND SPEED	m/s	5.6	4.2	5.4
TEMPERATURE	°C	37	36	26.5

For the dispersion result calculation, the single gas-phase leak and liquid-vapor leak were calculated. Single-phase dispersion calculation can run in parallel to a multi-core process. The Homogeneous Equilibrium Model (HEM) is a simpler modeling approach when it comes to two-phase chemical dispersion, which assumes local thermal and kinematic equilibrium. However, it cannot be computed in parallel with a FLACS engine.

2.4. Validation result

For the anhydrous ammonia field test, the Desert Tortoise was done in the same field in Nevada, USA. It was validated by Ichard's thesis (Ichard, 2012). The concentration sensor was at 300 m, 1000 m, and 3000 m; however the sensor at 3000 m did not catch the concentration peak of clouds in GF2. Like Ichard's thesis, only 300 m and 1000 m were tested. Table 2 shows the validation result. Out of the six validation points, single-phase simulation provides all six, and two-phase simulation provides five points within the factor of two. There was not much difference between the single-phase and two-phase simulation results. Thus, the single-phase simulation is set as the base case scenario and used in the validation result comparison and in the modeling of the hydrogen fluoride gas leak. The mean relative error was 0.336 and mean relative square error was 0.134. Therefore, it satisfies the $-0.4 < \mathrm{MRB} < 0.4$, and $\mathrm{MRSE} < 2.3$ criteria, meaning that the FLACS hydrogen fluoride dispersion model qualifies as a useful model (Ivings et al., 2013).

2.5. Comparison with other well-known dispersion models

The validity of the Goldfish and Desert Tortoise models are proven by those found in Hanna et al. (1991). Fig. 2 is the plot of mean relative bias (MRB) and mean relative square error (MRSE) for the result of two combined tests. FLACS has a MRB of 0.135 and MRSE of 0.068. It is near the origin, which means this CFD engine provides a good representation of the field test. The Britter and Mcquaid (B&M) model is the closest one among dispersions, but it is based on a set of simple equations and nomogram suggested in the 'Workbook on the Dispersion of Dense Gases', which fits curves

Table 2
Goldfish time averaged across an arc specified radius (Averaging time: 66.6 s).

	Position	Observed	FLACS (Single phase)	FLACS (Two phase)
GF1	300 m	25,473	18,628	15,070
GF1	1000 m	3098	2025	1895
GF2	300 m	19,396	13,131	12,120
GF2	1000 m	2392	1326	1073
GF3	300 m	18,596	16,565	15,795
GF3	1000 m	2492	2012	1662
		MRB	0.336	0.463
		MRSE	0.134	0.246

MRB: Mean Relative Bias.
MRSE: Mean Relative Square Error.