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# A study on effective mitigation system for accidental toxic gas releases

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A B S T R A C T

Hydrogen fluoride (HF) is a strong, pervious gas that acts as a stimulus for some parts of the human body, such as the respiratory system and the skin. HF is widely used as a polisher and disinfectant in electronics manufacturing. Safety considerations for using HF have been gaining interest after the accidental release of the HF in Gumi, South Korea, 2012, and studies have emphasized the importance of creating a management system for this gas. Chlorine is another widely used chemicals in the world, especially for water purification plants near populated areas.

In this study, ANSYS FLUENT, a computational fluid dynamics (CFD) program, is used to assess the efficiency of installing a physical barrier as a mitigation action against HF and chlorine leaks from industrial facilities. In a typical industrial facility, a barrier is usually set to separate the workplace from the outside environment, but it is not sufficient to prevent the release of hazardous substances outside the facility. Therefore, we analyzed the efficiency of various heights of physical barriers (3 m, 6 m, and 9 m) for mitigating toxic gas releases using simulation. The results of this study were compared to the experimental data obtained by Goldfish in 1986 to verify the results of HF. These results were also compared to the data obtained by Jack Rabbit in 2010 to verify the results of chlorine. The mitigation effectiveness factors of HF and chlorine were derived, and the results indicated that the increase in the barrier height decreases the concentrations of these gases in the surrounding area. In addition, it was proven that the proposed mitigation system can reduce the possibility of an offsite exposure to toxic gases in case of a release and enhance the effectiveness of the emergency plans.

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## 1. Introduction

Currently, the amount of toxic gases used in South Korea is increasing (with 39% annual average increase) as a result of the development in high-tech industries, such as semiconductor, LCD, and solar cell industries. However, following the Gumi Hube Global hydrogen fluoride release in 2012, concerns were raised about the safety measures involved in using toxic gases. Furthermore toxic gas accidents represent a large part (25%) of the total high pressure gas accidents that have occurred over the last six years (84 accidents), and the damage caused by these accidents was very severe. Therefore, there is a necessity for establishing systems to mitigate the impact of accidents involving toxic gas release.

Several models are currently utilized to predict possible toxic gas releases from tanks, containers, or pipes, in which toxic gases are stored at high pressure. However, these models rely on simple calculation formulas without considering the surrounding topography, situations, or barriers (Jung, 2016). In addition, they overestimate the values in case of long distances and underestimate the values in case of short distances from the release point (Qial and Zhang, 2010), (Van den Berg and Lannoy, 1993).

Considering the surrounding environment and conditions in the accident impact evaluation is still difficult. Therefore, models with more precise accident prediction are required for risk evaluation, because the released toxic gases can cover very long distances with far-reaching effects and are greatly affected by various variables, such as the surrounding topography, temperatures, and wind speed and direction. Thus, methods employing computational fluid dynamics (CFD) analysis, which can consider such conditions, were investigated.

Several studies investigated the actual gas dispersion and the effects of mitigation systems using various dispersion modeling techniques that employ CFD. Filippo Gavelli et al. studied the formation of LNG pools based on the ground characteristics using a CFD code called Fluent in addition to comparing and analyzing the effects of LNG when released on ground and water surfaces. The

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study revealed that LNG evaporation rates were higher in the case of LNG release on water surface (Gavelli and Kytomaa, 2008). A. Mack et al. analyzed the behavior of heavy gases using OpenFoam and verified the results through wind tunnel experiments and the commercial code (Fluent) (Mack and Spruijt, 2013). Further, P. Gousseau et al. compared and analyzed the performances of the RANS and LES turbulence models in predicting pollutant dispersion around buildings and found that the RANS model was faster compared to the LES model, but the LES model was more accurate, which helps in the selection of dispersion prediction models using CFD codes (Gousseau and van Heijst, 2011). Steven Hanna et al. studied and simulated the data from the chlorine release field experiments conducted by Jack Rabbit using the SLAB model (Hanna et al., 2012). On the other hand, Robert N. Meroney investigated various mitigation systems for heavy gas dispersion to determine the factors affecting the dispersion process, and formulated equations to predict the concentration results of dispersion (Meroney, 1991).

In the present study, the behaviors of hydrogen fluoride and chlorine when released were first simulated, analyzed to match with experiment results done by Goldfish (1986) and Jack Rabbit (2006) tests using Fluent. And then, the effects of physical barriers, based on their heights, on these behaviors were analyzed in addition.

## 2. CFD simulation

### 2.1. Simulation tool

Recently, the frequency of using CFD simulations in the analyses of accidental releases of inflammable or toxic gases from industrial facilities has been increasing in order to obtain more precise results. CFD software can predict the possibility of accidents over time while taking into consideration the surrounding topography in order to make the results closer to reality. The flame acceleration simulator (FLACS) of GexCon and the ANSYS Fluent are representative software suitable for evaluating the impacts of accidents. In the present study, the latter one, Fluent 13.0 of ANSYS Co., was used.

Fluent is a fluid flow analysis software that can analyze the entire flow area including incompressible, compressible, and transonic flows. In addition, it can analyze the diverse physical and chemical phenomena, such as laminar flows, turbulence, heat transfer, chemical reaction, and multiphase flow problems. Therefore, it is highly reliable and used in all sectors of flow analyses, such as process design and product design. In addition, GAMBIT 2.4.6, a dedicated grid generation software program, was used in the modeling of surrounding topography (ANSYS Inc., 2010).

### 2.2. Actual experiments used in validation(field test)

#### 2.2.1. Hydrogen fluoride release experiment (Goldfish test)

The first experiment modeled in this study is based on 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 experiment, pressurized liquid HF was released at a height of 1 m from the ground. HF gas was released 3 times under different conditions. The conditions used in the individual experiments are shown in Table 1. The experiments were conducted with no surrounding topography other than the experimental apparatuses, and the studied scenario was: releasing the gas through a 4-inch diameter line from a 5000 gallon tank. The concentrations of the released gases were measured using concentration sensors at points that are 300 m, 1000 m, and 3000 m away from the release point in the direction of the release (Hannaet al, 1991; 1993).

#### 2.2.2. Chlorine release experiment (Jack Rabbit test)

The chlorine release experiment was conducted in Dugway Proving Ground, Utah in 2010 with the support of the Department of Homeland Security-Transportation Security Administration and was called the Jack Rabbit Test. The released space was an approximately 2 m deep and 50 m diameter dug area, and the experimental substances were released at a 2 m height from the ground toward the bottom of the pit. In the Jack Rabbit test, many substances, such as ammonia were released along with chlorine, and the sensors were arranged in circles at various distances (25, 50, 100, 30 0, and 500 m, etc.) from the point of release to measure the concentrations of the substances. In the test, 1 or 2 tons of chlorine were released at different wind speeds ranging from 1.6 m/s to 6.2 m/s as shown in Table 2 (Hanna et al., 2012; 2016).

### 2.3. Numerical analysis model

#### 2.3.1. Governing equation

The governing equations of CFD simulations with 3D steady state incompressible turbulence flow are equation (1) and equation (2).

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{1}$$

$$\frac{\partial U_i}{\partial t} + U_j\frac{\partial U_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \nu\frac{\partial^2 U_i}{\partial x_i \partial x_j} - \frac{\partial}{\partial x_i}\left(\overline{u\prime_i u\prime_j}\right) \tag{2}$$

where $-\overline{u\prime_i u\prime_j}$ is defined as follows:

$$-\overline{u\prime_i u\prime_j} = \frac{\mu_t}{\rho}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}K \tag{3}$$

where $\mu_t$ is a turbulence viscosity coefficient that can be inferred through dimensionless analysis of flows with high Reynold's number. When the turbulence energy generation rate and dissipation rate are assumed to be almost in equilibrium, $\mu_t$ is expressed as follows:

$$\mu_t = f_\mu C_\mu \rho \frac{K^2}{\varepsilon} \tag{4}$$

where $f_u$ is a coefficient determined by the turbulence model. K and $\varepsilon$ are the turbulent kinetic energy and turbulent energy dissipation, respectively, and they can be determined by the K-$\varepsilon$ model. The standard k-epsilon model, which is the most commonly used, was employed for the simulation, and the SIMPLE algorithm was used as a scheme for speed and pressure coupling. (Kim and Yoon, 2003)

#### 2.3.2. Grid generation

The grids that are necessary for the simulations were generated using GAMBIT 2.4.6, a dedicated grid generation software program, and the mesh volume was specified by generating polygonal cells using the Tet/Hybrid tab. The fluid simulated was assumed to be a mixture of air and toxic gases. The optimum grid was found by conducting grid dependency simulation using 3 different grids within the range that does not affect the result.

In the first simulation, which analyzed the Goldfish test, the total volume of the studied area (3500 * 250 * 500 m$^3$) was simulated by modeling half of the studied area and then using symmetric conditions to simulate the total volume, because the left and right sides of the release point are symmetric. A 0.5 m thick barrier was installed vertically at a distance of 100 m in the x direction from the release point. In addition, the sizes of the grids closer to

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