Assessment of Dispersion Coefficients and Downward Positions of Water Spray for Small-Scale Release of Chlorine Gas

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Abstract - To assess downward positions of water spray for the small-scale release of chlorine gas, dispersion coefficients for the Gaussian dispersion model were validated at the small-scale release experiment. And the downwind distances of water spray were assessed with the simulated results. As results, the Gaussian plume model using the Briggs’ dispersion coefficient well estimated the dispersed characteristics for small-scale release of chlorine gas. The best adequate downwind position of water spray is the position of the maximum concentration of chlorine at the ground level. And the adequate vertical and horizontal dimensions of water spray consider the maximum width and height of cloud.

Key words : dispersion coefficient, water spray, chlorine, small-scale release, dispersion model

I. INTRODUCTION

Accidental dangerous release of toxic or flammable compounds can occur during process, storage or transportation, and can magnify serious risks to both people and property[1-3]. The mitigation of accidental release of dangerous toxic or flammable vapor cloud is a serious concern in industries.

The dispersion of these clouds can be controlled by using more or less expensive techniques as thermal inactivation, fans, specific foams, water or air sprays[4]. Recently, the water curtain is recognized as a useful technique to mitigate a heavy gas cloud[5]. Also, water sprays appear to be a good technique to mitigate heavy gas clouds and also for protection of small storages where other mitigation means are economically or technically unachievable[6].

The actions of water sprays are threefold, and consist mainly in reducing the density difference between the ambient air and the dense gas[7]. The mechanical dilution of the cloud by entrainment of the pollutant and ‘clean’ air in the spray consist in momentum exchange between the droplets and the gas phase[8]. And the forced dispersion of the toxic cloud is enhanced by physicochemical absorption of the pollutant in the water droplets and finally by cloud heating[6].

Effectiveness of the water spray depends on its own characteristics such as droplets distribution, types of nozzles, width and height, water pressure, etc. or extrinsic parameters, such as cloud features, gas nature, wind speed, atmospheric stability[6]. Generally, release experiments for toxic gases were carried out at large-scale release that is very lower likelihood and very higher accidental effect. But respectively small-scale release experiments, which are very lower accidental effect and very higher likelihood, were carried out nearly.

The Gaussian plume model is probably the most widely used one in estimating pollutant dispersion. Most parameters in the Gaussian plume equa-
tion are straightforward. However, this does not apply to plume rise or the dispersion coefficient, which seldom can be measured. One must often resort to the use of empirical formulae, of which many have been proposed. The influence of the lateral and vertical dispersion coefficients is assumed that no turbulence measurements are available[2]. Several well-known sets of empirical formulae for the dispersion coefficient are tested under different simulated dispersion conditions and results are compared. The comparison should necessarily be carried out between the concentrations computed with the dispersion coefficient scheme being tested and those obtained through a “model” or standard computation under identical atmospheric conditions. Because the general characteristics of our area prevent an ideal experiment with a single point source and flat ground, the latter approach has been used.

Therefore, dispersion coefficients for the Gaussian dispersion model could need to validate at small-scale release experiment. This paper gives results of validated dispersion coefficients for the Gaussian plume model at the small-scale release experiment and assessment of various downward distances of water spray.

II. THEORETICAL

2.1. Atmospheric stability and wind speed
A large number of parameters affect the dispersion of gases. These include atmospheric stability, wind speed, local terrain effects, height of the release above the ground, release geometry, momentum of the material released, buoyancy of the material released, etc.[9].

Weather conditions, especially atmospheric stability and wind speed, have a major influence on the extent of dispersion. Generally, atmospheric stability suggested to the Pasquill-Gifford Stability and Pasquill-Mohan-Siddiqui Stability. The Pasquill-Gifford Stability[10] considers an angle of sun and the Pasquill-Mohan-Siddiqui Stability[11] considers a radiation of sun.

Also, a wind speed with a release height used Hanna’s formula[12].

\[ u_z = u_{10} \left( \frac{z}{10} \right)^p \]  \hspace{1cm} (1)

where \( u_z \) (m/s) is a wind speed at \( z \) height and \( p \) is a power coefficient (-) which is a function of atmospheric stability and surface roughness.

2.2. Gaussian plume model
The Gaussian plume model describes a continuous release of material. The solution depends on the rate of release, the atmospheric conditions, the height of the release above the ground, and the distance from the release. In its simplest form, the Gaussian plume equation for the average concentration for this case is:

\[
< C > (x,y,z) = \frac{G}{2\pi\sigma_y\sigma_z u} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \times \\
\left\{ \exp \left[ -\frac{1}{2} \left( \frac{z-H}{\sigma_z} \right)^2 \right] + \exp \left[ -\frac{1}{2} \left( \frac{z+H}{\sigma_z} \right)^2 \right] \right\} \] \hspace{1cm} (2)

where \( < C > (x,y,z) \) is the average concentration, \( G \) is the continuous release rate (kg/s), \( u \) is the wind speed (m/s), \( \sigma_y \) and \( \sigma_z \) are the dispersion coefficients in the \( y \) and \( z \) directions (m), \( H \) is the height of the source above the ground level plus plume rise (m), \( y \) is the cross-wind direction (m), and \( z \) is the distance above the ground (m).

Generally, various dispersion coefficients are suggested. This paper used various dispersion coefficients appeared on Briggs[13], Pasquill-Gifford[14], Burt[15], and Vogt[16].

III. RESULTS AND DISCUSSION

3.1. Suitability of dispersion coefficients for small-scale release of chlorine gas
This study adopted the experimental results for the small-scale release of chlorine gas by Dandrieux et al.[17] at Champclauson(Gard, France). Especially, experimental results of trials 3 and 4 were carried out at similar meteorological conditions. This study assessed the suitability of various dispersion coefficients at experimental result of trials 3 in absence of the water curtain. The ex-
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Table 1. Experimental conditions (meteorological conditions and release rates)[17]

| Classification                      | Distance (m) |
|-------------------------------------|--------------|
|                                     | 5 | 10 | 15 |
| Experimental (by Dandrieux et al.[17]) | 488 | 54 | 17 |
| Dandrieux et al.[17]                | 13 | 7  | 5  |
| UIC A                               | 754 | 189 | 84 |
| UIC B                               | 284 | 90  | 46 |
| DN                                  | 233,000 | 54,000 | 27,000 |
| ALOHA A                             | 218,000 | 50,500 | 25,400 |
| This study                          | 419 | 117 | 53 |
| Briggs A                            | 732 | 251 | 118 |
| Briggs B                            | 394 | 118 | 51 |
| Vogt A                              | 372 | 111 | 51 |
| Vogt B                              | 15,354 | 7,755 | 3,677 |
| Pasquill-Gifford A                  | 29,073 | 10,362 | 5,131 |
| Pasquill-Gifford B                  | 15,747 | 5,167 | 2,515 |
| Pasquill-Gifford & Burt A           | 29,163 | 10,429 | 5,161 |

Table 2. Comparisons of experimental and theoretical concentrations of chlorine gas [unit : ppm]

| Classification                      | Distance (m) |
|-------------------------------------|--------------|
|                                     | 5 | 10 | 15 |

Experimental conditions for trials 3 and 4 are shown in Table 1.

At meteorological conditions of trial 3, there were two stability categories A and B by the Pasquill-Mohan-Siddiqui[11]. Therefore power coefficient is 0.07, respectively, and wind speed was calculated 1.59 m/s by equation (1). Also, the average concentrations with downward distance were calculated by equation (2) for various dispersion coefficients that indicated by Briggs, Pasquill-Gifford, Burt, Vogt, and combined Paquill-Gifford & Burt[2].

Dandrieux et al.[17] calculated the average concentration with downward distance of chlorine gas by the software ALHOA (Areal Locations of Hazardous Atmospheres) Ver. 5.0 based on the DEGA-DIS (Dense Gas Dispersion) model and Gaussian
The results of this study and Dandrieux et al. are shown in Table 2. The predicted results very differ from various dispersion coefficients and dispersion models. Carrascal et al.[2] recommended the use of several sets of standard deviations to study dispersion because of large differences in the predictions according to the chosen parameterization.

The ALOHA DEGADIS model predicts concentrations far higher than those measured for distances. The main reason for this discrepancy between experimental and calculated concentrations is that the model may not be appropriate for the distances used in this study that are considerably lower than 100 m and it may not be validated for such short distances[17].

The UIC A of Gaussian model predicts concentrations far lower than those measured for distances and UIC B of Gaussian model predicts concentrations far higher than those measured for distances. And the Pasquill-Gifford and Pasquill-Gifford & Burt of the Gaussian model predicts concentrations far higher than those measured for distances.

Comparison of various dispersion coefficients (excepted the aforementioned it) of the Gaussian model is shown in Fig. 1.

At Fig. 1, with meteorological stability classes (A, B), dispersion coefficients of Briggs are far sensitive than dispersion coefficients of Vogt and DN. Also, dispersion coefficients of Briggs, Vogt, and DN are similar suitability near the source. Therefore, as the results, we found that the dispersion of chlorine gas was fairly varied with dispersion coefficient and meteorological stability and that chlorine concentrations were well estimated by the Gaussian plume model using the Briggs’ dispersion coefficient and meteorological stability class A.

3.2. Assessment of downward position of water spray

Using the Briggs’ dispersion coefficient from the results of part 3.1, first we calculated the average concentrations with downward distances of chlorine gas at the ground level for trial 4. At aforementioned conditions, the calculated average concentration profile with downward distance is shown in Fig. 2.

As presented in Fig. 2, the calculated concentrations of chlorine nearby source show steep increase; thereafter its tendency with downward dis-
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Fig. 3. The calculated 3D profile with IDLH of chlorine.

...tance shows exponential decrease. At the ground level, the maximum concentration of chlorine and downwind distance are 1176 ppm and 2 m, respectively.

To assess downward positions of water spray, we calculated the 3-distances (downwind, crosswind and above the ground) with IDLH (immediately dangerous to life or health) of chlorine, which is 10 ppm. At aforementioned conditions, the calculated 3-distance profiles with IDLH are shown in Fig. 3.

In Fig. 3, the maximum downward distance of IDLH is 35 m. And the maximum crosswind distance and maximum distance above the ground level are about 10 and 6 m at 21 m of downwind distance, respectively. Also, the width and the height of chlorine cloud are 2 and 1.8 m at 2 m (downward distance at the maximum concentration of chlorine), respectively.

Also, the water curtain (trial 4) by Dandrieux et al.[17] is a peacoak tail spray (Pons DSP65). Water is thus directed upwards, forming a fan. The flow rate of water was measured and found to be equal to an average of 0.730 kl/min, with a functioning pressure of 8 bars. Its vertical and horizontal dimensions are 8 and 20 m, respectively. Therefore, at 4 m of downwind distance, we calculated the width and the height of chlorine for IDLH. Thus, the width and the height of chlorine are about 4 and 2.7 m, respectively.

Therefore, because the maximum width and height appeared at 21 m, the vertical and horizontal dimensions of water spray must be, respectively, 6 and 10 m at least. And, at 4 m of downwind distance, the vertical and horizontal dimensions of water spray must be, respectively, 2.7 and 4 m at least. Also, because of the maximum concentration of chlorine at 2 m, the vertical and horizontal dimensions of water spray must be, respectively, 1.8 and 2 m at least. From aforementioned results, we found that downwind position of water spray over 21 m is inadequate and the best adequate downwind position of water spray is 2 m.

IV. CONCLUSIONS

To assess downwind position of water spray for the small-scale release of chlorine gas, dispersion coefficients for the Gaussian dispersion model were validated at small-scale release experiment. And downwind distances of water spray with simulated results were assessed. The results were as follows:

(1) The dispersion of chlorine gas was fairly varied with dispersion coefficient and meteorological stability and that chlorine concentrations were well estimated by the Gaussian plume model using Briggs’ dispersion coefficient.

(2) The best adequate downwind position of water spray is the position of the maximum concentration of chlorine at the ground level.

(3) The adequate vertical and horizontal dimensions of water spray consider the maximum width and height of cloud.

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