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A modified steady-state model for evaluation of ammonia concentrations behind a water curtain

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ABSTRACT

Water curtain system has been proved an effective mitigation measurement for ammonia spill dispersion. Calculating of ammonia cloud concentration with water curtain was less studied. This paper presents a steady-state calculation model to calculate open and forced ammonia spill dispersion. The formula of ammonia absorption was built and integrated into the calculation model. The calculated downwind ammonia concentrations for open and forced spill dispersion were reproduced and compared with literature using a statistical method. In addition, the relationship between ammonia concentration in water droplet and the droplet diameter was studied. The results display that the formula of ammonia absorption is suitable for calculating mass transfer process between the ammonia cloud and the water curtain. The calculation model presents good performances for open and forced ammonia spill dispersion. This study indicates that the calculation model can be satisfactory in determining the impact of open and forced ammonia spill dispersion and the design of water curtain mitigation system.

1. Introduction

As a common cooling agent, ammonia is frequently used in the chemical industry. Being a toxic gas, the potential public consequence from an accidental ammonia release is very serious due to the increasing transportation and storage of ammonia. Water curtain mitigation system has been recognized as one of the most effective and economic mitigation measurement for accidental chemical gas spill dispersion (Hald et al., 2003; Rana, 2008; Rana et al., 2010). The effectiveness of water mitigation system mainly depends on mass, momentum and heat exchange between gas cloud and water curtain. However, for the water-soluble gas, such as ammonia (the solubility of ammonia is 530 g/L at 25 °C), the mass transfer mechanism between gas cloud and water droplets was less studied.

Several mathematical models have been built for calculating the gas concentrations behind water curtains. Moore and Rees (1981) built a model based on the hydrodynamics of the water sprays. The model does not take physic-chemical absorption, initial jet process, and atmospheric stability into account. Dandrieux-Bony et al. (2005) modified the model by taking the initial jet process and atmospheric stability into account to calculate the chlorine concentrations and was named RED model. Diaz-Ovalle et al. (2012) developed a simplified steady-state model based on momentum, heat and mass transfers between the cloud and the environment. But, this model has large errors with the CFD simulation. Palazzi, Curro', & Fabiano (2007) developed an n-Compartment mathematical model for transient behavior of water curtain in mitigating an accidental chlorine spill dispersion. Most of the mathematical models were built for chlorine or heavy gas cloud release dispersion. However, the model for calculating ammonia concentration behind water curtain has not been reported in literature. Since ammonia is water-soluble gas, the influence of ammonia absorption should not be neglected.

In this paper a steady-state model for evaluation of open and forced ammonia spill dispersion was built based on RED model. The formula of ammonia absorption was built using the two-film theory and integrated into the model by a factor $\sqrt{R}$ (R is the ammonia concentration in water droplet). First, the ammonia concentrations in water droplets were compared with experimental results to validate the ammonia absorption model. Then, the calculated concentrations of open and forced ammonia spill dispersion were validated with experimental results. Finally, the potential and the limitations of the calculation model were evaluated.

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2. Theoretical modeling based on existing model

RED model was developed by Dandrieux-Bony et al. (2005) based on the hydrodynamics of the water curtain, especially on air entrainment in the water curtain which can be either measured or calculated (Briffa and Dombrowski, 1966; Heskestad et al., 1976; McQuaid, 1975). In RED model, three zones are defined: the first one before the water curtain (open field dispersion), the second one where the cloud interacts with the water curtain, and the third zone where the dispersion of the plume is again due to atmospheric turbulences (open field dispersion) (Seen in Fig. 1). RED model was built to calculate open and forced chlorine spill dispersion as shown in Eq. (1).

$$C(x) = \frac{Q}{\pi u(x)} \frac{1}{r^2(x)} \tag{1}$$

where $C(x)$ is gas concentration in x m location, Q is gas release rate, $u(x)$ is wind speed in x m location, $r(x)$ is the gas cloud radius in x m location. r can be calculated as follow.

$$\text{Zone 1}: r = r_o + c_{atm}\, x$$

$$\text{Zone 2}: r = r_o + c_{atm}\, x_2 + \left(\frac{c_s v_a D_w}{u(x_2)}\right)$$

$$\text{Zone 3}: r = r_o + c_{atm}\, x + \left(\frac{c_s v_a D_w}{u(x_2)}\right)$$

The polynomial expression r contains the diameter of release source r_o, the atmospheric dispersion parameter c_{atm}, the air entrainment coefficient c_s et al. The model does not take the gas absorption into consideration due to the low solubility of chlorine in water (7.3 g/L). However, the solubility of ammonia in water is very high (the solubility of ammonia is 530 g/L at 25 °C), the effect of ammonia absorption cannot be neglected. For considering the effect of ammonia absorption, the formula of ammonia absorption should be integrated into the polynomial expression r.

The mass transfer between ammonia cloud and water droplets can be calculated using "two-film theory" (Cheng et al., 2014). The mass transfer coefficient k_Y can be calculated using the Eq. (2) (Harriott, 1962).

$$\frac{k_Y d_p}{D} = 2 + 0.6\mathrm{Re}^{1/2}\mathrm{Sc}^{1/3} \tag{2}$$

where $Re = d_p v/\nu_g$, $\mathrm{Sc} = \nu_g/D$, d_p is the diameter of water droplet, D is the molecular diffusivity coefficient, v is the velocity of water droplet, ν_g is the Kinematic viscosity of air.

Considering an ideal behavior, the water drops were assumed to be spherical and have a constant density, specific heat, constant

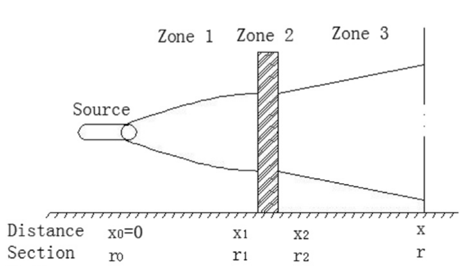

Fig. 1. Schematic representation of the dispersion process in presence of a water curtain. (From the work of Dandrieux-Bony et al. (2005)).

diameter. The mass of ammonia absorption into a water droplet during the duration of the water droplet movement from the nozzle exit to falling on the ground can be calculated as the Eq. (3).

$$m_p = 0.001 k_Y A_p M_{NH3} C_{vap} T \tag{3}$$

$$C_{vap} = (p_{atm} c_a)/(8.314 T_{atm}) \tag{4}$$

$$A_p = \pi d_p^2 \tag{5}$$

where C_{vap} is the mole concentration of ammonia in air, M_{NH3} is the mole mass of ammonia, T_{atm} is atmospheric temperature, c_a is the mole fraction of ammonia in air, p_{atm} is the atmospheric pressure, T is duration of water droplets in the ammonia cloud. For an upward nozzle, the movement of water droplets can be simplified as uniform accelerated motion and the T can be calculated as Eq. (6).

$$T = 2h/v_o \tag{6}$$

where h is the height of water curtain, v_o is the initial velocity of water droplet.

The ammonia concentration in water droplet can be calculated as follow.

$$R = m_p/m_w \tag{7}$$

where m_w is the mass of a water droplet.

The ammonia concentration in water droplet R provides an indicator of ammonia absorption. The coefficient R is assessed and the factor $\sqrt{R}$ represents acceptable agreement with experimental results. So, the modified polynomial expression r is expressed as follow.

$$\text{Zone 1}: r = r_o + c_{atm}\, x$$

$$\text{Zone 2}: r = r_o + c_{atm}\, x_2 + \left(\frac{c_s v_a D_w}{u(x_2)}\right) + \sqrt{R}$$

$$\text{Zone 3}: r = r_o + c_{atm}\, x + \left(\frac{c_s v_a D_w}{u(x_2)}\right) + \sqrt{R}$$

3. Assessment of the model parameters

3.1. Assessment of the coefficient c_{atm}

Due to the different physical properties between chlorine and ammonia, the atmospheric dispersion parameters c_{atm} built by Turner, D.B. (1994) used for open and forced chlorine dispersion is not suitable for open and forced ammonia dispersion. So, a set of new coefficient c_{atm} is estimated with a set of atmospheric dispersion parameter built by Briggs (1973) for short distance (50 m). The c_{atm} can be assessed for each stability class and for different distances, as shown in Table 1.

3.2. Assessment of air entrainment velocity v_a

Based on the literature (Dandrieux-Bony et al., 2005), air entrainment velocity in the water curtain v_a is deduced from the total entrained air Q_a with Eq. (8) (Briffa and Dombrowski, 1966; Heskestad et al., 1976; McQuaid, 1975, 1976; Rasbah and Stark, 1962). The Q_a can be obtained from a correction of the ratio of the volumetric air rate to volumetric water rate as function of "Flow number" (Atallah et al., 1988).