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Consequence analysis of aqueous ammonia spill using computational fluid dynamics

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ABSTRACT

A mathematical model to calculate the dimensions of toxic impact zones due to evaporation from the aqueous ammonia emergency spill surface is presented. The mathematical model is based on the numerical solution of mass, momentum, species, and energy transport equations. The computational procedure was implemented by using FLUENT program. The special feature of the model proposed in this manuscript is the ability to calculate simultaneously both binary solution pool evaporation and gas dispersion. The evaporation model takes into account the nonstationarity of pool evaporation process due to changes of liquid composition and temperature. The additional equations were implemented in FLUENT program by means of user-defined functions (UDF). A numerical analysis of the wind speed and obstacle influence on the evaporation characteristics and toxic dose distribution is carried out.

1. Introduction

A consequence analysis of accidental spills of toxic and flammable liquids is based on the use of the mathematical models describing the evaporation of hazardous substance from the pool surface and its advective-diffusive transport in the atmosphere. Most of the research has been focused either on the gas dispersion or the pool evaporation as two separate problems. There are many papers such as (Blocken, Stathopoulos, Saathof, & Wang, 2008; Labovsky, & Jelemensky, 2010; Santos, Reis, Goulart, & Mavroidis, 2009; Tauseef, Rashtchian, & Abbasi, 2011; Tominaga & Stathopoulos, 2010) devoted to the investigation of gas dispersion in the atmosphere. In some papers the models to describe the evaporation of pure (Brighton, 1990; Desoutter, Habchi, Cuenot, & Poinsot, 2009), binary solution (Leonelli, Stramigioli, & Spadoni, 1994; Mikesell, Buckland, Diaz, & Kives, 1991) and multicomponent liquids (Cavanaugh, Siegell, & Steinberg, 1994; Fingas, 2004; Okamoto, Watanabe, Hagimoto, Miva, & Ohtani, 2010; Smith, 2011) are considered. In such studies the researchers isolated specific physical phenomena and developed ad-hoc models that were not interconnected to describe the complete phenomenology (Brambilla & Manca, 2009).

There are some models that describe a series of events and processes accompanying the accidental release. In the paper (Brambilla & Manca, 2009) the modeling of accidents involving spreading, evaporation and burning of liquid pools by using semi-analytical and semi-empirical equations is considered. This model only laid down the input data of the gas dispersion module. The computational fluid dynamics (CFD) model FLACS (Hansen, Melheim, & Storvik, 2007) deserves special attention. In this methodology the dispersion of the two phase jet, the rain-out, the pool spreading and evaporation are modeled. The CFD model is presented in the paper (Galeev, Starovoytova, & Ponikarov, 2012) which describes the dynamics of toxic cloud formation during instantaneous release of liquefied ammonia by interconnecting and tackling the different phenomena, viz. the evaporation of aerosol in the cloud, vaporization during boiling and evaporation of pool, dispersion of gas with droplets in the atmosphere, water vapor condensation in the cloud. Abovementioned complex models do not account for multicomponent releases and spills. In the work (Pontiggia, Derudi, Alba, Scaioni, & Rota, 2010) the results of CFD modeling of 10% w/w aqueous ammonia spill consequences in urban terrain are presented. However, in this study the computation of pool evaporation was made without taking into account the changes in the liquid composition and temperature.

The accurate estimation of the evaporation rate from multicomponent liquid spills is important to provide reliable estimates of the toxic impact zones or sizes of the flammable cloud. Most of

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the existing evaporation models are based on the use of expression (Kawamura & Mackay, 1987):

$$\frac{dm_g}{dt} = -\frac{k_g \cdot M_g \cdot P_{g,s}\left(X_g, T_{liq}\right)}{R_0 T_{liq}} \quad (1)$$

where mass transfer coefficient k_g is calculated according to the relation:

$$k_g = 0.0048 \cdot U^{0.78} \cdot d^{-0.11} \cdot Sc^{-0.67} \quad (2)$$

The Equations (1) and (2) do not take the influence of a number of effects on the evaporation into account:

- the changing of the driving force of the evaporation due to changes of liquid composition or the accumulation of the evaporating component above the pool;
- the changing in the turbulent structure of the flow over the spill surface when the evaporating component has molecular weight of M_g, which differs from the molecular weight of environment air M_a. When $M_g < M_a$ the density-driven convection may take place and that accelerates the evaporation (Dil'man, Lotkhov, Kulov, & Naidenov, 2000; McBain, Suehrcke, & Harris, 2000), and when $M_g > M_a$ the suppression of turbulence and the evaporation reduction due to the effect of stable stratification may be observed (Desoutter et al., 2009);
- the degree of stability of the atmosphere;
- the presence of buildings, fences, height difference in terrain.

Taking into consideration the above, the spill evaporation process depends on a great amount of factors that, in aggregate, are extremely problematic to be taken into account in simplified analytical and empirical relationships. Therefore, to solve this problem the using of numerical simulation method is preferable.

In this paper the CFD model is presented to determine the toxic impact zones due to the evaporation from the aqueous ammonia pool surface. An aqueous ammonia solution is widely used in chemical industry. Ammonia water is mainly used to produce nitrogen fertilizers (nitrate and ammonium sulfate, urea), as well as for the production of nitric acid, soda, polymers and production of explosives and other chemical products. The process of aqueous ammonia solution evaporation is transient in nature due to changes in the liquid composition and temperature.

The feature of the model proposed in this manuscript is the ability to calculate simultaneously both binary solution pool evaporation and gas dispersion. The mass flow rate from the pool surface was determined using standard wall functions and taking the correction for Stefan flow into account. The heat balance equation for the liquid layer was introduced into the model to take the heat and mass transfer coupling into account. For discretization of the differential equations a control volume approach implemented in the FLUENT code was used.

The influence of the wind speed and obstacle presence on the characteristics of evaporation and toxic dose distribution was investigated.

2. Mathematical model

2.1. The mathematical model of evaporation

When developing the model of evaporation from the spill of aqueous ammonia solution the following assumptions have been made:

- the liquid is assumed to be well-mixed in the layer height;
- the free surface of the liquid during evaporation is motionless;
- evaporation of water from pool is not taken into account.

The latter assumption is reasonable because in the initial period of the evaporation the water vapor partial pressure at the interface an order of magnitude lower than the partial pressure of dissolved gas. In addition, the presence of the certain amount of water vapor in the ambient air reduces the driving force for the water evaporation.

The concentration of the ammonia on the pool surface was calculated on the basis of the hypothesis of the thermodynamic equilibrium between liquid and vapor at the interface. Thus, the mole fraction of component at the interface is:

$$Y_{g,s} = \frac{P_{g,s}\left(X_g, T_{liq}\right)}{P_0}. \quad (3)$$

The partial pressures of ammonia $P_{g,w}$ above the surface of the aqueous ammonia solution depending on the temperature T_{liq} and the ammonia mass fraction in the liquid X_g are given in Table 1.

The partial pressure at intermediate values of temperature and mass fraction of ammonia in solution were calculated by linear interpolation.

The evaporation rate of ammonia from the spill surface has been calculated on the basis of the standard wall functions (Fluent, 2006) taking into account the correction for Stefan flow (Law, 2006, Chapter 6; O'Rourke & Amsden, 1996) (convective flow of the gas-vapor mixture, induced by the diffusion of component at the impermeable interface and directed from the liquid surface into the gas-vapor medium):

$$J_{g,s} = K\frac{(Y_{g,s} - Y_{g,P})\rho C_\mu^{0.25} k_P^{0.5}}{Y^+}; \quad (4)$$

$$Y^+ = \begin{cases} Sc \cdot y^+ & (y^+ < y_C^+) \\ Sc_t(u^+ + P_C) & (y^+ > y_C^+) \end{cases}; \quad (5)$$

$$y^+ = \frac{\rho C_\mu^{0.25} k_P^{0.5} y_P}{\mu}; \quad (6)$$

$$u^+ = \frac{1}{\kappa}\ln\left(Ey^+\right) - \Delta B; \quad (7)$$

Table 1
The partial pressures of ammonia $P_{g,s}$ above the surface of the aqueous ammonia solution (Pa) (Wilson, 1925).

Temperature, °C	Ammonia content in aqueous solution X_g, (% by weight)					
	4.74	9.5	14.29	19.1	23.94	28.81
0	758	2758	6205	10,411	17,513	28,544
4.4	1516	3999	7860	13,238	21,787	35,370
10	3240	6136	10,411	17,444	28,682	45,712
15.5	4274	8205	13,789	22,822	36,956	58,467
21.1	5722	9101	18,547	29,509	45,988	74,188
26.6	7308	13,652	23,028	37,576	59,915	93,217
32.2	9377	17,375	29,303	47,436	75,084	115,487
37.7	11,859	22,063	36,818	59,295	93,286	142,583