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Are dispersion models suitable for simulating small gaseous chlorine releases?

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Abstract

Dispersion models are mostly validated on the basis of historical dispersion experiments. The latter imply large quantities of hazardous products (flammable or toxic gases), and are dedicated to study the dispersion of the resulting clouds on great distances from the source to reach a better knowledge of the different phases of gas dispersion (slumping, creeping, passive dispersion…).

However, dispersion models have hardly been validated on small releases and therefore require more validation on small plumes of dangerous gases. Indeed, what is their reliability in case of accidents involving small amounts (e.g., chlorine leakages at swimming pools' installations), and for small distances downwind the gas source? This information is of prime interest in so far as small releases are more likely to occur than larger ones.

This paper reports on chlorine small-scale dispersion experiments and deals with the comparison between experimental data of ground level concentrations in the plume and predicted concentrations obtained from several dispersion models.

Keywords: Chlorine; Dispersion models; Toxic gases

1. Introduction

The development of more and more complex industrial facilities is coupled with an increase of the quantities of dangerous materials transported by road, rail etc. (Lees, 1986).

Therefore, accidental dangerous gas discharges, either flammable or toxic, are more likely to occur during manufacture, storage or transport (Brockhoff, Petersen, & Haastrup, 1992; Khan & Abbasi, 1999).

This paper focuses on chlorine which is a highly toxic gas produced and used in large quantities all over the world (Eurochlor, 2001; SHD, 2002).

Chlorine has a wide range of uses. Indeed, it is a chlorinating agent in the manufacture of various chemical products of our daily life (such as plastics, medicines…) for bleaching paper or textile…

Due to its high oxidizing and germicidal potential, it is also widely used for water disinfection at drinking water treatment installations (White, 1999) or at public swimming pools (while domestic pools typically use hypochlorite solutions). For these uses, chlorine is generally transported and stored as a liquefied compressed gas in bottles of several dozens of kilograms.

Despite the efforts conducted to achieve a high degree of safety in the production, transportation and handling of chlorine (Dicken, 1974), accidental releases still occur (BARPI, 2002) on fixed installations (Schwartz, Smith, & Lakshminarayan, 1990), or during the transportation (Dicken, 1974; Harris, 1978; Mansot, 1998; Marco, Pena, & Santamaria, 1998; Ramachadran, Chawla, & Khokhar, 1990).

Quantities of chlorine released to the atmosphere may vary from several hundreds of kilogrammes till tons (BARPI, 2002).

Accidents involving small quantities of chlorine (several dozens of kilograms) mainly occur at swimming pools or at water treatment installations (BARPI, 2002; Bessix, 2000; Decker, 1988; Decker & Koch, 1978; Fleta, Calvo, Zuniga, Catellano, & Bueno., 1986; Martinez & Long, 1995; Mvros, Dean, & Krenzelok, 1993; Sexton & Pronchik,

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1998; Vinsel, 1990) and represent about 38% of the accidents involving chlorine in France (BARPI, 2002).

In these cases, accidental releases mainly occur during the replacement of spent bottles or as a result of equipment failures (flange, pipe, valve or seal) or human error (BARPI, 2002).

Even if the implicated quantities are small, a loss of containment accident may present a serious chemical hazard that is the potential to kill or injure large numbers of people considering the high toxicity of this product. Indeed, chlorine is a highly toxic element (immediately dangerous to life or health concentration value—IDLHCl_2: 10 ppm). Exposure results in irritation of the respiratory tract, eyes, and skin, and just a few breaths of 1000 ppm can be fatal (Lauwerys, 2003; Sexton & Pronchik, 1998; SHD, 2002; The Chlorine Institute, 1999; Tissot & Pichard, 2000).

Moreover, the high vapor density (2.49 at 20 °C) of chlorine leads to the development of denser than air cloud, which dispersion and dilution are lower than that of passive ones (Koopman, Ermak, & Chan, 1989). Such dense clouds may stay and persist at ground level, which corresponds to human breath level and thus magnifies its harmful potential to people.

2. Problematic

The assessment of the subsequent dispersion of such a cloud is therefore of great interest for the competent authorities in charge of the accident (emergency squad).

The dispersing cloud of a heavy jet gas release can be divided into four major phases (as sketched in Fig. 1). First, there is an expansion zone that corresponds to the jet phase. Then the plume is dominated by the gravity during the so-called slumping phase. It is followed by the transition phase and by the atmospheric turbulence dominated phase (passive dispersion).

The purpose of atmospheric dispersion modeling is to provide, if all the input data are known, the observed concentrations downwind of the source of release.

Dispersion models can be classified into three categories, which are, from the less to the more complex, Gaussian models, box models and three-dimensional or computational fluid dynamics (CFD) models. Their application domains are in a few words the following:

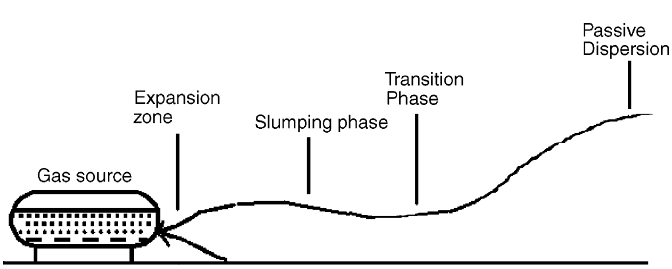

Fig. 1. Stages in the dispersion of a heavy gas jet.

Three-dimensional models solve conservation of mass, momentum and energy equations, and can be used to model the dispersion of clouds in presence of obstacles even of complex geometry. Moreover, they can deal with heavy, neutral or light gas dispersion.

Most of the heavy gas models treat the cloud as a cloud with uniform properties (box or slab models). They are especially designed for taking into account the different stages of the heavy gas dispersion: slumping and creeping, transition phase and finally passive dispersion.

Gaussian models are specific to passive clouds and therefore occur in heavy gas models for the last stage of dispersion (passive dispersion). They assume that the pollutant concentration follows a Gaussian distribution, which standard deviations are dependent on the atmospheric turbulence and the distance from the source (Pasquill standard deviations, Beychok 1994) or the duration since the beginning of the release (Doury standard deviations, Doury, 1988).

These models are well adapted to passive gas, medium meteorological conditions, in the far field from the source (distance higher than 100 m), for homogenous conditions of wind, on flat ground etc. Even if Gaussian models are not adapted, they are sometimes used to assess heavy gas dispersion.

However, dispersion models are mostly validated on the basis of past dispersion experiments. The latter imply large quantities of hazardous products (flammable or toxic gases), and are dedicated to study the dispersion of the resulting clouds on great distances from the source to reach a better knowledge of the different phases of gas dispersion (slumping, creeping, passive dispersion…).

However, dispersion models have hardly been validated on small releases and therefore require more validation on small plumes of dangerous gases. Indeed, what is their reliability in case of accidents involving small amounts e.g., chlorine leakages at swimming pools' installations, and for small distances downwind the gas source? This information is of prime interest in so far as small releases are more likely to occur than larger ones.

The scope of this study is therefore restricted to the case of a small accidental release of gaseous chlorine, particularly on the assessment of the consequences of such accidents.

This paper reports on chlorine small-scale dispersion experiments and deals with the comparison between experimental data of ground level concentrations in the plume and predicted concentrations obtained from several dispersion models.

3. Methodology

3.1. Database on chlorine dispersion experiments

Feedback information on small chlorine cloud dispersion is rare and often incomplete (concentrations are unknown). Moreover, few publications about experiments