Journal of Loss Prevention in the Process Industries 36 (2015) 20–29

Contents lists available at ScienceDirect

Journal of Loss Prevention in the Process Industries

journal homepage: www.elsevier.com/locate/jlp

An improved model for heavy gas dispersion using time-varying wind data: Mathematical basis, physical assumptions, and case studies

Yue Li [b], Dongsheng Chen [a,*], Shuiyuan Cheng [a], Tingting Xu [a], Qing Huang [c], Xiurui Guo [a], Xin Ma [d], Nan Yang [a], Xiangxue Liu [a]

[a] Key Laboratory of Beijing on Regional Air Pollution Control, College of Environmental & Energy Engineering, Beijing University of Technology, Beijing 100124, PR China
[b] Transport Planning and Research Institute, Ministry of Transport, Beijing 100028, PR China
[c] Department of Environmental Engineering, Jinan University, Guangzhou 510632, PR China
[d] National Meteorological Center, Beijing 100081, PR China

ARTICLE INFO

Article history:
Received 1 April 2014
Received in revised form
19 April 2015
Accepted 5 May 2015
Available online 5 May 2015

Keywords:
Dispersion model
SLAB
SLABi
Toxic gases
Time-varying wind vectors

ABSTRACT

This study developed an improved model for the dispersion of released toxic gases, SLABi, based on the widely used model SLAB. Two major improvements enhanced the model's ability to represent observations. First, SLAB was upgraded to account for temporal variation in wind vectors. Thus, real-time changes in meteorological conditions can be considered in dispersion forecasting. Second, a source term module was developed and embedded in SLABi to standardize the procedure of emission calculation. Both the standard SLAB model and the SLABi model were applied to a case study to evaluate the impact of time-varying winds on the dispersion of released gases. The results showed that meteorology has a significant influence on the dispersion of released gases. The SLABi model can provide decision makers with timely and accurate guidance, so as to minimize hazards to people and the environment.

1. Introduction

Many industrial substances are toxic, flammable, or both. Accidental release of such substances can cause mass casualties and huge economic losses (Bellasio and Bianconi, 2005). An example of such a case occurred in Huai'an (Jiangsu, China), where a traffic accident released 40 tonnes of pressurized liquid chlorine from a storage tank. The incident killed 28 people and injured 350 (Gao, 2011). To establish emergency plans and appropriate land-use policies in industrial areas, it is crucial to be able to predict the dispersal of toxic gas releases. Accurate predictions of toxic gas distribution can also aid in evacuating affected areas and rescuing victims (Bellasio and Bianconi, 2005).

Mathematical models are useful for predicting the consequences of accidents and planning measures to decrease damages. A number of models have been applied to support decision making regarding the accidental release of toxic and/or flammable substances in gas or liquid phase (Bellasio and Bianconi, 2005). To provide decision makers with timely advice on an accident's possible impact, toxic gas dispersion models must be computationally efficient and applicable to various types of dangerous gas. Ideally, the calculation should take only a few seconds to a few minutes.

Current models include Gaussian models, the INtegrated PUFF Model (INPUFF) (U.S. Environmental Protection Agency), the Air Force Toxics Model (AFTOX; U.S. Air Force), and the Terrain Responsive Atmospheric Code (TRAC) Emergency Response Model developed by the Rocky Flats Environmental Technology Site (Colorado, USA),. These models perform well when predicting the dispersion of toxic gases with molecular weight similar to the air (i.e., neutrally buoyant gases, NBG). However, toxic gases released in accidents usually form clouds denser than the air. These clouds are composed of quasi-gaseous substances, such as chlorine, ammonia, and hydrogen fluoride, and exist in a gaseous or aerosol state. The diffusion mechanism of these heavy gases is essentially different from that of NBG. To predict their dispersion, a dense gas dispersion model with a mechanism for simulating dense cloud collapse is needed (Van Ulden, 1974).

Hundreds of dense air dispersion models are available, but most

* Corresponding author.
E-mail address: dschen@bjut.edu.cn (D. Chen).

http://dx.doi.org/10.1016/j.jlp.2015.05.010
0950-4230/

have not yet been fully validated against experimental data. These dense gas dispersion models can be grouped into five categories: empirical models (Britter and Mc-Quaid, 1988), box models (Kaiser and Walker, 1978; Britter, 1990), similarity models (Havens, 1988) three-dimensional finite element models (Ermak and Chan, 1986), and shallow layer models (Ermak, 1990). Empirical models are computationally efficient but have low accuracy. Box models are also called integral models. They use a combination of conservation laws applied to the cloud, supplemented by semi-empirical relations derived from dispersion research. Box and similarity models are not computationally demanding and are easy to use, but the prediction results are relatively less accurate because some unreasonable assumptions are used in the simulations. Three-dimensional finite element models like CFD models have outstanding accuracy. Tauseef et al. (2011) applied CFD method to simulating dense gas dispersion in presence of obstacles. Kassomenos et al. (2008) modeled the dispersion of a Vinyl Chloride Monomer at a workplace. Generally, the modeling area of these studies is confined to very small scales, i.e. hundreds of meters. Few studies apply this method to the simulation of toxic dispersion on an urban scale. Besides, CFD method is computationally intensive and very complicated. Hence application this type of model is confined to very small scale research and is not suitable for practical use. The shallow layer approach is a compromise between the complexity of finite element models and the simpler Gaussian models and box models. This type of model is widely used because it simplifies the controlling equations of dense air dispersion but keeps the advantages of the other four model types.

The SLAB model, an outstanding representative of the shallow layer model type, is an atmospheric dispersion model designed for denser-than-air releases. After the full evaluation of various dense air dispersion models, the US Environmental Protection Agency recommended SLAB as the regulatory model for the prediction and consequence analysis of toxic gas release (US EPA, 1999). SLAB is also used for risk assessment in Canada, Mexico, Japan, China, and other countries. SLAB is capable of predicting the dispersion of hazardous gases of different molecular weights and can be applied to both neutrally buoyant and dense gases. It is easy to use and computationally efficient. Furthermore, its source code is open, allowing for convenient modification and improvement of the model. In recent years, SLAB predictions have been compared with a wide range of data obtained from both laboratory and field-scale heavy gas dispersion experiments (Ermak, 1997). SLAB is often used as a standard for model verification, and the prediction performances of other models have been evaluated against its results.

Although SLAB has many advantages, it has also some substantial disadvantages, the most important one being the assumption of constant wind speed in all horizontal directions, neglecting the impact of wind variation on the prediction. However, for small-scale toxic gas dispersion, different wind directions and speeds can lead to completely different dispersion paths. Tiny differences in predicted dispersion paths may have serious consequences in rescue operations, resulting in casualties and property losses. Changes in wind direction and speed must be taken into account when SLAB is used for real-time prediction. Another disadvantage of SLAB is that it does not include a source term module to estimate the source emission rate of toxic gases and related parameters. This means the source emission rates of various toxic gases have to be estimated by the users, making use of the model inconvenient. Furthermore, a lack of uniform emission rate estimation procedures tends to cause errors and uncertainties in the results.

We developed an improved version of SLAB, SLABi, to address the two disadvantages discussed above. SLABi takes the variation in wind vectors into account when predicting the dispersion of toxic gases, while keeping the advantages of SLAB. This approach enables the model to reflect the real-time changes in meteorological conditions during dispersion forecasting. In addition, a source term module was also developed and embedded in the model. These two major improvements enhance on the prediction accuracy and make SLABi more applicable than SLAB for predicting the consequences of toxic gas release. This model can provide decision makers with timely and accurate guidance, so as to minimize the damages to people and the environment.

2. Methodology

2.1. Standard SLAB

SLAB is an atmospheric dispersion model for denser-than-air releases developed by the Lawrence Livermore National Laboratory, with support from the U.S. Department of Energy, U.S. Air Force Engineering and Services Center, and the American Petroleum Institute. The model can treat various types of releases, including a ground-level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet, and an instantaneous volume source. Transport and dispersion are calculated by solving conservation equations of mass, momentum, energy, species, and the cloud half-width. Solution of the spatially-averaged conservation equations for a dispersion mode yields the spatially-averaged cloud properties (Ermak, 1997). SLAB uses the assumption of air entrainment to calculate the mixing of atmospheric turbulence clouds and vertical wind speed changes due to the influence of ground friction. More information on SLAB is given in the user's manual (Ermak, 1990).

2.2. SLABi's improvements to SLAB

2.2.1. Release amount calculation module for toxic gases

In this study, a source term sub-model was developed to calculate the source emission rate and related parameters. This sub-module was developed primarily based on risk management program guidance for offsite consequence analysis (US EPA, 1999), technical guidelines for environmental risk assessment of projects (MEP of China, 2004), and other literature (Tixier et al., 2002; Bellasio and Bianconi, 2005). The source model evaluates the release rate in case of a gas, pressurized gas, a liquid, or a two-phase fluid leak. The calculation methods are as follows:

(1) Gas phase release

This study used

$$Q = C_d A P \sqrt{\frac{Mk}{RT}\left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}} \quad (1)$$

Eq. (1) is based on the Bernoulli equation (MEP of China, 2004; Mills and Paine, 1990; Tixier et al., 2002).

(2) Liquid phase release

Disregarding the hydrostatic pressure in the tank and assuming a breach in the inner wall (with no charge loss),

$$Q = C_d A \rho \sqrt{\frac{2(P-P_0)}{\rho} + 2gh_l} \quad (2)$$

We used Eq. (2) to simulate a flow in the liquid phase based on the Bernoulli equation (MEP of China, 2004; Ziomas et al., 1989; Tixier et al., 2002).