Journal of Loss Prevention in the Process Industries 46 (2017) 1–12

Contents lists available at ScienceDirect

Journal of Loss Prevention in the Process Industries

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

Simulation of heavy gas dispersion in a large indoor space using CFD model

Longxiang Dong, Hongchao Zuo*, Liang Hu, Bin Yang, Licheng Li, Liyang Wu

Key Laboratory for Semi-Arid Climate Change of PRC Ministry of Education, College of Atmospheric Sciences, Lanzhou University, Lanzhou 730000, China

ARTICLE INFO

Article history:
Received 15 August 2016
Received in revised form
12 January 2017
Accepted 12 January 2017
Available online 16 January 2017

Keywords:
Indoor dispersion experiment
Heavy gas
CFD
Model performance
Ventilation rate

ABSTRACT

Accurate prediction of the associated hazards resulting from accidental leakage in a large indoor environment is essential for risk analysis and emergency response. Although computational fluid dynamics (CFD) is seen as a promising tool to model complex dispersion scenarios, it is necessary that it be fully validated against reliable experimental data before the predictions can be used with confidence. This paper presents a comprehensive and systematic evaluation of the performance of four commonly used Reynolds Averaged Navier-Stokes (RANS) turbulence models (i.e., standard k-ε, Realizable k-ε, standard k-ω, and shear-stress transport (SST) k-ω) for predicting heavy gas dispersion in a factory building with various obstacles. The predicted concentrations were compared with tracer (SF_6) concentrations measured from a full-scale indoor tracer test, in which 14 sampling sites were distributed around the release source. Several statistical measures were applied to quantify the model performance in and above the breathing zone. The results suggest that the standard k-ω model and the SST k-ω model show the best performance in the breathing zone according to Chang's criteria, producing 78% of predictions (paired in time and space) within a factor of two of the observations. However, none of the RANS models are satisfactory in predicting the spatial-temporal variation of tracer clouds above the breathing zone. Additionally, the SST k-ω model was employed to reproduce the heavy gas dispersion in the building and to analyze the relationship between ventilation rate and concentration in the breathing zone.

1. Introduction

A hazardous chemical leakage accident may occur in the process of production, transportation, and storage. Once these hazardous substances are released into the atmosphere, they are likely to cause serious injury to human health or cause other disasters (Sklavounos and Rigas, 2004; Li et al., 2015), especially in a semi-enclosed indoor environment. To avoid accidents and minimize harm to people, it is necessary to take preventive measures, including environmental risk assessment, monitoring method improvement, and emergency plan establishment (Britter, 1989). In the implementation of these countermeasures, a quantitative description of the associated hazards is needed. Consequently, mathematical models that can be used to simulate and predict pollutant dispersion have become increasingly significant (Hanna et al., 1993; Markiewicz, 2012).

Over the past few decades, various dispersion models have been established for modeling the flow and dispersion of heavy gas, which has a density greater than air, because most of the toxic or flammable materials (e.g., Cl_2, H_2S, SO_2) derived from leakage accidents are heavy gases (Blackmore et al., 1982; Britter, 1989; Markiewicz, 2012; Sun et al., 2013). The computational fluid dynamics (CFD) model is the most popular model because it can well describe the influence of complex terrain and obstacles on gas flow and diffusion, although it consumes more computation time (Scargiali et al., 2005; Tauseef et al., 2011; Liu et al., 2016). The rapid development of computer hardware and numerical algorithms has enabled the CFD model to be used extensively in indoor pollutant dispersion studies. Wang et al. (2013) analyzed the effect of the release rate, wind speed, and obstacles on carbon dioxide dispersion in indoor space using the FLUENT model. Kassomenos et al. (2008) investigated toxic vinyl chloride monomer dispersion in a geometrically complex industrial area and estimated the exposure of the workers to this dangerous substance. Ricciardi et al. (2008) performed multidimensional simulations of heavy gas (i.e., SF_6) dispersion in a ventilated room and compared model results with experimental data. They concluded that the higher the air flow rate,

* Corresponding author.
E-mail address: zuohch@lzu.edu.cn (H. Zuo).

http://dx.doi.org/10.1016/j.jlp.2017.01.012

the more satisfactory the comparison between predicted and experimental values. Finlayson et al. (2004) demonstrated that the agreement between CFD predictions and ensemble averaged experimental measurements was satisfactory for both the transient and steady-state conditions. Recently, the CFD model was also applied to the study of indoor risk assessment, ventilation design, and occupant comfort (Siddiqui et al., 2012; Chen, 2009; Zhu et al., 2015).

The accuracy of model results is a main concern, and experimental validation studies are imperative before the predictions can be used with confidence (Chen and Srebric, 2002; Schleder and Martins, 2016). A tracer experiment, which has the advantage of a real situation being taken into account, can provide experimental data for the model validation; however, full-scale field experiments addressing heavy gas dispersion in a large indoor environment are very rare. To the our knowledge, only a few scaled experiments have been conducted, and scale modeling may suffer from incompatible similarity requirements (Thatcher et al., 2004). Furthermore, the CFD model performance in predicting heavy gas dispersion in a large indoor environment with various obstacles is not well known, as existing simulation studies were carried out under simple configurations with few or no obstacles (Ricciardi et al., 2008; Tauseef et al., 2011; Xing et al., 2013).

Moreover, many previous CFD studies have indicated that the appropriate choice of Reynolds Averaged Navier-Stokes (RANS) turbulence models is important in reproducing heavy gas dispersion, but there is not a consistent conclusion regarding which model is better for simulating heavy gas dispersion (Tauseef et al., 2011; Cheng et al., 2014). For example, Sklavounos and Rigas (2004) found that the standard $k-\varepsilon$ and shear-stress transport (SST) k-ω models appeared to overestimate maximal concentrations recorded in the trials. Xing et al. (2013) showed that the results from the standard k-ε and SST k-ω models were in acceptable agreement with the experimental data, while the predicted values from the RNG k-ε model were unsatisfactory.

The major objective of this investigation was to evaluate the adequacy of a set of commonly used RANS turbulence models for predicting heavy gas dispersion in a large indoor environment with various obstacles. Numerical simulations were performed in a transient form using four RANS turbulence models (i.e., standard k-ε, Realizable k-ε, standard k-ω, and SST k-ω). The CFD predictions were validated via a full-scale heavy gas tracer test conducted in an industrial factory building in which SF_6 tracer gas was released from a point source near the ground level and concentrations were measured at 14 sampling sites distributed around the release source. Several statistical measures were introduced to quantitatively evaluate the model performance in and above the breathing zone. Then, the validated model is employed to present the spatial-temporal evolution of heavy gas dispersion in the factory building and to analyze the relationship between ventilation rate and concentration in the breathing zone.

2. Description of heavy gas tracer test

The Indoor Hazardous Gas Diffusion Test (IHGDT) was conducted in a typical industrial factory building in Lanzhou City, China, in April 2015. As the main component of the IHGDT, a full-scale tracer test was designed to imitate heavy gas leakage in a large building, especially for complex configurations with multiple obstacles, and to provide experimental data for the model validation. Fig. 1a shows the ichnography of the factory building, which has a volume larger than 10 000 m^3. The dimensions of the building are 48 m long by 18 m wide by 13 m high, and there are four natural ventilation holes 0.4 m in diameter located at the top of the building. The lightly shaded region at the left side of Fig. 1a is an office area with a height of 3 m; a door (5 m wide, 6 m high) is located on the right side, and both sides of the door with gray shading are storage regions, 2.8 m high.

SF_6, the density (6.164 kg/m^3) of which is approximately 5 times that of air, is a non-toxic and highly inert gas. The background concentration of SF_6 is quite low and can be easily detected; thus, SF_6 was used as a heavy gas tracer in our tests. The exact locations of the release source and the tracer sampling sites are marked in Fig. 1a. Fourteen sampling sites were distributed around the release source to monitor the variation of the tracer cloud concentration in time and space. As shown in Table 1, the sampling height at the half of the sampling sites (i.e., L1D-L6D, T1) is within the breathing zone, defined as height between 1 and 2 m above ground level (AGL) in this study. The sampling height at the other half sites is above the breathing zone, including five sites (i.e., L1U, L3U, L4U, L6U, J) with a sampling height of 4 m AGL, and two sites (i.e., T2, T3) with a sampling height of 5.5 and 8 m mounted on a tower inside the building (Fig. 1b).

The total duration of the tracer test was 24 min, from 11:20 to 11:44 Beijing Time (BJT=UTC+8 h). The tracer SF_6 was released continuously at 1 m AGL from a point source during the first 12 min. The tracer was sampled at all 14 sites simultaneously using a 0.5-L sample bag, and sequential 3-min-averaged concentrations of SF_6 were measured. A total of 112 valid samples were collected, 4 of which were used to measure the background concentration. The SF_6 tracers were analyzed using a gas chromatography-electron capture detector (GC-ECD, HP-5890II) in the laboratory (Fig. 1b), with a lower detection limit of 1.0 × 10^{-12} (V/V). The detailed concentration detection method can be found in the literature (Geller et al., 1997).

3. Numerical simulation

3.1. CFD model description

The commercial software ANSYS FLUENT 15.0 (ANSYS Inc., 2014) was employed for the simulation of SF_6 dispersion in a factory building in this study. Considering the balance between computational time and accuracy, the RANS model was used for the simulations. The RANS model includes the continuity and momentum equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{1a}$$

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{\partial x_j} - \rho\overline{u_i' u_j'}\right) \tag{1b}$$

where ρ is the density; t is time; u_i and u_j are the mean velocity components in the x_i and x_j directions, respectively; and μ is dynamic viscosity. The overbar and prime indicate the mean and fluctuating components of the velocity, respectively.

The relationship between the Reynolds stresses $-\rho\overline{u_i' u_j'}$ and the mean velocity gradients is shown in formula (2):

$$-\rho\overline{u_i' u_j'} = \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\left(\rho k + \mu_t \frac{\partial u_i}{\partial x_i}\right)\delta_{ij} \tag{2}$$

here, μ_t is turbulent viscosity, k is turbulent kinetic energy, and δ_{ij} is the Kronecker delta. The k and its rate of dissipation ε are obtained from the following transport equations: