Journal of Hazardous Materials 271 (2014) 266–274

Contents lists available at ScienceDirect

Journal of Hazardous Materials

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

A new numerical formulation of gas leakage and spread into a residential space in terms of hazard analysis

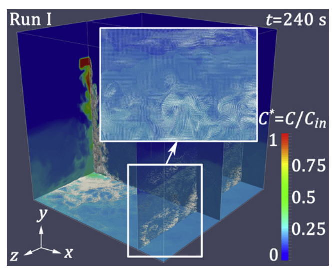
Ryuichi S. Nagaosa *

AIST, Research Center for Compact Chemical System (CCS), 4-2-1 Nigatake, Miyagino, Sendai 983-8551, Japan

HIGHLIGHTS

- A new numerical approach of the spread of leaked gases is proposed.
- A computational fluid dynamics technique without a turbulent model is employed.
- Numerical solutions without uncertainties produced by turbulent model are shown.
- A series of case studies of gas spread is demonstrated.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 11 November 2013
Received in revised form 14 February 2014
Accepted 20 February 2014
Available online 2 March 2014

Keywords:
Flammable gas leakage
Extended two-compartment model
Gas density
Computational fluid dynamics (CFD)
Hazard analysis

ABSTRACT

This study proposes a new numerical formulation of the spread of a flammable gas leakage. A new numerical approach has been applied to establish fundamental data for a hazard assessment of flammable gas spread in an enclosed residential space. The approach employs an extended version of a two-compartment concept, and determines the leakage concentration of gas using a mass-balance based formulation. The study also introduces a computational fluid dynamics (CFD) technique for calculating three-dimensional details of the gas spread by resolving all the essential scales of fluid motions without a turbulent model. The present numerical technique promises numerical solutions with fewer uncertainties produced by the model equations while maintaining high accuracy. The study examines the effect of gas density on the concentration profiles of flammable gas spread. It also discusses the effect of gas leakage rate on gas concentration profiles.

1. Introduction

The spread of a flammable gaseous substance into a residential space has significant possibility to cause a hazardous event by an ignition and subsequent combustion or explosion. For example, the lower and upper flammability limits of propane at 296.2 K and 1.013×10^5 Pa have been reported as very low concentrations of 2.03 and 10.10 vol%, or, 0.835 and 4.16 mol m^{-3}, respectively [1]. Considering its low minimum ignition energy of 0.48 mJ at a concentration of 5.2 vol% [2], or, 2.14 mol m^{-3}, only a small amount of leakage of propane in an insufficiently ventilated space will be hazardous. Utilization of a flammable gas in home-use electrical appliances is therefore regulated strictly by international standards, i.e., IEC 60335-2-40 [3], to avoid hazardous events.

A hazard assessment of the flammable gas leakage into the indoor environment has been obtained extensive research in the field of heating, ventilating, and air conditioning for the following reason [4]. Several traditional refrigerants such as hydrofluorocarbons (HFCs) have been found to have extensive global warming impacts. A typical value of the global warming potential (GWP) of HFCs is in the order of 10^3; hence, the Kyoto Protocol [5] has specified quantitative targets of emission reductions of six greenhouse

* Tel.: +81 29 861 8227.
E-mail address: ryuichi.nagaosa@aist.go.jp

http://dx.doi.org/10.1016/j.jhazmat.2014.02.033
0304-3894/

gases, including HFCs [6,7]. It has also been revealed that emissions of high-GWP refrigerants into the atmosphere will accelerate global warming significantly if no actions to mitigate the emissions are taken [8]. HFC-based refrigerants should be replaced by other substances with low global-warming impacts to comply with the Kyoto Protocol. Several substances have been considered as alternatives to phase out the high-GWP refrigerants [7,9]. While these candidates have very low global-warming impacts, many of them are categorized as flammable [4], and their practical applications in the residential space are regulated by the IEC standard [3].

Extensive laboratory and in situ measurements of the concentration profiles are necessary to evaluate the potential hazard posed by flammable gas spread. These measurements require a lot of experimental work to quantify gas flow velocities and concentrations in the residential space [10–12], since the profiles depend strongly on many parameters and leakage scenarios. Assessing the hazard can be achieved in a more efficient manner by utilizing the numerical data based on computational fluid dynamics (CFD) technique [13,14]. For example, Minor et al. [15] carried out a series of numerical experiments on flammable refrigerant spread in a mobile fleet for assessing the hazard posed by an accidental leakage. They predicted the spread of a low-GWP flammable refrigerant based on six leakage scenarios, exhibiting notable advantages of numerical experiments [16]. The numerical works by Minor et al. [15,16] are a good example that demonstrates the critical role of a theoretical, or numerical approach to assess the hazard, providing a series of case studies of the flammable refrigerant spread in enclosed spaces, with details of leaked gas concentrations.

This study proposes a new numerical formulation of the gas spread into the residential space, and combines it and a CFD approach for obtaining unsteady concentration profiles of the leaked gas. An open-source CFD software package for transparent and traceable hazard analysis is employed. The CFD technique does not implement a turbulent model, and uncertainties produced by the model equations are not included. The accuracy of the present numerical solutions is sufficiently high, since all the essential scales of fluid motions are resolved by sufficient number of meshes with a sufficiently small time step. The numerical technique, without using a turbulent model, has been applied to environmental sciences by the author, and the usefulness of the model-free methodology has already been demonstrated in several references [17–19].

The leakage process of the flammable gas is modeled by a mass balance based formulation, and the leakage concentration is determined by the formulation. This study performs three numerical runs of flammable gas spread using two gases with different density as a series of case studies, and compares the effect of gas density on the three-dimensional spread of these gases in the residential space. The effect of the gas leakage rate on the spread of the gases leaked into the three-dimensional enclosed space is also demonstrated.

2. Numerical method

2.1. Mathematical formulation of leaked gas spread

Fig. 1 shows a schematic representation of the newly proposed two-compartment concept. This concept is flexible to establish a mathematical formulation in many fields of environmental sciences, and an example of applications is found in Ref. [19]. Compartment I is the storage of the flammable gas whose charge is expressed by S in mol. Molecular mass of the gas is designated by M in kg mol^{-1}, therefore, the mass based charge of the gas is expressed by $S_m = M \times S$ in kg. Compartment II is the residential space, which is filled initially with ambient air of zero velocities at pressure p_0 in

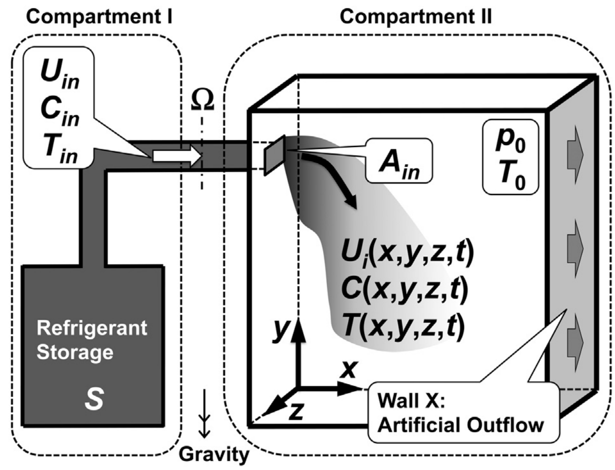


Fig. 1. A schematic representation of an extended compartment model for mathematical formulation of a dense gas leakage into the indoor environment.

Pa, and temperature T_0 in K. Molecular mass of ambient air is given by $M_0 = 0.029$ kg mol^{-1} as a reference value. The gas is assumed to be discharged into Compartment II through the leakage window, whose area is A_{in} in m^2. Its leakage velocity, concentration, and temperature are designated by $U_{in}(t)$ in m s^{-1}, $C_{in}(t)$ in mol m^{-3}, and $T_{in}(t)$ in K, respectively. The volume flow rate of the leaked gas, which is a mixture of the flammable refrigerant and air, is given by $Q(t) = A_{in} \times U_{in}(t)$ in m^3 s^{-1}. It is also assumed that all the charged gas is leaked between $t = 0$ and t_L in s.

We consider the mass balance of the gas discharged through the leakage window, and the following equation is obtained,

$$S = A_{in} \int_0^{t_L} U_{in}(t) C_{in}(t) \mathrm{d}t \tag{1}$$

Eq. (1) can be reduced to the following equation by assuming that both $U_{in}(t)$ and $C_{in}(t)$ are constant in time, respectively

$$C_{in} = \frac{\mathrm{d}S/\mathrm{d}t}{A_{in} U_{in}} = \frac{W}{Q} \tag{2}$$

where $W \equiv \mathrm{d}S/\mathrm{d}t = S/t_L$ is the leakage rate of the gas in mol s^{-1}. Eq. (2) shows that the leakage concentration of the flammable gas can be estimated using W and Q only.

2.2. Numerical procedure for CFD analysis

A CFD technique is implemented to evaluate the unsteady three-dimensional details of concentration, velocity, and temperature profiles. It is assumed that an air-refrigerant mixture is an ideal gas, whose viscosity, ν, molecular diffusivity of gas in air, D, and thermal diffusivity, α are constant. Under the assumption that the leaked gas is incompressible Newtonian fluid, the governing equations are expressed as follows,

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{3a}$$

$$\frac{\partial U_i}{\partial t} = \frac{\partial}{\partial x_j}\left(\nu \frac{\partial u_i}{\partial x_j} - U_j U_i\right) - \frac{\partial}{\partial x_i}\left(\frac{p}{\rho_0}\right) + \left\{\frac{M_0(r-1)}{\rho_0} C + \beta T_0 \left(1 - \frac{T}{T_0}\right)\right\} g_i \tag{3b}$$

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_j}\left(\frac{\nu}{\mathrm{Sc}} \frac{\partial C}{\partial x_j} - U_j C\right) \tag{3c}$$