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Influence of concentration distribution of hydrogen in air on measured flammability limits

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ABSTRACT

There is a clear difference between exiting data on the measured flammability limits of hydrogen-air mixture. The non-uniformity of concentration distribution of hydrogen in air is a contributor to deviations of the upper flammability limit (UFL) and the lower flammability limit (LFL) measured in different experiments. This paper presents a numerical model to simulate the gas mixing process from start to stability, to predict the concentration distribution, and to research the influence of concentration distribution of hydrogen in air on measured UFLs and LFLs. The commercial software package Fluent was used to carry out the numerical simulation for the concentration distribution of hydrogen in air in the vessels with length-to-diameter ratios (L: D) of 1:1, 3:1, 5:1 and 7:1 respectively. Based on the numerical simulation and analysis, the influence of concentration distribution on measured flammability limits was demonstrated for hydrogen in air in the vessel. It is found that the deviations of measured flammability limits of hydrogen in air are the minimum in the vessel with length-to-diameter ratio of 1:1, and augment with the augmentation of vessel length-to-diameter ratio. Moreover, it is presented that the deviations of measured flammability limits of hydrogen in the center of the vessel are lower than that in the top and the bottom.

1. Introduction

A premixed fuel-air mixture will explode as long as the fuel concentration is between the upper and lower flammability limits, i.e. UFL and LFL. The UFL and LFL are important in an evaluation of the explosive hazards of fuel-air (Bjerketvedt et al., 1997). The wide flammable range of hydrogen tells us that it is easy to get a flammable cloud of hydrogen in air. The UFL and LFL of hydrogen in air are key parameters for predicting fire, assessing the possibility of explosion, and designing protection systems.

The UFL and LFL of hydrogen in air have been studied for many years (Bjerketvedt et al., 1997, Le et al., 2012, Nga, Leeb, 2008, Razus et al., 2004, Sánchez and Williams, 2014). Previously published works focus on the experimental results of UFL and LFL of hydrogen in air and its corresponding parameters (Bjerketvedt et al., 1997, Zlochower, Green, 2009). However, it is found that the results of measured LFLs or UFLs are not exactly the same. At room temperature and under atmospheric pressure, the measured UFLs of hydrogen in air are 75% (Coward, Jones, 1952), 74.7% (Wierzba, Wang, 2006), 75.1% (Schröder,Molnarne, 2005), 75.8% ± 0.2% (Schröder,Molnarne, 2005), 76.6% ± 0.2% (Schröder,Molnarne, 2005) and 75.73% ± 0.15% (Cashdollar, A Zlochower et al., 2000); and the measured LFLs of hydrogen are 4%(Kuznetsov et al., 2012), 4% ± 0.5% (Liu,Zhang, 2014), 4.2%(Ishizuka, 1991), 5% ± 0.5% (Cashdollar, A Zlochower et al., 2000), 6% ± 0.5%, 6.5% ± 0.5% and 7.5% ± 0.5% (Cashdollar, A Zlochower et al., 2000). It is generally considered that these deviations of measured LFLs or UFLs are caused by experimental device system (Takahashi et al., 2003) or ignition energy (Britton, 2002, Hertzberg et al., 1988, Pfahl et al., 2000, Zhang et al., 2013). In experiments and numerical simulations, the concentration distribution of hydrogen in air was deemed homogenous (Appel et al., 2002, Azatyan et al., 2010, Bane et al., 2013, Biet et al., 2008, Griffiths, Phillips, 1990, Grune et al., 2013a, Grune et al., 2013b, Gurney, 1966, Liu et al., 2006, Liu, Zhang, et al., 2014, Salzano et al., 2012, Shu et al., 1998, Takahashi et al., 2003, Wierzba, Wang, 2006). However, due to the gravity, homogeneous gas mixture is fairly rare. Usually, homogeneous mixture composition in the vessel is achieved by using a stirrer. It is found that stratified hydrogen-air mixtures have influence on combustion

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pressure and flame speeds(D. Makarov, Verbecke, et al., 2009, Whitehouse et al., 1996). The non-uniformity of concentration distribution of premixed gas is another contributor to the deviations of UFL and LFL measured in different experiments. Nevertheless, this contributor hasn't received much attention. It may be difficult to measure concentration distribution in gas mixing process because that concentration distribution varies greatly.

The subject of this present study involved the influence of concentration distribution of hydrogen in air on measured flammability limits. The commercial software package Fluent was used in this study to carry out numerical simulation of the concentration distribution of hydrogen in air in vessels. Novel aspect of modeling is that it could simulate the gas mixing process from start to stability, and predict the concentration distribution. Based on the numerical simulation and analysis, the influence of concentration distribution of hydrogen in air in the vessels with different length-to-diameter ratios was obtained.

2. Numerical model

The commercial software package Fluent, a finite element computational code for fluid dynamics simulation, was used to carry out the numerical simulation process. The Fluent provides a mixture model that could be used to model multiphase flow where the phases move at different velocities. Physical phases of matter are gas, liquid, and solid, but the concept of phase in a multiphase flow system is applied in a broader sense(Inc, 2006). In multiphase flow, a phase can be defined as an identifiable class of material that has a particular inertial response to and interaction with the flow and the potential field in which it is immersed(Inc, 2006).

2.1. Governing equations

The mixture model solved the continuity equation and the momentum equation for the mixture, and the volume fraction equation for the secondary phases, as well as algebraic expressions for the relative velocities.

(1) Continuity equation

The continuity equation for the mixture is

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \vec{v}_m) = 0, \tag{1}$$

where $\rho_m = \sum_{k=1}^{n} \alpha_k \rho_k$, $\vec{v}_m = \frac{\sum_{k=1}^{n} \alpha_k \rho_k \vec{v}_k}{\rho_m}$, $\nabla = \frac{\partial}{\partial x}\vec{i} + \frac{\partial}{\partial y}\vec{j} + \frac{\partial}{\partial z}\vec{k}$, and ρ_m is the mixture density, kg/m^3; t is time, s; $\vec{v}_m$ is the mass-averaged velocity, m/s; α_k is the volume fraction of phase k; ρ_k is the density of phase k; $\vec{v}_k$ is the mass velocity of phase k, m/s.

(2) Momentum equation

The momentum equation for the mixture can be obtained by summing the individual momentum equations for all phases. It can be expressed as

$$\frac{\partial}{\partial t}(\rho_m \vec{v}_m) + \nabla \cdot (\rho_m \vec{v}_m \vec{v}_m) = -\nabla p + \nabla \cdot \left[\mu_m \left(\nabla \vec{v}_m + \nabla \vec{v}_m^{\,T}\right)\right] + \rho_m \vec{g}_m + \nabla \cdot \left(\sum_{k=1}^{n} \alpha_k \rho_k \vec{v}_{dr,k} \vec{v}_{dr,k}\right) \tag{2}$$

where $\mu_m = \sum_{k=1}^{n} \alpha_k \mu_k$, $\vec{v}_{dr,k} = \vec{v}_k - \vec{v}_m$, and n is the number of phases; and μ_m is the viscosity of the mixture; $\vec{v}_{dr,k}$ is the drift velocity for secondary phase k; p is static pressure, Pa; $\vec{g}_m$ is gravity, m/s^2.

(3) Relative (slip) velocity and the drift velocity

The relative velocity (also referred to as the slip velocity) is defined as the velocity of a secondary phase (p) relative to the velocity of the primary phase (q):

$$\vec{v}_{pq} = \vec{v}_p - \vec{v}_q \tag{3}$$

The drift velocity and the relative velocity are connected by the following expression:

$$\vec{v}_{pq} = \vec{v}_p - \vec{v}_q \tag{4}$$

(4) Volume fraction equation for the secondary phases

From the continuity equation for secondary phase p, the volume fraction equation for secondary phase p can be obtained:

$$\frac{\partial}{\partial t}(\alpha_p \rho_p) + \nabla \cdot (\alpha_p \rho_p \vec{v}_m) = -\nabla \cdot \left(\alpha_p \rho_p \vec{v}_{dr,p}\right) \tag{5}$$

(5) Standard k-ε Model

$$\frac{\partial}{\partial t}(\rho_m k) + \nabla \cdot \left(\rho_m k \vec{v}_m\right) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_i}\right] + G_k + G_b - \rho_m \varepsilon - Y_m \tag{6}$$

and

$$\frac{\partial}{\partial t}(\rho_m \varepsilon) + \nabla \cdot \left(\rho_m \varepsilon \vec{v}_m\right) = \nabla \cdot \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_i}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}(G_k + C_{3\varepsilon} G_b) + C_{2\varepsilon} \rho_m \frac{\varepsilon^2}{k} \tag{7}$$

where G_k represents the generation of turbulence kinetic energy due to the mean velocity gradients; G_b is the generation of turbulence kinetic energy due to buoyancy; Y_m represents the contribution of the fluctuating dilatation incompressible turbulence to the overall dissipation rate; $C_{1\varepsilon}$, $C_{2\varepsilon}$, and $C_{3\varepsilon}$ are constants, $C_{1\varepsilon} = 1.44$, $C_{2\varepsilon} = 1.92$, $C_{3\varepsilon} = 0.09$; δ_k and δ_ε are the turbulent Prandtl numbers for k and ε, respectively, $\delta_k = 1.0$, $\delta_\varepsilon = 1.3$.

Fluent code solves these equations by the finite volume method. The computational domain is subdivided into a finite number of tetrahedral control volumes. The SIMPLE method (Patankar, 1980)