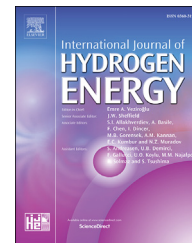




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Dilution of hazardous vapor cloud in liquid hydrogen spill process under different source conditions

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ABSTRACT

Dilution of hydrogen vapor cloud formed by the liquid hydrogen spills under different spill amounts, spill rates and liquid mass fractions at the exit were numerically investigated. Three dimensional CFD simulations were performed with ANSYS FLUENT using Realizable $k-\epsilon$ turbulence model. Time variation of the maximum hydrogen concentration ($t = 0$ s at the end of the spill) is most sensitive to the liquid mass fraction, followed by the spill rate, and finally the spill amount. The dilution process is nearly unaffected by the spill amount. With the increment of spill rates, the dilution speed first decreases and then remains approximately unchanged, which can be attributed to the combined effects of the gaseous hydrogen generated per unit time and the source disturbances generated by the spill and evaporation process. In addition, the dilution accelerates with the increment of liquid mass fraction at the exit. The turbulence induced by the evaporation of liquid hydrogen promotes the mixing and dilution processes, while the temperature drop in the ground and the ambient air due to liquid evaporation has little influence on the overall dilution of the vapor cloud. The durations of detonation and flammability when the liquid mass fraction is 0% are 1.65 and 1.88 times of those when liquid mass fraction is 100%, respectively.

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Introduction

With the environmental degradation and the depletion of non-renewable resources, alternative energy has been attracting more and more attention [1,2]. Hydrogen has so far been widely used in the manufacture of ammonium and methanol, aerospace propulsion technology, hydrogen-

powered vehicles, fuel cells, etc. For large-capacity storage and long-distance transportation of hydrogen, liquid hydrogen (LH₂) is commonly preferred in view of economics and efficiency [3]. However, in case of material failure, corrosion attack or human errors, LH₂ may spill out and cause a series of accidental events, such as the explosion or flammability hazards exerted by the hydrogen vapor cloud, and the extremely low temperature [4].

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Experimental, theoretical and computational studies concerning LH₂ spills have been reported by a number of researchers. National Aeronautics and Space Administration (NASA) [5], Federal Institute for Materials Research and Testing (BAM) [6], and U.K. Health and Safety Laboratory (HSL) [7] have carried out LH₂ spill experiments under different scenes, including spills in open environment, of the presence of buildings and under pipe ruptures conditions. For the theoretical and computational studies, a sensitivity investigation on the influence of atmospheric stability on the dispersion of a hydrogen plume was performed [8], and the stable configuration gave the most consistent results with the experimental observations. Jin et al. [9] numerically analyzed the influence of wind speed, wind temperature and ground temperature on the spreading behavior of the LH₂ pools and vapor clouds with ANSYS FLUENT. The increased wind speed was found to expand the downwind distance of flammable cloud, while the increased wind temperature retarded the hydrogen diffusion. Verfondern et al. [10,11] used the LAUV code to investigate the different pool spreading and vaporization behaviors of LH₂ on water and solid ground, respectively, and found that the pool spread a larger area on water surface than on the solid ground. Giannissi et al. [12] simulated the LH₂ spill experiments carried out by the HSL with the ADREA-HF code, and concluded that the humidity along with the slip effect influenced the buoyancy of the cloud to a great extent. Different boiling regimes, including film boiling, transition boiling and nucleation boiling were implemented in the commercial CFD code ANSYS CFX for the same HSL spill tests [13], and the calculated pool distributions were consistent with the experimental data. The ADREA-HF code were applied to simulate LH₂ spill experiment carried out by NASA, and the downward two-phase jet, compared with pool, produces results that were more consistent with the experiment [14]. Schmidt et al. [15] simulated the behavior of hydrogen clouds formed by accidental hydrogen gas release with the commercial CFD code ANSYS FLUENT. High velocities caused high concentrations of hydrogen near the ground and a wider range of explosive mixtures. Ichard [16] conducted a sensitivity study on the effects of gas volume fractions at the exit on the flow field with the CFD tool FLACS, and showed that their influence on the flow field was not negligible.

The source condition is one of the basic factors that affect the LH₂ spill behavior. However, there are fewer studies concerning the spills under different spill amounts and spill rates. Also, the fraction of the liquid or gas phase at the source exit has demonstrated to have non-negligible influences on the flow field [16], and further analysis is still needed. Moreover, previous studies were mainly focused on the concentration distribution or the spread of the hydrogen vapor cloud, that is, the regions covered by the hazardous cloud. However, durations of the potential hazards (detonation or flammability) are at least as important as the hazardous regions from the safety perspective. Consequently, the present investigation mainly focuses on the dilution of hazardous vapor cloud in LH₂ spill process and the corresponding source effect.

Behaviors of spilled LH₂ in the open environment can be influenced by many factors, including the wind, the ground property, the spill source and etc. The experimental method is costly to investigate the various scenarios. The Computational

Fluid Dynamics (CFD) method has been demonstrated to be useful tools to predict the behaviors of LH₂ pools and the spread and dispersion of hydrogen vapor cloud [8–16]. Systematic sensitive study is allowed in CFD to study the spills under different spill amounts, spill rates and liquid mass fractions at the exit (the ratio of liquid mass and total mass). Besides, compared with discrete sampling points in field study, CFD study provides easy access to all data, for example, the dilution of hydrogen concentration at different locations, the variation of the maximum hydrogen concentration in the flow field, and the time needed for the vapor cloud to be diluted below the hazardous levels.

Numerical methods

Mathematical equations

In the present work, LH₂ spill occurs at the open environment under atmospheric pressure. The liquid phase and the gas phase are both assumed to be incompressible, and the single fluid mixture approach is adopted in the simulation for describing the two-phase flow. Reynolds time-averaged N-S equations closed by Realizable *k-ε* turbulence model are used, i.e., the two-phase flow for LH₂ spills is predicted by solving the three-dimensional, transient conservation equations for mixture mass, mixture momentum and mixture enthalpy. The density, the velocity and the kinetic viscosity of the mixture are expressed as $\rho_m = \alpha_l \rho_l + \alpha_g \rho_g$, $\vec{v}_m = (\alpha_l \rho_l \vec{v}_l + \alpha_g \rho_g \vec{v}_g) / \rho_m$ and $\mu_m = \alpha_l \mu_l + \alpha_g \mu_g$, respectively. The subscripts *l* and *g* represent liquid phase and gas phase, respectively, and α is the phase's volume fraction. The liquid phase and gas phase are assumed to be in thermal equilibrium state but with different velocities. To prescribe an algebraic relation for the relative velocity, a local equilibrium between the phases over a short spatial length scale is assumed. In addition, the air humidity is ignored in the simulation. The governing equations are:

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

$$\begin{aligned} \frac{\partial}{\partial t} (\rho_m \vec{v}_m) + \nabla \cdot (\rho_m \vec{v}_m \vec{v}_m) = & -\nabla p + \nabla \cdot [\mu_m (\nabla \vec{v}_m + \nabla \vec{v}_m^T)] \\ & + \rho_m \vec{g} + \nabla \cdot \left(\sum_{i=1}^2 \alpha_i \rho_i \vec{v}_{dr,i} \vec{v}_{dr,i} \right) \end{aligned} \quad (2)$$

$$\frac{\partial}{\partial t} \sum_{i=1}^n (\alpha_i \rho_i h_i) + \nabla \cdot \sum_{i=1}^n (\alpha_i \vec{v}_i (\rho_i h_i + p)) = \nabla \cdot (k_{eff} \nabla T) \quad (3)$$

where $\vec{v}_{dr,i}$ is the drift velocity for phase *i*, and k_{eff} is the effective heat conductivity. The subscripts *i* and *m* represent either liquid phase or gas phase, and mixture phase, respectively. The slip velocity takes the form of Mahnomen et al. [17]:

$$\vec{v}_{pq} = \frac{\tau_p}{f_{drag}} \frac{\rho_p - \rho_m}{\rho_p} \vec{a} \quad (4)$$

where the drag force is:

$$f_{drag} = \begin{cases} 1 + 0.15Re^{0.687}, & Re \leq 1000 \\ 0.0183Re, & Re > 1000 \end{cases} \quad (5)$$

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