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CFD modeling and analysis of the influence factors of liquid hydrogen spills in open environment

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ABSTRACT

A three-dimensional model has been built for the simulation of liquid hydrogen (LH_2) spill on the ground, where the source of LH_2 was modeled as a jet and placed near the ground. The model was firstly validated by the experimental results from the large-scale test of LH_2 spill carried out by NASA at New Mexico in 1981, and then used to analyze the vaporization time of LH_2 and the spreading range of gaseous hydrogen. The numerical calculation and analysis was carried out in a domain of 200 m × 60 m × 80 m. The variation of hydrogen concentration distribution at different time nodes and different environmental conditions are presented. The influences of wind velocity, wind temperature and ground temperature on the concentration distribution have also been analyzed.

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Introduction

Hydrogen energy is widely considered as one of the most promising energies, with high mass-related energy density but zero air pollution, and has many applications, such as rocket fuel, hydrogen-powered vehicles, and proton exchange membrane fuel cell [1–4]. Liquid hydrogen (LH_2) is an efficient and economically effective solution for hydrogen transportation and storage [5,6]. However, there are also many disadvantages when using liquid hydrogen as our daily used energy. One of the problems is that the release of low-temperature gaseous H_2 from the storage tank due to the unavoidable heat leakage, which may form a potentially hazardous cloud around the tank. The release could also damage the facilities in the surroundings due to its low temperature [7–9]. Thus, the safety issue is one of the main concerns during its production, transportation, storage and application, which has also been one of the hot topics in the research and industry fields for decades [10–12]. One of basic scientific problems is the spreading of LH_2 and the diffusion of gaseous hydrogen during an accidental release, which deserves efforts on both simulation and experimental studies.

In the past decades, several experimental attempts have been made to obtain basic information regarding the physical phenomena governing the dispersion of flammable clouds formed as the result of large-scale spills of LH_2. In 1981, NASA (National Aeronautics and Space Administration, USA)

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conducted a series of experiments to investigate the generation and dispersion of flammable clouds [13,14]. The results showed that the ground-level cloud could travel approximately 50–100 m from the LH_2 source, and the cloud rising rate was approximately 0.5–1.0 m/s. In 1994, BAM (Federal Institute for Materials Research and Testing, Germany) carried out a series of large-scale LH_2 spill experiments with the presence of buildings [15,16]. The hydrogen concentration changing over time around the buildings, as well as the ground's temperature changing over time was obtained. In 2011, HSL (Health and Safety Laboratory, UK) performed both unignited and ignited LH_2 releases to investigate the spills of LH_2 at a rate of 60 L/min [17–19]. The clouds of hydrogen produced by the release of LH_2 were fairly difficult to ignite even if four 1 kJ chemical igniters were fired within it. The release of hydrogen in contact with the concrete surface produced a solid deposit of oxygen and nitrogen once the substrate was sufficiently cooled. Besides the experimental results, simulations have also been conducted to analyze the overall behavior features of the liquid spreading and the gaseous diffusion process. Chitose et al. simulated the LH_2 spill tests using the CHAMPAGNE code by performing two-dimensional (in the symmetry plane) two-phase flow calculations [20]. The evaporation model and turbulent mixing model were built in the CHAMPAGNE code and the parametric analysis was performed to discuss the instability of vapor film and the effect of ground roughness. Verfondern et al. simulated the cryogenic liquid pool spreading during the LH_2 spill tests using the LAuV shallow layer code [21]. Schmidt et al. simulated hydrogen gas releases between buildings using the Batelle code BASSIM [22]. The simulation results showed that the release of hydrogen at high velocities results in a much more hazardous situation than a release at low exit velocities, and the approach of the hydrogen cloud to walls or other obstacles influences the pattern of the concentration field. In other studies, parametric analyses were also performed by changing hydrogen flow rate, liquid droplet radius, vapor film thickness and ground roughness [23–25]. As for the model building tests, much work has been done on the setting of air humidity [26], the choosing of LH_2 source model [27] (say liquid pool or downward flow), and the influence of fence presence around the spill site [27]. However, the agreement between the simulation and experimental results of the previous studies needs to be improved, and the influence of some important environmental parameters to the LH_2 spill results also needs to be further analyzed [23].

In the present work, the overall LH_2 spill process will be modeled with the help of CFD software FLUENT, and the simulation results will be compared with the NASA Test 6 experiment for validation. The effect of wind velocity, wind temperature and ground temperature to the essential parameters, such as total vaporization time, farthest downwind height and farthest downwind distance to the flammable cloud, will then be analyzed.

Physical and mathematical model

Physical description

The physical model of LH_2 spill process is presented in Fig. 1. As soon as the LH_2 leaves the storage tank, part of it vaporizes immediately by the heat from the ambient while part of it drops to the ground and vaporizes gradually by the heat absorbed from the ground. Shortly after the cease of the LH_2 spill, all spilled LH_2 will turn into gas, and then the gaseous hydrogen will continue to disperse.

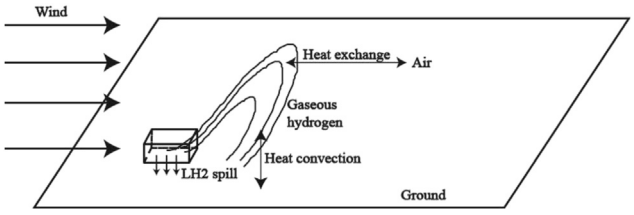

Fig. 1 – Physical model of LH_2 spill process.

Mathematical formulation

The mean flow was modeled using the three-dimensional, transient, fully compressible conservation equations for mixture mass, mixture momentum, mixture enthalpy and hydrogen mass fraction.

The continuity equation for the mixture is [27].

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

Assuming that there is no slip between the phases, the momentum equation for the mixture is [25].

$$\frac{\partial \rho u_i}{\partial t}+\frac{\partial \rho u_j u_i}{\partial x_j}=-\frac{\partial P}{\partial x_i}+\rho g_i+\frac{\partial}{\partial x_j}\left((\mu+\mu_t)\left(\frac{\partial u_j}{\partial x_i}+\frac{\partial u_i}{\partial x_j}\right)\right) \tag{2}$$

The hydrogen mass fraction (liquid plus vapor) equation is [27].

$$\frac{\partial \rho q_l}{\partial t}+\frac{\partial \rho u_j q_l}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\left(\rho d+\frac{\mu_t}{Sc_t}\right)\frac{\partial q_l}{\partial x_j}\right) \tag{3}$$

The energy equation for the mixture is [27].

$$\frac{\partial \rho H}{\partial t}+\frac{\partial \rho u_j H}{\partial x_j}=\frac{\partial}{\partial x_j}\left(\frac{\mu_t}{Pr_t}\cdot\frac{\partial H}{\partial x_j}\right)+\frac{dP}{dt}+\frac{\partial}{\partial x_j}\left(\lambda\frac{\partial T}{\partial x_j}+\rho d H_i\frac{\partial q_i}{\partial x_j}\right) \tag{4}$$

The modeled transport equations for k and ε in the realizable k–ε model are [28].

$$\frac{\partial}{\partial t}(\rho k)+\frac{\partial}{\partial x_j}(\rho k u_j)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_k}\right)\cdot\frac{\partial k}{\partial x_j}\right]+G_k-\rho\varepsilon \tag{5}$$

$$\frac{\partial}{\partial t}(\rho \varepsilon)+\frac{\partial}{\partial x_j}(\rho \varepsilon u_j)=\frac{\partial}{\partial x_j}\left[\left(\mu+\frac{\mu_t}{\sigma_\varepsilon}\right)\cdot\frac{\partial \varepsilon}{\partial x_j}\right]+\rho C_1 E\varepsilon-\rho C_2\frac{\varepsilon^2}{k+\sqrt{\nu\varepsilon}} \tag{6}$$

where $C_1=\max\left[0.43,\ \frac{\eta}{\eta+5}\right]$, $\eta=\sqrt{2S_{ij}\cdot S_{ji}}\cdot\frac{k}{\varepsilon}$, and $S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)$.

The liquid–vapor mass transfer (evaporation/condensation) is governed by the vapor transport equation [26]:

$$\frac{\partial}{\partial t}(\alpha_v \rho_v)+\nabla\cdot\left(\alpha_v \rho_v \overrightarrow{V_v}\right)=\dot{m}_{l\to v}-\dot{m}_{v\to l} \tag{7}$$

As given in the right side of Equation (6), FLUENT defines the positive mass transfer as being from the liquid to the

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