INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2014) 1–7

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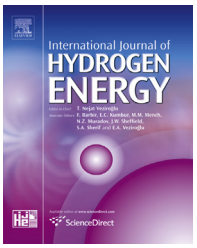

CFD based simulation of hydrogen release through elliptical orifices

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ARTICLE INFO

Article history:
Received 20 January 2014
Received in revised form
24 March 2014
Accepted 27 March 2014
Available online xxx

Keywords:
Hydrogen
Computational fluid dynamics
Under-expanded jet
Elliptical orifice
Enlarging orifice

ABSTRACT

Computational Fluid Dynamics (CFD) is employed to investigate the hydrogen jet exiting through different shapes of orifices. The effect of orifice geometry on the structure, development and dispersion of a highly under-expanded hydrogen jet close to the exit is numerically investigated. Various shapes of orifices are evaluated, including holes with constant areas such as elliptical and circular openings, as well as, enlarging circular orifices. A three-dimensional in-house parallel code is exploited to simulate the flow using an unstructured tetrahedral finite volume Euler solver. The numerical simulations indicate that, for a high pressure reservoir hydrogen release, the area of the orifice is the main geometric parameter influencing the centerline pressure at the hydrogen-air interface and the transient peak temperature, while the elliptical or expanding orifices slightly mitigate the auto-ignition risks associated with the accidental release of hydrogen. Therefore, circular openings represent the most conservative geometry for the study of auto-ignition of hydrogen.

Introduction

The accidental release of hydrogen from a high-pressure reservoir into the low-pressure surrounding results in the formation of the under-expanded jet and can lead to auto-ignition or to the dispersion of a hydrogen cloud. Investigations of hydrogen dispersion are reported in various numerical and experimental studies [1–3]. Some studies have focused on the calculation of the hydrogen concentration and its relation to dimensions of the circular exit [1,2]. Han et al. [4] studied the concentration distribution and the mass flux of hydrogen released from a pressurized tank through different hole sizes (less than 1 mm) and storage pressures (less than 400 bar). They defined the dilution length of a specific hydrogen mole fraction as a distance from the hole. Results represented a consistent decrease of the centerline hydrogen concentration and the dependency of mass reduction ratio on 1/d for different storage pressures less than 400 bar.

Other studies have focused on the evaluation of the ignition and the auto-ignition possibility of the hydrogen release. Radulescu et al. [5,6], analyzed the effect of the volumetric expansion on the ignition of high-pressure hydrogen release in a diffusion layer by applying the Lagrangian unsteady diffusion-reaction model. It was demonstrated that the strong expansion can lessen the ignition possibility. Furthermore, it was shown that for each storage pressure there exists a size of the hole that separates the non-ignition region from the auto-

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http://dx.doi.org/10.1016/j.ijhydene.2014.03.226

ignition region. Many studies have been conducted to clarify the effects of tube length and tube diameter on the auto-ignition possibility of the high-pressure hydrogen release [7–10]. Golub V. et al. [7] investigated the hydrogen auto-ignition in tubes both numerically and experimentally. The effect of the shape of the release tube on the auto-ignition was analyzed. Two different shapes of the tube were considered, circular and rectangular. It was shown that the auto-ignition in a rectangular tube occurred at a lower pressure compared to its equivalent circular tube.

Yamada E. et al. [9,10] carried out a direct numerical simulation (DNS) with a detailed chemical model to study the ignition of high-pressure hydrogen (40 MPa) discharging into the air. For a given tube diameter, the effect of varying tube lengths was evaluated. It was found that there is a relation between the length of the tube and the auto-ignition. A longer tube provides enough space for hydrogen and air to mix before the exit, and in turn, a higher possibility of auto-ignition. Very detailed direct numerical simulation DNS, which is made for smaller release pressures and longer release tubes, lead to similar conclusions [11,12]. Furthermore, it was recognized that longer tubes increase the ignition probability and for a higher release pressure, an auto-ignition can occur inside the release tube. This effect is related to the better mixing of hydrogen and air through molecular diffusion. Khaksarfard R. et al. [13] numerically investigated the expanding of the release area with different expansion rates. It was shown that the pressure on the contact surface is sensitive to the opening speed. The higher the opening speed, the higher the expansion of the hydrogen jet.

Most of the studies about hydrogen safety issues have focused on circular nozzles and the development of a hydrogen jet exiting from a standard round exit hole. Thus, owing to the lack of study of the hydrogen dispersion and its auto-ignition possibility under different conditions in terms of geometrical layout, this work aims to numerically investigate the effect of the orifice geometry on the behavior and development of the hydrogen jet issuing from different types of release exits. The novelty of this work is that various types of exits including elliptical, expanding and circular are considered, and jet characteristics and expansion are compared between these different cases.

Computational domain and model

The 3D computational domain consists of a circular cylinder as a reservoir containing hydrogen gas at a high pressure and a 2 mm straight nozzle leading to the exit at the ambient pressure. To examine the influence of the orifice geometry on the jet behavior and the ignition possibility, three different shapes of orifices are considered including fixed circular, fixed elliptic and an expanding exits.

Computational model

In this study, a three-dimensional in-house parallel code is exploited to simulate the flow. This code has been extensively validated with experimental results for a wide variety of CFD problems [14]. Abrupt discharging of hydrogen from a high-pressure tank into a low-pressure quiescent environment causes a highly under-expanded jet. Due to the high Reynolds number in the vicinity of the release hole, convection dominates over viscosity and diffusivity and the flow is modeled by the compressible Euler equations [3,6].

$$\frac{\partial \vec{U}}{\partial t} + \vec{\nabla}.\vec{\vec{F}}(U) = 0, \tag{1}$$

Since a dynamic mesh algorithm based on the spring analogy is employed to simulate the enlarging orifices, the Euler equations must be modified. This method was described in Ref. [13]. Considering the dynamic mesh formulation in which the convection velocity components are the relative velocity between fluid and coordinates for a time-dependent system, the modified conservative fluxes in the Euler equations will be as follows:

$$\vec{\vec{F}} = \left(\begin{bmatrix} \rho(u-w_x) \\ \rho(u-w_x)u+P \\ \rho(u-w_x)v \\ \rho(u-w_x)w \\ \rho(u-w_x)E+uP \end{bmatrix} \begin{bmatrix} \rho(v-w_y) \\ \rho(v-w_y)u \\ \rho(v-w_y)v+P \\ \rho(v-w_y)w \\ \rho(v-w_y)E+vP \end{bmatrix} \begin{bmatrix} \rho(w-w_z) \\ \rho(w-w_z)u \\ \rho(w-w_z)v \\ \rho(w-w_z)w+P \\ \rho(w-w_z)E+wP \end{bmatrix} \right) \tag{2}$$

where w_x, w_y, w_z are the grid speeds along the coordinate directions. In the case of a fixed mesh, the grid velocities are not considered and the cell volume is not time-dependent. A discrete form of the Euler equations based on the implicit finite volume method can be written as:

$$|V_i| \frac{\vec{U}_i^{n+1} - \vec{U}_i^{n}}{\Delta t} + \sum_{\text{over } \partial V_i} \vec{\vec{F}}_{\partial V_i}^{n+1} \cdot \vec{n}_{\partial V_i} \Delta S_{\partial V_i} = 0 \tag{3}$$

The system of linear equations is solved by means of a fully implicit scheme which has an accuracy of the first and second orders in time and space, respectively. Convective fluxes are evaluated using the Roe-MUSCLE scheme. To avoid oscillations generated near the shock or discontinuity regions, the Van Leer–Van Albada limiter is used to control the accuracy of special approximation at the thin layer near the exit hole where the second-order approximation is switched to the first-order accuracy to prohibit the numerical instabilities in this region.

The system of Euler equations is completed by the Abel Nobel equation of state which is defined as follows [11] [13]:

$$p = \frac{R_{mix}T}{(v-b)} = (1-b\rho)^{-1}\rho R_{mix}T = \zeta \rho R_{mix}T, \;\; b = 0.00775\,\mathrm{m^3/kg} \tag{4}$$

Then the system of equations is solved using an iterative GMRES solver and MPI parallel processing.

To describe the convection of hydrogen into the ambient air and track the shape and the location of the contact surface between hydrogen and air, the advection equation is implemented. The modified form of the transport equation for the dynamic mesh model is written as follows:

$$\frac{\partial c}{\partial t} + \frac{\partial (c(u-w_x))}{\partial x} + \frac{\partial (c(v-w_y))}{\partial y} + \frac{\partial (c(w-w_z))}{\partial z} = 0 \tag{5}$$

where c is a fraction function. A unit value of the fraction function ($c = 1$) corresponds to a cell occupied only by air, and a zero value ($c = 0$) indicates a cell full of hydrogen. The

Please cite this article in press as: Shishehgaran N, Paraschivoiu M, CFD based simulation of hydrogen release through elliptical orifices, International Journal of Hydrogen Energy (2014), http://dx.doi.org/10.1016/j.ijhydene.2014.03.226