INTERNATIONAL JOURNAL OF HYDROGEN ENERGY XXX (2014) 1–6

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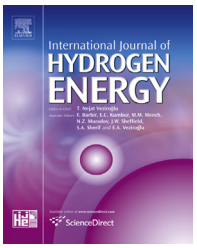

The effect of tube internal geometry on the propensity to spontaneous ignition in pressurized hydrogen release

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Keywords:
Spontaneous ignition
Shock reflection
Numerical simulation

ABSTRACT

Spontaneous ignition of compressed hydrogen release through a length of tube with different internal geometries is numerically investigated using our previously developed model. Four types of internal geometries are considered: local contraction, local enlargement, abrupt contraction and abrupt enlargement. The presence of internal geometries was found to significantly increase the propensity to spontaneous ignition. Shock reflections from the surfaces of the internal geometries and the subsequent shock interactions further increase the temperature of the combustible mixture at the contact region. The presence of the internal geometry stimulates turbulence enhanced mixing between the shock-heated air and the escaping hydrogen, resulting in the formation of more flammable mixture. It was also found that forward-facing vertical planes are more likely to cause spontaneous ignition by producing the highest heating to the flammable mixture than backward-facing vertical planes.

Introduction

As a possible next-generation energy carrier, hydrogen's safe transport and utilization is of particular importance. A potential hazard of such system is the high pressure hydrogen releases which are prone to spontaneous ignition [1–14].

Experimental [2–4] and numerical [5–14] investigations have revealed that a possible mechanism of hydrogen spontaneous ignition is shock-induced diffusion ignition. As compressed hydrogen is suddenly released into the ambient environment, a shock wave is generated ahead of the emerging jet and driven into air. The air behind the shock is heated to a level well above the hydrogen auto-ignition temperature. The shock-heated air exchanges mass and energy with hydrogen at contact region, leading to an ignition under specific release conditions. Most previous experimental studies [2–4] focused on phenomenological observations of pressurized releases through a length of tube. According to these experimental observations, release pressure and length of release tube are two major factors affecting the occurrence of the spontaneous ignition: a higher release pressure would facilitate the occurrence of ignition by producing a higher shock-heated temperature, while a longer

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http://dx.doi.org/10.1016/j.ijhydene.2014.04.141

Please cite this article in press as: Xu BP, Wen JX, The effect of tube internal geometry on the propensity to spontaneous ignition in pressurized hydrogen release, International Journal of Hydrogen Energy (2014), http://dx.doi.org/10.1016/j.ijhydene.2014.04.141

tube would provide a longer mixing time to make ignition more readily happen. Dryer et al. [2] also emphasized the importance of the internal geometry downstream of the burst disk and the multi-dimensional shock formation/reflection/interaction resulting from the rupture process of the bursting disk, and postulated that both factors were responsible for significant mixing occurring at the contact surface.

The majority of the previous numerical studies were concerned with releases through a length of tube with constant cross-section except that Xu et al. [6] numerically investigated the effect of a local contraction inside the release tube on the spontaneous ignition. Their study revealed that a local contraction significantly facilitate the occurrence of spontaneous ignition by producing elevated flammable mixture and enhancing turbulent mixing from shock formation, reflection and interaction. Here our previous study [6] is extended to include more general types of internal geometry: local contraction, local enlargement, abrupt contraction and abrupt enlargement.

Numerical methods

For details of the numerical methods, the readers should refer to our previous publication [11]. Briefly, an arbitrary Lagrangian and Eulerian (ALE) method [16] is adopted to treat convective terms separately from diffusion terms in the transport equations considering the substantial scale difference between diffusion and advection. A second-order Crank–Nicolson scheme is used for the diffusion terms and the terms associated with pressure wave propagation, a 3rd-order TVD Runge–Kutta method [17] is used to solve the convection terms. For spatial differencing, a 5th-order upwind WENO scheme [15] is used for the convection terms and the 2nd-order central differencing scheme for all the other terms.

A mixture-averaged multi-component approach [18] is used for the molecular transport with consideration of thermal diffusion for non-premixed hydrogen combustion. For autoignition chemistry, Saxena and Williams' detailed chemistry scheme [19] which involves 21 elementary steps among eight reactive chemical species is used. The scheme was previously validated against a wide range of pressures up to 33 bar. It also gave due consideration to third body reactions and the reaction-rate pressure dependent "fall-off" behaviour. To deal with the stiffness problem of the chemistry, the chemical kinetic equations are solved by a variable-coefficient ODE solver [20].

Problem descriptions

It was revealed in our previous study [11] that spontaneous ignition firstly occurs inside release tubes and gradually evolves into a partially pre-mixed flame before jetting out of tube exits. Therefore, the present study is limited to the flow inside the tube. The computational domain is composed of a cylindrical high-pressure vessel of large diameter and a release tube with varied cross-sections as shown in Fig. 1. The pressurized cylinder is set up to be sufficiently large to ensure that pressure drop during simulations does not exceed 3% of the initial pressure. The release tubes have an initial diameter D of 3 mm and a length L of 6 cm. The contraction and expansion ratios are fixed to be 0.6 and 1.5, respectively in this study. The distance of the internal geometries to the rupture plane is chosen as 5 times of the initial diameter to allow the incident shock to reach a nearly constant shock velocity before it transmits into the abrupt change in flow area. The width of the local contraction/enlargement is set to be the tube diameter. Our previous study [11] has revealed that the rupture process of the initial pressure boundary is crucial to the spontaneous ignition. An Iris model [21] was used to simulate the rupture process of the pressure boundary. It assumes that the pressure boundary, which is mimicked by a thin diaphragm with a thickness of 0.1 mm placed at the left plane of the release tube in the simulations, ruptures linearly from the centre at a finite pre-determined rate as the computations start. To obtain a fast increase rate of the shock velocity, in this study the rupture time, which is the time for a full bore opening of the thin diaphragm, is fixed as 5 μs. A release pressure of 50 bar was chosen which is lower than that required to produce a spontaneous ignition with a tube of constant cross section (Fig. 2).

All the simulations start from still with the tube filled with ambient air and the pressurized cylinder region with pure pressurized hydrogen separated by a thin diaphragm with a thickness of 0.1 mm. All the wall surfaces are assumed to be non-slip and adiabatic. Non-uniform grids are used for the pressurized cylinder while and uniform grids are used for the tube region. Since flame is firstly initiated at the thin contact region, a very fine grid resolution is required to resolve the species profiles in the ignited flame. Following our previous study [11] a 15 μm grid size is used. The non-uniform grids are clustered around the two ends of the tube and the grid sizes range from 15 μm to 150 μm inside the region of the pressurized cylinder. The total grid points are approximately two millions. The key parameters of the computed release scenarios are summarized in Table 1.

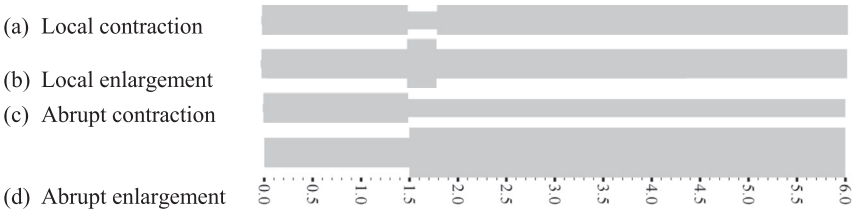

Fig. 1 – Release tubes with varied cross-sections.

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