The Effects of Local Expansion on the Propensity to Spontaneous Ignition in Pressurized Hydrogen Release via a Length of Tube

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1 Introduction

As a possible next-generation energy carrier, safe transport and utilization of compressed hydrogen is of particular importance. A potential hazard of such system is high pressure hydrogen jet originating from either a pressure relief valve or a small crack in the piping of a storage vessel. It is generally accepted that the pressurized hydrogen release can lead to spontaneous ignition [1-15], which could potentially lead to jet fires, rapid flame acceleration and explosions in confined areas.

The spontaneous ignition has been experimentally [2-5] and numerically [5-15] proven to be due to shock-induced diffusion ignition. Most previous experimental studies [2-5] 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 important factors affecting the occurrence of the spontaneous ignition. Dryer et al. [2] emphasized the importance of the internal geometry downstream of the burst disk and the multi-dimensional shock formations/reflections/interactions resulting from the rupture process of the burst disk, and postulated that both factors were responsible for significant mixing occurring at the contact surface. In their experimental observation the minimum release pressure to induce an ignition for a release through a tube with internal geometries is as low as 20.4bar. In a recent study by Maxwell et al. [5] the turbulence-enhanced mixing at the contact surface due to the shock reflections from the confinement walls was also expermentally and numerically confirmed.

All the aforementioned previous numerical studies were concerned with releases through a length of tube with constant cross-section. In the present study, numerical simulations of spontaneous ignition in pressurized hydrogen release through a length of tube with a local expansion is conducted using our previously developed numerical model [12].

2 Numerical Methods

Numerical study of the spontaneous ignition is of particular challenge because of the substantial scale difference between diffusion and advection and the reactive flow accompanied by strong shock waves. To explicitly resolve physical diffusion at the contact region, high-order numerical schemes

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along with fine grid resolution are required to prevent it from being smeared by numerical diffusion. For applications involving rich shock structures, high-order WENO shock-capturing schemes are more efficient than low order total variation diminishing (TVD) schemes and can help to reduce numerical diffusion [16].

Considering the substantial scale difference between diffusion and advection, an arbitrary Lagrangian and Eulerian (ALE) method [17] was adopted to treat convective terms separately from the diffusion terms and the pressure-related terms in the transport equations. For time differencing, a second-order Crank-Nicolson scheme is used for the diffusion terms and the terms associated with pressure wave propagation in the Lagrangian phase and a 3rd-order TVD Runge–Kutta method [18] is used to solve the convection terms in the rezone stage. For spatial differencing, a 5th-order upwind WENO scheme [16] is used for the convection terms and the second-order central differencing scheme is used for all the other terms including the diffusion terms and the pressure-related terms.

A mixture-averaged multi-component approach [19] was used for the calculation of molecular transport with consideration of thermal diffusion which is important for non-premixed hydrogen combustion. For autoignition chemistry, Saxena and Williams' detailed chemistry scheme [20] which involves 21 elementary steps among eight reactive chemical species was 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 were solved by a variable-coefficient ODE solver [21]. More detailed description of the numerical models and validations can be found in Wen et al. [12].

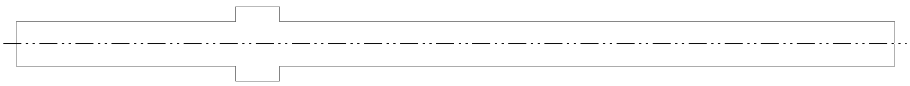

Figure 1. Geometries of release tube with a local expansion.

3 Problem Descriptions

Table 1: Computational details

Parameters	Values
Rupture time (μs)	5
Release pressure (bar)	50, 25
Initial Temperature (K)	293
Diameter of tube (mm)	3
Length of tube (mm)	60
Expansion ratio	1.5
Thickness of film(mm)	0.1
Minimum grid spacing (μm)	15

It was revealed in our previous study [12] that spontaneous ignition firstly occurs inside the release tube and gradually evolves into a partially pre-mixed flame before jetting out of the tube exit. Therefore, the present study is limited to the flow inside the release tube. The computational domain is composed of a cylindrical high-pressure vessel of large diameter and a release tube with a local expansion as shown in Fig. 1. The pressurized cylinder was set up to be sufficiently large to ensure that pressure drop during simulations does not exceed 3% of the initial pressure. The release tube has a diameter D of 3 mm and a length L of 6 cm. The expansion ratio is fixed to be 1.5. The distance of the local expansion to the rupture plane is chosen as 5 times of the tube diameter, which ensures that the incident shock reaches a nearly constant shock velocity before transmitting into the expansion section if the finite opening time of the pressure boundary is taken into account. The width of the local expansion is set to be the tube diameter. In our previous study [12] it was found that the rupture process of the initial pressure boundary is crucial to the spontaneous ignition. An Iris model [22] is 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 simulations start. It was revealed [12] that although the shock velocity finally stabilizes at approximately the same value after the rupture for different rupture times, the longer the rupture time, the slower the increase rate of the shock velocity. 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. Two release pressures of 50 bar and 25 bar, which are not sufficiently high to produce a spontaneous ignition for a tube of a constant cross-section, are considered in this study.

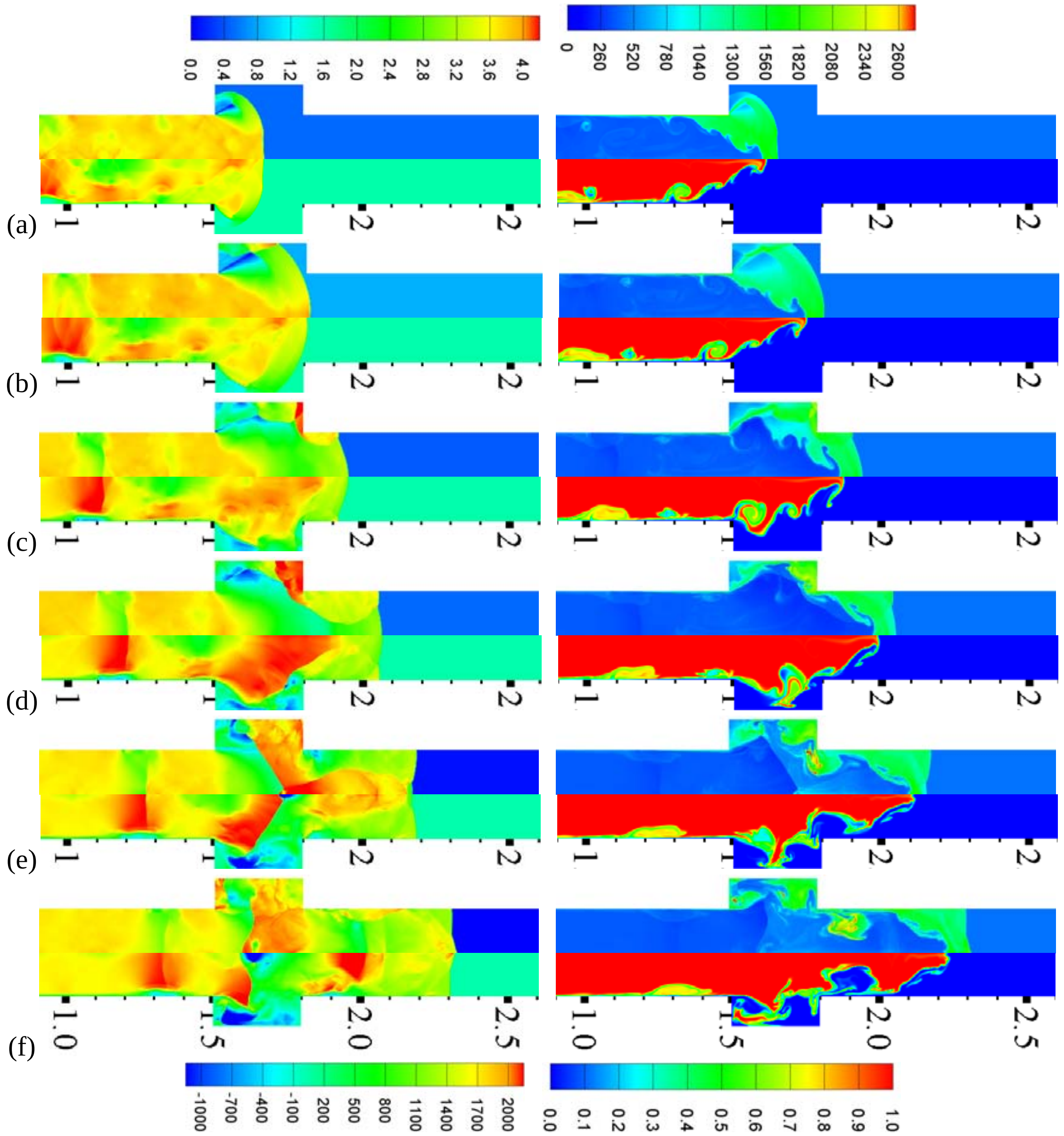

Figure 2. Predicted contours of the Logarithm of pressure (bar) and axial velocity (m/s) listed in the left column, temperature (K) and hydrogen mass fraction listed in the right column at a time interval of 1 μs starting from 14 μs for the case of 50 bar. (Pressure and temperature are shown in the upper half of each frame; while axial velocity and mass fraction are shown in the lower half of each frame.)

All the simulations were started from no flow condition 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 were assumed to be non-slip and adiabatic. Non-uniform grids were applied to the regions of pressurized cylinder and uniform grids to the tube region. Since ignition is first initiated at the thin contact region, a very fine grid resolution is required to resolve the species profiles in the ignited flame. According to our previous study [12] a 15 μm mesh size is sufficient to resolve the species profiles hence used in this study. The non-uniform grids were clustered around the two ends of the tube and the grid sizes range from 15 μm ~150 μm inside the region of pressurized cylinder. The total grid points are then approximately two millions in the current simulations. The key parameters of the computed release scenarios are summarized in Table 1.

4 Results and Analysis

It was revealed in our previous study [12] that a curvilinear incident shock is quickly generated and reflected from the tube wall. The reflected shock converges at the axis of symmetry creating shock focusing. The repeating processes of shock reflection and focusing create an intermittent flow pattern of circular and central flows causing a tongue-shaped contact region (see Figure 2(a)). Following rupture, the shock velocity reflecting the strength of the incident shock gradually reaches maximum and then slowly decreases. For the current release conditions, the maximum shock velocity is reached at a distance of approximately 5 times the tube diameter downstream the rupture plane, i.e. the location of the local expansion.

Figure 2 shows a close-up of flow development at the local expansion using the predicted contours of pressure, axial velocity, temperature, and hydrogen mass fraction. As the planar incident shock moves into the expansion section, it quickly diffracts into a semi-spherical shock once the diffraction wave originating from the left edge of the expansion section reaches the axis of symmetry at t=15 μs (Figure 2(b)). Meanwhile the semi-spherical shock is reflected back first from the side wall of the expansion tube and then from the right vertical wall and the downstream tube wall. Two reflected shock waves merges near the left corner at t=16 μs (Figure 2(c)) raising the fluid temperature behind them (see Figure 2(c-d)). The second reflected shock having a curvilinear shape is much stronger and part of it converges on the axis creating two jet flows moving in the opposite directions (see Figure 2(e-f)). The upper part of the second reflected shock impacts on the left vertical wall and bounces back and forth between two vertical walls. As the flow passes the expansion section, a large low-speed recirculation flow sustains between two vertical walls. Both the shock reflections and the recirculation flow between two vertical walls create favorite conditions for the ignition. The reflected shock from the downstream tube wall also creates an annular Mach stem (see Figure 2(c-d)) in the form of a von Neumann Mach reflection. Ignition is first observed at t=17 μs (Figure 2(d)) at the contact region near the right edge of the expansion section and then the initial flame extends along the contact region propagating downstream. At t=19 μs (Figure 2(f)) another two ignition locations emerges inside the recirculation zone.

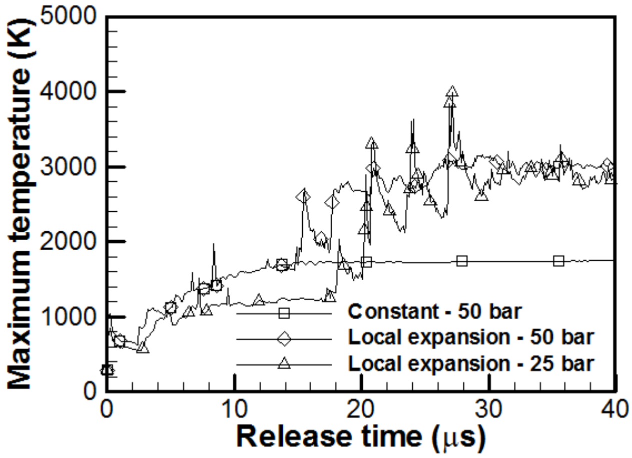

Figure 3. Maximum temperature versus release time.

Figure 3 shows the maximum temperature versus release time. For the cases of 50 bar release, the maximum temperature jumps to 1046K at t=0.2 μs after the rupture due to the shock heating and then drops to 624K at t=2.3 μs due to the flow divergence. After t=2.3 μs it quickly increases again due to the shock reflection. Two spikes at t=6.6 μs and 8.3 μs are caused by shock focusing. For the case with a constant cross-section, it finally stabilizes a value of 1653K from t=13 μs and no ignition occurs. For the case with a local expansion, it jumps to 2715K at t=15.5 μs due to the strong shock reflection from the right vertical plane. After the reflection, it decreases to 1945K at t=16.7 μs and then jumps to 2703K due to the ignition at t=18 μs. After the ignition, it fluctuates but still remains at a very high value. The spikes appearing after the ignition are caused by shock reflections and focusing. For the cases of 25 bar, as the incident shock reaches the right vertical wall, it increases to 2028K at t=18.2 μs resulting in an ignition at t=20.2 μs. It is revealed that both temperature behind the reflected shock from the vertical wall and the ignition time decrease with the release pressure. For the cases of both 25 bar and 50 bar, the maximum temperature stays well above 2000K after the ignition indicating that the flames are sustained in the tube.

5 Conclusion

The effect of a local expansion inside the release tube on the propensity to spontaneous ignition is investigated. As the planar incident shock moves into the expansion section, it quickly diffracts into a semi-spherical shock. The semi-spherical shock is then reflected back first from the side wall of the expansion tube and then from the right vertical wall. Two reflected shock waves merges near the left corner raising the fluid temperature behind them. The second stronger reflected shock converges on the axis creating jet flows. As the flow passes the expansion section, a large low-speed recirculation flow sustains between the two vertical walls. Both the shock reflections and the recirculation flow between the two vertical walls create favorite conditions for the ignition, which is firstly observed at the contact region near the right edge of the expansion section and then the initial flame extends along the contact region propagating downstream.

The present study suggests that the internal geometry of a local expansion can significantly increase the propensity to spontaneous ignition by raising the temperature of the flammable mixture and enhance turbulent mixing due to the shock reflections and interactions.

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