

# Effect of Burst Pressure on the Spontaneous-Ignition of High-Pressure Hydrogen Released through a Tube

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## 1 Introductions

Utilization of high-pressure hydrogen has been extended to various industries, but there are still safety problems in real applications. It is because pressurized hydrogen released into the air by accident or during technical operation can undergo spontaneous ignition and/or explosions. In fact, many accidents by hydrogen leaks have been occurred over the last century and any specific ignition source was not revealed in many cases [1]. Many plausible causes had been suggested on this issue, but in present, a diffusion ignition model is universally accepted as the most influential mechanism through several studies using pressurized hydrogen released into air by the failure of rupture disk through extension tubes to simulate practical systems. This is also supported by the fact that most of hydrogen accidents have been initiated from a plumbing system such as pipes, flanges and valves [2].

Studies on the diffusion ignition model have been conducted through experimental and numerical investigations using a rupture disk and an extension tube [3-12]. Dryer et al. [4] suggested that both a sufficiently high burst pressure and a downstream geometry for fast mixing of the hydrogen and air is necessary from the experimental investigation. Mogi et al. [7,8] also showed the similar results that the ignition depends on the tube length and the burst pressure. Wen et al.[9] and Lee and Jeung [10] conducted numerical simulations on this issue. Wen et al.[9] conducted the parametric study through the numerical simulation. They investigated the various influencing factors such as rupture time, burst pressure, tube diameter and tube length on the spontaneous ignition of high-pressure hydrogen in detail. Lee and Jeung [10] focused a mixing process by the multi-dimensional interactions inside the tubes. Lee et al. [11] showed that there are two reaction regions from the visualization images at the exit of the tube, and the flame cannot be sustained when two reaction regions are not merged due to short tube length.

From these previous results, it seems that the ignition mechanism is quite clear, but it remains imperfect. In fact, most of above experimental and numerical results were obtained from the burst pressure of about 10 MPa and less than 20 MPa. However, there can be a strong possibility that the feature of shock interactions and mixing can be different largely and the mechanism can be also different if the burst pressure is higher than 20 MPa.

At these points, it is needed to confirm that the previous conclusions are still valid in all burst pressure. In this study, it was tried to analyze the effect of shape of the rupture disk and higher pressure of

above 20 MPa on the spontaneous ignition mechanism inside the tube. To do this, the numerical simulations have been conducted for the various rupture conditions, which the burst pressure of maximum 70 MPa were applied for one tube with the diameter of 10.9 mm and length of 100 mm. The numerical results are suggested as being classified into three types such as low, high and extremely high, with burst pressures in this paper. As the numerical results, flow formations, ignition process and flame propagation inside the tube were analyzed in detail and the paper suggested the different ignition features with a burst pressure.

## 2 Numerical methods

The governing equations are the unsteady, compressible two dimensional axi-symmetric Navier–Stokes equations for a chemically reactive multi-species mixture of ideal gases.

For solving multidimensional problems, the finite volume approach is employed. The solution is updated including all the intercell fluxes in a single step. Using the rotational invariance property of Euler equations, the local Riemann problem becomes a one-dimensional system in the rotated frame. The resulting numerical flux is rotated back to obtain the required intercell flux at each side. The convective numerical fluxes are evaluated by the HLLC scheme [13]. HLLC scheme is switched to HLL scheme in the vicinity of such regions [14,15]. The second-order upwind finite volume scheme is achieved using the weighted average flux (WAF) scheme [15]. Total Variation Diminishing (TVD) modification of the WAF flux is evaluated by the MINBEE (Minmod) limiter. The viscous fluxes are solved by the Crank-Nicolson method. Thermodynamic properties of the species are obtained from the thermodynamic database of NASA [16]. The transport properties of pure species--the viscosity coefficient, thermal conductivity, and mass diffusion coefficient--are obtained from the classical kinetic theory. The properties in a gas mixture are obtained from the mixture-averaged methods [17,18]. For the reaction source terms, the stiff ODEs are solved by RADAU5 [19]. A comprehensive kinetic model of hydrogen combustion, updated by Li et al. [20] and based on the mechanism of Mueller et al. [21], is used for describing the reaction kinetics with nine species and nineteen reactions. The second-order time accuracy of the multi-dimensional system with reaction source terms is achieved by the operator splitting method--Strang splitting [22].

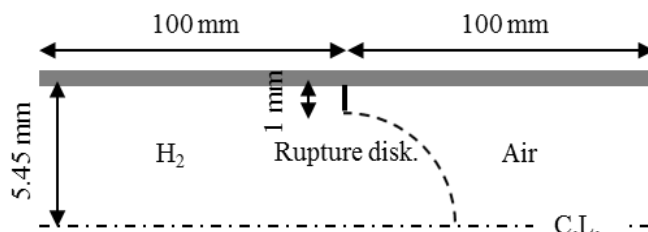


Figure 1. Computational domain with the geometry

Figure 1 shows the computational domain with the geometry of the pressure boundary that represents the shapes of the rupture disk. The computed tube length from the plane of the rupture disk is 100 mm, and the inner radius is 5.45 mm. The upstream part of the tube from the plane of the rupture disk is 100 mm, which is sufficient for the present simulation, since an expansion wave moves only to the left-hand side and does not affect the rest of the domain. The radius of the hemispherical part of the rupture disk is assumed to be about 4.45 mm. A thin vertical wall with a height of 1 mm is remained. For the boundary conditions, adiabatic non-slip conditions for the tube wall, transmissive conditions for both ends of the computational domain, and slip conditions for the axis of symmetry are applied. The initial temperature is set at 300 K for both the hydrogen and air, and the initial pressure on the air side is set at 0.1 MPa. A Cartesian grid system with a uniform size of 10  $\mu\text{m}$  is used downstream of the plane of the rupture disk. The total number of cells is about 8 million.

### 3 Results and discussions

Figure 2 shows the numerical images for the low burst pressure,  $P_b=10$  MPa. Equivalence ratio (ER), the concentration of OH radical and local Mach number are presented in the figure. The results show the ignition process in detail, and observed mechanism is very similar with the previous results [10]. The moment of the disk failure is time 0. The spherical leading shock wave is formed by the spherical shape of pressure boundary, which impacts the side wall of the downstream tube and is reflected back. Subsequently, the shock focusing is observed at the axis of symmetry, which causes a strong jet and flow instability. The jet is strong enough to intrude the preceding shock along the axis of symmetry and starts to form a vortex ring at the center of the tube, as shown in the images of 10  $\mu\text{sec}$ . From the results, we can see there are the two separate reaction regions, boundary layer and core region, at the initial stage. The reaction region within the boundary layer is due to a volume of mixture formed within the heating boundary layer as the contact surface of expanding hydrogen and ambient air interacts with the developing boundary layer. The reaction in this region grows into the hot shocked region along the junction of boundary layer and the contact surface. On the other hand, the reaction in the core region is also observed along the mixing region by a generated vortex ring. Reaction region by spontaneous ignition is observed as the low-density area, which corresponds to the high temperature area and the local distribution of OH radicals. These two ignition regions grow and eventually meet each other forming a complete section of flame at 40  $\mu\text{sec}$ . After that this complete flame over the cross section is sustained and propagates along the downstream tube.

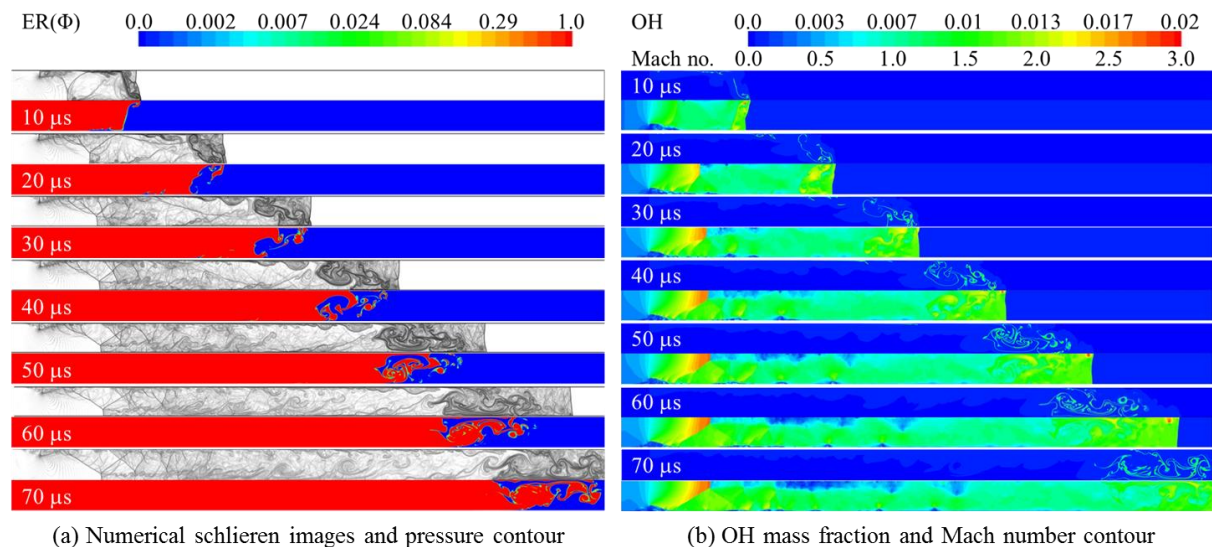


Figure 2. Numerical results for the low burst pressure ( $P_b=10$  MPa)

In this paper, high pressure was defined from the burst pressure of 20 MPa to 40 MPa. Figure 3 shows the numerical results at the high burst pressure,  $P_b=30$  MPa. The numerical results from 20 to 40 MPa are shown the same tendency. Generally, the flow formation for the high burst pressure is very similar with that of low burst pressure in the initial stage after a failure of rupture disk. There is reaction in the core region, and reaction region near the boundary layer is developed gradually as the flow is propagated downstream. However, compared to the results for the low burst pressure of 10 MPa, the different ignition feature is observed. The flow is formed very similarly until 10  $\mu\text{sec}$  after a failure of disk. A vortex ring is generated from the multi-dimensional shock interactions and a strong reaction is also observed in the core region. Simultaneously, the reaction region near the boundary layer is also

developed well. But, two reaction regions are not merged together and two regions apart from each other gradually as the flow near the vortex ring is propagated downstream very fast as shown in the Mach number contours. As the flow is propagated downstream, the reaction in the core region disappears and only reaction region generated from the boundary layer is developed widely. Consequently, the reaction in the core region does not play a key role to initiate the spontaneous ignition any more when the burst pressure is high.

The results show the same tendency for explaining the spontaneous ignition patterns as the burst pressure increases. The speed that a flame is generated and propagated is getting faster as a burst pressure increases. As the burst pressure is higher, a large vortex ring and a strong reaction are observed in the core region at the initial stages after a failure of a disk, but they are disappeared soon. Instead, the reaction region developed from the boundary layer grows up gradually and becomes a complete flame filling the cross section of the tube. That is, when the burst pressure is high, two reaction regions are generated by the multi-dimensional shock interactions because of spherical pressure boundary, however, it is observed that the reaction of the core region is not important to initiate the ignition. Rather than this, the reaction region developed from the boundary layer plays a main role for spontaneous ignition inside the tube. Therefore, some tube length is necessary to initiate the spontaneous ignition even though the burst pressure is high sufficiently, because the ignition mechanism depends on the reaction region developed from the boundary layer which is slower than the mixing and reaction region of the core region.

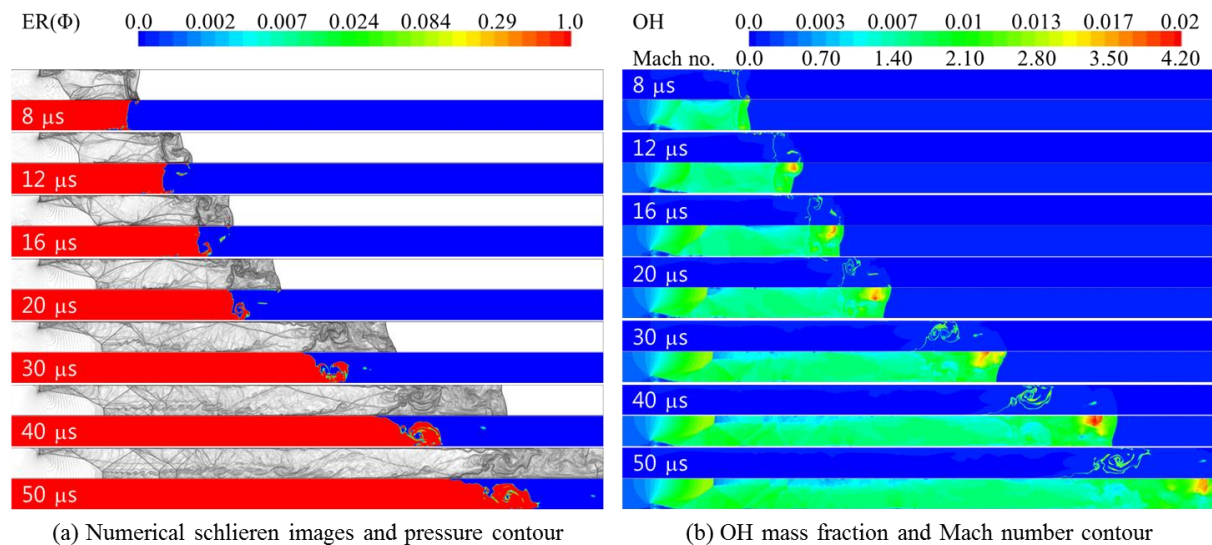


Figure 3. Numerical results for the high burst pressure ( $P_b = 30$  MPa)

Figure 4 is the results for the extremely high burst pressure,  $P_b$  of 70 Mpa. A high-pressure of hydrogen is usually used to 40 Mpa in present, but its utilization is expected to extend upto about 70 Mpa as like a fuel cell car. For this reason, it is needed to check the ignition feature at the very high burst pressure. In the initial stage after a failure of rupture disk, the feature of flow formaion is very similar with that of low and high burst pressure. Two mixing and reaction regions, in the core region and near the boundary layer, are induced by a multi-dimensional shock interactions. And it seems that two regions are taken apart separately until 12  $\mu$ sec as like the results of high burst pressure. However, after that, two reaction regions are merged again as the reaction region developed from the boundary layer moves very fast. The reaction region generated from the boundary layer already fills the tube

fully at 20  $\mu\text{sec}$  and then it develops with the reaction in the core region together to 30  $\mu\text{sec}$ . From the next, it is difficult to distinguish two reaction region and the reaction region is developed widely.

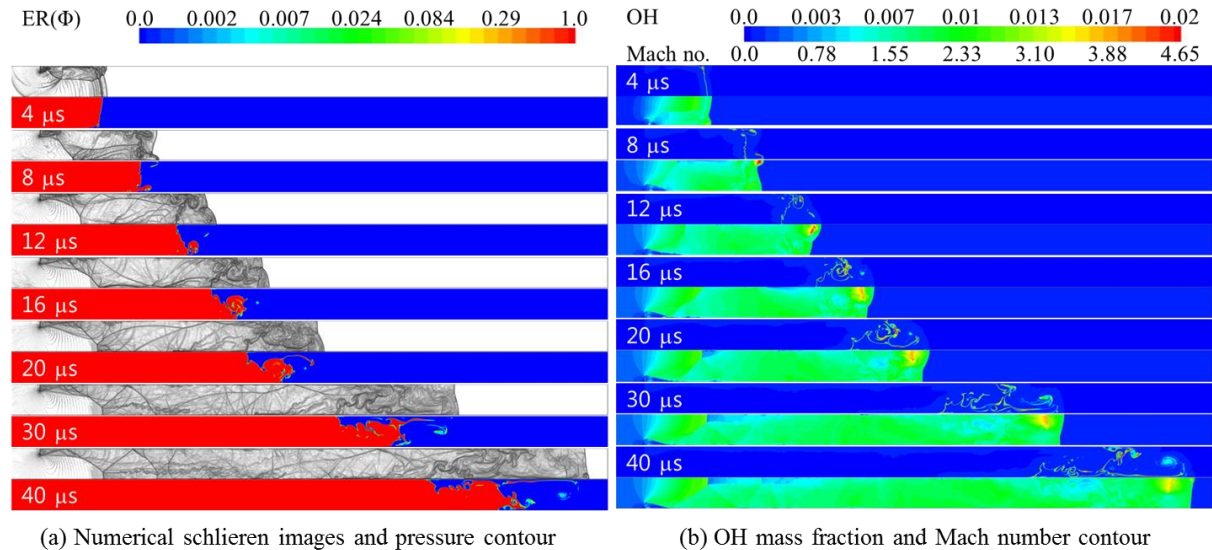


Figure 4. Numerical results for the extremely high burst pressure ( $P_b=70$  MPa)

## 4 Summary

The numerical simulations allow for detailed visualization of the flow development and spontaneous ignition features of hydrogen released through a tube for various burst pressures. The numerical simulation was conducted up to the burst pressure of 70 MPa. In this paper, the burst pressure was classified by three types with the values such as low (about 10 MPa), high (up to 40 MPa) and extremely high (70 MPa) burst pressure. The numerical results showed that ignition mechanism is closely connected with flow formation inside the tube which is strongly affected by the burst pressures. From the results, it is possible to reconsider the ignition mechanism and its concept postulated from previous studies.

It is obvious that the multi-dimensional shock interactions can play a critical role for the ignition as making separated two mixing regions inside the tube. However, the reaction induced by a vortex ring in the core region or the merge of two reaction regions is not essential necessity to initiate a spontaneous ignition as the burst pressure is higher. For the low burst pressure, the ignition feature is very similar with the previous results as showing that the reaction in the core region is important. However, if the burst pressure is higher than 20 MPa, the spontaneous ignition could be initiated by only reaction region developed from the boundary layer as a reaction in the core region is disappeared. In this case, the reaction in the core region cannot play any role to initiate the spontaneous ignition as it disappears soon after a failure of disk. The complete flame is formed by a reaction region developed from the boundary layer and the spontaneous ignition can be initiated from it. When the burst pressure is extremely high it seems that the two reaction region is merged again because the reaction generated from the boundary layer also moves very fast. The reaction region near the boundary layer is developed fast enough to fill the tube and spread widely inside the tube. Consequently, the reaction region near the boundary layer is very important to initiate the ignition when the burst pressure is high.

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