Research paper

Numerical simulation on hydrogen fuel jetting from high pressure tank

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Abstract

In this paper, direct numerical simulations are performed in order to investigate whether an ignition will happen when a small hole is opened suddenly on the wall of an extremely high pressure hydrogen tank and a hydrogen jet is ejected out of the tank into the air. Two-dimensional axisymmetric Euler equations with a full chemical mechanism of hydrogen-air mixture are employed, where the detailed chemical mechanism consists of 9 species and 18 elementary reactions. Mass diffusion and heat conduction terms are included in the governing equations. The diameter of the hole is 1 mm. Three cases of tank pressures, 10, 40 and 70 MPa, are simulated. The results show that a local combustion occurs at the tip region of the contact surface at 10 μs after hydrogen jetting out from the hole for the 40 and 70 MPa tank pressure cases. This local combustion is caused by the strong shock wave which heats up the air in front of the hydrogen jet to a very high temperature. However, as the jet propagates away from the tank wall, its strength drops off and the local combustion is quenched quickly. The results demonstrate that the local combustion is blown off and it can not develop into a stable jet flame under the pressure and the diameter of the hole being examined in this study.

Keywords: Hydrogen jet, Auto-ignition, Shock wave, High pressure, Numerical simulation

1. Introduction

Fuel cell for automobile industry has been developed recently and the safety issue of the high pressure hydrogen becomes important[1]. It is concerned about whether a high pressure hydrogen jet can be ignited if there is an accidental leak. For a high pressure hydrogen tank, its pressure is more than 10 MPa and a typical speed of a sonic jet is about 1,300 m s^{-1}. The accidental emission of the hydrogen into the air produces a strong shock wave. The strong shock wave compresses and heats up the air in front of the hydrogen jet. Under such conditions, the temperature of the air considerably exceeds the over-all temperature of the hydrogen jet. This can lead to an explosion even if the temperature of the hydrogen is considerably below its ignition temperature[2)~3)]. The aim of the present work is to study the diffusion ignition mechanism of the high pressure hydrogen jet to determine the conditions under which such an ignition is possible.

In this paper, we conduct direct numerical simulations to investigate the ignition mechanism of the high pressure hydrogen jet. Two-dimensional axisymmetric Euler equations and a detailed chemical mechanism are used to simulate the hydrogen ignition. Mass diffusion and heat conduction terms are considered in the governing equations. A small hole with a diameter of 1 mm is assumed to be opened on the wall of a tank suddenly and a sonic hydrogen jet is injected into the air. The pressure of the tank is taken to be 10, 40 and 70 MPa, respectively.

2. Numerical setup and method

Two-dimensional axisymmetric Euler equations and a detailed chemical reaction mechanism are employed to simulate the ignition of the hydrogen jet at the early stage of the leakage. The detailed chemical reaction mechanism

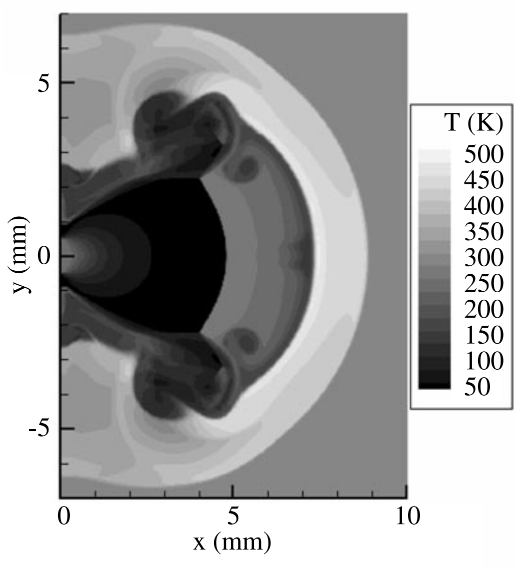

Fig. 1 Temperature contours at 10 μs of 10 MPa case.

of hydrogen-air mixture is constituted by 9 species (H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, and N_2) and 18 elementary reactions[4]. Mass and heat diffusion terms are considered in the governing equations. A Harten-Yee type Non-MUSCL TVD scheme is used for the convection term integration and the central difference for the mass and heat diffusion terms. The time discretization is implemented by a Strang-type fractional step method. Especially, chemical reactions are treated by a point implicit way to avoid stiffness.

Stagnation pressures of the hydrogen in the tank are 10, 40 and 70 MPa with a stagnation temperature of 300 K. A rectangular computational domain is selected of which the left boundary condition is a solid wall. Slip boundary conditions are imposed on the wall and the other three boundary conditions are free stream conditions. A small hole with a diameter of 1 mm is located at the center of the left wall. The jet is choked at the hole and its Mach number is unity. The initial ambience is air at 0.1 MPa, 300 K, and at rest.

A uniform grid size of $dx = dy$ =10 μm is accepted in the simulations because the grid size resolution study shows that the coarse grid size gives lower temperature prediction. It is necessary and reasonable to use such small grid size to simulate high pressure hydrogen jet combustion.

3. Results and discussions

3.1 The case of 10 MPa tank pressure

Figure 1 shows the temperature contours at 10 μs after hydrogen jetting out from the hole for the case of 10 MPa tank pressure. We can see from Fig. 1 that the maximum temperature is about 450 K. The maximum temperature decreases to about 350 K at 60 μs (see Fig. 2). The results demonstrate that the ignition of the hydrogen jet does not occur under the conditions of this case.

3.2 The case of 40 MPa tank pressure

In the case of 40 MPa tank pressure, the temperature contours at 10 μs after hydrogen jetting out from the hole are plotted in Fig. 3. We can see from Fig. 3 that the maximum temperature at the contact surface region is up to 2,000 K. The high temperature region appears at the contact surface region because the hydrogen mixes with the high temperature air and a local combustion takes place there. Figure 4 shows the contours of OH mass fraction at 10 μs. A large number of OH molecules are found at the contact surface region (see Fig. 4), which means that the local ignition of the hydrogen and air mixture occurs there.

Figure 5 shows the pressure and temperature profiles along the axis at 10 μs. From Fig. 5 we can study the ignition mechanism of the high pressure hydrogen jet. The high pressure hydrogen jet produces a semi-spherical shock wave in the air. The strength of the shock wave is very strong at the central part at the early stage. Under

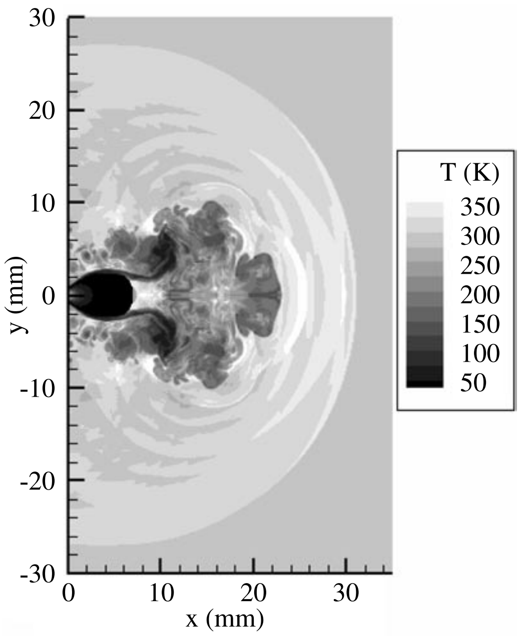

Fig. 2 Temperature contours at 60 μs of 10 MPa case.

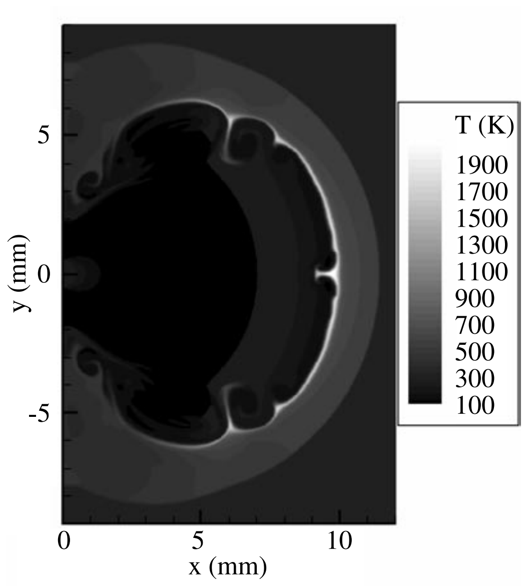

Fig. 3 Temperature contours at 10 μs of 40 MPa case.

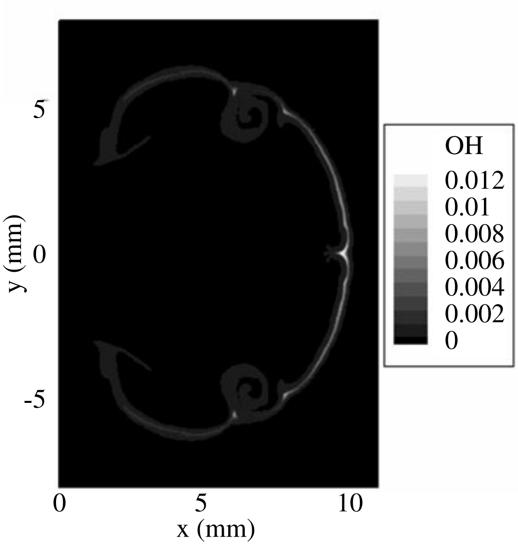

Fig. 4 OH mass fraction contours at 10 μs of 40 MPa case.

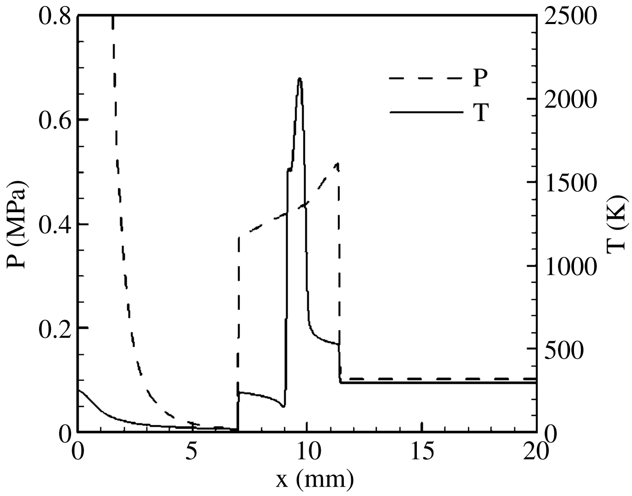

Fig. 5 Pressure and temperature profiles along the axis at 10 μs of 40 MPa case.

certain conditions, the temperature of the air, which is heated up in the shock wave, may exceed considerably the over-all temperature of the emitted hydrogen. Between the emerging hydrogen and the heated air there is a moving diffusion contact surface, through which there is mass exchange and heat conduction from the cold hydrogen to the hot air, which results in ignition. At the side parts of the jet, the shock wave is weaker and the temperature of the hydrogen is very low because of over-expansion. Therefore, there is no ignition at the sides of the hydrogen jet although there are stronger vortexes.

However, the local ignition can not develop into a steady hydrogen jet flame. As the jet propagates and expands further away from the tank, the temperature at the contact surface decreases quickly and the local combustion is blown off. Figure 6 shows the temperature contours at 100 μs. The temperature at the contact surface drops to under 700 K. This demonstrates that the local combustion is extinguished. There are two mechanisms of the quenching. The first mechanism is that the strength of the shock wave becomes weaker and the temperature of the hydrogen and air mixture becomes lower than its ignition temperature. The heat release at the diffusion surface is negligible because its amount is very little and its time is very short. This little heat release can not ignite the hydrogen and air mixture at the sides of the jet. The second mechanism is that the diffusion at the tip of the contact surface is not strong enough so that the equivalence ratio of the combustible hydrogen and air mixture is not satisfied. Figure 7 shows the hydrogen and oxygen mass fraction contours

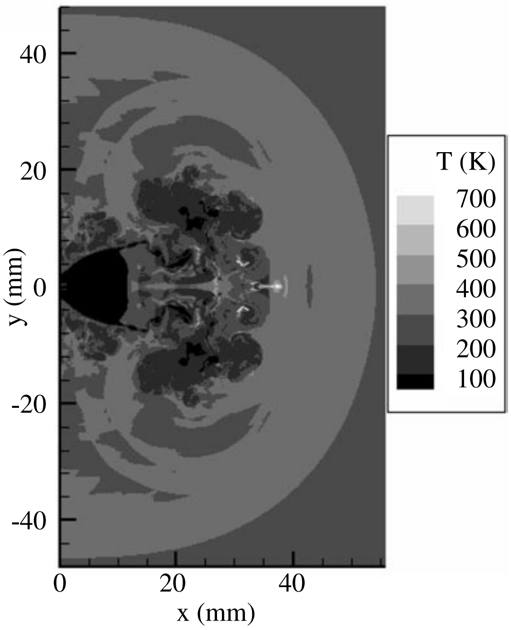

Fig. 6 Temperature contours at 100 μs of 40 MPa case.

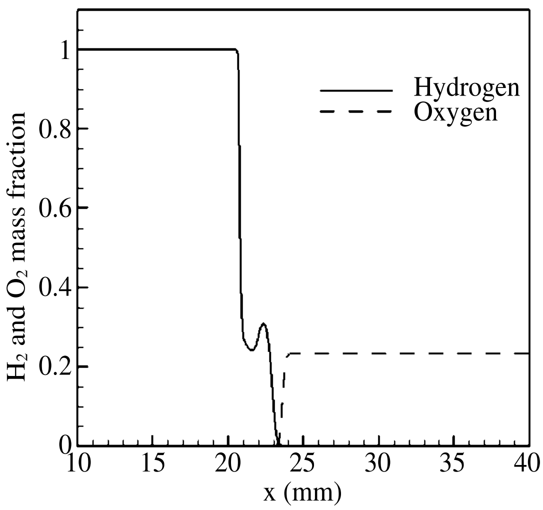

Fig. 7 Hydrogen and oxygen mass fraction contours along the axis at 50 μs of 40 MPa case.

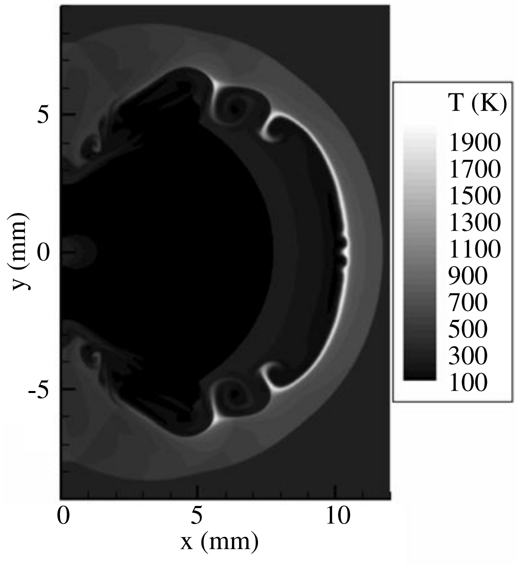

Fig. 8 Temperature contours at 9 μs of 70 MPa case.

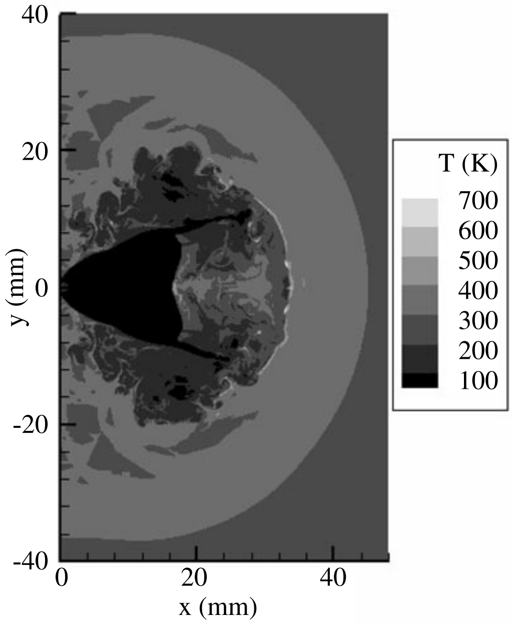

Fig. 9 Temperature contours at 70 μs of 70 MPa case.

along the axis at 50 μs. We can see from Fig. 7 that the hydrogen and air are separated from each other by the combustion products. The first mechanism is the main mechanism because we can find that the temperature of the hydrogen and air mixture is very low in the vortex region.

3.3 The case of 70 MPa tank pressure

In this case, the pressure of the hydrogen tank is 70 MPa. The local ignition at the diffusion surface also occurs at 9 μs like the 40 MPa case (see Fig. 8). The maximum temperature is higher and the distance from the wall is longer than that of the 40 MPa case because the semi-spherical shock wave is stronger. However, the result shows that the maximum temperature drops to below 700 K at 70 μs (see Fig. 9). In this case, the local ignition is also blown off and can not develop into a stable jet flame even if the stagnation pressure is very high.

3.4 Resolution study

Resolution study is conducted before the direct simulations. Two grid sizes of 10 and 100 μm are studied and the temperature contours are presented in Figs. 10 and 11,

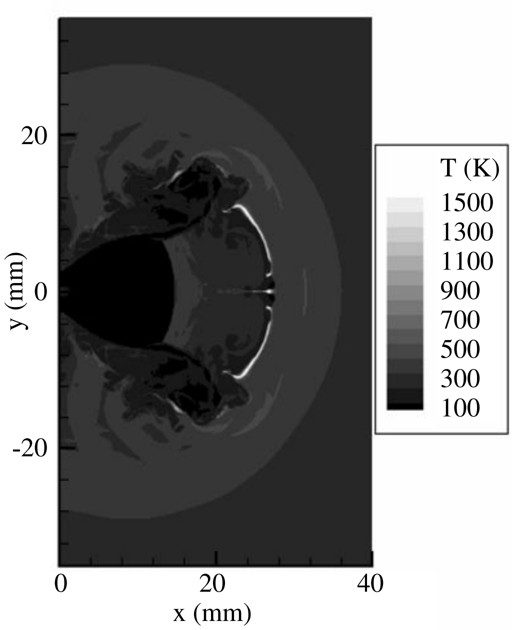

Fig. 10 Temperature contours at 50 μs using 10 μm grid size of 70 MPa case.

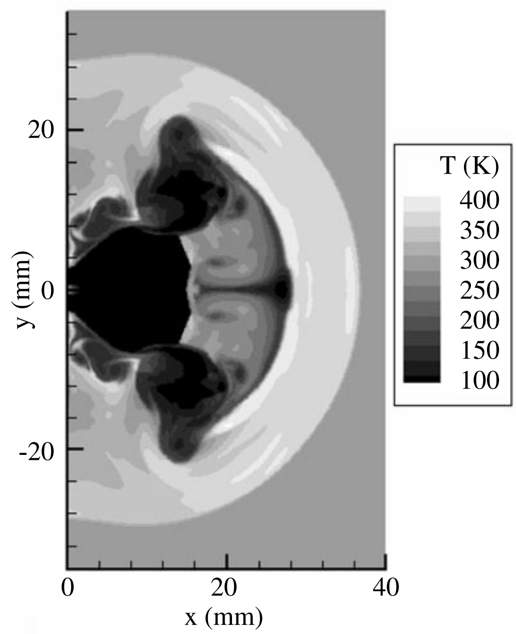

Fig. 11 Temperature contours at 50 μs using 100 μm grid size of 70 MPa case.

respectively. There is a big difference between them. This resolution study shows that the grid size influences the simulation results very much. The ignition does not happen if the 100 μm grid size is used. For the hydrogen jet ignition simulation, the grid size of 10 μm is fine enough, but the grid size of 100 μm is too coarse to be used.

4. Conclusions

The ignition phenomena of a high pressure hydrogen jet are numerically simulated by using two-dimensional axisymmetric Euler equations with a full chemical mechanism, where the detailed chemical mechanism contains 9 species and 18 elementary reactions. The mass and heat diffusion terms are considered in the Euler equations. The diameter of the small hole is 1 mm. Three tank pressures, 10, 40 and 70 MPa, are studied, respectively. The hydrogen jet is choked at the hole and its Mach number is unity. Especially, the uniform grid size of $dx = dy = 10$ μm is used because the resolution study shows that the grid size influences the temperature prediction very much.

(1) For the 40 and 70 MPa tank pressure cases, the local ignition of the hydrogen and air mixture at the contact surface region occurs at about 10 μs after hydrogen jetting out from the hole. The local combustion increases the temperature at the contact surface up to 2,000 K. The mechanism is that the high pressure hydrogen jet produces a stronger semi-spherical shock wave. This shock wave heats up the air in front of the jet to a very high temperature. If the temperature of the hydrogen and air mixture at the diffusion surface is higher than the ignition temperature and the time is longer than the ignition time, ignition occurs. For the 40 and 70 MPa cases, the ignition conditions are satisfied at the tip region of the contact surface, therefore, the local combustion happens there. But for the 10 MPa case, the shock wave is not strong enough to ignite the hydrogen and air mixture. The maximum temperature of this case is only about 450 K at 10 μs.

(2) However, for the 40 and 70 MPa tank pressure cases, the maximum temperature decreases quickly and the local combustion is quenched as the jet propagates away from the tank wall. The local ignition can not develop into a stable jet flame. There are two mechanisms of the quenching. The first mechanism is that the strength of the shock wave decreases quickly because the diameter of the hole is only 1 mm. This results in the rapid decrease in the temperature of the heated air. The heat release at the diffusion surface is negligible because its time is very short. The temperature of the hydrogen and air mixture at the diffusion surface quickly drops to below its ignition temperature. The heat release is too little to ignite the low temperature hydrogen and air mixture in the vortex region. The second mechanism is that the diffusion at the tip of the contact surface is not strong enough so that the equivalence ratio of the combustible hydrogen and air mixture is not satisfied. Therefore, the local ignition is blown off under the conditions being considered in the simulations.

Acknowledgments

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