

Direct Numerical Simulation on Hydrogen Fuel Jetting from High Pressure Tank

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Introduction

Fuel cell for automobile industry has been developed recently and the safety issue of the high pressure hydrogen emerges from behind the application to the safety of high pressure hydrogen tanks (Hayashi 2004). We are concerned about the behavior of the hydrogen jet if there is a leak in the tank and whether the high pressure hydrogen jet can be ignited by itself or not. However, little attention has been paid to this topic. Some numerical studies on the ignition of the non-premixed counter-flowing hydrogen and hot air streams were performed (Balakrishnan et al. 1995; Kreutz and Law 1996; Mastorakos et al. 1997; Uejima et al. 1998); however, the pressure was one atmosphere and the maximum jet velocity was 50 m s^{-1} . For a high pressure hydrogen tank for fuel cell purposes, its pressure is more than 10 MPa and a typical speed of a choked jet is about $1,300 \text{ m s}^{-1}$. Hence, their results do not apply to the cases of the fuel cell and high pressure hydrogen tanks directly.

In this paper, we conduct direct numerical simulation to investigate the behavior of the high pressure hydrogen jet. Two-dimensional axisymmetric Euler equations and detailed chemical mechanisms are used to simulate the hydrogen ignition and combustion. A small hole with a diameter of 1 mm is assumed to be opened on the wall of a tank suddenly and a choked hydrogen jet is injected into the air. The pressure of the tank is taken to be 10, 40 and 70 MPa, respectively.

Numerical Setup and Method

Two-dimensional axisymmetric Euler equations and detailed chemical reaction mechanisms are employed to simulate the behavior of the hydrogen jet at the early stage of the leakage. The detailed chemical reaction mechanism 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 (Petersen and Hanson 1998). A Harten-Yee type Non-MUSCL TVD scheme is used for the convection term integration and 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 hydrogen in the tank are 10, 40 and 70 MPa with a stagnation temperature of 300 K. A rectangular computational domain is selected, where the left boundary condition is a solid wall and the other three boundary conditions are free stream conditions. A

small hole with a diameter of 1mm is located at the center of the left wall. The jet is choked at the hole and the Mach number is unity. The initial ambience is air at 0.1 MPa, 300 K, and at rest.

A uniform grid size of $dx = dy = 10 \mu\text{m}$ is accepted in the simulation because our grid size resolution study before the simulation shows that the coarse grid size gives lower temperature prediction. It is necessary and reasonable to use such small grid size to simulate high temperature hydrogen combustion.

Results and Discussions

The case of 10 MPa tank pressure

In this case, the pressure of the hydrogen tank is 10 MPa. Figure 1 shows the temperature contours at $10 \mu\text{s}$. We can see from Fig. 1 that the maximum temperature is about 450 K. The high temperature region appears at the jet front. No OH molecule is found in the results of this case, which means no combustion occurs without any ignition source.

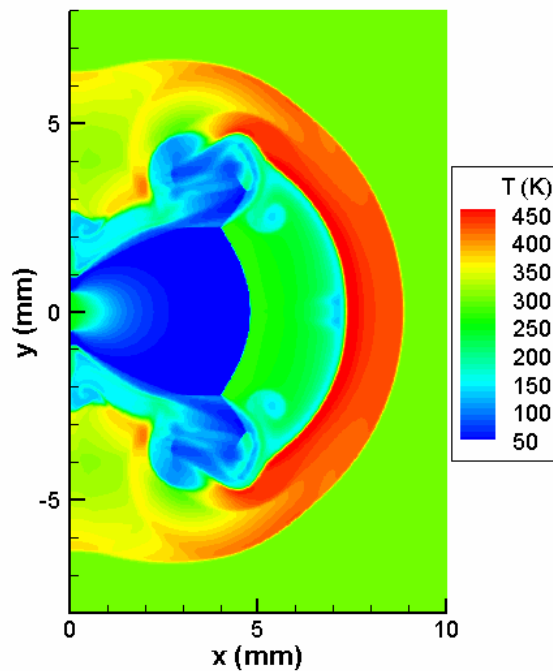


Figure 1. Temperature contours at $10 \mu\text{s}$ in 10 MPa tank pressure case

The case of 40 MPa tank pressure

In this case, the pressure of the hydrogen tank is 40 MPa. The temperature contours at $10 \mu\text{s}$ are plotted in Fig. 2. We can see that the maximum temperature at the contact surface region is up to 1,750 K at $10 \mu\text{s}$. The high temperature region appears not at the shock wave front but at the contact surface region because hydrogen mixes with oxygen and combustion takes place there. Fig. 3 shows the OH mass fraction at $10 \mu\text{s}$. A large number of OH molecules are found at the contact surface region (see Fig. 3), which means the local combustion of hydrogen-air mixture occurs there.

The shock wave produced by the hydrogen jet itself is simulated in order to study the mechanism of local combustion. The temperature contours are presented in Fig. 4. Fig. 4 shows that the maximum temperature at the shock wave front at $2 \mu\text{s}$ is higher than 1,400 K. This result demonstrates that the combustion at the contact surface is caused by the high temperature behind the shock wave.

However, the hydrogen jet can not be ignited by the local combustion at the contact surface region. As the jet propagates and expands further away from the tank, the temperature at the contact surface decreases quickly and the local combustion is quenched. Figure 5 shows the temperature contours at 100 μ s. The temperature at the contact surface drops to under 1,000 K at 100 μ s. This demonstrates that the local combustion is extinguished and it can not lead to a hydrogen flame only by itself without any ignition source. The reason will be discussed in the next subsection.

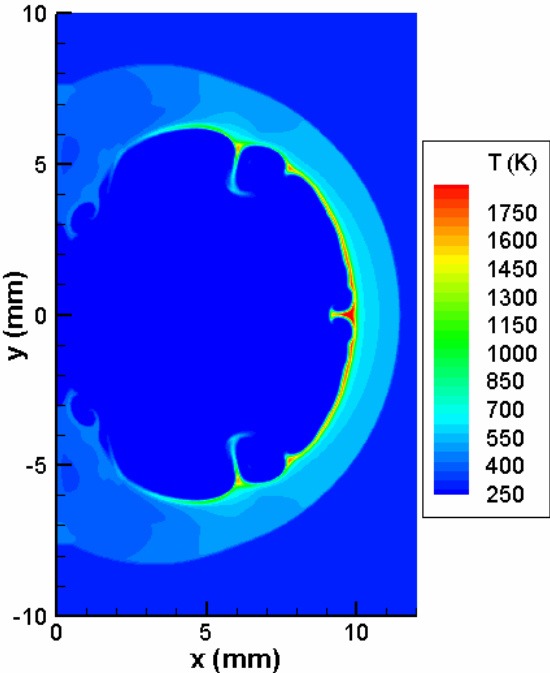


Figure 2. Temperature contours at 10 μ s in 40 MPa tank pressure case

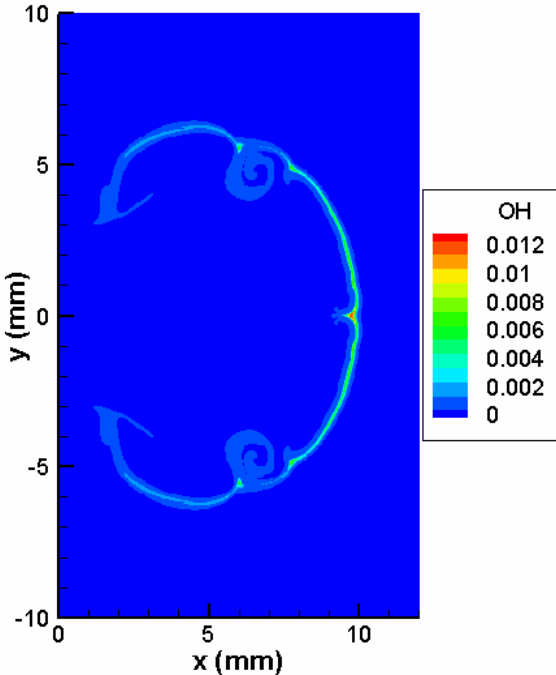


Figure 3. OH mass fraction contours at 10 μ s in 40 MPa tank pressure case

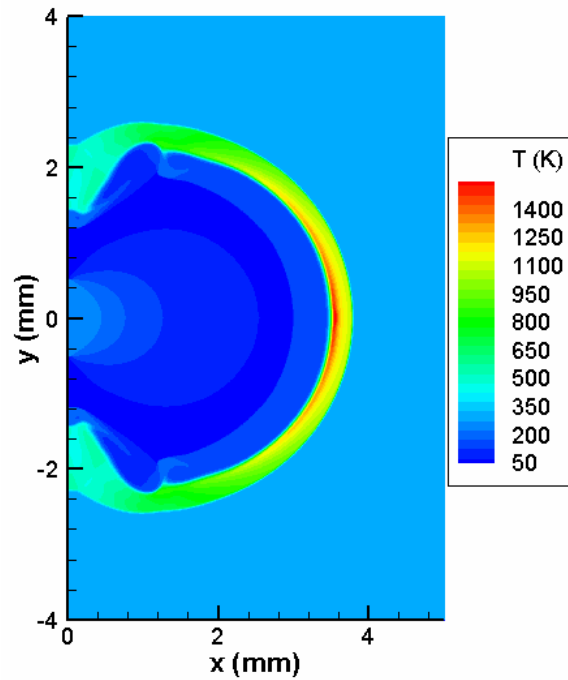


Figure 4. Temperature contours of shock wave at 2 μ s in 40 MPa tank pressure case

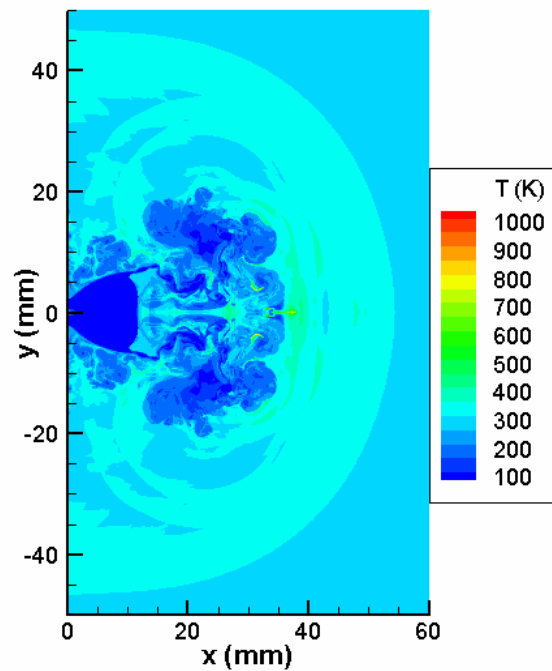


Figure 5. Temperature contours at 100 μ s in 40 MPa tank pressure case

The case of 70 MPa tank pressure

In this case, the behavior of the hydrogen jet from a 70 MPa tank is simulated. The local combustion at the contact surface region also occurs at the early stage of the leakage like 40 MPa case (see Fig. 6). The maximum temperature is higher and the distance from the wall is longer than that in 40 MPa case because the shock wave is stronger. However, this stronger jet can not be ignited only by itself and the local combustion also dies out 100 μ s later. Figure 7 shows that the maximum temperature decreases to 1,150 K and the local combustion almost disappears at 110 μ s. The nonpremixed flame does not take place in this case.

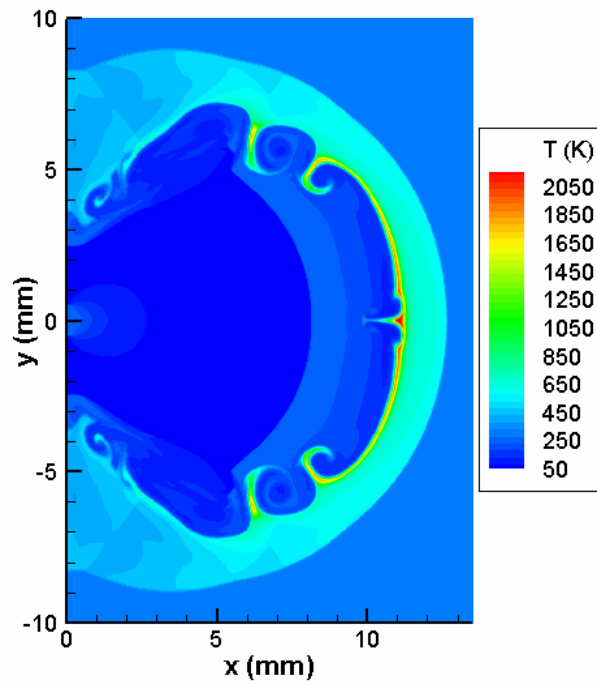


Figure 6. Temperature contours at 10 μ s in 70 MPa tank pressure case

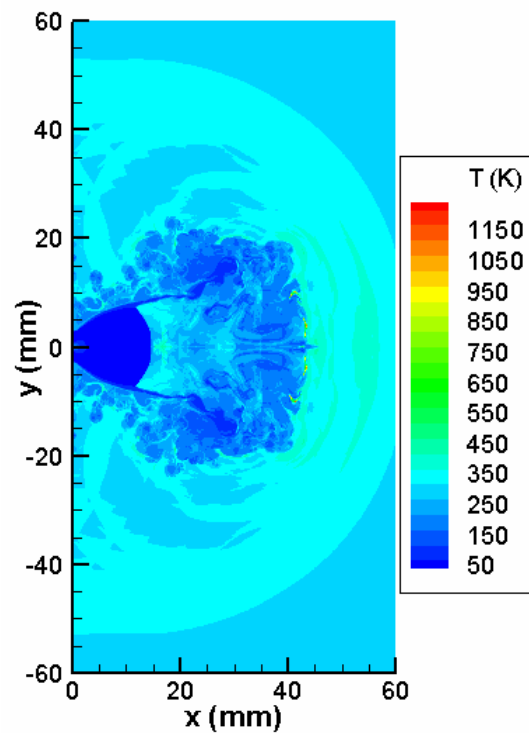


Figure 7. Temperature contours at 110 μ s in 70 MPa tank pressure case

Two mechanisms of local combustion quenching are discussed here on the basis of the simulation results. The first mechanism is that why the local combustion can not develop into a nonpremixed flame in the time period of 100 μ s. The second is that why the local combustion is quenched 100 μ s later. The main reason for the first question is that the local combustion occurs at the tip region of the contact surface to move together with the jet and its position is always in

front of the hydrogen gas. It can not form a steady ignition source. Hydrogen and oxygen mixes with each other at the side boundaries and the temperature of the mixture is very low because of the over-expansion. The position of the mixture is always behind the high temperature local combustion products. Therefore, the local combustion can not be held to ignite the hydrogen-air mixture.

The main reason for the second question is that H_2O is produced by the local combustion and its amount increases at the contact surface continuously. Figure 8 shows the mass fraction of H_2O and hydrogen, where the colors represent the mass fraction of hydrogen and the black lines represent H_2O . From Fig. 8 we can find that H_2O stays between hydrogen and air and propagates together with the jet. It prevents hydrogen and air from well mixing and puts the local combustion out.

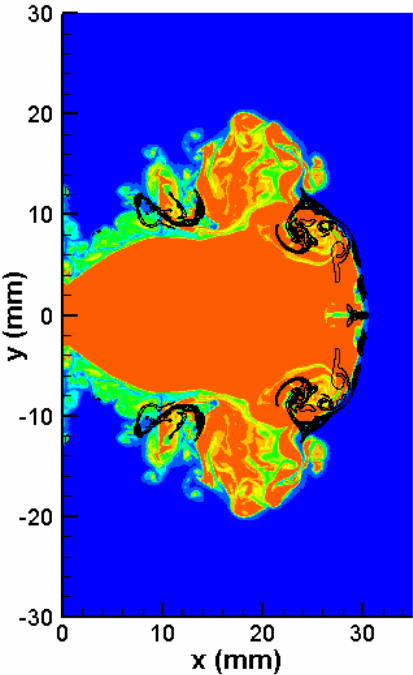


Figure 8. Mass fraction contours of H_2O and H_2 at $60 \mu s$ in 70 MPa tank pressure case (the colors represent H_2 and the black lines represent H_2O)

Resolution study

Resolution study is conducted before the direct simulation. Two grid sizes of 10 and 100 μm are studied and the results are presented in Figs. 9 and 10. This study shows that the larger grid size influences the simulation results very much. No local combustion occurs if the 100 μm grid size is used. For combustion simulation, the grid size of 10 μm is fine enough. But the grid size of 100 μm is too coarse to simulate the hydrogen combustion.

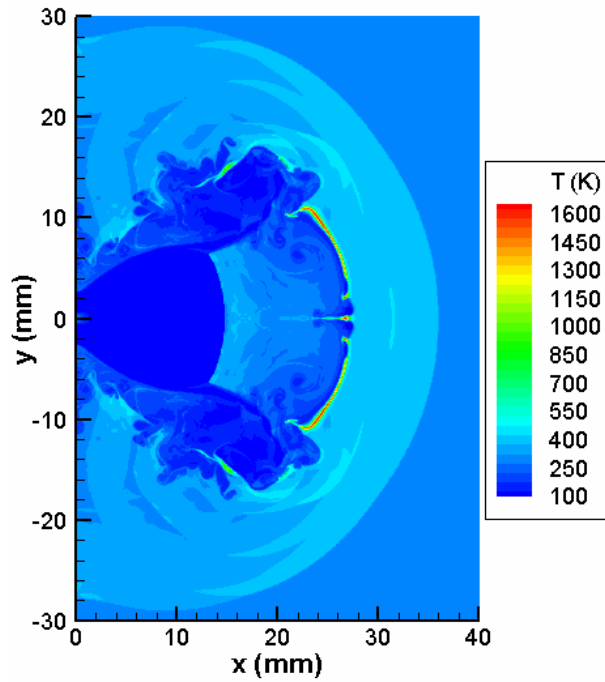


Figure 9. Temperature contours at 50 μ s using 10 μ m grid size in 70 MPa tank pressure case

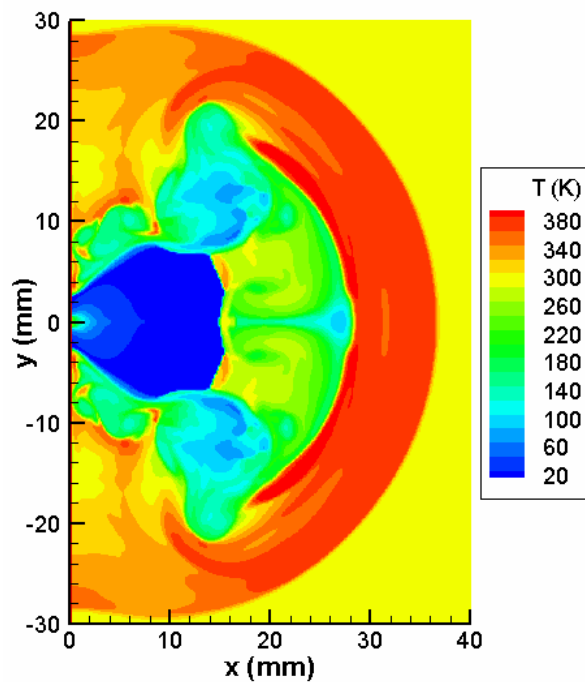


Figure 10. Temperature contours at 50 μ s using 100 μ m grid size in 70 MPa tank pressure case

Conclusions

We investigate the behavior of a hydrogen jet coming into the air from 10, 40 and 70 MPa high pressure tanks by the direct simulation using two-dimensional axisymmetric Euler equations with the full chemical mechanism, where the detailed chemical mechanism contains 9 species and 18 elementary reactions. Especially, the uniform grid size of $dx = dy = 10 \mu$ m is used

because our resolution study shows that the larger grid size influences the temperature at the jet front very much.

(1) For 40 and 70 MPa tank pressure cases, the local combustion of hydrogen-air mixture at the contact surface region occurs at the early stage of hydrogen jet propagation. This local combustion is caused behind the shock wave induced by the high pressure hydrogen jet. The local combustion increases the temperature at the contact surface up to 2,000 K. But for 10 MPa case, the shock wave is not strong enough to ignite the local mixture. The maximum temperature for this case is about 450 K at the early stage.

(2) However, the maximum temperature decreases to 1,000 K at 100 μ s and the local combustion is quenched as the jet propagates and expands away from the tank. The main reason is that H₂O produced by the local combustion stays between hydrogen and air and prevents them from well mixing. H₂O puts the local combustion out.

(3) The hydrogen jet itself can not become a nonpremixed flame either in 40 or 70 MPa cases although the local combustion occurs. The main reason is that the position of the local combustion is always in front of the mixture. It moves together with the jet and can not form a steady ignition source. Therefore, a hydrogen flame does not take place without any additional ignition source.

Acknowledgments

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