Numerical study on auto-ignition of a high pressure hydrogen jet in a tube having a gap

Naoki Kitabayashi[1], Eisuke Yamada[1], A. Koichi Hayashi[1] Nobuyuki Tsuboi[2]

[1]Department of Mechanical Engineering, Aoyama Gakuin University, 5-10-1 Fuchinobe, Sagamihara, Kanagawa 229-8558, Japan

[2]Institute of Space and Astronautical Science, Japan Aerospace Exploration Agency, 3-1-1 Yoshinodai, Sagamihara, Kanagawa 229-8510, Japan

1 Introduction

Hydrogen is concerned as an alternative renewable source of energy, practically inexhaustible source of energy and absolutely clean energy, as well. Some are interested in hydrogen usage as a new energy source. Others are interested in scientific and technological points of the hydrogen energy. Industrial companies of power generation and transportation are also interested in the technology and the business of the hydrogen infrastructure, which replaces the fossil fuel. Many governments regard hydrogen technologies to be a priority matter in their social and economic development. Hydrogen energy is one of the answers for the environmental issue.

However, there are problems when we use hydrogen energy safety and efficiently. One of the serious problems is that hydrogen might lead to an accidental explosion. High pressure tank is often used to store hydrogen. It is necessary to compress hydrogen gas to decrease its volume since hydrogen energy density is low. However, it is well known that the accidental release of hydrogen from a high-pressure tank into the air can produce a strong shock wave that heats up air to a high temperature to ignite hydrogen. The auto-ignition of hydrogen leads to an explosion under a certain condition. From the safety point of view, this problem is important in practical cases such as a pressure vessel containing high-pressure hydrogen or an automobile fuel cell, etc.

For this reason, studies have been performed to clarify the mechanism of an explosion induced by high pressure hydrogen jet spouting from a tube [1–8]. Auto-ignition of hydrogen jet at the tip of the contact surface is confirmed, but the mechanism of extinction or stabilization is under discussion. The different jet conditions in these studies show different results. E.g., Golub et al. [5] and Mogi et al. [6] present a relationship between hydrogen inlet pressure and a tube length. They said auto-ignition using a long tube is easier than that using a short one.

When a hydrogen jet is spouted into a tube connected to the air, the shock wave yields in front of hydrogen contact surface in the tube. When the shock wave reaches the exit of the tube, the gas begins to expand widely and vortices grow up around the tube exit, therefore the hydrogen-air mixture is generated and an explosion of hydrogen is induced [8]. If the high pressure hydrogen goes through a long tube connected to the air, it is predicted that an explosion is also occurred in the tube. Although this prediction is not sure, the study of the mechanism must be required from the safety point of view.

Correspondence to: yamada@me.aoyama.ac.jp

2 Aims

In the present work, a direct numerical simulation (DNS) with a detailed chemical model has been performed to clarify the ignition mechanism of high pressure hydrogen jet spouting from a tube connected to the large hydrogen tank. We noticed the phenomena of hydrogen explosion in a tube having a gap. The purpose of this analysis is to investigate whether there is an ignition inside the tube caused by an interaction between shock wave and boundary layer. In this paper, we calculated about the case of having a gap and no gap.

3 Method

The numerical simulations are performed by solving the equations of compressible reactive gas dynamics to clarify the explosion mechanism of high pressure hydrogen. The governing equations for this work are the conservation equations of mass, momentum, energy, and chemical species together with the equation of state. These equations are considered on the (r, z) plane under the assumption of axial symmetry for the cylindrical coordinate system. The governing equations are given in discrete forms with a finite difference method with the grid size of 2–10 μm to evaluate an effect of boundary layer in the tube.

Figure 1 shows the flow field model and boundary condition used for the present numerical simulation. It is assumed that high-pressure hydrogen provided from a tube is injected into the still air. The tube is connected to the large hydrogen reservoir at the left-hand side in the figure. The diameter of the tube is 4.8 mm and the diameter of the hole on the reservoir wall is 4.5 mm: that is, there is a small gap at the inlet. The hydrogen jet from the hole spreads a little vertically. Pressure at the inlet of hydrogen is 41 MPa which is estimated by the choked condition. In this case, the pressure of reservoir corresponds to 77.6 MPa. To save the CPU cost, the numerical domain along the z-axis is extended gradually with the propagation of shock wave induced by high pressure hydrogen.

The detailed kinetic mechanism includes nine chemical species (H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, and N_2) and 18 elementary reactions [9]. This mechanism has a good performance for ignition delay time and heat release within a wide pressure range from 0.1 to 60 MPa. The diffusion flux is evaluated using the Fick's law with binary diffusion coefficients. The transport coefficients of each chemical species, namely, viscosity, heat conductivity, and binary diffusion, are evaluated using the Lennard–Jones intermolecular potential model [10], and those of the gas mixture are calculated by the Wilke's empirical rule [11]. The enthalpy of each chemical species is derived from the JANAF table [12]. The buoyancy, bulk viscosity, and Soret and Dufour effects are neglected.

The convective terms are evaluated using the second-order explicit Harten–Yee non-MUSCL modified-flux type TVD scheme, considering the properties of the hyperbolic equations. The viscous terms are evaluated with the standard second-order central difference formulae. The time integration method is the second-order Strang type fractional step method. The chemical reactions are treated by a point implicit method to avoid stiffness.

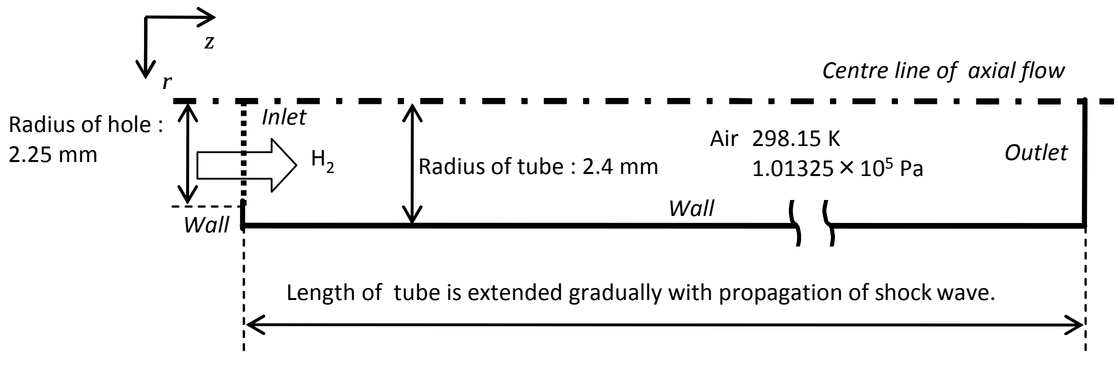

Figure 1 Analytical model and boundary condition of numerical simulation

4 Results & Discussion

Figure 2 shows the sequential temperature distributions in the tube. The time in μs shown in the figure indicates the time after the hydrogen gas begins to break into the tube. From the left side of the figure, high pressure hydrogen is spouted into the tube. Although the temperature of the air rapidly increases between shock wave and contact surface, it is found that the high temperature region decreases as the shock wave propagates. Therefore it is thought that an ignition is not occurred in this region. At first of this calculation, the shape of the contact surface is spherical, and it gradually becomes flat or reverse spherical shape. There are two low temperature regions behind the contact surface. These changes are caused by the pressure wave which is made by inlet wall.

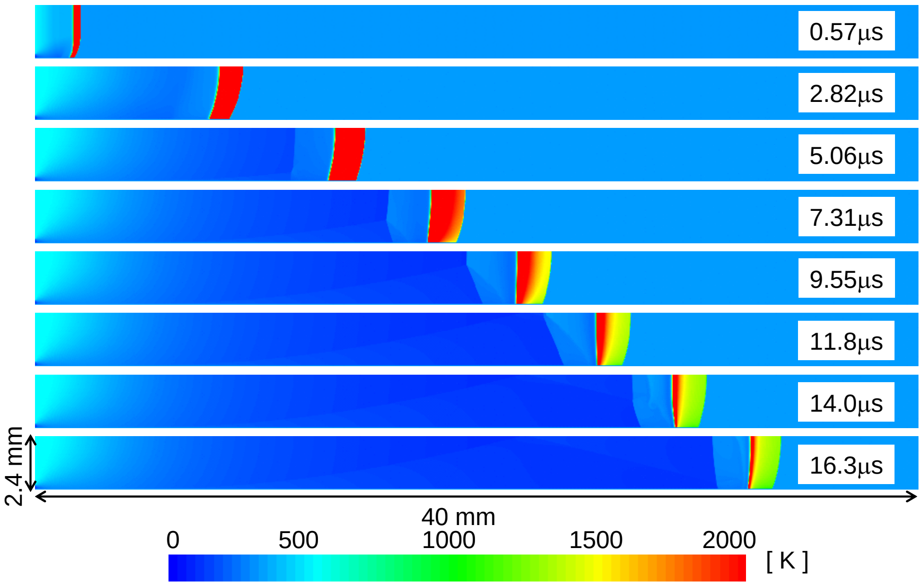

Figure 2 Temperature distributions in the tube

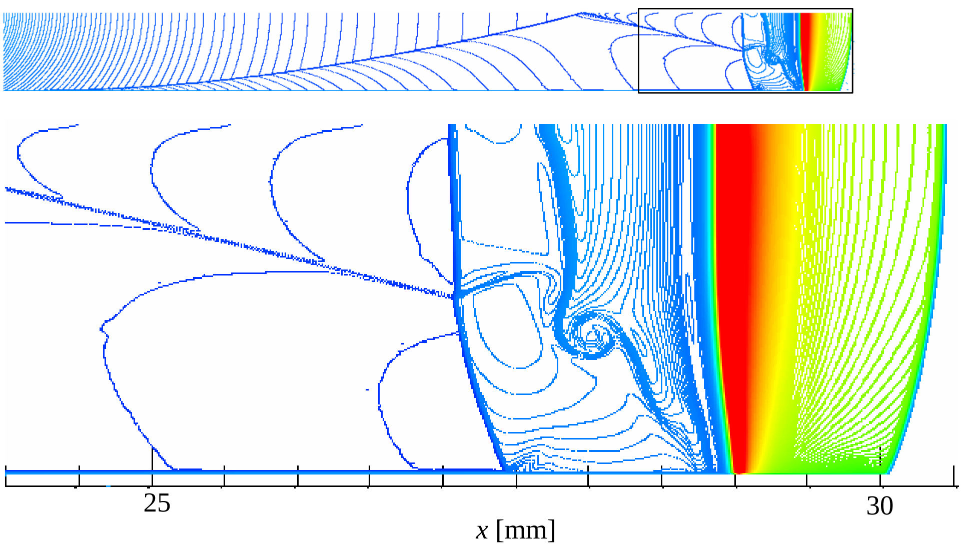

Figure 3 Temperature contours in the tube and around the contact surface at 14.0 μs

Figure 3 shows the temperature contours around the shock wave at 14.0 μs. The bottom contour is the enlargement figure of upper one. It is found that an eddy occurrs behind the contact surface. Many vertical lines including the eddy are concentrated just behind the contact surface. It is expected that the eddy mixes hydrogen and air to ignite easily. However, the eddy behind the contact suraface is not observed at the other time shown in Fig. 2.

Furthermore, the lateral line which separates two waves is recognized apparently in the figure. The line gradually aparts from the wall, crosses the axis, and moves toward the wall. The eddy is generated ahead of the lateral line. The small gap at the inlet of the tube caused this phenomenon. The two divided waves might affect the formation of the eddy.

4 Conclusions

In this work, the high pressure hydrogen jet spouting from a tube having a gap at the inlet of the tube is calculated with a direct numerical simulation using a detailed chemical model and considering viscosity. The present calculation needs more to see an auto-ignition. The different gap system in the will be checked for the full paper, which may cause auto-ignition.

Acknowledgement

The authors wish to thank the JAXA Supercomputer System for calculation.

References

[1] P. Wolański and S. Wójcicki, Proc. Combust. Inst. 14 (1973) 1217–1223.

[2] Y.F. Liu, H. Sato, N. Tsuboi, F. Higashino, A.K. Hayashi, Sci. Technol. Energ. Mater. 66 (2005) 233–239.

[3] T.V. Bazhenova, M.V. Bragin, V.V. Golub, S.B. Scherbak, V.V. Volodin, Twenty-fifth International Symposium on Shock Waves, 2005, Paper 1118_1a.

[4] F.L. Dryer, M. Chaos, Z. Zhao, J.N. Stein, J.Y. Alpert, C.J. Homer, Combust. Sci. Technol. 179 (2007) 663–694.

[5] V.V. Golub, D.I. Baklanov, S.V. Golovastov, M.F. Ivanov, I.N. Laskin, A.S. Saveliev, N.V. Semin, V.V. Volodin, J. Loss Prevent. Process Ind. 21 (2008) 185–198.

[6] T. Mogi, D. Kim, H. Shiina, S. Horiguchi, J. Loss Prevent. Process Ind. 21 (2008) 199–204.

[7] B.P. Xu, L. El Hima, J.X. Wen, S. Dembele, V.H.Y. Tam, T. Donchev, J. Loss Prevent. Process Ind. 21 (2008) 205–213.

[8] E. Yamada, S. Watanabe, A. K. Hayashi and N. Tsuboi, Proc. 32nd Int. Comb. Symp. 32 (2009) 2363-2369.

[9] E.L. Petersen, R.K. Hanson, J. Propul. Power 15 (4) (1999) 591–600.

[10] S. Chapman, T.G. Cowling, The Mathematical Theory of Non-Uniform Gases, Cambridge University Press, UK, 1970.

[11] C.R. Wilke, J. Chem. Phys. 18 (4) (1950) 517–519.

[12] D.R. Stull, H. Prophet, JANAF Thermochemical Tables, Clearinghouse for Federal Scientific and Technical Information, Washington, DC, 1965.