Numerical Simulation of High Pressure Hydrogen Emerges to Air

Mohamed H. Elhsnawi, Mesbah M. Salem, Saleh B. Mohamed

***Abstract*—**Numerical simulation performed to investigate the behavior of the high pressure hydrogen jetting of air. High pressure hydrogen (30–40 MPa) was injected to air at atmospheric pressure through 2mm orifice. Numerical simulations were performed with Kiva3V code with 2D axisymmetric geometry. Numerical simulations showed that auto ignition of high pressure hydrogen to air are possible due to molecular diffusion. Auto ignition was predicted at hydrogen-air contact surface due to mass and energy exchange between high temperature hydrogen and air heated by shock wave.

***Keywords*—**Spontaneous Ignition, Diffusion Ignition, Hydrogen ignition, Hydrogen Jet.

I. Introduction

THE risk of high pressure hydrogen release to auto-ignite is of great safety concern. The auto ignition of high pressure hydrogen release was previously observed in laboratory tests [1], [2] and suspected as possible cause of some accidents. Historically, there were incidents where sudden releases of high pressure hydrogen were ignited with no clearly identifiable ignition source [3]. Several ignition mechanisms have been examined in literature [2], [3]. Among them there are reverse Joule-Thomson effect, static electricity, diffusion ignition, sudden adiabatic compression, hot surface ignition, mechanical friction and impact ignition. The principal concern in this paper is diffusion ignition. The mechanism of diffusion ignition was first proposed by Wloanski and Wojciki [3]. They found that the ignition was caused by a temperature increase of combustible mixture due to the mass and heat diffusion between hydrogen and shock heated oxygen, and they referred to this phenomenon as diffusion ignition. Dryer et al. [1] demonstrated diffusion ignition of compressed releases of hydrogen into air by experiments. Auto ignition occurred for release pressures above 20 bars. Golub et al. [4] numerically and experimentally investigated the shock-induced ignition of high pressure hydrogen releases. Their numerical results revealed that the auto ignition of the jet release was related to the hole size and no combustion occurred for hole diameter less than 2.6mm. Liu et al [5] conducted two dimensional numerical simulation of high pressure hydrogen release into an oxidizer. Three tank pressures were considered, i.e. 10, 40 and 70 MPa. The predictions showed that the auto ignition occurred at the tip region of the contact surface separating hydrogen and air after 10 us for 40 MPa and 70 MPa cases. However, the local combustion was quenched quickly due to the cooling effect of under expansion of hydrogen jets.

In the present study, we conducted numerical simulation to investigate the diffusion ignition mechanism when high pressure hydrogen is released directly into an open ambient environment. Numerical simulations were performed with Kiva3V. The code was developed in Las Alamos National Laboratory for internal combustion engine modeling. The solver is based on ALE method (Arbitrary Lagrangian-Euler) used for the models with moving meshes and unsteady flows. More information about the solver is described in reference reports [6] and [7]. The detailed chemical-kinetics mechanism developed by Peterson and Hanson [8] for hydrogen combustion is implemented. It involves 8 reactive species and 21 elementary reactions. The pressure of hydrogen at jet exit was 30 and 40 MPa with stagnation temperature of 300 K. A rectangular computational domain is selected, where the left boundary condition is solid wall and the other three boundary conditions are free stream conditions. Small orifice of 2mm is located at the centre of the left wall. The initial conditions of the air is 1 atm and 300K and at rest. The computational grids were uniform at jet exit with $dx = dy = 20\mu m$ is accepted because grid size resolution study before the simulation shows that the coarse grid size gives lower temperature prediction.

II. Results and Discussions

As the high pressure hydrogen is suddenly released into air, due to the strong under expansion of hydrogen a semi spherical shock is generated as shown in Fig. 1 for a release pressure of 30 MPa. Due to flow divergence, as the shock wave propagates away from the jet exit, its strength becomes weaker. At the same time another spherical shock wave generated inside the expanding hydrogen jet. As the shock wave propagates downstream, it intensifies due to strong under expansion of hydrogen and finally Mach disk is formed. The pressure decreased to about 15 Bars after 12 µs from starting of injection. Fig. 2 shows the pressure distributions for 40 MPa hydrogen jet. The flow pattern is similar to 30 MPa jet only the the pressure decreased to 17 Bars as a result of stronger shock wave generated.

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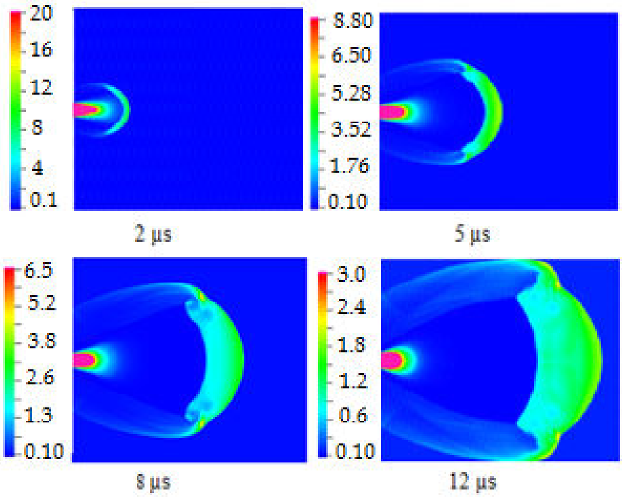

Fig. 1 Pressure contours for 30 MPa hydrogen jet

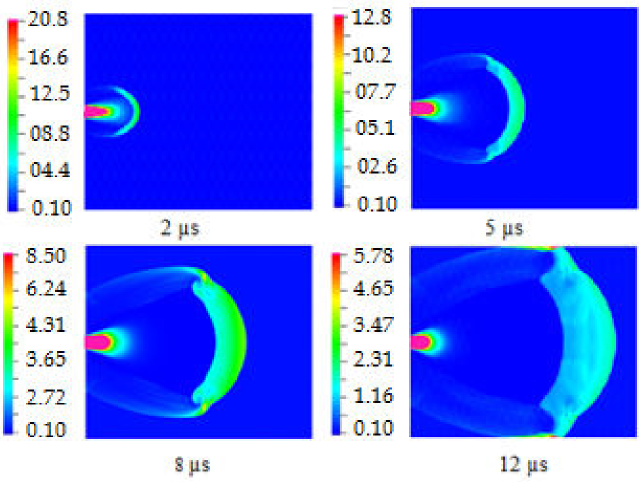

Fig. 2 Pressure contours for 40 MPa hydrogen jet

The temperature contours for 30 MPa jet at 5μs and 12μs are plotted in Fig. 3. It can be seen that the maximum temperature at the contact surface is up to 2500 K. The high temperature region appears at the contact surface region not the shock wave front as a result of mixing of hydrogen with air and combustion take place there. As the jet propagates and expands further away from the jet exit, the temperature at the contact surface decreases and the flame temperature drops to 1880 K. Fig. 4 shows the temperature contour as the jet pressure increased to 40 MPa. The maximum temperature after 5μs is almost similar to the case of 30 MPa case, but after 12μs from starting of injection the maximum temperature increased from 1880 K to 2220 K as a result of stronger shock created. Also Figs. 1 and 2 show that the shock wave generated by the hydrogen jet in front of the contact surface heated the hydrogen-oxygen mixture, chemical reaction initiated and combustion take place behind the shock wave.

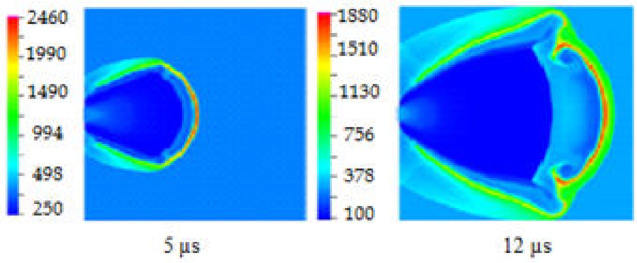

Fig. 3 Temperature contours (K) for 30 MPa hydrogen jet

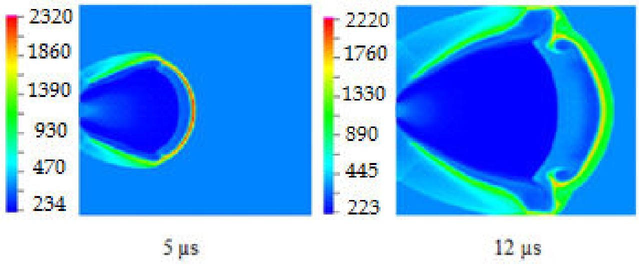

Fig. 4 Temperature contours (K) for 40 MPa hydrogen jet

Fig. 5 shows the OH mass fraction for 30 MPa jet. At 5μs large number of OH molecules are found at the contact surface region, which means the local combustion of hydrogen-air mixture occurs there. It is seen that although the reaction rate decrease with time, still there is a high OH mass fraction of 0.013 at 12μs. The main reasons are the temperature drop due to flow divergence and dilution of the mixture by combustion products. For 40 MPa jet as shown in Fig. 6 large numbers of OH molecules are also found after 5μs from starting of injection at the contact surface region which indicates existence of a flame and higher OH mass fraction of 0.017 at 12μs.

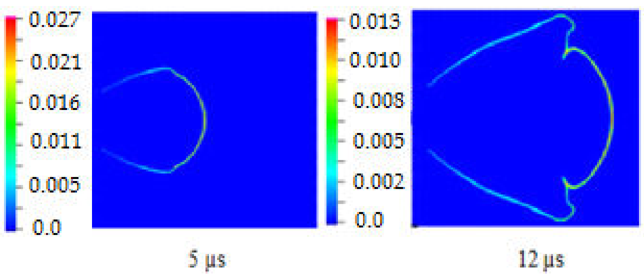

Fig 5 OH mass fraction for 30 MPa hydrogen jet

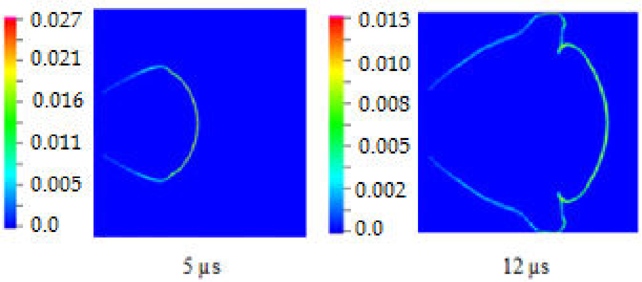

Fig. 6 OH mass fraction for 40 MPa hydrogen jet

Figs. 7 and 8 show the H_2O distribution for 30 and 40 MPa hydrogen jet. H_2O is produced by local combustion and its amount increases at the contact surface. High concentration of H_2O stays between hydrogen and air and propagates together with the jet which dilutes the mixture of hydrogen and oxygen in the contact surface and results of decreasing the maximum temperature of the combustion.

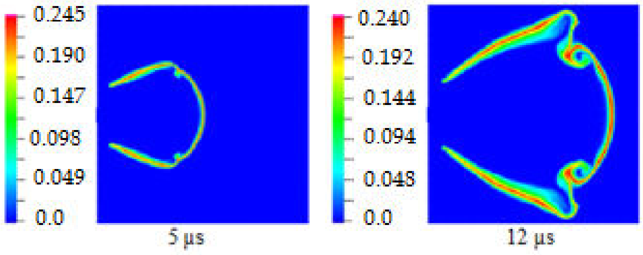

Fig. 7 H_2O mass fraction for 30 MPa hydrogen jet

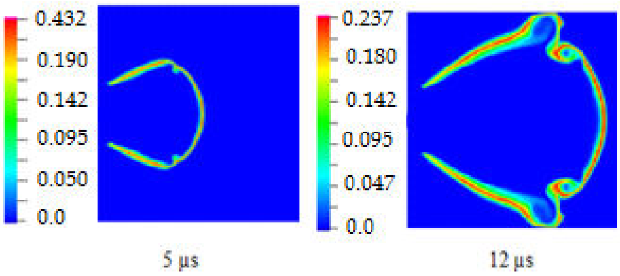

Fig. 8 H_2O mass fraction for 40 MPa hydrogen jet

III. Resolution Study

Resolution study is conducted before the direct simulation of high hydrogen emerges to air. Two grid sizes of 20 and 40 are studied and presented in Figs. 9 and 10. The study shows that the larger grid size influences the results too much. For 40 µm grid size no local combustion occurs and it's too coarse to simulate the hydrogen combustion, but for 20µm grids size is fine enough.

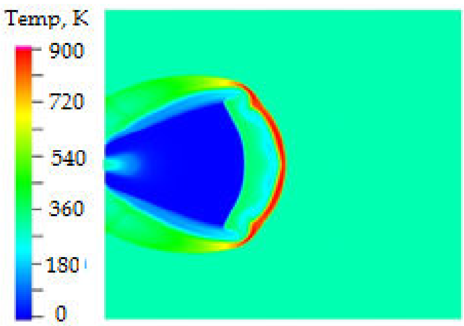

Fig. 9 Temperature contours at 8 µs using 40 µm grid sizes and 40 MPa

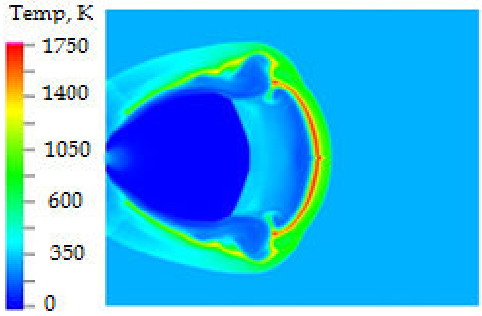

Fig. 10 Temperature contours at 8 µs using 20 µm grid sizes and 40 MPa

IV. Conclusions

Numerical simulations of high pressure hydrogen jetting into air are described. Auto ignition takes place at the tip region of the contact surface as a result of mass and energy exchange between low temperature hydrogen and air heated by shock wave in front of the contact surfaces induced by high pressure hydrogen jet. The combustion region extends downward along with the contact surface and the flame temperature drops with expansion. The main reason is that H_2O produced by the local combustion stays between hydrogen and air and prevents them from well mixing. Resolution study shows that the larger grid size than 20 µm influence the temperature at the jet front very much.

References

[1] Dryer, F.L., Chaos, M, Zhao Z. Stein, J.N., Alpert, J.Y. and Homer. C.J., Spontaneous Ignition of Pressurized Releases of Hydrogen and Natural Gas into Air, Combust. Sci. and Tech., 179:663-694, 2007.

[2] Wolanski, P. and Wojcicki, S., Investigation into the Mechanism of the Diffusion Ignition of a Combustible Gas Flowing into Oxidizing Atmosphere. Proc. Combust. Instit., 14 1217-1223, 1972.

[3] Astbury, G.R. and hawksworth, S.J., Spontaneous Ignition of Hydrogen leaks: a review of postulated mechanisms. International Conference on Hydrogen Safety, Pisa, Italy, 2005.

[4] Golub, V.V. , Baklanov, D.I. , Bazhenova, T.V. , Bragin, M.V. , Golovastov, S.V., Ivanov , M.F. , Volodin, V.V. (2007), Shock-Induced Ignition of Hydrogen Gas During Accidental or Technical Opening of High-Pressure tanks, Journal of Loss Prevention In the Process Industries, In Press, available on-Line.

[5] Liu, Y.F., Sato, H., Tsuboi, N., Hjigashino, F., and Hayashi, A.K., Numerical Simulation on Hydrogen Fuel Jetting from High Pressure Tank. Sci. Tech. Energ. Mater., 67,7-11, 2006.

[6] Amsden A. A., O'Rourke P.J., Butler T.D.: KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays. Los Alamos National Laboratory, New Mexico 87545, May 1989.

[7] Amsden A. A.: KIVA-3: A Kiva Program with Block-Structured Mesh for Geometries. Los Alamos National Laboratory, New Mexico 87545, March 1993.

[8] E.L. Peterson and R.K. Hanson 1999 "Reduced Kinetics Mechanisms for Ram Accelerator Combustion," J .prop. and Power, 15 (4): 591-600.