Numerical Simulations of Self-Ignition of Hydrogen in a Pipe by Rupture of Pressure Boundaries

Bok Jik Lee[1], **Hyoung Jin Lee**[1], **In-Seuck Jeung**[2]

[1]School of Mechanical and Aerospace Engineering, Seoul National University
Seoul 151-742, Korea

[2]Institute of Advanced Aerospace Technology, Seoul National University
Seoul 151-742, Korea

1 Introduction

It has been known that pressurized hydrogen released into the air by accident or during technical operation can undergo spontaneous ignition. Recently, several experimental observations to identify the limiting conditions of spontaneous ignition of hydrogen have been made on the case that pressurized hydrogen is released into air by the failure of rupture disks through extension pipes.

Dryer et al.[1] conducted more than 200 experiments with hydrogen for failure pressures ranging from 11.2 atm to 113.25 atm, using various downstream flow geometries. Their experiments showed that compressed hydrogen suddenly released into air by failure of a burst disk can produce spontaneous ignition if the burst disk failure pressure is sufficiently high, and the flow geometry after the burst disk results in sufficiently fast mixing of the escaping hydrogen and shocked air in contact with the expanding hydrogen. They postulated that the multi-dimensional shock caused by the geometry of pressure boundary and subsequent shock-boundary and shock-shock interactions within the downstream pipe play a key role for the spontaneous ignition to occur. The experimental observations of Golub et al.[2] and Mogi et al.[3] lead to qualitatively same interpretation though the range of bursting pressure and the diameter of extension pipe are different in their cases.

Xu et al.[4] and Yamada et al.[5] performed numerical studies relevant to above experiments. However, the mixing process within the pipe was not their primary concern, a slip boundary condition was assumed in the former and a uniform velocity profile of hydrogen was given for the inlet boundary in the latter study.

In the present study, direct numerical simulations with detailed reaction kinetics are conducted to investigate the mechanism of spontaneous ignition of hydrogen within a certain length of downstream pipe released by the failure of pressure boundaries of various geometric assumption to see their effect on the formation of flammable mixture volumes and the development of ignition sources.

2 Numerical Simulations

The governing equations are the unstready, compressible two-dimenstional axisymmetric Navier-Stokes equations for a chemically reactive multi-species mixture of ideal gases. The numerical scheme is based

Correspondence to : enjis@snu.ac.kr

on the cell-centered finite volume method. The convective numerical fluxes are evaluated by AUSM-DV scheme which is accurate and robust for resolving shock and contact(stationary and moving) discontinuities. Second-order spatial accuracy is attained by using MUSCL extrapolation on primitive variables with limited slopes by the Superbee limiter for Total Variation Diminishing(TVD) constraint. The viscous terms are evaluated with the second-order central differencing discretization. For time integration, the second-order Strang-type method splitting convection-diffusion terms and chemical source terms is employed. A memory efficient type of four-step Runge-Kutta scheme is used for the integration of convection and diffusion terms, while a stiff ODE solver named RADAU5[6], an implicit Runge-Kutta method of order 5 with step size control, is used in order to overcome the stiffness caused by the chemical source terms. A comprehensive kinetic model of hydrogen combustion recently updated by Li et al.[7] is used for describing the reaction kinetics with nine species(H_2, O_2, H, O, OH, H_2O, HO_2, H_2O_2, N_2) and nineteen reactions. The evaluation of thermodynamic properties, transport properties and chemical source terms are assisted by Cantera[8] library with its interface for Fortran.

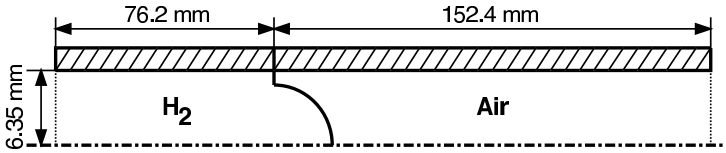

Figure 1: Computational domain

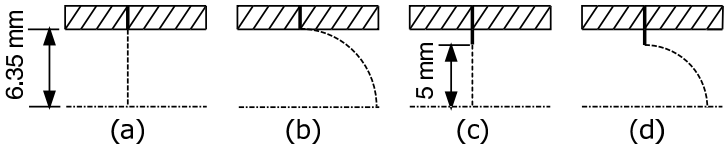

Figure 2: Geometries of pressure boundary

The computational domain is shown in Figure 1 with the geometry of one of pressure boundaries. Four geometries of pressure boundary considered for the present study are shown in Figure 2. As for the boundary conditions, adiabatic, non-slip condition for the tube wall, transmissive condition for both ends of computational domain, and slip condition for axis of symmetry are applied. The initial temperature is set as 300 K for both hydrogen and air. The bursting pressure of rupture disks is set as 86.1 atm. To keep the cell size within the order of Kolmogorov scale, a cartesian grid system of uniform size of 19 μm is accepted. Total number of cells is about 4 millions.

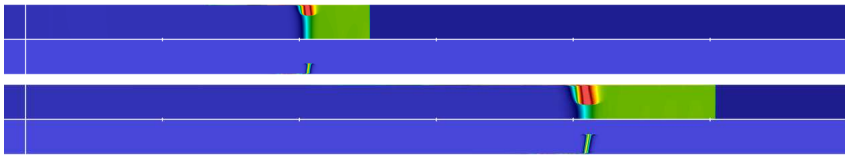

Figure 3: Case (a): Temperature(upper half) and Y_{OH}(lower half) at 43 μs and 86 μs

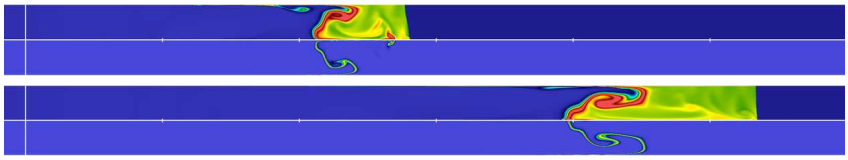

Figure 4: Case (b): Temperature(upper half) and Y_{OH}(lower half) at 43 μs and 86 μs

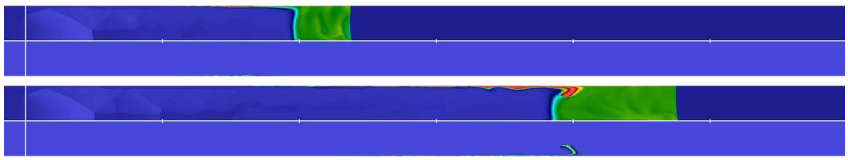

Figure 5: Case (c): Temperature(upper half) and Y_{OH}(lower half) at 43 μs and 86 μs

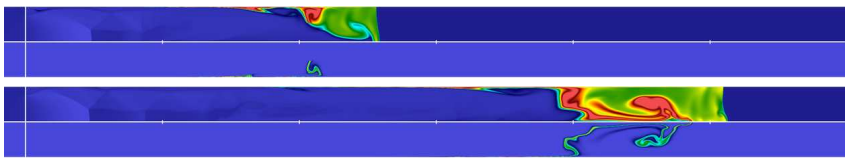

Figure 6: Case (d): Temperature(upper half) and Y_{OH}(lower half) at 43 μs and 86 μs

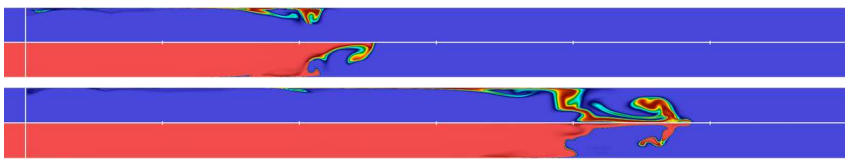

Figure 7: Case (d): Y_{H_2O}(upper half) and Φ(lower half) at 43 μs and 86 μs

3 Simulation Results

3.1 Case (a): Plane boundary of full radius

3.2 Case (b): Spherical boundary of full radius

3.3 Case (c): Plane boundary of partial radius

3.4 Case (d): Spherical boundary of partial radius

4 Summary

A series of numerical simulations on the effect of the geometry of pressure boundary at the moment of its failure on the development of flows downstream of the pipe and on the occurrence of spontaneous ignition of hydrogen. When the failure geometries are assumed as planar ones as in case (a) and (c), local ignition from the boundary layers is developed in limited area and the mixing of hydrogen and air is weak. On the other hand, with the failure geometries which represent realistic bursting geometries of type B rupture disks, as in case (b) and (c), the multi-dimensional shock-shock interaction and shock-boundary layer interaction take place, hence the flame fronts at the contact region of hydrogen and air are developed to the full radius of the pipes. It is found that the initial formation of multi-dimensional shock wave and sufficient length of downstream pipe which allows the sufficient time of mixing by shock interactions are necessary for the spontaneous ignition kernel is developed within the pipe length.

References

[1] Dryer FL, Chaos M, Zhao Z, Stein JN, Alpert JY, Homer CJ. (2007). Spontaneous ignition of pressurized releases of hydrogen and natural gas into air. Combust Sci Technol. 179(4):663-694.

[2] Golub VV, Baklanov DI, Golovastov SV, Ivanov MF, Laskin IN, Saveliev AS, Semin NV, Volodin VV. (2008). Mechanisms of high-pressure hydrogen gas self-ignition in tubes. J Loss Prevent Proc. 21(2):185-198.

[3] Mogi T, Kim D, Shiina H, Horiguchi S. (2008). Self-ignition and explosion during discharge of high-pressure hydrogen. J Loss Prevent Proc. 21(2):199-204.

[4] Xu BP, El H, Wen JX, Dembele S, Tam VHY, Donchev T. (2008). Numerical study on the spontaneous ignition of pressurized hydrogen release through a tube into air. J Loss Prevent Proc. 21(2):205-213.

[5] Yamada E, Watanabe S, Hayashi AK, Tsuboi N. (2009). Numerical analysis on auto-ignition of a high pressure hydrogen jet spouting from a tube. Proc. Combust. Inst. 32(2):2363-2369.

[6] Hairer E, Wanner G. Solving ordinary differential equations II: Stiff and differential-algebraic problems. Springer, 2004.

[7] Li JL, Zhao Z, Kazakov A, Dryer FL. (2004). An updated comprehensive kinetic model of hydrogen combustion. Int J Chem Kinet 36(10):566-575.

[8] Goodwin DG. (2003). An open-source, extensible software suite for CVD process simulation. In: Proceedings of CVD XVI and EuroCVD Fourteen. p.155-162.