Numerical Investigation of Hydrogen Release from Varying Diameter Exit

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Abstract

Computational fluid dynamics is used to simulate the release of high pressure Hydrogen from a reservoir with an exit of increasing diameter. Abel-Noble real gas equation of state is used to accurately simulate this high pressure release. Parallel processing based on Message Passing Interface for domain decomposition is employed to decrease the solution time. The release exit boundary is increased in time to simulate a scenario when the exit area increases during the release. All nodes and elements are moved accordingly at each time step to maintain the quality of the mesh. Different speeds of increasing diameter are investigated to see the impact on this unsteady flow.

Introduction

Hydrogen is considered to be the best candidate as a replacement for fossil fuels because fossil fuels are diminishing very rapidly and the utilization rate is higher than the generation rate while the potential for hydrogen production is almost infinite. Furthermore, hydrogen is not harmful to the environment since water is the result of burning Hydrogen. Although Hydrogen is a good source of energy, concerns about safety issues need to be addressed. Explosions like the one occurred in Stockholm [1], showed how easily hydrogen can cause a disaster. The main concern about the hydrogen use is the safe storage. Hydrogen is combustible at a very wide range of concentration (4% - 75%) and it may also auto-ignite. In case of failure of storage reservoir or pipes and connectors there is high possibility of explosion. Therefore, the flow pattern after this high pressure release is important to discuss.

Experiment work [2] is costly in this field and only a few experiment results are available. In most cases Hydrogen is replaced by Helium to avoid combustion while still providing the flow pattern. Analytical work is very limited and is only capable of giving us the steady state position of the Mach disk [3]. Numerical simulation based on computational fluid dynamics is less expensive than experiment and the accuracy is acceptable. In-house codes or softwares can be used to simulate this flow. Fluent is used by Pedro et al [4] to discuss the release from a 10MPa tank. Higher pressures are observed in the work of Liu et al [5] (pressure of 70MPa) and Radulescu et al [6] (pressure of 100MPa). The pressure of 10MPa is low enough to use ideal gas law as the state equation [7]. Higher pressures cannot be simulated by ideal gas law. Real gas simulation can be performed as reported by Cheng et al [8] and Mohamed et al [9]. The Beattie-Bridgeman state equation including five constants is applied in the work of Mohamed et al. Hydrogen is released from a 34.5MPa tank, and the properties at the jet exit are found. Abel-Noble state equation with only one constant is used in the work of Cheng et al [8]. They simulate the release from a 400 Bar tank and the difference between ideal and real gas simulations are

given. It is shown that the difference between ideal gas and real gas is not negligible. Also in [10] ideal gas and real gas results are compared which confirms the necessity of a real gas model for high tank pressures. Beattie-Bridgeman and Abel-Noble state equations are compared in [11] for the release of hydrogen in hydrogen. Results show that the difference between models is negligible. In reality the exit is opening in time. The failure of the tank or the pipes exit can be modelled as a hole with increasing diameter. Therefore, in this research a moving mesh is applied to accurately simulate the flow caused by an increasing diameter opening.

In this research, a three-dimensional in-house code is developed to simulate the release of high pressure hydrogen (70MPa). Abel-Noble state equation is used. Parallel processing (Message Passing Interface) is utilized, since the mesh uses a large number of nodes and elements. Without parallel processing we have a memory problem and also the solution time is very high. The geometry and mesh are generated by Gambit and the mesh is divided into 32 partitions by the Metis software. Hydrogen is released into air; a transport equation is solved at each iteration to find out the concentration of the hydrogen-air mixture. A moving mesh feature is added to the code to simulate the release from an increasing diameter opening which is the real case. In this case, the release area is expanded from different initial diameters. The results are discussed at different rates of opening. The final code is an accurate tool to find out the flow pattern in case of sudden release of high pressure hydrogen into ambient air. This tool is capable of applying the real gas equation, finding out the concentration of the hydrogen-air mixture, uses parallel processing and also an increasing diameter exit which is similar to real cases.

Governing Equations

The flow is simulated by Euler equations as follows

$$\frac{\partial U}{\partial t} + \nabla . F = 0$$

Where,

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix} \quad , F = \left\{ \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ \rho uw \\ \rho uH \end{bmatrix} \begin{bmatrix} \rho v \\ \rho vu \\ \rho v^2 + P \\ \rho vw \\ \rho vH \end{bmatrix} \begin{bmatrix} \rho w \\ \rho wu \\ \rho wv \\ \rho w^2 + P \\ \rho wH \end{bmatrix} \right\}$$

Euler equations can be used since the flow is very high speed and Reynolds number is high.

Implicit finite-volume is used for discretization:

$$|V| \frac{U^{n+1} - U^n}{\Delta t} + \sum_{surface} F^{n+1} . n \Delta A = 0$$

$$F^{n+1} = F^n + (\frac{\partial F}{\partial U})^n (U^{n+1} - U^n) = F^n + J^n (U^{n+1} - U^n)$$

To find out the concentration of hydrogen-air mixture a transport equation is applied:

$$\frac{\partial(\rho c)}{\partial t} + \nabla.(\rho u c) = 0$$

c is the concentration. It is 0 when there is no air and is 1 when there is no hydrogen. This equation is solved, at each iteration, with the same numerical approach as the Euler equations.

Abel-Noble equation of state including only one constant is used as the real gas equation :

$$P = \frac{RT}{(\upsilon - b)} = \frac{\rho RT}{(1 - b\rho)} = (1 - b\rho)^{-1}\rho RT = z\rho RT \quad , \quad b = 0.00775\, m^3/kg$$

z is the compressibility factor and equals one for an ideal gas but it deviates from one for the real gas as shown by this equation. In table (1) compressibility factor is given for hydrogen at T of 300K. The deviation from one becomes bigger as the pressure increases.

In order to apply the add the moving mesh feature, Euler equations are changed [12] :

$$U = \begin{bmatrix} \rho \\ \rho u_x \\ \rho u_y \\ \rho u_z \\ \rho E \end{bmatrix} \quad , \quad F = \left\{ \begin{bmatrix} \rho(u_x - w_x) \\ \rho(u_x - w_x)u_x + P \\ \rho(u_x - w_x)u_y \\ \rho(u_x - w_x)u_z \\ \rho(u_x - w_x)E + u_x P \end{bmatrix} \begin{bmatrix} \rho(u_y - w_y) \\ \rho(u_y - w_y)u_y \\ \rho(u_y - w_y)u_y + P \\ \rho(u_y - w_y)u_z \\ \rho(u_y - w_y)E + u_y P \end{bmatrix} \begin{bmatrix} \rho(u_z - w_z) \\ \rho(u_z - w_z)u_x \\ \rho(u_z - w_z)u_y \\ \rho(u_z - w_z)u_z + P \\ \rho(u_z - w_z)E + u_z P \end{bmatrix} \right\}$$

Where w is the velocity of each node in case of movement. Also the discretization is changed to the following equation :

$$\frac{U^{n+1}V^{n+1} - U^n V^n}{\Delta t} + \sum_{surface} F^{n+1}.n\,\Delta A = 0$$

which includes the volume of the control volume before and after each time step.

The new eigenvalues are calculated using the moving velocity:

$$\lambda_1 = \lambda_2 = \lambda_3 = (u_x - w_x)n_x + (u_y - w_y)n_y + (u_z - w_z)n_z$$
$$\lambda_4 = (u_x - w_x)n_x + (u_y - w_y)n_y + (u_z - w_z)n_z + a$$
$$\lambda_5 = (u_x - w_x)n_x + (u_y - w_y)n_y + (u_z - w_z)n_z - a$$

Table (1)- compressibility factor at different pressures for Abel-Noble equation

Pressure (MPa)	20	40	60	80	100
Compressibility factor (Abel-Noble)	1.12	1.25	1.37	1.50	1.62

Spring-based mesh moving

The mesh is moved based on spring method. Boundary nodes are moved and all the interior nodes are moved accordingly to reach the equilibrium state. Each edge acts like a spring. A movement on a boundary node causes a force along the edges connected to the node, This force based on the Hook's law is found as:

$$F = \sum k_i \ (\Delta x_i - \Delta x)$$

Where Δx , Δx_i are the node displacement and the displacements of neighbouring nodes. The total force on the each node is the sum of all forces along the edges connected to it. k_i is the stiffness of the edge and is found as follows:

$$k_i = \frac{1}{Edge \ \ Length}$$

Since the force on each node should be zero at equilibrium, the following iterative equation is solved:

$$\Delta x = \frac{\sum k_i \Delta x_i}{\sum k_i}$$

Finally the new position of each node is calculated by adding the displacement:

$$x^{n+1} = x^n + \Delta x$$

Geometry and mesh

Three different meshes of different release area diameters are created by Gambit. The meshes have initial release diameters of 2.0mm, 1.5mm and 1.0mm. In figure (1), the initial geometry and mesh for the release area of 2.0mm are given. For other diameters, the geometry is the same except the release area diameter. All three meshes include around 0.8 million nodes and 4 million tetrahedral elements. Each mesh is divided into 32 partitions by the help of Metis software and Cirrus, a supercomputer of Concordia University, is employed for the parallel processing. Boundary nodes are moved at each time step and all the other nodes are moving based on the spring method.

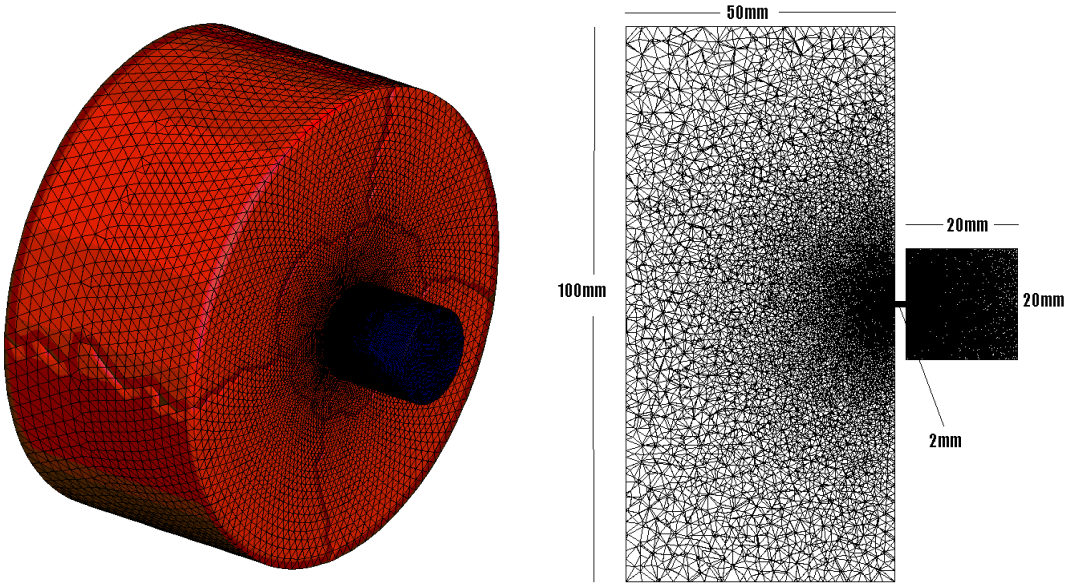
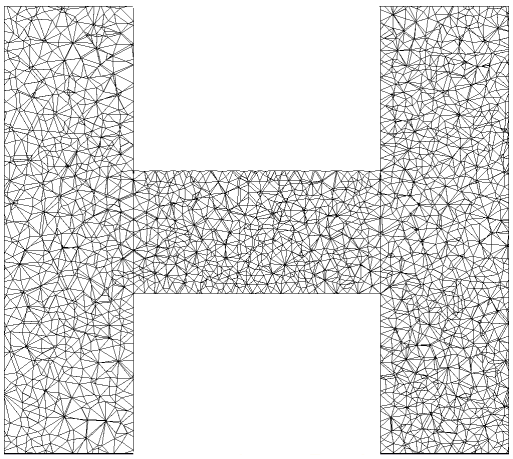


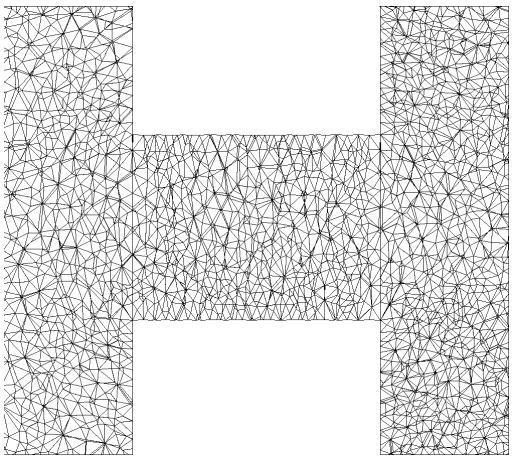
Figure (1) - 3D and 2D views of the mesh (dimensions are in metres).

Results

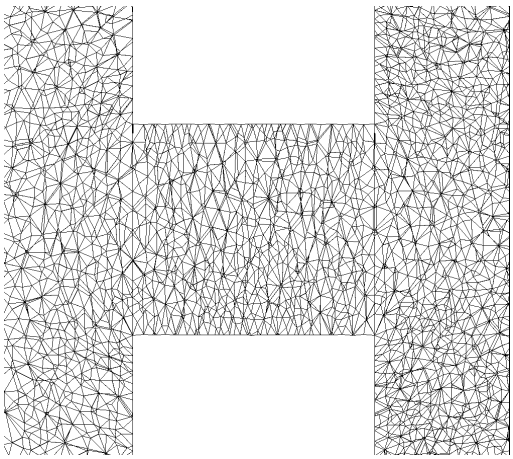
Three initial release area diameters of 1.0mm, 1.5mm and 2.0mm are tested. The tank pressure for all cases is 70MPa and the outside has ambient conditions. The initial temperature is 300K everywhere. For each case, three opening rates of 80m/s, 200m/s and 500m/s are examined. In figure (2), for the initial diameter of 1.0mm at the opening rate of 500m/s, the two-dimensional view of the release area mesh at different times of 1.0, 1.5, 2.0, 2.5 and 3.0 micro seconds after release is given. The mesh is moving based on the spring method and is a very high quality mesh. The final diameter (at time 3.0 micro seconds) for the initial diameters of 1.0mm, 1.5mm and 2.0mm at the opening rate of 500m/s are 2.5mm, 3.0mm and 3.5mm respectively. In figure (3), Mach contours for initial diameter of 1.0mm at the opening rate of 500m/s are given.



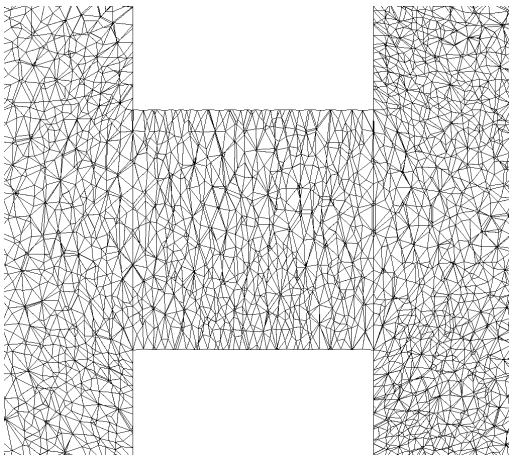
Initial diameter



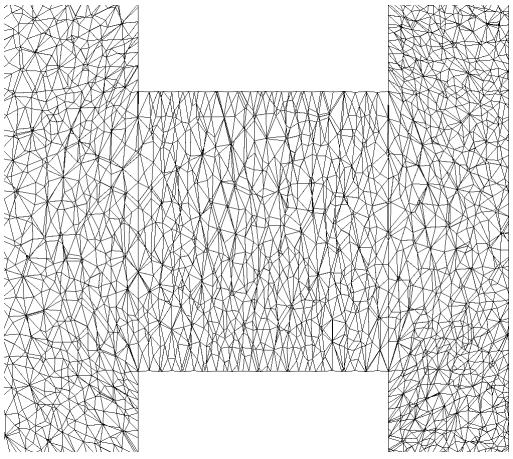
After 1.0 micro seconds



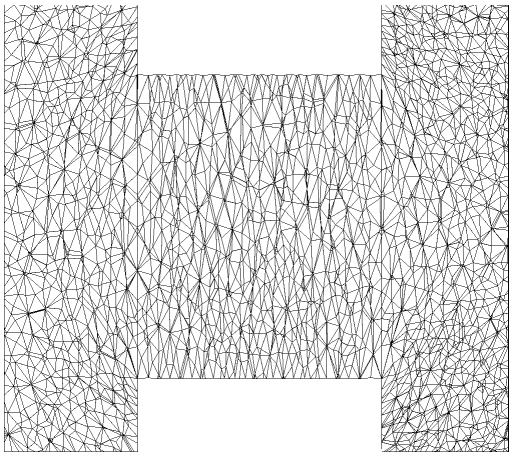
After 1.5 micro seconds



After 2.0 micro seconds

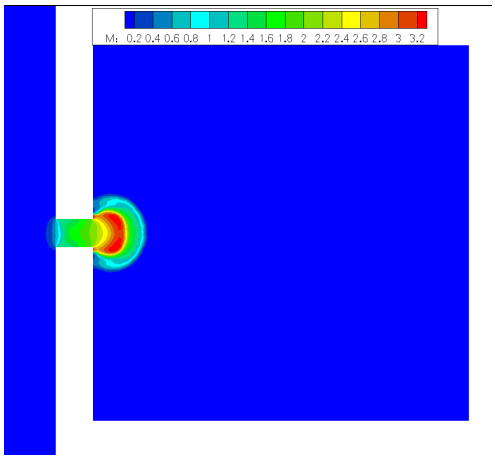


After 2.5 micro seconds

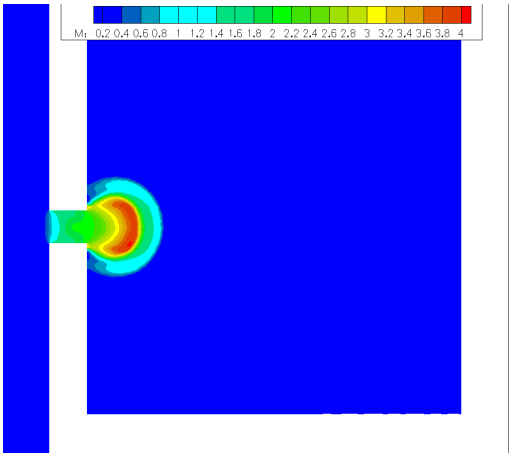


After 3.0 micro seconds

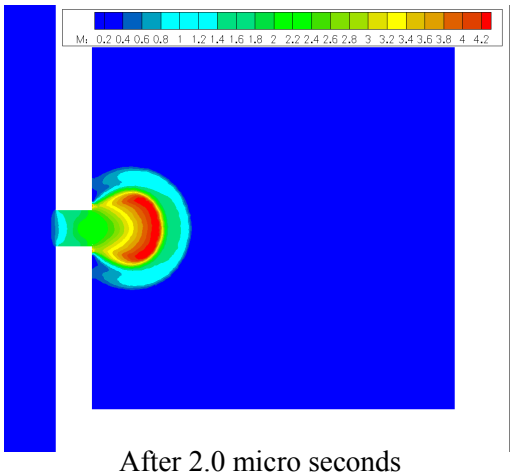
Figure (2) – Release area expanding for the initial diameter of 1.0mm at the rate of 500m/s.



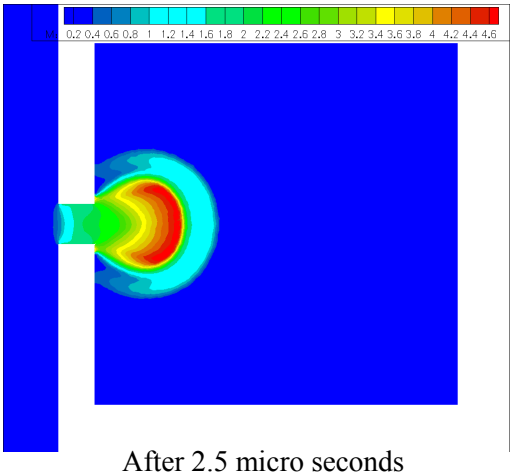
After 1.0 micro seconds



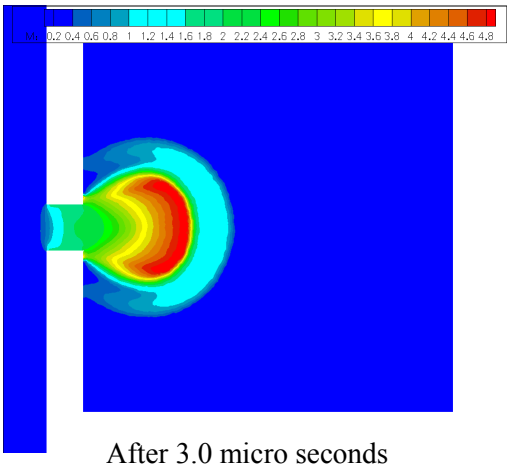
After 1.5 micro seconds



After 2.0 micro seconds



After 2.5 micro seconds



After 3.0 micro seconds

Figure (3) – Mach contours for the initial diameter of 1.0mm at the opening rate of 500m/s.

Properties on the contact surface are important for combustion discussion. In figure (4) Pressure versus time on the contact surface is given for initial release area diameter of 1.0mm at different opening rates and in figure (5) contact surface location is given. It is noticed pressure on the contact surface depends on the opening rate. For example, at time of 0.5 micro seconds the pressure is almost 2.0MPa for the opening velocity of 500m/s while it is almost 5.0MPa for the opening velocity of 80m/s. The main difference is noticed in almost the first micro second. There is also a small difference in contact surface location for different opening velocities.

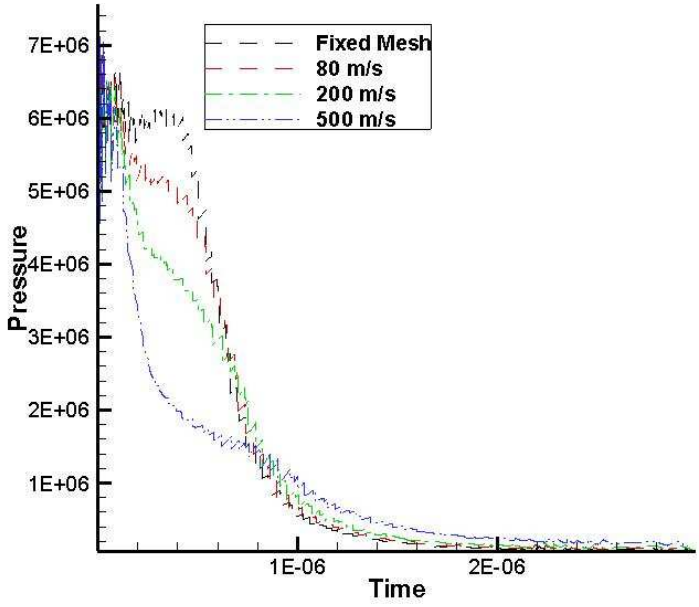


Figure (4) – Pressure on the contact surface for the initial diameter of 1.0mm at different opening rates

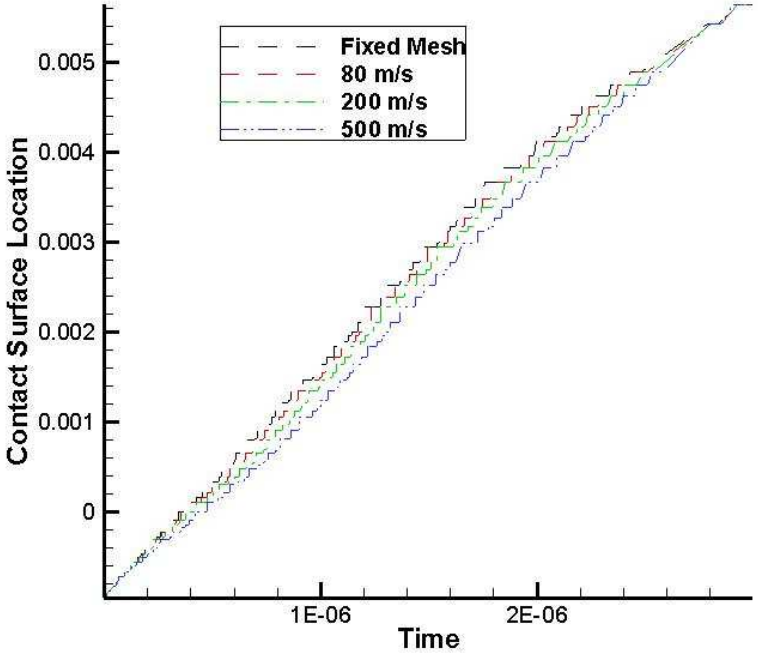


Figure (5) – Contact surface location for the initial diameter of 1.0mm at different opening rates

In figures (6) and (7) pressure and contact surface location versus time at opening rate of 200m/s for the initial release area diameter of 1.0mm, 1.5mm and 2.0mm are given. It is noticed pressure is higher for higher initial diameters and the difference is not negligible. Contact surface locations are similar up to 2.0 micro seconds and after that the difference appears. After 2.0 micro seconds, the flow advances faster for higher initial diameters.

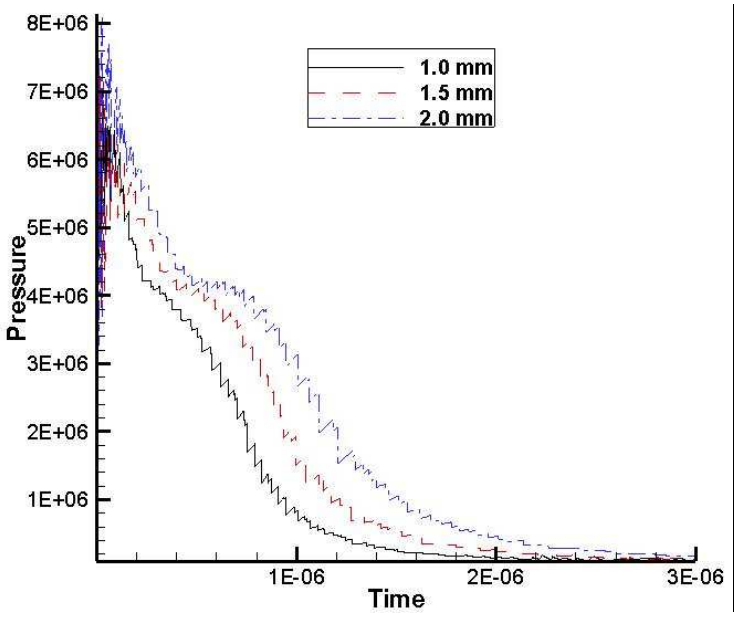


Figure (6) – Pressure on the contact surface for different initial diameters at the opening rate of 200m/s

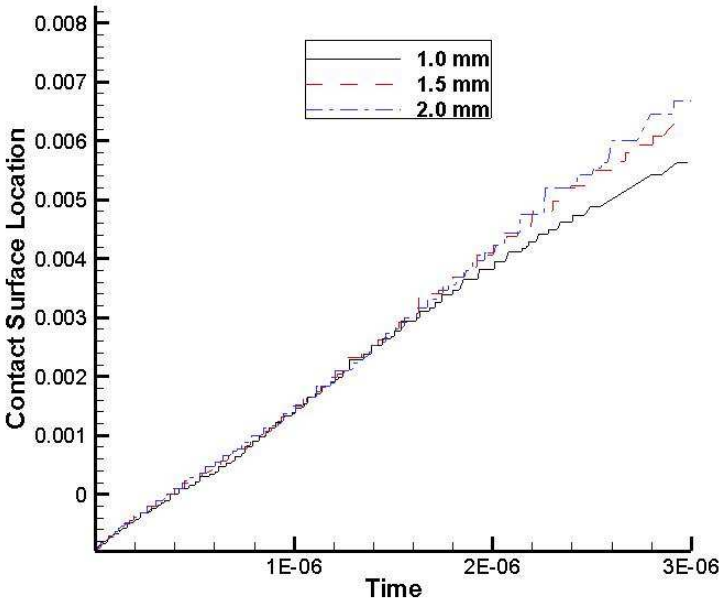


Figure (7) – Contact surface location for different initial diameters at the opening rate of 200m/s

Conclusion

An in-house code is developed to simulate the release of high pressure hydrogen into air through an expanding opening. Able-Noble is used as the real gas state equation since high pressure hydrogen cannot be accurately simulated by ideal gas equation. Parallel processing is applied to decrease the solution time. In reality, the release area expands and does not have a fixed diameter. Three cases of initial release diameter of 1.0mm, 1.5mm and 2.0mm are discussed. Each case is tested for three different opening speeds of 80m/s, 200m/s and 500m/s. Properties on the contact surface are important for combustion discussion, therefore pressure and contact surface location versus time are given for different cases. Each case is investigated until the release time of 3 micro seconds. We conclude that the pressure on the contact surface depends on both opening speed and initial release area diameter.

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