Numerical Investigation of Hydrogen dispersion into Air

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ABSTRACT

Computational fluid dynamics (CFD) is used to numerically solve the sudden release of hydrogen from a high pressure tank (up to 70MPa) into air. High pressure tanks increase the risk of failure of the joints and pipes connected to the tank which results in release of Hydrogen. The supersonic flow caused by high pressure ratio of reservoir to ambient generates a strong Mach disk. A three dimensional in-house code is developed to simulate the flow. High pressure Hydrogen requires a real gas law because it deviates from ideal gas law. Firstly, Beattie-Bridgeman and Abel-Noble real gas equation of states are applied to simulate the release of hydrogen in hydrogen. Then Abel-Noble is implied to simulate the release of hydrogen in air. Beattie-Bridgeman has stability problems in the case of hydrogen in air. A transport equation is used to solve the concentration of Hydrogen-air mixture. The code is second order accurate in space and first order in time, and uses a modified Van Leer limiter. The fast release of Hydrogen from a small rupture needs a very small mesh, therefore parallel computation is applied to overcome memory problems and to decrease the solution time. The high pressure ratio of the reservoir to ambient causes a very fast release which is accurately modeled by the code and all the shocks and Mach disk happening are observed in the results. The results show that the difference between real gas and ideal gas models cannot be ignored.

INTRODUCTION

Safety issue of hydrogen as a fuel is one of the main concerns. Explosions like the one in Stockholm, Sweden in 1983 [1] show the necessity to develop reliable and standard codes which can predict the hazards related to hydrogen use as a fuel. Hydrogen is combustible at concentrations between 4% and 75% and it needs a small amount of energy to ignite. Hydrogen may also auto-ignite under certain conditions. Hydrogen is stored in high pressure tanks since it has small amount of energy per unit volume. The pressure is increased up to 70MPa. The failure of the tank and release of this high pressure hydrogen may result in a huge explosion.

Analytical results are restricted to the location and diameter of the steady state Mach disk and they are not capable of solving the unsteady flow [2]. Experimental work can help to see the flow pattern and hazards related to this release [3]. The experimental results are mostly given by schlieren pictures and movies recorded during the release. Although experimental works are more accurate and reliable, the cost of such experiments forces researchers to use numerical methods. Computational fluid dynamics (CFD) is widely used in this area and is divided into two categories: commercial softwares like FLUENT and in-house codes. Pedro et al [4] use FLUENT to simulate a two dimensional flow. In their work, a structured grid is employed and adaptation is applied to refine the grid in necessary areas. The tank pressure is 10MPa and ideal gas law is used to simulate the release of hydrogen. Ideal gas law results are still at a good approximation for pressure of 10MPa [5], but higher pressure hydrogen cannot be treated as ideal gas and a real gas model is required. FLUENT does not have a real gas model for hydrogen.

In-house codes have the advantage of allowing the addition of a real gas model. Real gas equation of state can be modeled with the Beattie-Bridgeman equation of state with five constants, Van der waals with two constants or Abel Noble with only one constant. Mohamed et al [6] applies the Beattie-Bridgeman to model the release of hydrogen from a high pressure tank (34.5MPa). In their simulation only the tank and the release hole are modeled. The flow pattern after release is not discussed and simulated. Abel Noble state equation is seen in the work of Cheng et al [7]. Beattie-Bridgeman equation has been unstable to solve the release of hydrogen in air. Therefore only Abel Noble state equation is used in our work to simulate the case of hydrogen in air. In order to compare the accuracy, Beattie-Bridgeman is used for the simulation of hydrogen in hydrogen release and the results are in good agreement with Abel Noble results.

In this work, an in-house code is developed to simulate the release of high pressure hydrogen into air. Sudden failure of the tank results in discharge of hydrogen from the tank. Hydrogen pushes the air at the ambient condition and a highly under-expanded jet is generated. A Mach disk is formed which changes the high supersonic flow to subsonic. In some cases the Mach number behind this Mach disk reaches 10. High Mach number and high gradients caused by high pressure ratio along with the small release hole makes the simulation of this flow complicated and a very fine and high quality mesh is needed to accurately capture all the feature of the flow and overcome the stability problems. The mesh is unstructured and is generated by GAMBIT. High number of elements and nodes requires lots of memory and it is not possible by a single processor. Furthermore, the solution time is very high if only one processor is employed. The in-house code is developed for parallel processing. Message Passing Interface (MPI) method is used in the parallel code. The code uses a three-dimensional finite volume solver and an implicit scheme. The accuracy is second order in space and first order in time. High gradients caused by a high pressure ratio make the flow unstable in areas such as the shock regions and contact surface. MUSCL scheme and a modified Van leer limiter are used for the second order accuracy. The solver implies Euler equations i.e. viscous terms are negligible since the flow is very high speed. However, in areas of high gradients, viscous terms become higher. Navier-Stokes equations will be applied in the future to have more accurate results.

NUMERICAL METHOD

Euler equations are used to solve this flow. Although in high gradient areas viscous terms cannot be neglected, these terms are still small compared to convective terms and Euler equations can give acceptable results. Therefore, governing equations are as follows:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u)}{\partial x}+\frac{\partial(\rho v)}{\partial y}+\frac{\partial(\rho w)}{\partial z}=0$$

$$\frac{\partial(\rho u)}{\partial t}+\frac{\partial(\rho u^2+P)}{\partial x}+\frac{\partial(\rho v u)}{\partial y}+\frac{\partial(\rho w u)}{\partial z}=0$$

$$\frac{\partial(\rho v)}{\partial t}+\frac{\partial(\rho u v)}{\partial x}+\frac{\partial(\rho v^2+P)}{\partial y}+\frac{\partial(\rho w v)}{\partial z}=0$$

$$\frac{\partial(\rho w)}{\partial t}+\frac{\partial(\rho u w)}{\partial x}+\frac{\partial(\rho v w)}{\partial y}+\frac{\partial(\rho w^2+P)}{\partial z}=0$$

$$\frac{\partial(\rho E)}{\partial t}+\frac{\partial(\rho u H)}{\partial x}+\frac{\partial(\rho v H)}{\partial y}+\frac{\partial(\rho w H)}{\partial z}=0$$

The discretization scheme is implicit finite-volume:

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

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

Therefore,

$$\left(\frac{|V|}{\Delta t} I + \sum_{surface} (\frac{\partial F}{\partial U})^n .n\,\Delta A\right)\delta U^{n+1} = -\sum_{surface} F^n .n\,\Delta A$$

Two real gas equation of state are analysed.

Beattie-Bridgeman

This equation includes five constants and the constants are given in table (1).[6]

$$P = \frac{RT}{\upsilon} + \left(\frac{-cR}{T^2} + B_\circ RT - A_\circ\right)\frac{1}{\upsilon^2} + \left(-\frac{B_\circ cR}{T^2} - B_\circ bRT + \alpha A_\circ\right)\frac{1}{\upsilon^3} + \frac{B_\circ bcR}{T^2}\frac{1}{\upsilon^4}$$

Table (1)- constants of Beattie-Bridgeman equation for hydrogen

$A_\circ$ (m^5/Kg.s^2)	$10^{+3}\,\alpha$ (m^3/Kg)	$10^{+2}\,B_\circ$ (m^3/Kg)	$10^{+2}\,b$ (m^3/Kg)	$10^{-2}\,c$ (m^3 .K^3/ Kg)
4924	-2.510	1.034	-2.162	2.500

Abel-Noble

This equation is simpler and uses only one constant:

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

z is compressibility factor and is one in the ideal gas law. In order to compare ideal gas law and Abel-Noble, in table (2) compressibility factor is given for hydrogen at T=300K. The difference between real gas and ideal gas becomes higher when the pressure is increased. For the pressure of 100Mpa there is almost 60 percent difference. Therefore for this flow, the real gas equation is necessary to accurately capture all the features. All the relations are found by Abel-Noble equation. Some relations like $c_p - c_v = R$ are the same for ideal gas and Abel-Noble gas but some like speed of sound differ. For example, for ideal gas, speed of sound equals $\sqrt{\gamma RT}$ while for an Abel-Noble gas is:

$$a_{AN} = \frac{v}{v-b}\sqrt{\gamma RT}$$

Table (2)- 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

Transport equation

Hydrogen is released into air. Therefore, soon after release a mixture of hydrogen-air exists in the flow. A transport equation is solved to find the concentration of each species:

$$\frac{\partial(\rho c)}{\partial t}+\frac{\partial(\rho cu)}{\partial x}+\frac{\partial(\rho cv)}{\partial y}+\frac{\partial(\rho cw)}{\partial z}=0$$

c gives the concentration and varies from 0 to 1. It initially equals 0 where the concentration of Hydrogen is 100 percent and equals 1 where the concentration of air is 100 percent. The transport equation is solved at each iteration separately. R of mixture is found by concentration as follows:

$$R_{mix}=R_{H_2}(1-c)+R_{Air}c$$

where,

$$R_{H_2}=4124(J/kgK)$$

$$R_{Air}=287(J/kgK)$$

RESULTS

Two cases of release of hydrogen in hydrogen and hydrogen in air are discussed in this section. Firstly, Abel-Noble and Beattie-Bridgeman equation of states are applied for hydrogen in hydrogen release, and Accuracy is compared for these two real gas equations, then Abel-Noble is used to simulate the hydrogen in air release. Beattie-Bridgeman shows stability problems for this case, therefore it is not applied.

The mesh required for the simulation is created by GAMBIT. Symmetry of the problem allows us to restrict the simulation to a 60-degree cut of the domain. Initially, smaller cuts were tried but the mesh had low quality. The diameter of release area is 5mm. The external environment is 150mm long or 30 times the release area diameter. This long area is needed since the release speed is very high and it should be noticed that we are only interested in the release time of the order of micro seconds. A bigger space in the external environment is required for higher release times. The mesh is very small and includes high number of elements and nodes. Three-dimensional tetrahedral elements are used. Three-dimensional mesh is necessary for future work since gravity will be added to the code and also large eddy simulation (LES) will be considered as the turbulence model.

Two different domain sizes and meshes are tried. Figure (1) shows a small domain with a coarse mesh. This mesh contains almost 2.8 million elements and 0.5 million nodes. This mesh is divided into 16 partitions to run the parallel code. CIRRUS, a supercomputer of Concordia University is employed to run the parallel code. This supercomputer has the capacity to run on 64 CPUs. Different partitions of the mesh are observed in the figure. Figure (2) shows a bigger domain with a finer mesh. This mesh contains almost 15.3 million elements and 2.6 million nodes, and uses 64 partitions. The tank shape is a little different in these two domains but it does not affect the results. In both cases the mesh is very small in the release area and it gets coarser as the distance from the release area increases. In the tank the mesh coarsens at a much higher rate compared to the external environment. Gradients in the tank are much smaller, therefore the mesh in the tank does not need to be very small. This helps to have fewer elements and decrease the solution time.

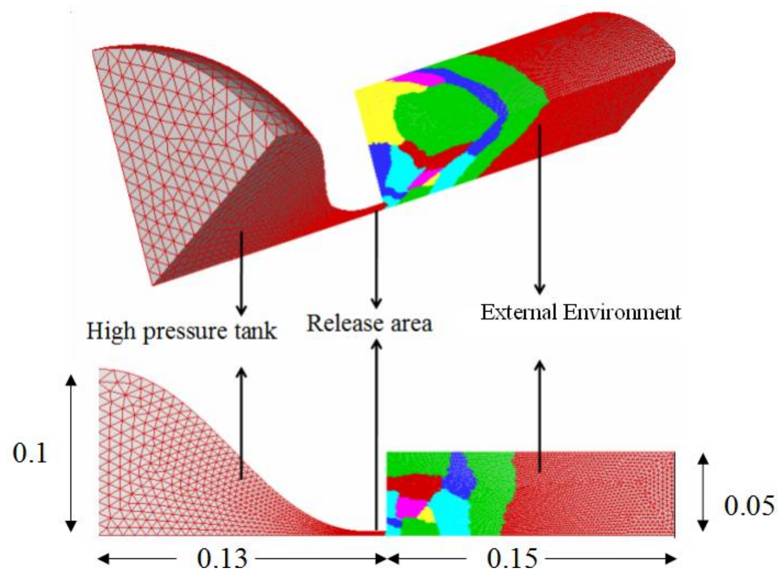


Figure (1)- Three-dimensional and two-dimensional view of a coarse mesh divided into 16 partitions

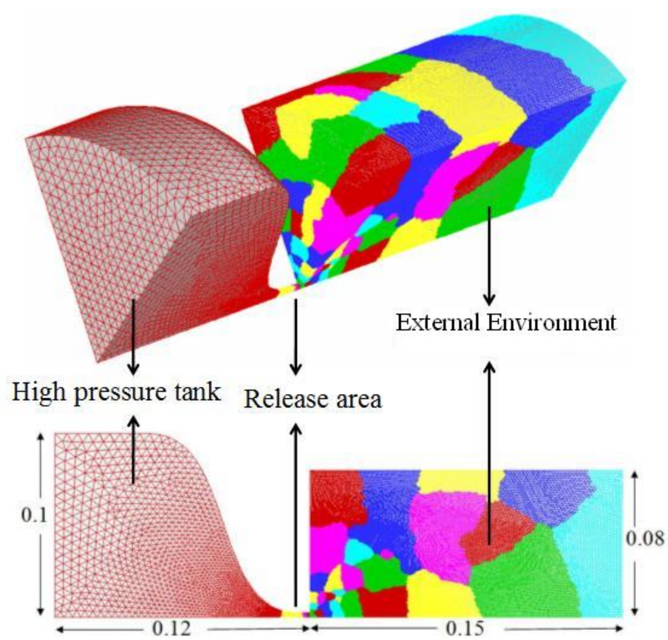


Figure (2)- Three-dimensional and two-dimensional view of a fine mesh divided into 64 partitions

Hydrogen in Hydrogen

In this case both Beattie-Bridgeman and Abel-Noble are applied. Hydrogen is released in still hydrogen therefore initial velocity is zero in the whole domain. Initial pressure of hydrogen in the tank is 34.5MPa and is released in hydrogen at 101325Pa. Initial temperature is 300K everywhere in the domain. Initial density depends on the equation of state. In table (3) Initial tank density is given for different equations.

Table (3)- initial tank density for different equations at initial pressure and temperature of 34.5 MPa and 300K

Equation of state	Ideal gas	Abel-Noble	Beattie-Bridgeman
Initial tank density	27.88	22.93	22.32

After release, high pressure causes chocked flow in the release area, Mach number becomes one and the velocity equals the speed of sound. In the external area, a highly supersonic flow is generated in just a few micro seconds and a Mach disk is formed. In figure (3) the Mach contours are shown for Beattie-Bridgeman at t=40 micro seconds. The mesh of 2.8 million elements is employed. Barrel shock and Mach disk are captured well and the flow is advancing very fast. Mach disk takes place at a distance of almost 40mm. In figure (4) Mach number along the centerline is compared for Beattie-Bridgeman and Abel-Noble. The initial interface is located at z=-2.5 mm. In table (4), release temperature, velocity and density at t=40 micro seconds are compared. It is noticed the difference between results of these two equations is negligible but the real gas results are different from ideal gas. Beattie-Bridgeman was tried for the pressure of 70MPa but due to stability problems no results were achieved. The very small difference between Beattie-Bridgeman results and Abel-Noble results allows us to imply Abel-Noble for the remaining cases.

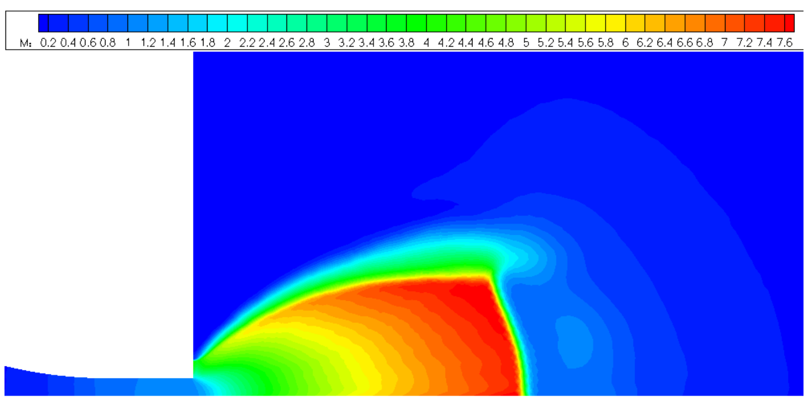


Figure (3)- Mach contours for pressure of 34.5MPa at time of 40 micro seconds by Beattie-Bridgeman equation

Table (4)- Release properties at z=-2.5mm for different equations (Pressure of 34.5MPa and time of 40 micro seconds)

Equation of state	Ideal gas	Abel-Noble	Beattie-Bridgeman
Release temperature (K)	233	235	234
Release velocity (m/s)	1287	1431	1446
Release density(kg/m^3)	14.69	13.35	13.42

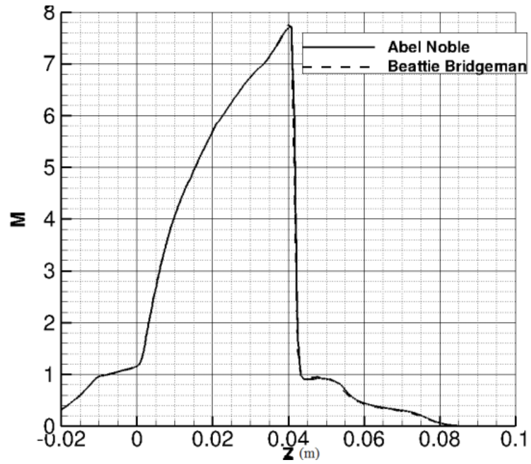
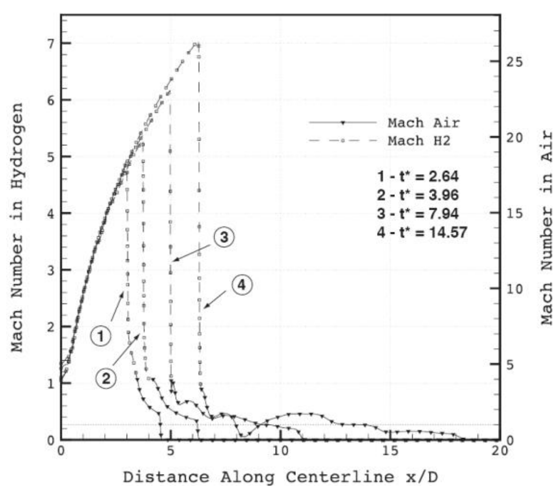


Figure (4)- Mach number along the centerline for pressure of 34.5MPa
at time of 40 micro seconds (Beattie-Bridgeman and Abel-Noble)

Experimental results have a limited use to validate the code since most of them discuss the results qualitatively. Analytical results are also not accurate enough. In this work, the numerical results of [4] are used to compare the results. The tank pressure is 10MPa. For our simulation the mesh of 15.3 million elements is used. Abel-Noble is used as the real gas equation. Ideal gas is employed in the work of [4], but the pressure is 10MPa and the difference of ideal gas and real gas is negligible. Figure (5) shows the comparison at four different times. Comparison shows good agreement between the results. Time is non-dimensionalized by release area diameter over hydrogen speed of sound for ideal gas at T=300K.



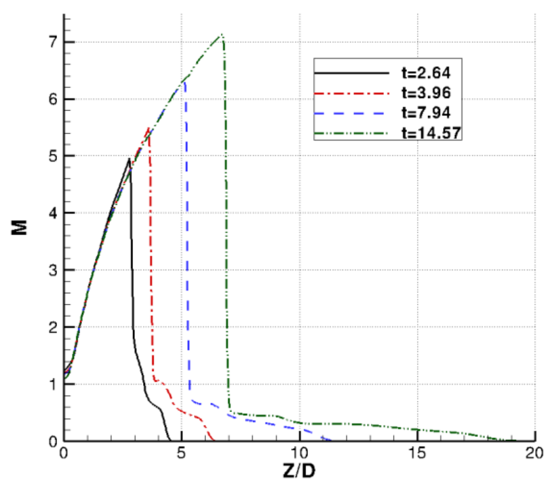


Figure (5)- Mach number along the centerline for pressure of 10MPa at four non-dimensional times.
Left: results of [4]
Right: Abel-Noble results of our code

Hydrogen in Air

For our application of interest, hydrogen is released into air. Beattie-Bridgeman shows stability problems in this case and since it showed no advantage over Abel-Noble for the hydrogen in hydrogen scenario, only Abel-Noble is applied to simulate the release of hydrogen in air. A transport equation is solved to find the concentration of hydrogen-air mixture. Molecular mass of air is almost 29 while it is almost 2 for hydrogen. Therefore for equal pressure and temperature, density of air is higher than hydrogen. At the same time of release, Mach disk is stronger for hydrogen in hydrogen release. Also the flow advances faster in this case. In figure (6), Mach number along the centerline is given for hydrogen in air and hydrogen in hydrogen release. The tank pressure is 70MPa and the time is 70 micro seconds.

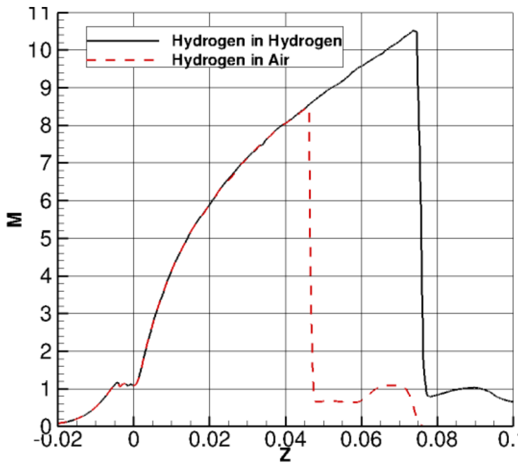


Figure (6)- Mach number along the centerline for pressure of 70MPa at time of 70 micro seconds (hydrogen in hydrogen and hydrogen in air)

In figure (7), for the case of hydrogen in air, concentration and Mach number contours are given together for the pressure of 70MPa at t=70 micro seconds. Different features of the flow are shown in the figure. The lead shock is a weak shock happening ahead of the contact surface. This shock diffuses in the air very fast. Comparison between concentration and Mach number contours shows the Mach disk takes place in the area of no air.

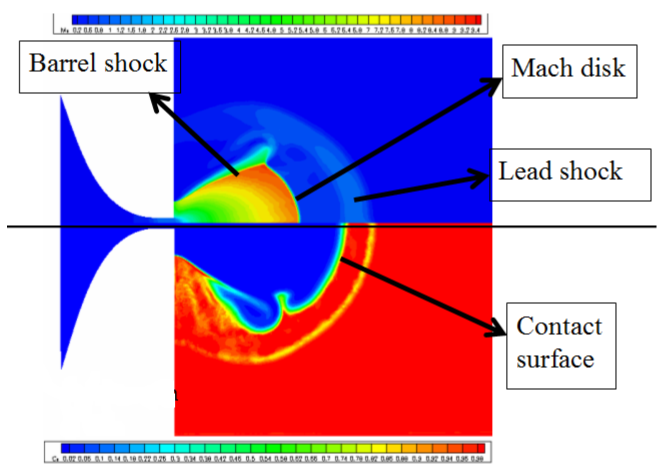


Figure (7)- Mach contours (upper half) and concentration contours (lower half) for pressure of 70MPa at time of 70 micro seconds

In figure (8), Mach number along the centerline is given for ideal gas and Abel-Noble real gas for pressure of 70MPa at t=70 micro seconds. Mach disk is stronger and faster in the case of real gas. Although the Mach disk location is only almost 2mm more for the real gas, it is expected to be more in longer times.

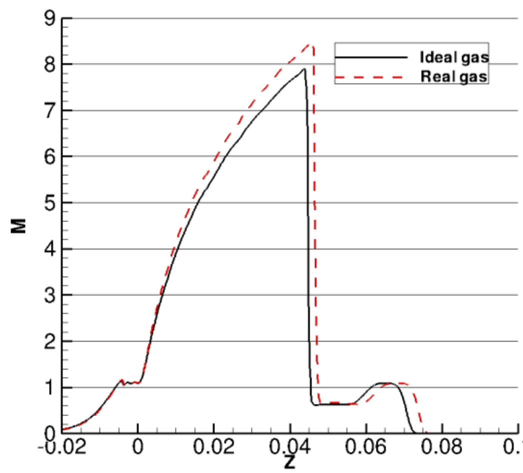


Figure (8)- Mach number along the centerline for pressure of 70MPa at time of 70 micro seconds (ideal gas and Abel-Noble real gas)

CONCLUSION AND FUTURE WORK

An in-house code is developed to simulate the release of high pressure hydrogen into air at ambient condition. High pressure hydrogen deviates from ideal gas law. Two scenarios of hydrogen in hydrogen and hydrogen in air release are discussed. Two real gas equation of state; Beattie-Bridgeman and Abel-Noble are applied for the case of hydrogen in hydrogen release. Beattie-Bridgeman equation shows stability problems in case of hydrogen in air release, therefore only Abel-Noble is applied for the case of hydrogen release in air. Results show that the difference between ideal gas and real gas is not negligible. A very strong Mach disk is generated after release and changes the high supersonic flow to subsonic. The Mach disk takes place in the area of no air. Besides the Mach disk, a very weak shock happens ahead of the contact surface. This shock diffuses into air very fast. This fast changing flow demands for a very small mesh to be well captured. Parallel processing is used to overcome memory problems and to decrease the solution time. In the future work, viscous terms and a turbulence model, large eddy simulation, will be added to the code.

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REFERENCES

1. A.G. Venetsanos, T. Huld, P. Adams, and J.G. Bartzis, Source, dispesion and combustion modeling of an accidental release of hydrogen in an urban environment, Journal of Hazardous Material, A105, 1-25, 2003.
2. W.S Young, Derivation of the free-jet Mach-disk location using the entropy-balance principle, Physics of Fluids, vol. 18, p. 1421-1425, Nov. 1975.

3. L. C. Shirvill, P. Roberts, C. J. Butler, T. A. Roberts, M. Royle, Characterisation of the hazards from jet releases of hydrogen, Proceedings of International Conference on Hydrogen Safety, paper 120005, Pisa, Italy, September 8-10 2005.
4. G. Pedro, F. Peneau, P. Oshkai, and N. Djilali, Computational Analysis of Transient Gas Release from a High Pressure Vessel, Conference CFD, Kingston, Canada, 2006
5. R.W. Schefer, W.G. Houf, T. C. Williams, B. Bourne, J. Colton, Characterization of high-pressure, underexpanded hydrogen-jet flames, International Journal of Hydrogen Energy 32 (2007) 2081 – 2093
6. K. Mohamed, and M. Paraschivoiu, Real gas simulation of hydrogen release from a high-pressure chamber, International journal of hydrogen energy, vol. 30, no8, pp. 903-912, 2005.
7. Z. Cheng, V. Agranat, A. V. Tchouvelev , W. Houf, S. V. Zhubrin, PRD hydrogen release and dispersion; a comparison of CFD results obtained from using ideal and real gas law properties, First international conference on hydrogen safety, Pisa, Italy September 8–10, 2005,
8. M. R. Kameshki, Simulation of Hydrogen Jet Exiting a High Pressure Reservoir, M. Sc. Thesis, Concordia University, 2007.