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**RESEARCH ARTICLE**

# SIMULATION OF HIGH PRESSURE HYDROGEN RELEASE IN AIR

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**ABSTRACT**

Hydrogen have the potential that can replace fossil fuels which is the primary source of environmental pollution. Hydrogen should be stored in high pressure reservoirs for any practical purpose. In this work hydrogen leak from a high pressure vessel by means of a 2mm tube length and 4.8mm diameter of pipe in atmospheric air is simulated using FLUENT 13. A strong shock wave is formed during the flow of high pressure hydrogen in a tube filled with atmospheric air which leads to heating of hydrogen behind the shock wave. This is mainly because of compression effect and which leads to an auto ignition. The simulated results are not in agreement with the results obtained by Yamada Eisuke *et al*. (2010).



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## INTRODUCTION

Energy is one of the most important sources in human development, an effort to meet the demands of a world in energy and however hydrogen is widely concern as the next generation energy fuel, one of the most important characteristics of hydrogen is low density when compared to other gas. It's necessary to compress hydrogen for storage in high pressure vessel for any practical application and it is a very clean energy source with very low amount emission. Hydrogen is a widespread energy source; this could help to address the concern about energy security, global climate change, and air quality. Fuel cells is an important enabling technology for the Hydrogen Future and have the potential to revolutionize the way we power our nation, offering cleaner, more-efficient alternatives to the combustion of gasoline and other fossil fuels. When the high hydrogen gas enters in to an atmospheric air, soon it leads to auto ignition. because hydrogen is more reactive and it prefers to join the molecular pair of $H_2$ and when it is mixed in sufficient quantity of oxidant air, $O_2$ becomes a combustible mixture. At $25^0$c of atmospheric density of air is 1.225 kg $m^{-3}$ while hydrogen is 0.0838 kg $m^{-3}$, making it 14.6 times lighter than air so hydrogen gas is dissipate quickly which leads to diffusion ignition, sudden adiabatic compression, hot surface ignition. High pressure Hydrogen leak might leads to an accidental explosion, when Hydrogen is leaking into atmospheric air at high pressure, soon its produced an strong shock wave and behind the shock wave the atmosphere air is heats up to maximum 2000K. This heat is enough source for auto ignition. Air behind the leading of shock is heated and mixes with hydrogen in the contact region, to form a significant amount of flammable mixture due to enhanced turbulent mixing. In this work, Computational Fluid Dynamics (CFD) based numerical simulations have been performed to study the shockwave structure and finding the physical change when high pressure hydrogen is released in atmospheric air.

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**Problem description and numerical setup:** Investigation on the behavior of high pressure hydrogen leakage in atmospheric air. Governing equation namely the conservation of mass, momentum, energy and the species transport equations are solved using ANSYS FLUENT 13.0. Simulations are performed by solving the following full unsteady compressible Navier-Stokes equation of a chemically non reactive multi-component mixture of ideal gases; schematic diagram of the computational domain is rectangle with dimensions of 60mm in the axial direction and 40mm in the radial direction. Radius of the tube is assumed to 2.4mm, the flow field is analyzed by both 2D axis symmetric and 3D geometry, and also tried both structured mesh and unstructured mesh .There are six boundaries for the present calculation an inlet boundary, two wall boundaries, symmetry condition & outlet condition. The inlet pressure and temperature are 21.1 Mpa and 507K, which are estimated by the chocked condition. The reservoir pressure corresponding to 40.0Mpa (Yamada, 2011).

In the schematic diagram of the computational domain is a rectangle with dimensions increased by 600mm in the axial direction and increased by 400mm in the radial direction. the radius of the tube is assumed to be 2.4mm, the flow field is analyzed both 2D axis symmetric and 3D geometry ,both structured mesh and unstructured mesh were used.

**Grid generation:** ICEMCFD is used to generate the mesh required for the numerical simulation, Structured mesh was developed to lead very efficient numerical method by using multi-block O-grids have been generated and studied. O-Grid tool used to make it easy to accomplish even for complicated geometry

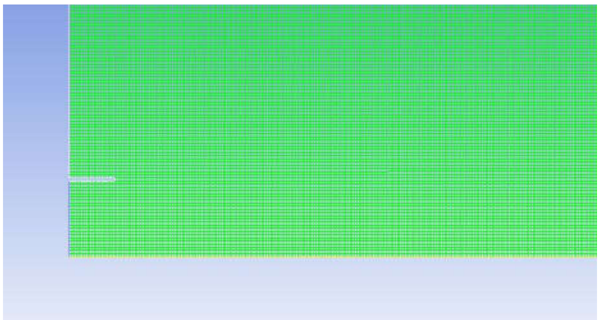


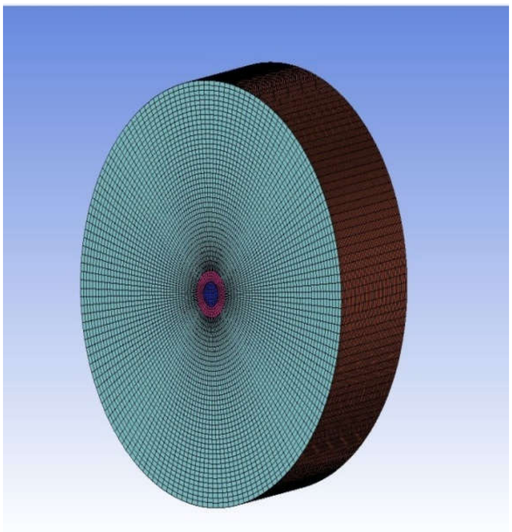
**Fig 2D meshed computational domain**

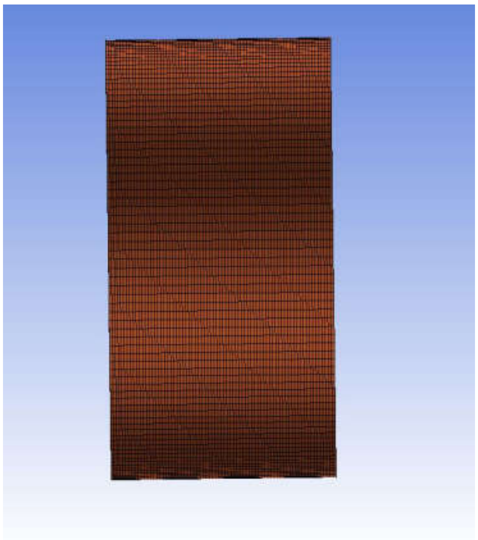
### 2D Structured Mesh

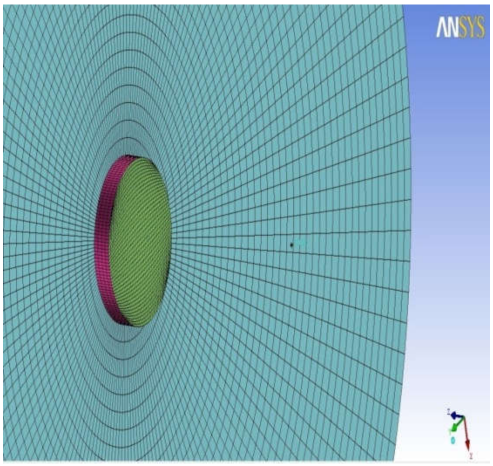
structured mesh is comprised of hex elements that flow a uniform pattern structured grid have been generated and studied ,the problem is associated with a moving shock wave, the uniform grid size is taken to be very small size dy = dx = 100 µm and total grid is around 2.5 million grid to resolve the shock structure . It is necessary and reasonable to use such small grid size to simulate high temperature hydrogen combustion.

### 3D Structured Mesh

3D grid generation have been generated and studied by using multi block "O" grid method for reality of an geometry the uniform grid size is taken to be very small size dy = dx = 100 µm and total grid is around 4 million grid generated to resolve the shock structure .







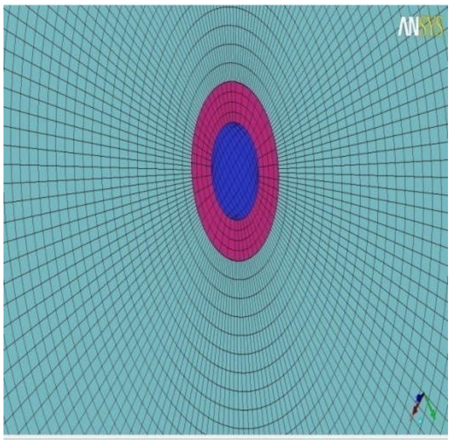


**Fig The meshed computational domain**

### 2D Unstrucured Mesh

2D unstructured mesh is generated with more fine in the inlet region and more coarse in outlet region ,grid generated by un uniform grid size and total grid is around 3 million to resolve the shock structure . In this geometry outer domain value is increased by 400 in Y-axis and 600 inX-axis.

### 3D Unstructured Mesh

3D unstructured mesh also generated by more fine in the inlet region and more coarse in outlet region , grid size is generated by non uniform method and total grid is around 4 million grid.

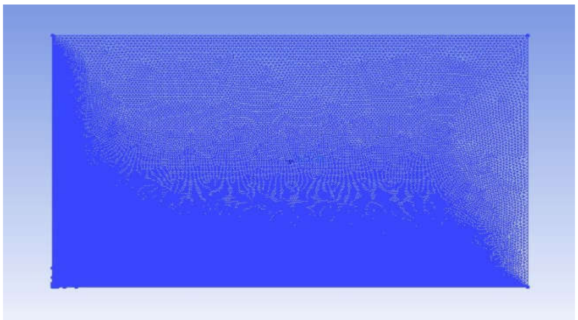


**Fig 2D. Non uniform meshed computational domain**

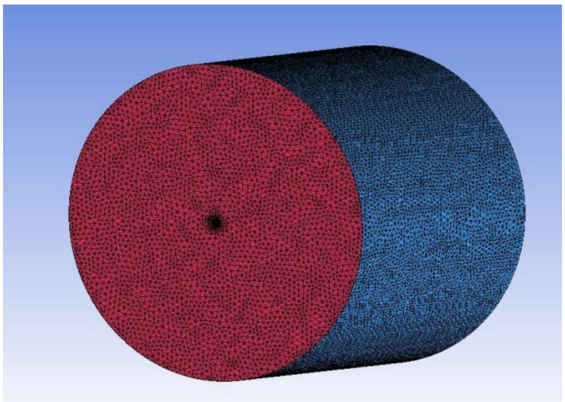


**Fig 3D. Non uniform meshed computational domain**

**Procedure for creating 3d structured mesh in icemcfd**

**Step 1:** Create geometry by using an explicit coordinate tool to create point
**Step 2:** Create line from joining the point
**Step 3:** Create surface by using surface tool
**Step 4:** Create material point by selecting two 2 centric points
**Step 5:** Create 3D blocking - initialize blocks , entities click icon to right, red message appears, select all geometry on screen using marquee select ,middle click to save selection, right click to de-select mode.
**Step 6:** Split blocking using 'O' grid block
**Step 7:** Blocking association with wanted edges
**Step 8:** Move Vertices with automatic blocking
**Step 9:** Mesh Edges and give Number of Nodes
**Step 10:** Select pre-mesh tool from the side bar tree
**Step 11:** Right click the pre-mesh, select tool convert in to unstructured mesh
**Step 12:** Edit mesh, Display Quality (at top)
**Step 13:** check the mesh quality is very good ,since this is a simple structured hex mesh with O-grid
**Step 14:** Edit Mesh, smooth hexahedral mesh quality
**Step 15:** Hide the mesh, select the lower bars in the histogram. Bad quality mesh areas appear
**Step 12:** Save as Ansys Fluent v6 file
**Step 13:** Create parts and create boundary condition
**Step 14:** Final convert fluent mesh file

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**Step 1:** Create geometry by using an explicit coordinate tool to create point
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**Step 4:** Create material point by selecting two 2 centroid points
**Step 5:** Create 2 D blocking
**Step 6:** Split blocking using 'H' grid block
**Step 7:** Blocking association with wanted edges
**Step 8:** Move Vertices with automatic blocking
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## RESULT AND DISCUSSION

The simulation results are presented for varying combinations of boundary condition for 2mm tube length case and Standard k-ε turbulence model is used, two additional transport equation are solved for the two turbulence quantities. the turbulent kinetic energy k and the energy dissipation rate ε.

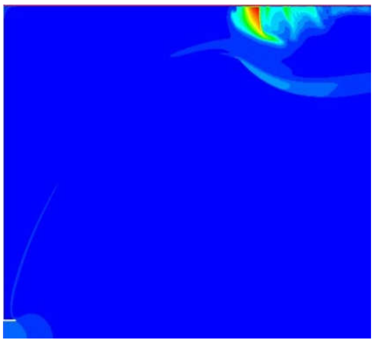
**Boundary condition**

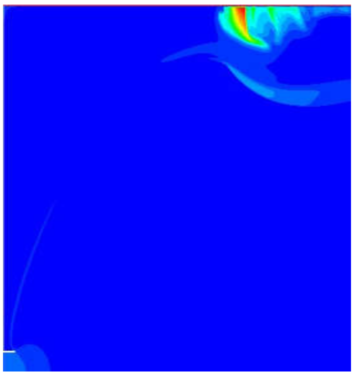
Solver- Density based solver
Model - Energy
Viscous model - Standard k-e
- Standard wall function
Species - Species transport - Hydrogen-air
Reaction -Non reactive flow

**Hydrogen Properties**

Density - Ideal gas
Cp (Specific Heat )- mixing law
Inlet - gauge total pressure (4e+07)Pascal
Supersonic /initial gauge pressure (2.21e+07)pascal
- Temperature - 507 k
- Hydrogen mass fraction 1
Turbulent specific method - Intensity & hydraulic diameter
- Turbulent intensity - 5%
- Hydraulic diameter - 0.0048m
Inner surrounding wall - Adiabatic Wall condition or no slip wall condition
- Temperature - 300k
Outer surrounding wall - Symmetry

**Outlet** - Pressure outlet 101325 Pascal
- Back flow temperature 300K
- Species oxygen mass fraction 0.23





**Temperature Contour**
Time -0.83 µs

**Boundary condition**

Solver- Density based
Model - Energy
Viscous model - standard k-e
- standard wall function
Species - species transport -- Hydrogen-air
Reaction - non reactive flow

**Hydrogen Properties**

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- Temperature - 300k
Outer surrounding wall - Pressure Outlet 101325
- Back flow temperature 300K
- Species oxygen mass fraction 0.23

**Outlet - Pressure Outlet 101325**

- Back flow temperature 300K
- Species oxygen mass fraction 0.23

**Conclusion**

In this work, the CFD based simulations have been applied to analyze the non-reactive characteristics of high pressure hydrogen leak in atmospheric air. The CFD simulations, taking in to account of fluid dynamics, shockwave structure and detailed of auto ignition mechanics, are investigated the effects by various boundary conditions. The boundary conditions were referenced from a Yamada Eisuke *et al.* (2010) work and variations were found after simulating using the solver FLUENT. The results show that the values obtained from journal Yamada Eisuke *et al.* (2010) work are a few order of magnitudes lesser. The difference in the results were mainly because of difference in computation error. Hence the feasibility of the simulations with the result is very less.

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