Simulation of Hydrogen Release from Reservoirs with Irregular and Variable Openings

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Challenges with CFD

- What is the cost of CFD?
  - Create the mesh
  - Solve the problem
- Solve the cost of solving the problem
  - Develop specific CFD for Hydrogen safety
- Accuracy of CFD?
  - Development accuracy
  - Research accuracy
- Improving Research accuracy
  - More accurate geometry
  - Ignition model

Improving Research Accuracy

Developing an in-house code to numerically (by computational fluid dynamics) solve the flow after sudden release of Hydrogen from a high pressure tank into air including features as:

- ✓ Real Gas Model
  - ➢ Abel-Noble equation of state
- ✓ Two Species (Hydrogen and Air)
  - ➢ Transport equation to find out the concentration
- ✓ Irregular and Expanding Reservoir Outlet
  - ➢ Moving mesh feature and spring-based method

Numerical Challenges

- High gradients caused by high pressure ratio
  - An accurate solver and a good quality mesh are required to overcome stability problems
- High number of nodes and elements are needed to capture all the features of the flow
  - Parallel processing is used to overcome memory problems and to decrease the solution time
- High pressure Hydrogen deviates from ideal gas law
  - Real gas equation is applied as the equation of state

Moving Mesh Equations

- Euler equation is changed according to the moving mesh velocity

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

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

Transport Equation

- A transport equation is solved to find the concentration of hydrogen and air

$$\frac{\partial(\rho c)}{\partial t}+\frac{\partial(\rho c(u_x-w_x))}{\partial x}+\frac{\partial(\rho c(u_y-w_y))}{\partial y}+\frac{\partial(\rho c(u_z-w_z))}{\partial z}=0$$

- c gives the concentration and varies from 0 to 1.
- c equals 0 where the concentration of Hydrogen is 100 percent

Discretization

- The equation is discretized as follows:

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

- The eigenvalues are as follows:

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

Spring-based method

- 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:

$$F = \sum k_i \ (\Delta x_i - \Delta x) \qquad k_i = \frac{1}{Edge \ \ Length}$$

- The force on each node should be zero at equilibrium

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

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

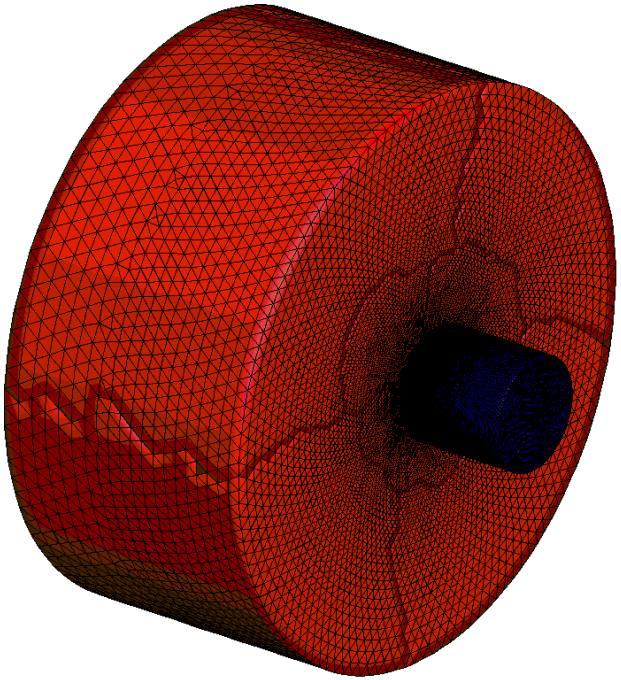
$$x^{n+1} = x^n + \Delta x$$

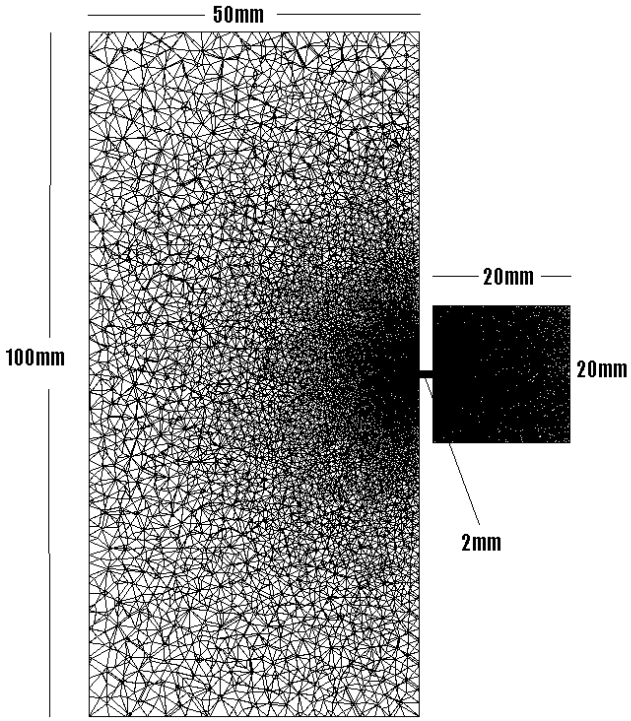
Parallel Processing

- Message passing interface
- Processors communicate with one another by sending and receiving messages
- Concordia super computer Cirrus
- Up to 64 CPUs
- Metis software is used to break the mesh into similar parts (node-based)
- An in-house code is generating the mesh partition files for the solver

Geometry and Mesh

- Three meshes of 0.8, 2 and 3 million nodes are tested
- Same geometry for all meshes
- Three- and two- dimensional views of 0.8 million node mesh are presented



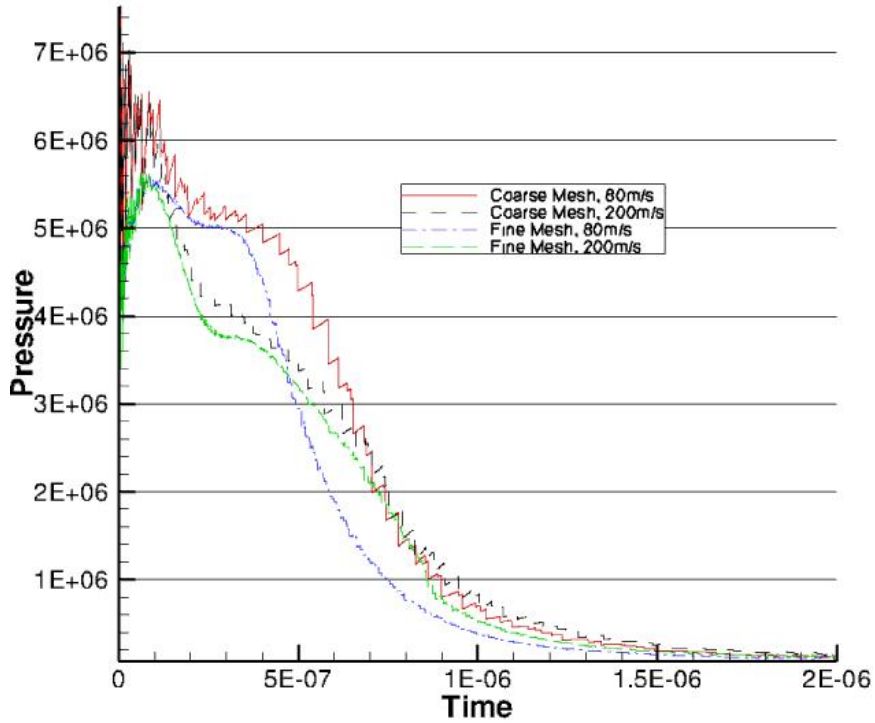


Results

- The tank pressure for all cases is 70 MPa
- The outside has ambient conditions
- The initial temperature is 300 K everywhere
- Three initial release area diameters of 1.0 mm, 1.5 mm and 2.0 mm are tested
- For each case, three opening rates of 80m/s, 200m/s and 500m/s are examined

Mesh Study

➢2 million and 0.8 million node meshes at the opening rates of 80m/s and 200m/s



Mesh Study

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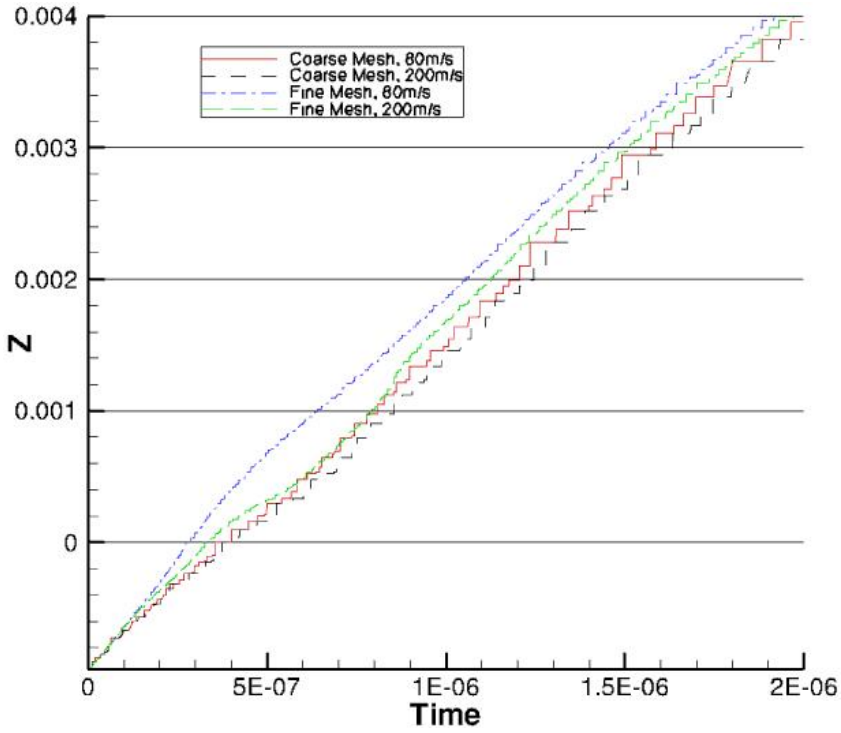
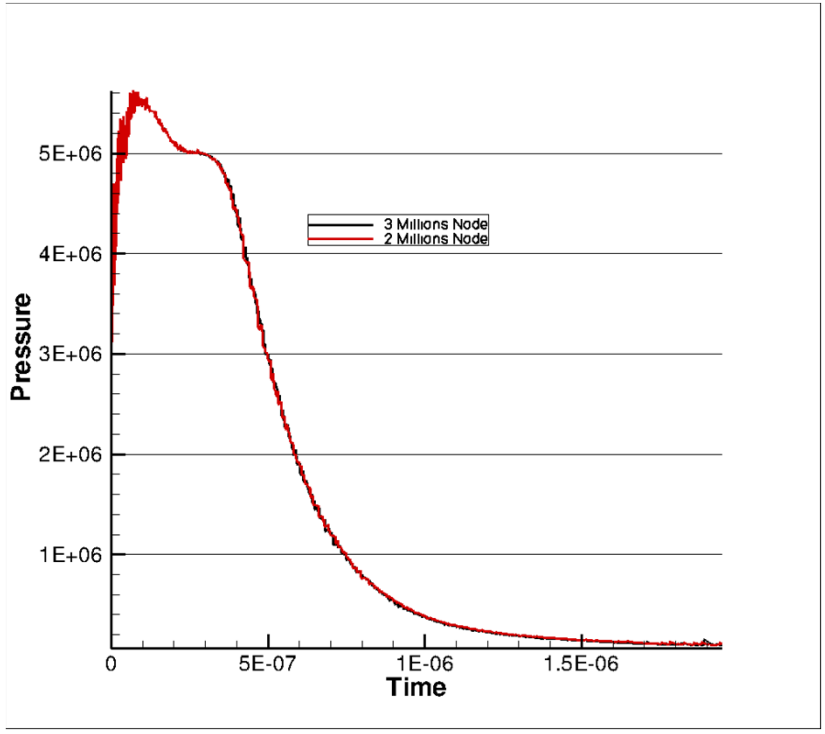


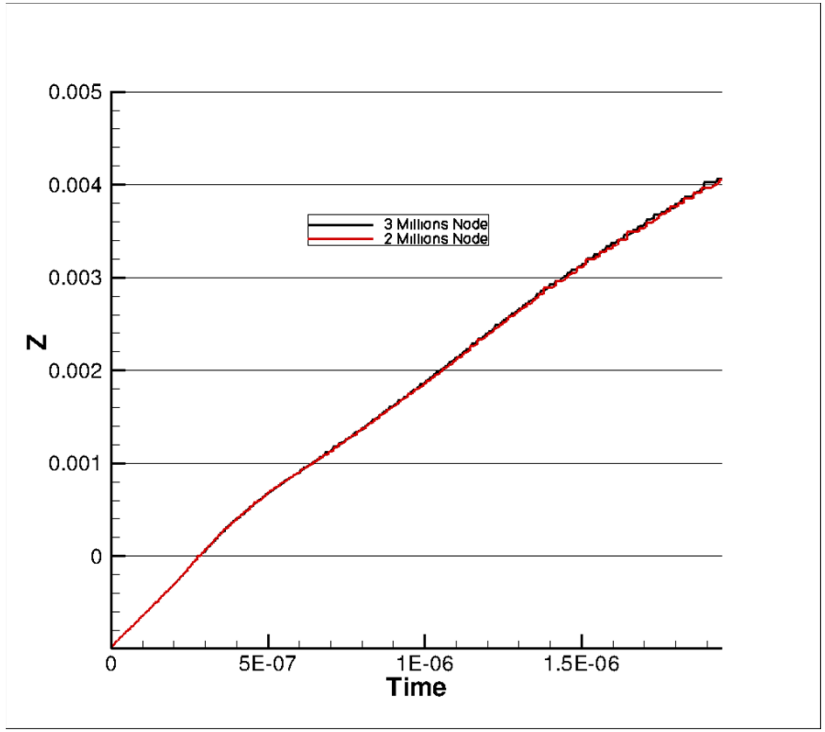
Mesh Study

➢The opening rate of 80m/s



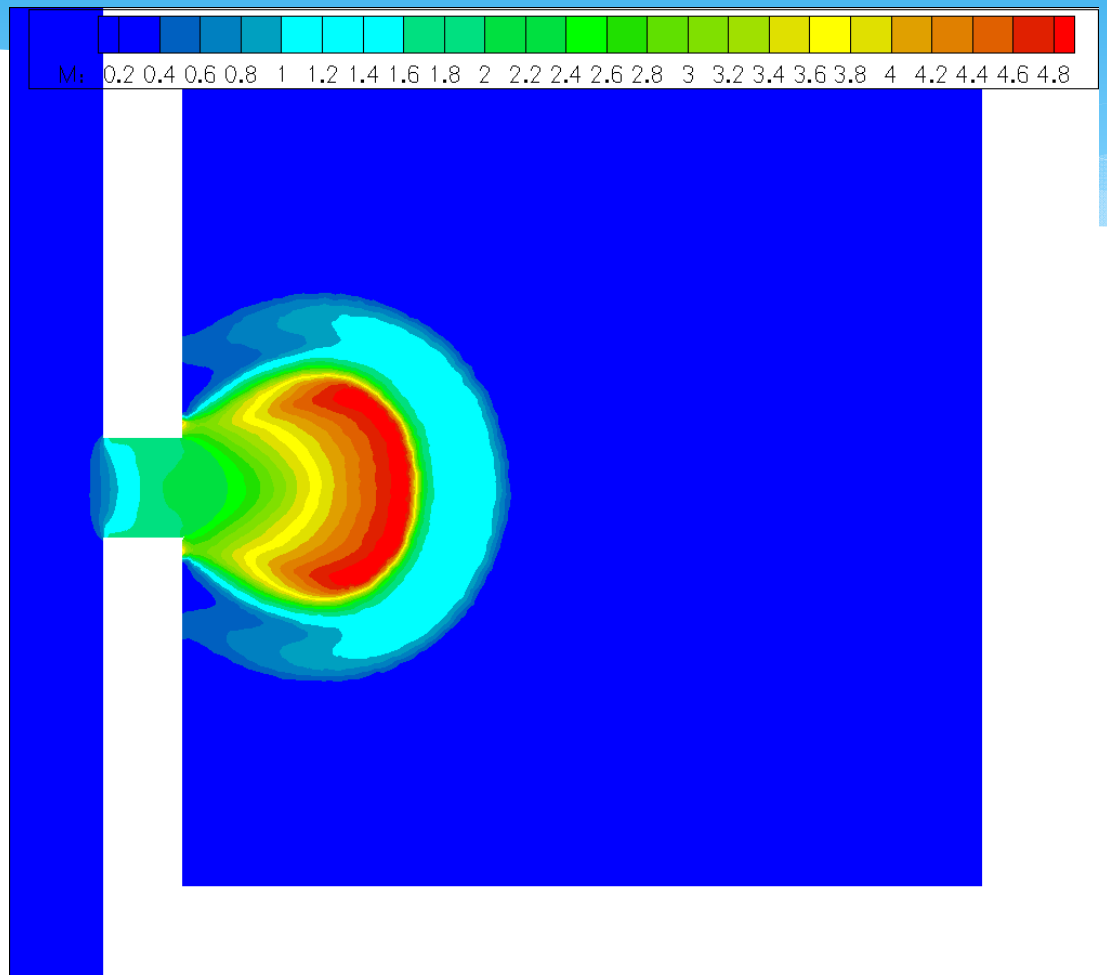
Mesh Study

➢The opening rate of 80m/s



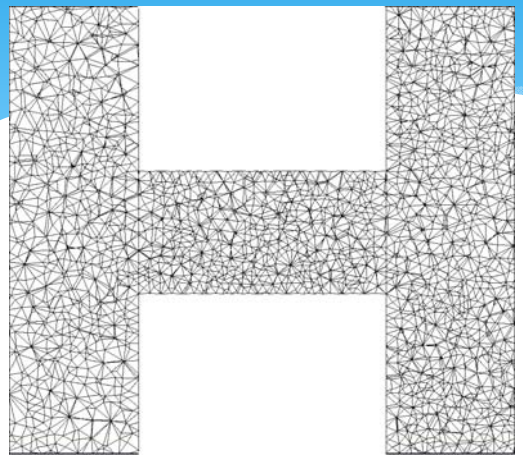
Mach contours for the initial diameter of 1.0mm

- The opening rate of 500m/s after 3.0 micro seconds

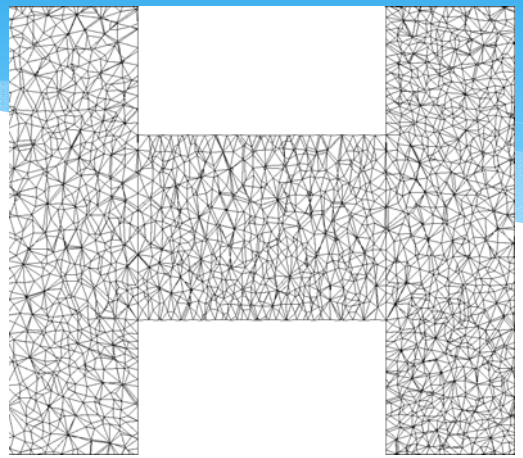


Release area expanding

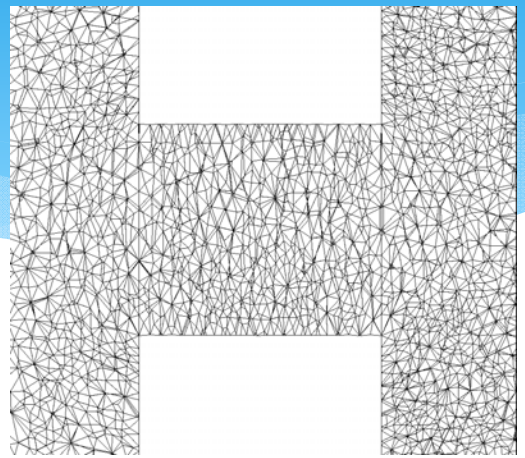
- The initial diameter of 1.0mm at the rate of 500m/s.



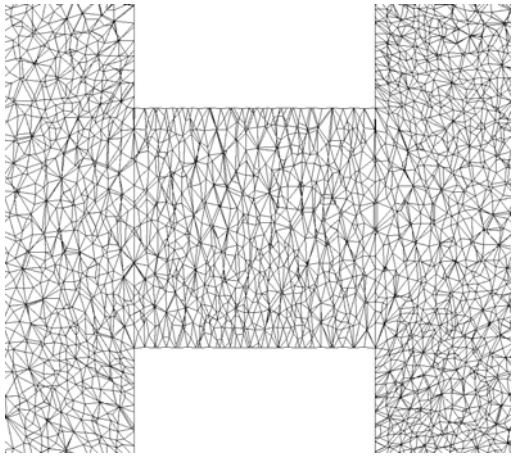
Initial diameter



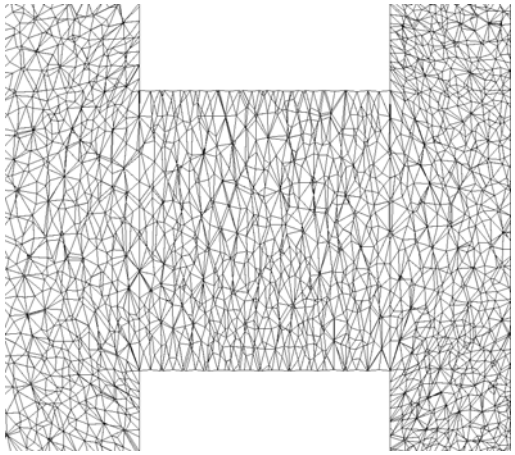
After 1.0 micro seconds



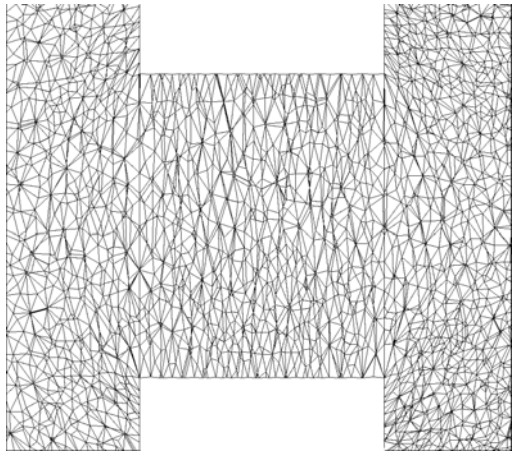
After 1.5 micro seconds



After 2.0 micro seconds



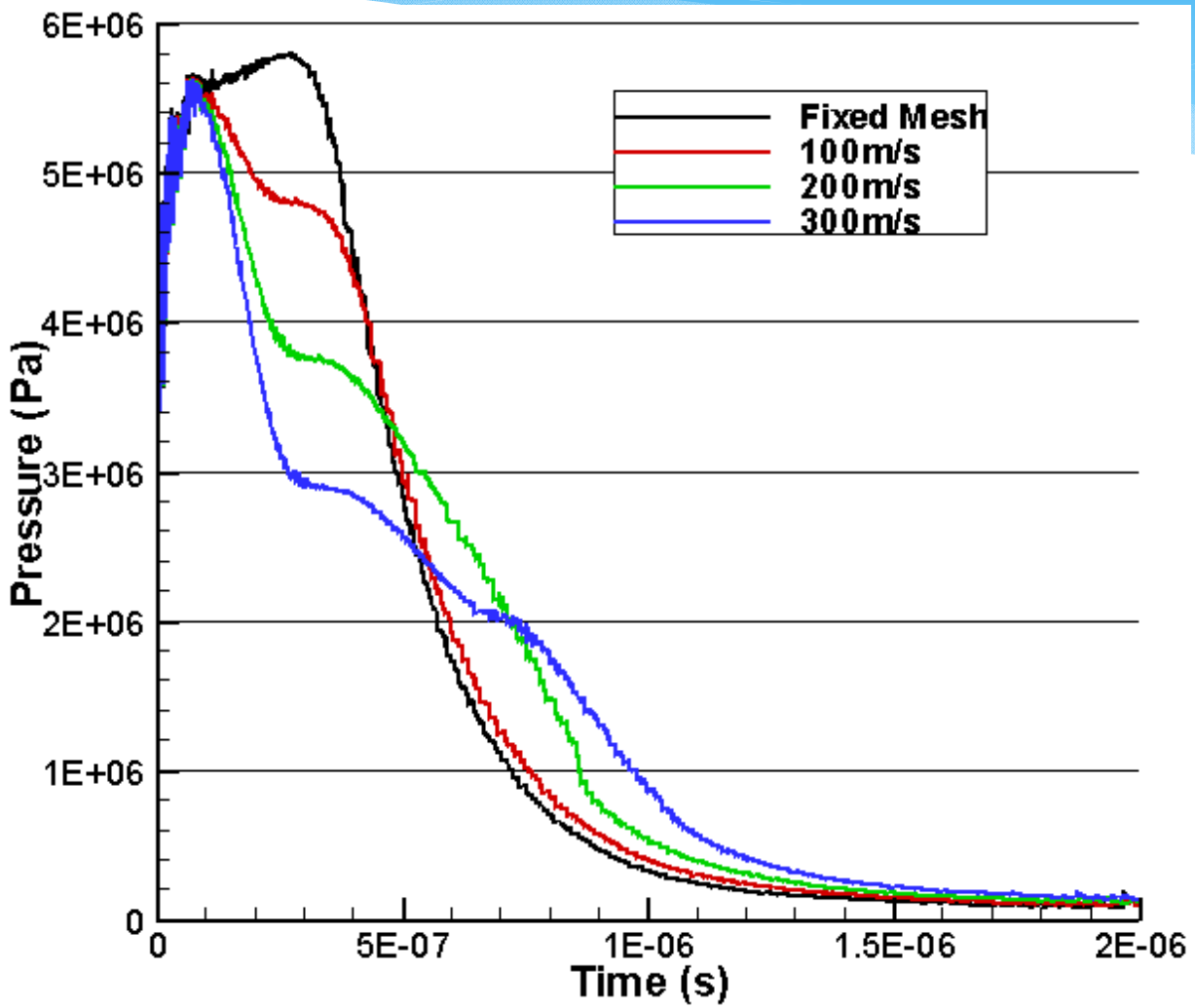
After 2.5 micro seconds



After 3.0 micro seconds

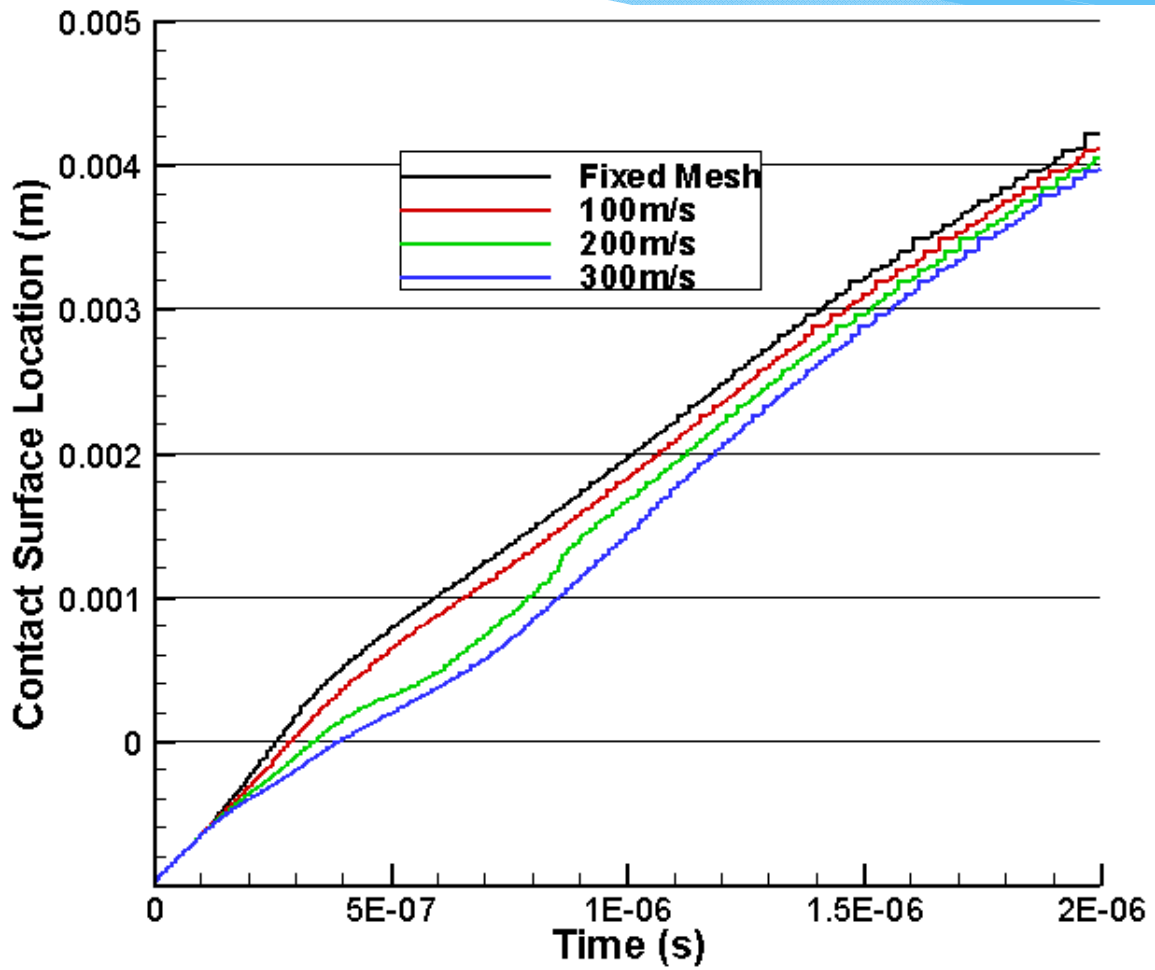
Pressure on the contact surface

- The initial diameter of 1.0mm at different opening rates



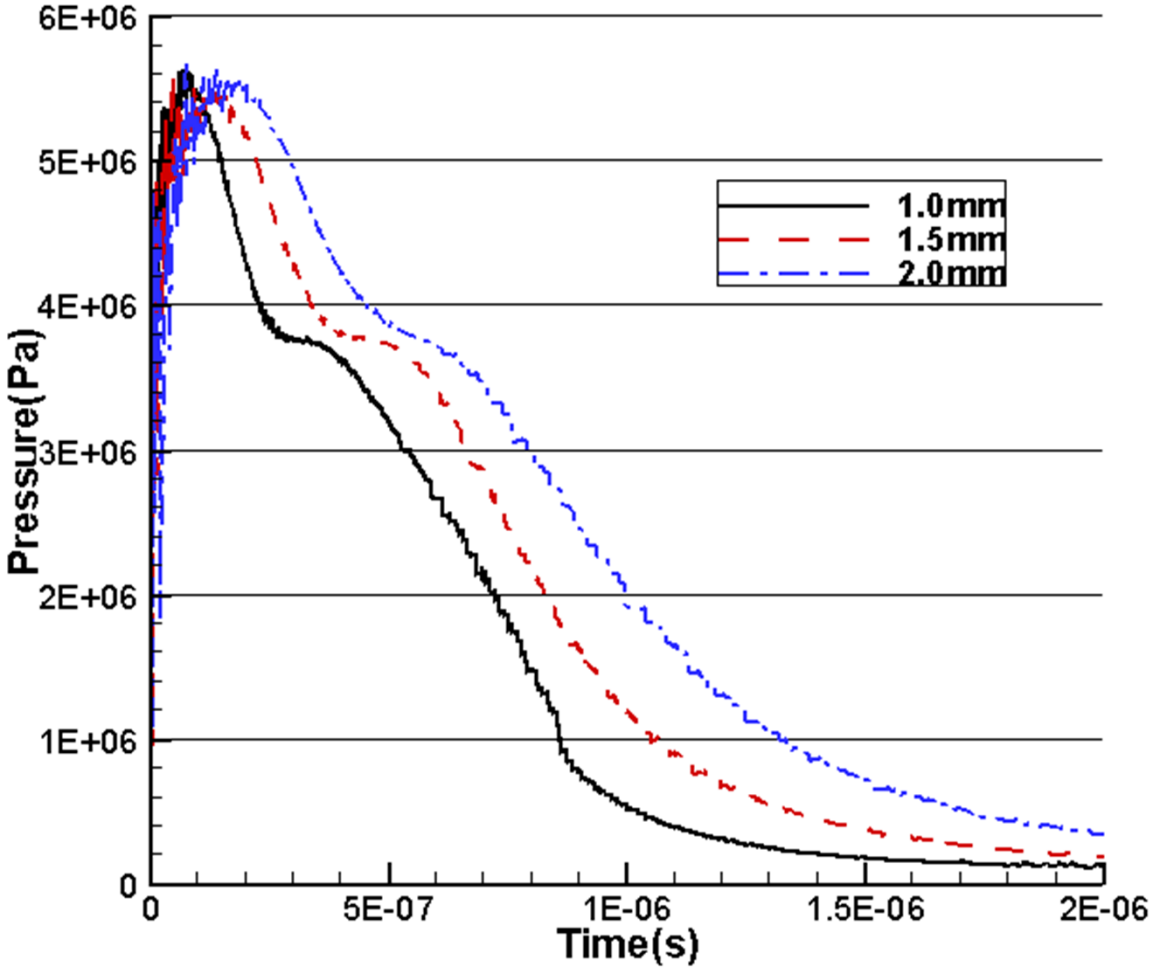
Contact Surface Location

- The initial diameter of 1.0mm at different opening rates



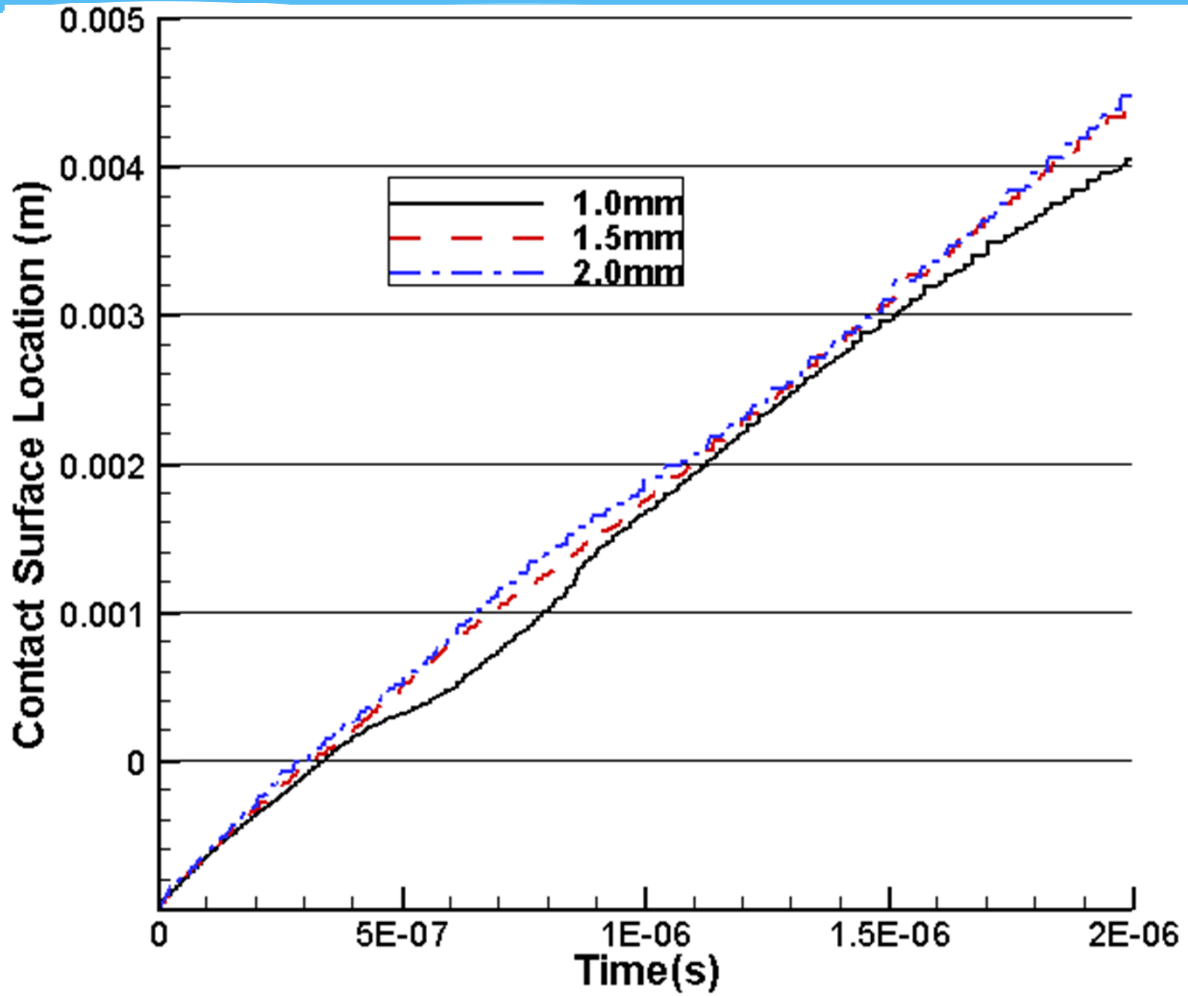
Pressure on the contact surface

- Different initial diameters at the opening rate of 200m/s



Contact Surface Location

- Different initial diameters at the opening rate of 200m/s

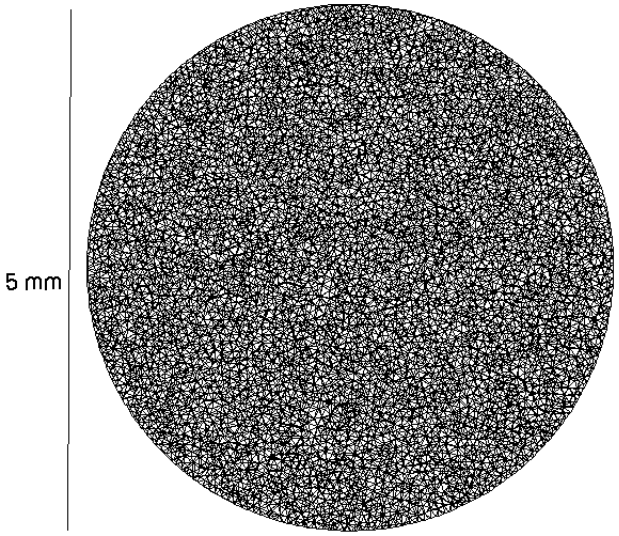


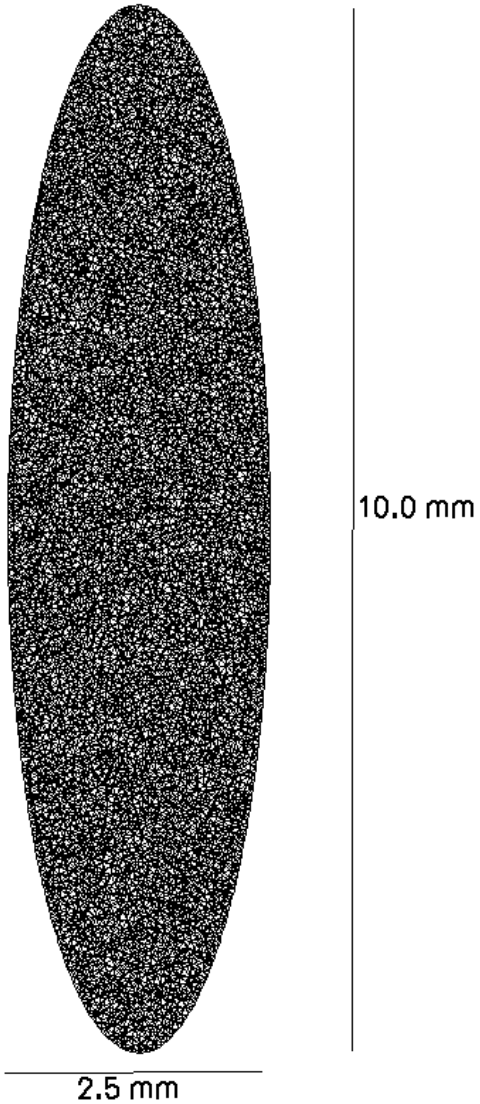
Flow Simulations through elliptical and circular outlets

- The tank pressure for all cases is 70 MPa
- The outside has ambient conditions
- The initial temperature is 300 K everywhere
- Equal section area equivalent to a 5 mm diameter
- Mesh containing 1 million nodes

Mesh of the outlet orifice

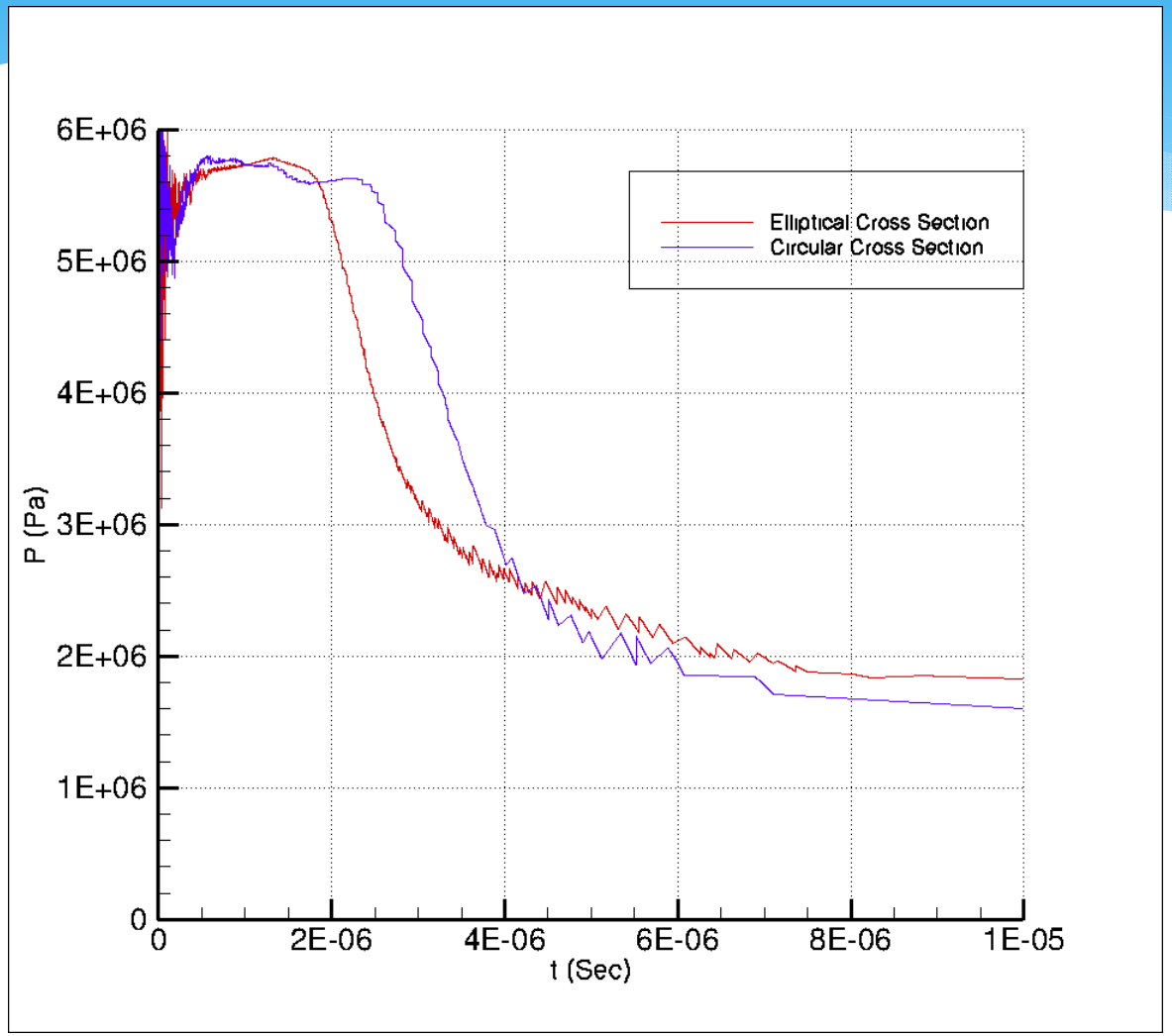
- Equal section area of 19.64 mm^2





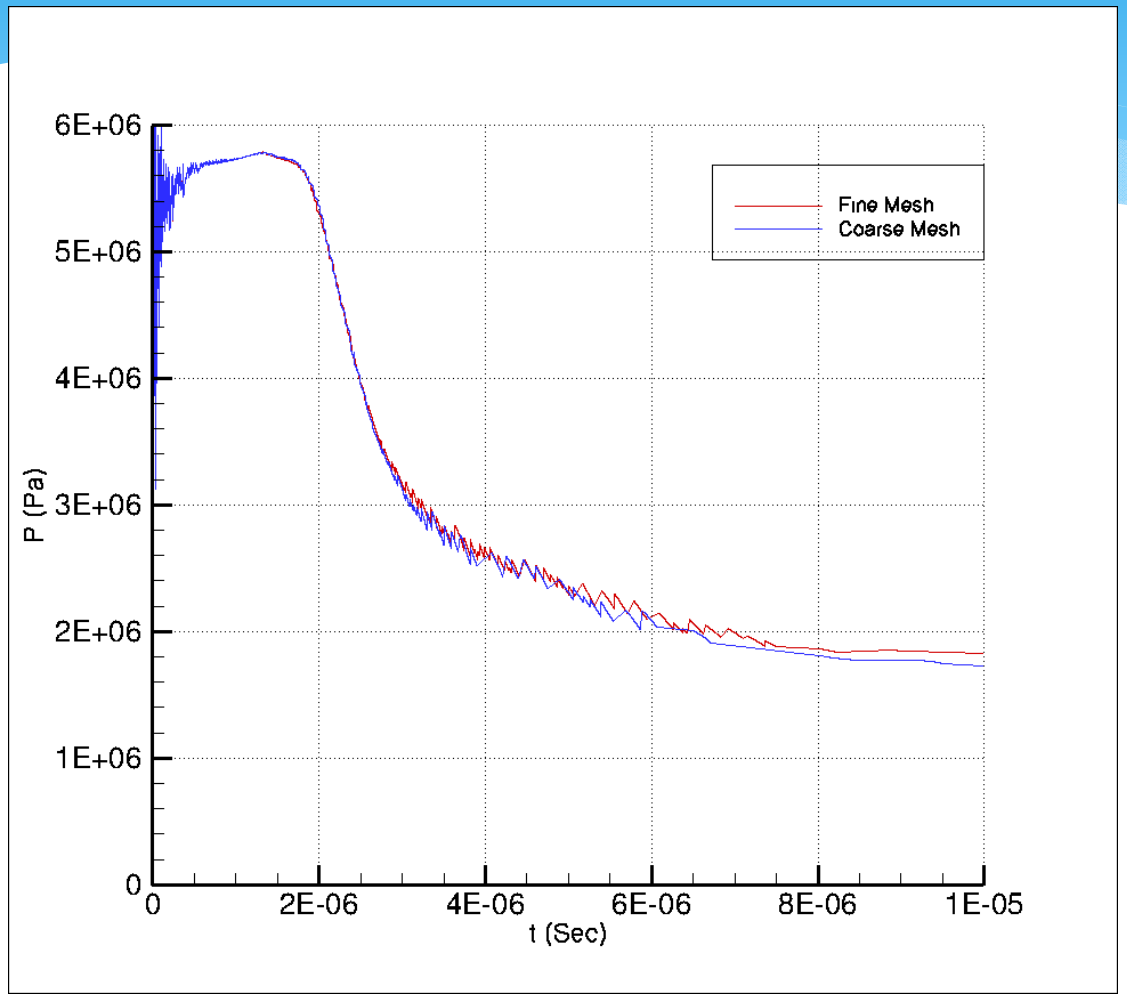
Pressure on the contact surface

- Elliptical and Circular outlet orifice



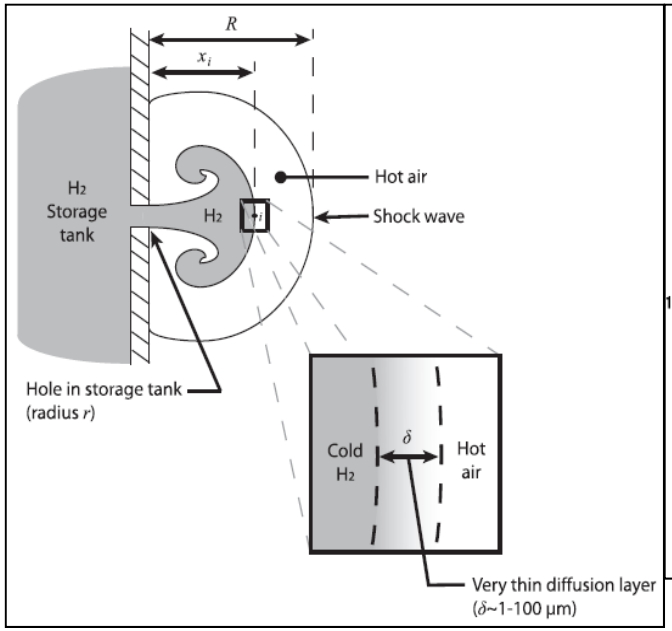
Pressure on the contact surface

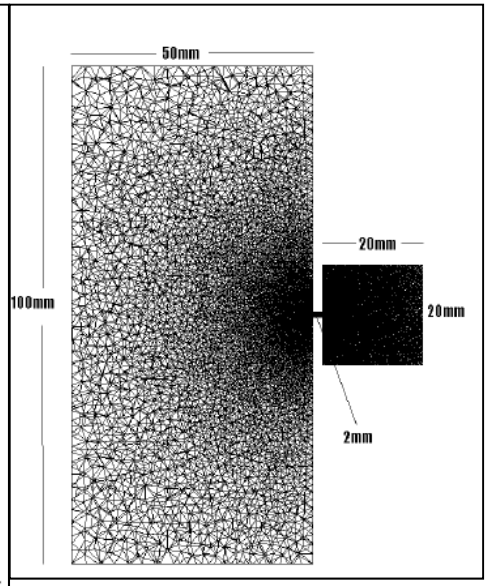
- Elliptical and Circular outlet orifice

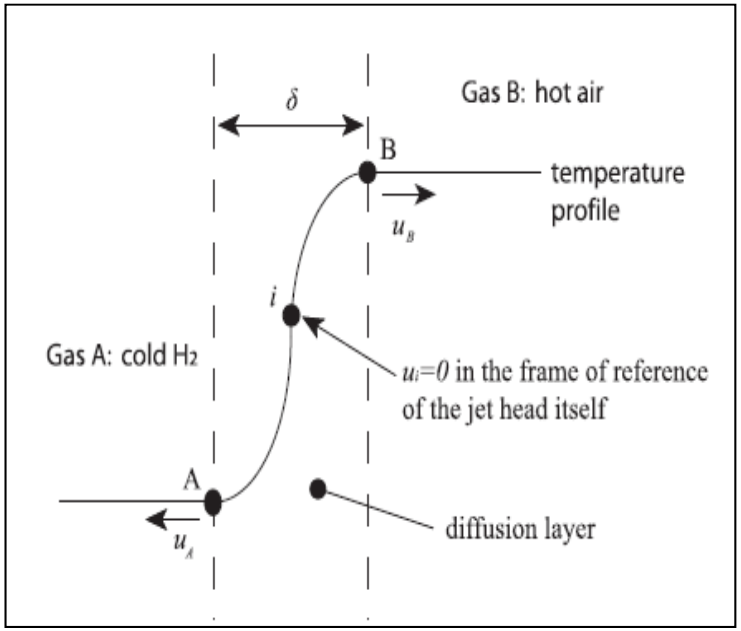


Ignition model from Radulescu

Contact Surface Pressure - Pcontact
Hot Air Temperature - T[High]
Cold H2 Temperature - T[low]
Pressure – Time Derivative – dP/dt

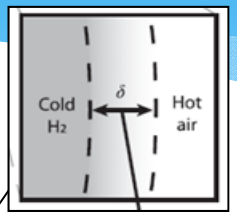






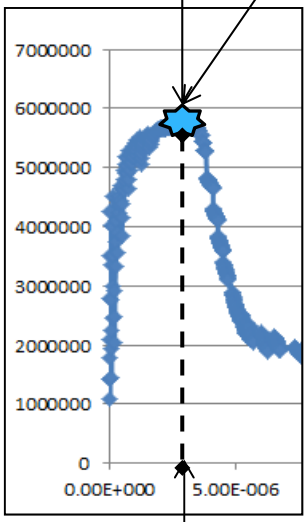
Input Parameters - Pressure Source Term

- T[low] ≈ 250 - 1500 K



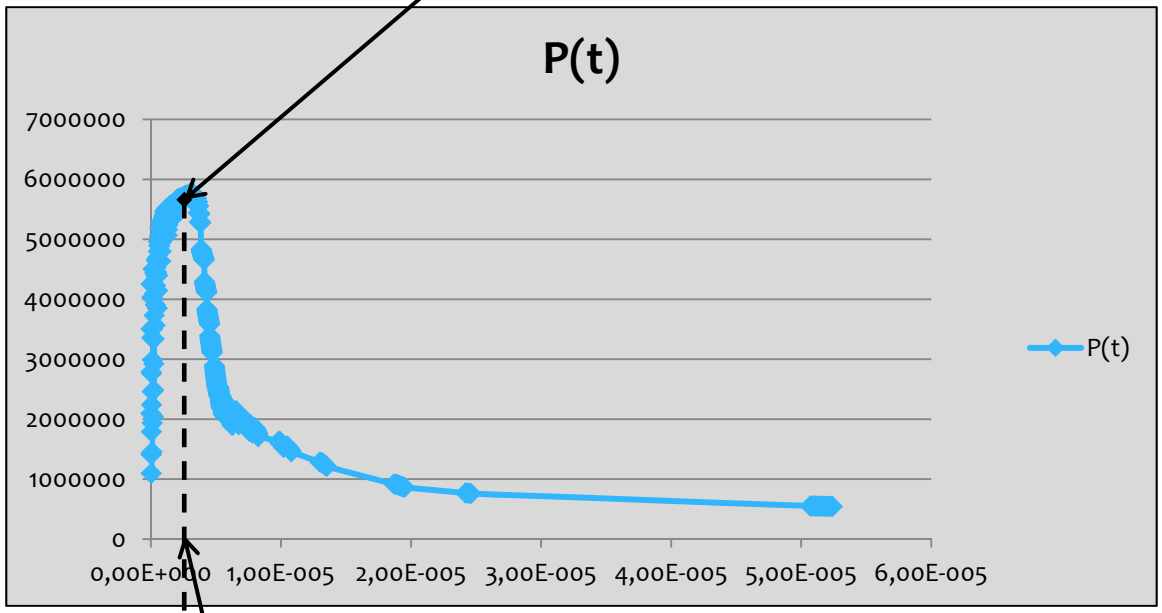
- T[High] ≈ 1250 - 2500 K

- Pcontact ≈ 4.5 – 6 MPA



Start of Decay

Pressure Decay Point



dP/dt =0

Pressure Decay Time

dP/dt is computed

Source Term [dp/dt] - Decay Time – Curve Fit

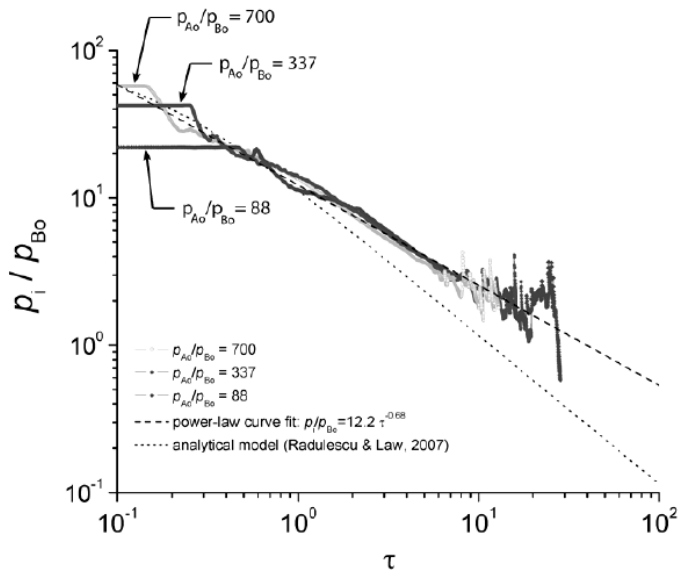
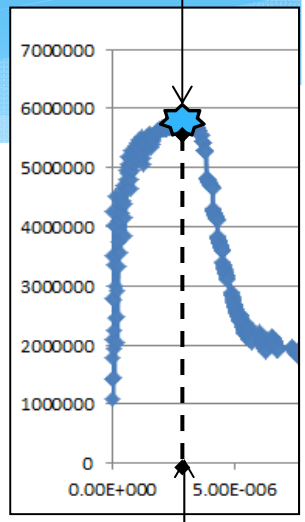


Figure 2.12: Evolution of the contact surface pressure along the jet axis for round jets. Results were obtained numerically for various storage pressure to ambient pressure ratios from Radulescu and Law (2007).

- Pcontact ≈ 4.5 – 6 MPA



Start of Decay

Start of Decay

Directly determined from The P(t) curve

Start of Decay

*Tao_i = pow(((12.2*P1)/(pGas->P)),(1/0.68));*

Pressure-Time Derivative

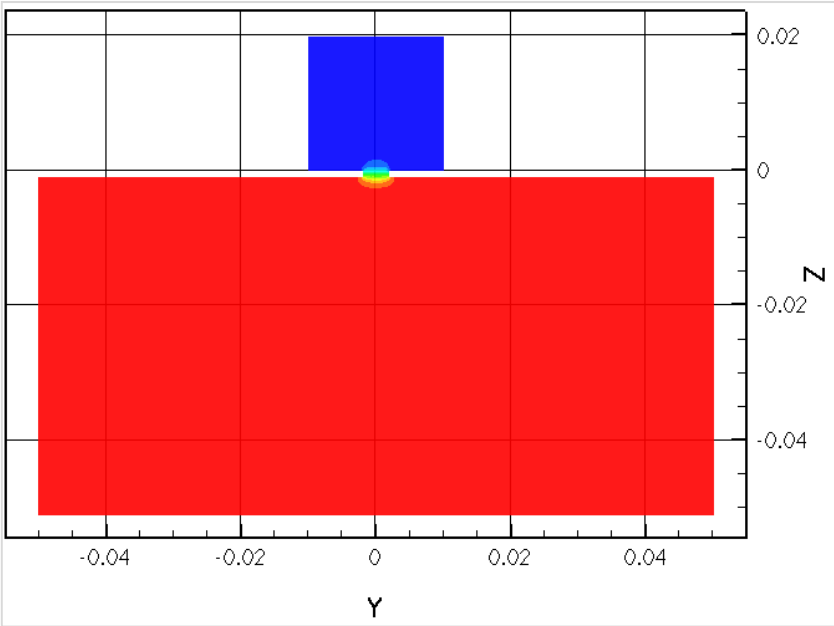
$$\frac{\partial p}{\partial z} = \frac{\partial p_i}{\partial \tau}\frac{\partial \tau}{\partial z} = -8.3 p_{Bo}\tau^{-1.68}\frac{\partial \tau}{\partial z}$$

Pressure-Time Derivative

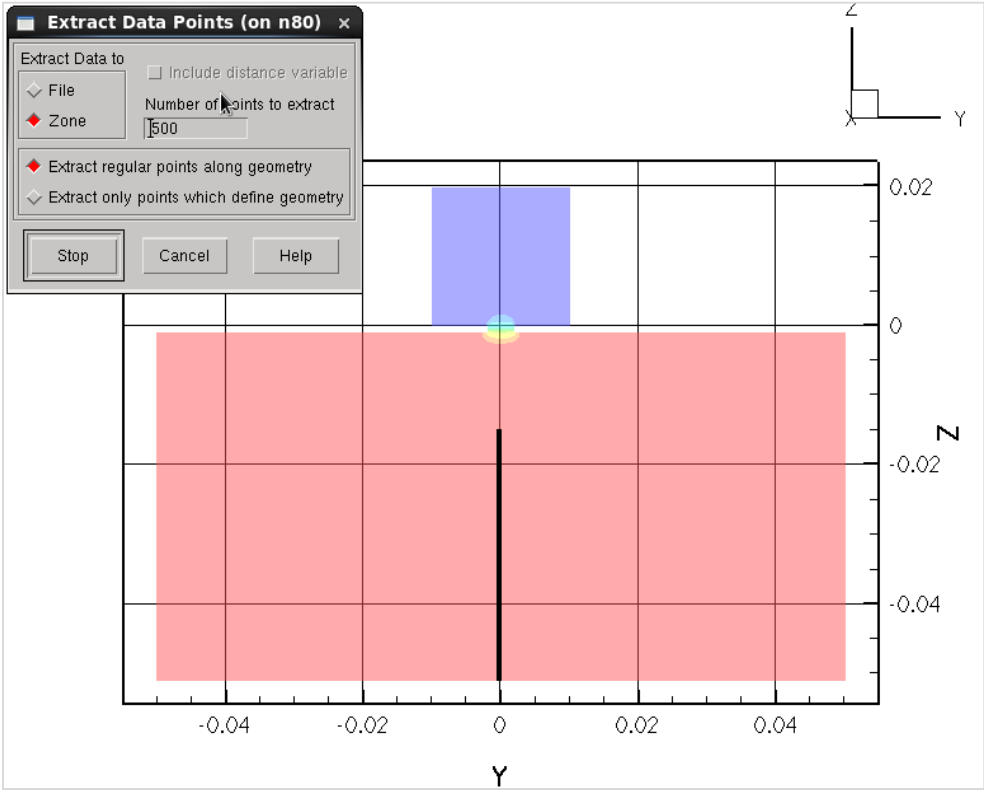
$P(t) = 6E{+}45t^6 - 3E{+}40t^5 + 5E{+}34t^4 - 5E{+}28t^3 + 3E{+}22t^2 - 7E{+}15t + 9E{+}08$

$dP/dt = 6E{+}45t^5 - 1.5E{+}41t^4 - 2E{+}35t^3 + 1.49E{+}29t^2 - 6E{+}22t + 7E{+}15$

Case Study : 4mm Dia – 1mm Length

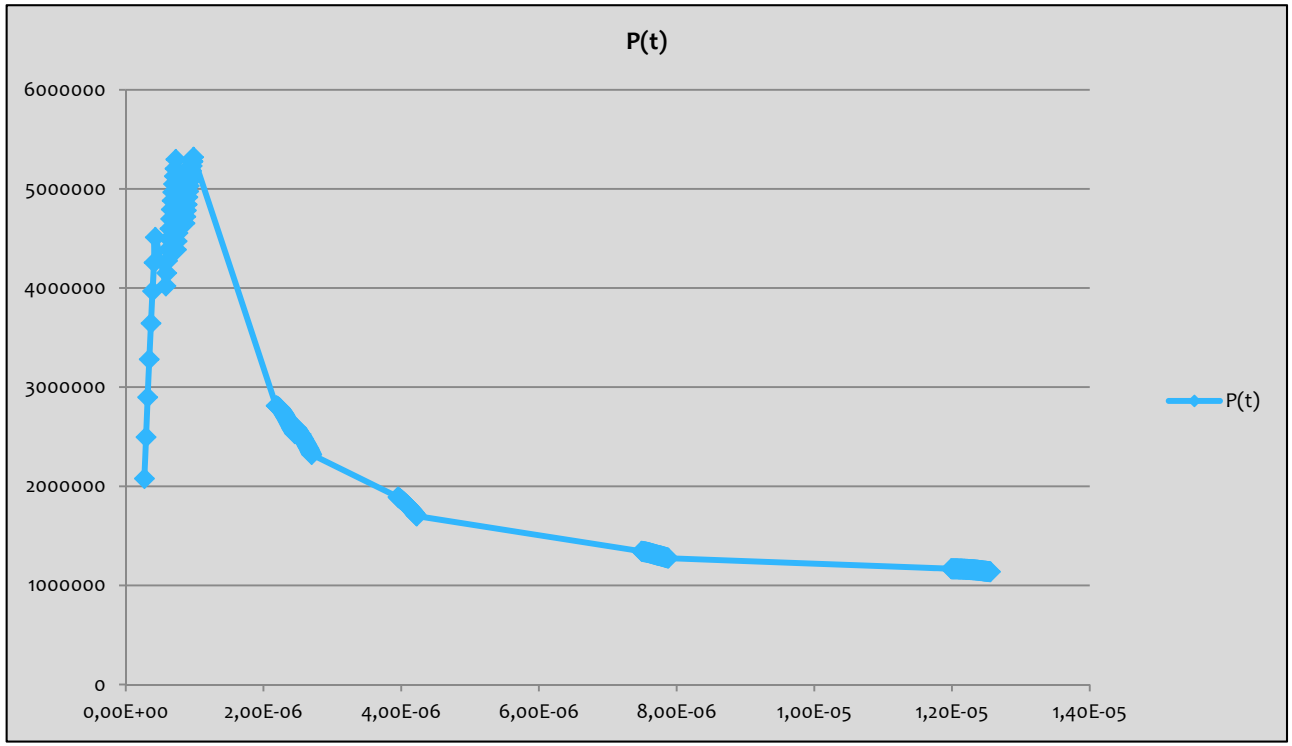


Case: 4mm Dia – 1mm Length	
Parameters	Values
Time-To-Decay - to [sec]	9.85E-07
P-contact - P(To) [MPa]	5.32
$T_{low\text{-}H_2}$ [K]	200
$T_{high\text{-}Air}$ [K]	668



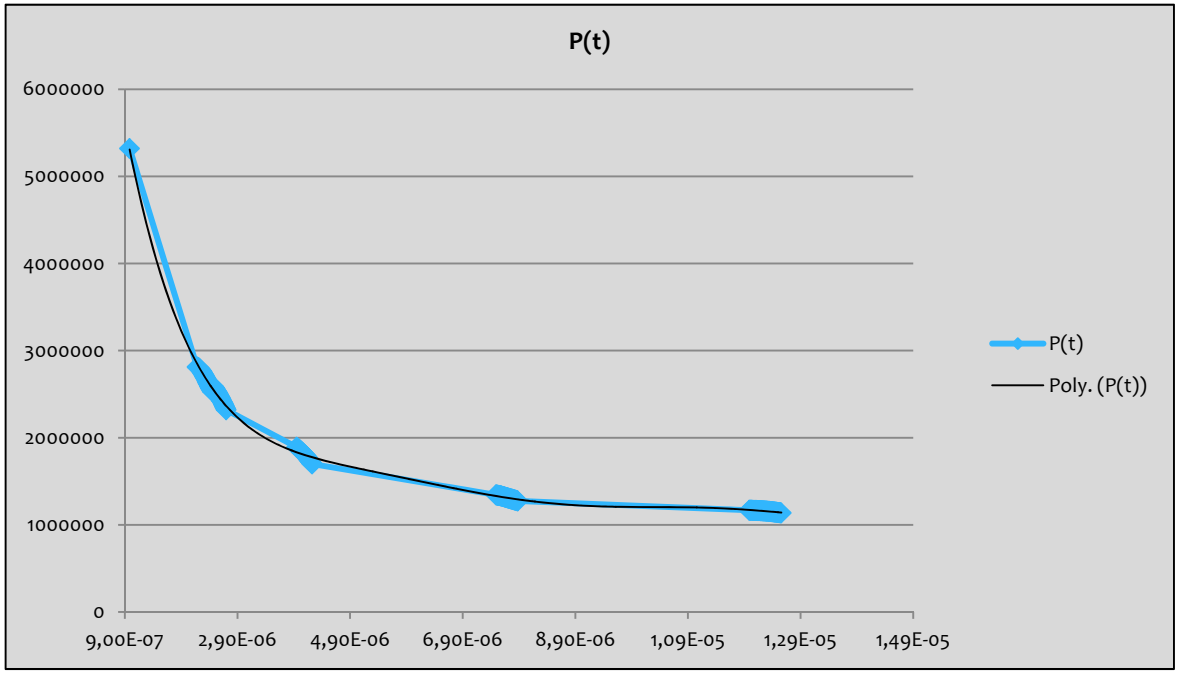
Case Study : 4mm Dia – 1mm Length

Contact Line Pressure – P(t,z) – x=y=0;



Case Study : 4mm Dia – 1mm Length

Source Term [dp/dt] - Decay Time – Curve Fit

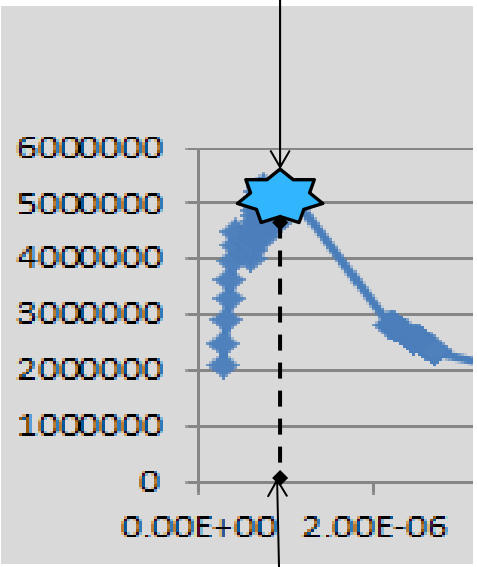


$$P(t) = (3E+37)*t^6 - (2E+33)*t^5 + (3E+28)*t^4 - (4E+23)*t^3 + (2E+18)*t^2 - (6E+12)*t + 1E+07$$

$$dP/dt = P'(t) = (1.8E+38)*t5 - (1.0E+34)*t4 + (1.2E+29)*t3 - (1.2E+24)*t2 + (4.0E+18)*t - 6.0E+12$$

Case Study : 4mm Dia – 1mm Length

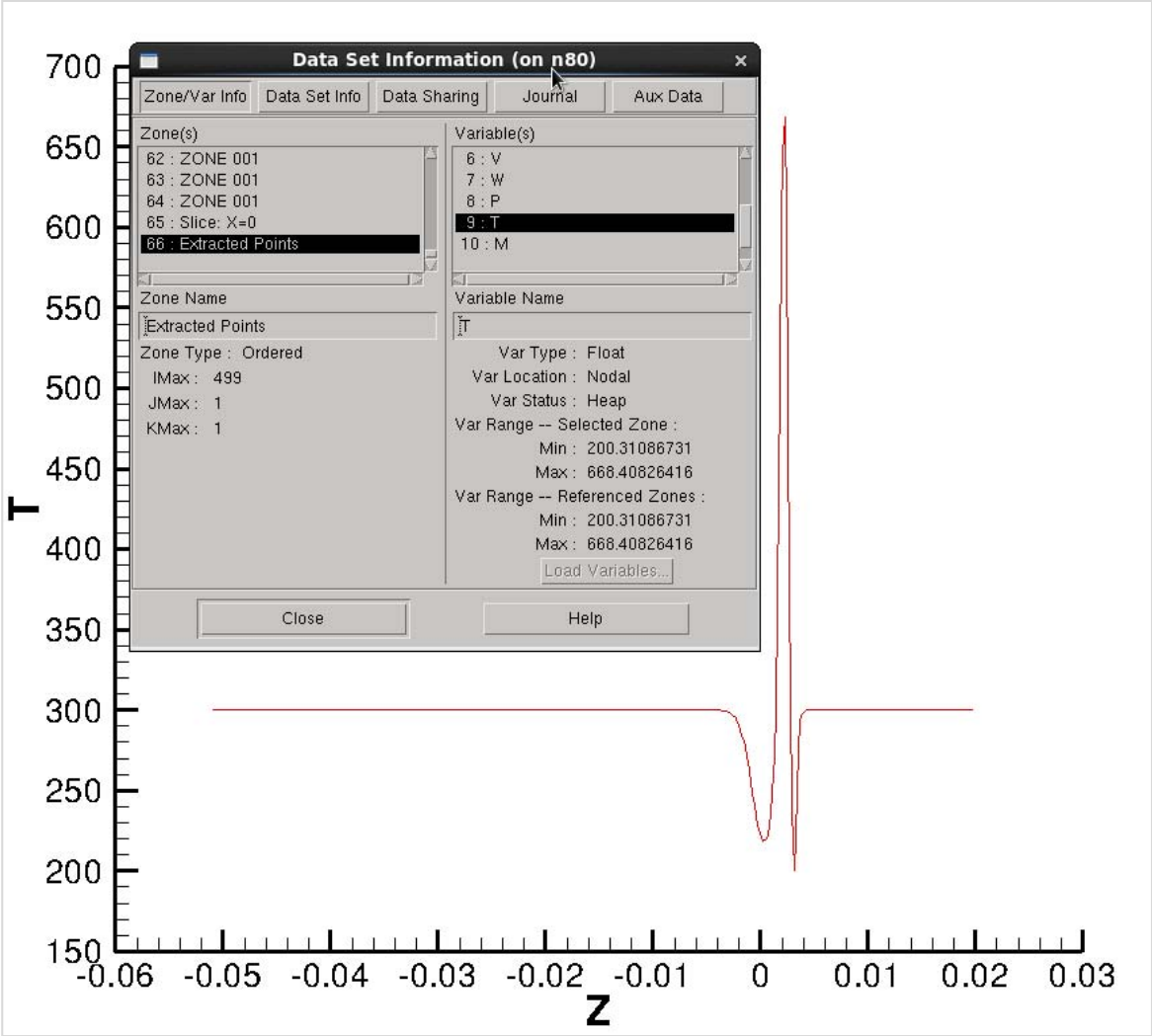
- $P_{contact} \approx +5.32E+06$



Case: 4mm Dia – 1mm Length	
Parameters	Values
Time-To-Decay - to [sec]	9.85E-07
P-contact - P(To) [Pa]	5320401.294

Time-To-Decay - t0 ≈ 9.85E-07

Case Study : 4mm Dia – 1mm Length



Ignition Model

Case: 4mm Dia – 1mm Length	
Parameters	Values
Time-To-Decay - to [sec]	9.85E-07
P-contact - P(To) [Pa]	5320401.294
Tlow [K]	200
Thigh[K]	668

Y[OH-ignite] = 10^-3
Y[OH-Max-4D1L] = 10^-21

./ldr

Enter the hole radius (mm): 2

Enter the tubelength (mm): 1

starting the gas-master 6000...

13 species detected...

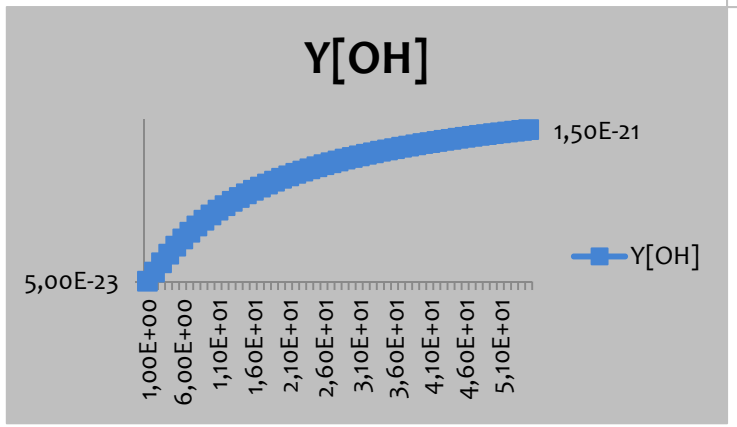
filename = ./output/RAD0000000.L0000000.P0000.0000.csv

creating gas containers...

ngas[1] = 501

ngas_tot = 2502

RAD = 0.002



OH production is very small and is below standard ignition production limits

filling gas containers... done.

creating reaction/diffusion/output modules...

Tao_i = 0.116878

dTao = 500943

tube time = 0s

Pressure ratio: **5.32e+06**

filename = ./output/RAD2.0E-03.L1.0E-03.P5320.0000.csv

getting inital conditions...

Enter Contact Surface Pressure: **5.32E+06**

Enter Contact Surface fuel temperature: **200 K**

Enter Contact Surface Oxidiser temperature: **668 K**

Conclusion

- ✓ Hydrogen release from a high pressure chamber is numerically simulated with computational fluid dynamics
- ✓ Real gas equation of state is necessary for high pressure hydrogen
- ✓ Abel Noble is recommended as the real gas equation
- ✓ The pressure on the contact surface depends on both opening speed, initial diameter and shape of the orifice
- ✓ The Pressure temporal derivative on the contact surface and the high and low temperature on both side of the contact surface are used in the ignition model to determine self ignition