CFD Based Simulation of Hydrogen Release through Elliptical Orifices

Nasim Shishehgaran and Marius Paraschivoiu

Concordia University

The 5th International Conference on Hydrogen Safety (ICHS)
Brussels, Belgium
September 9-11, 2013

Research Goal

- Numerically investigate the effect of orifice geometry on the behavior and development of hydrogen jet escaping from a high pressure reservoir.

Objectives

- Fixed elliptical and circular orifices with varying aspect ratios and sizes and under different storage pressures.
- Expanding circular holes with uniform radial growth rates effective before the release of hydrogen (t=0)
- Expanding circular holes with uniform radial growth rates effective after the release of hydrogen
- Deformation of circular holes to elliptic openings

Euler Equations:

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

$$\vec{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}, \qquad \vec{\vec{F}} = \left(\begin{bmatrix} \rho(u-w_x) \\ \rho(u-w_x)u + P \\ \rho(u-w_x)v \\ \rho(u-w_x)w \\ \rho(u-w_x)E + uP \end{bmatrix} \begin{bmatrix} \rho(v-w_y) \\ \rho(v-w_y)u \\ \rho(v-w_y)v + P \\ \rho(v-w_y)w \\ \rho(v-w_y)E + vP \end{bmatrix} \begin{bmatrix} \rho(w-w_z) \\ \rho(w-w_z)u \\ \rho(w-w_z)v \\ \rho(w-w_z)w + P \\ \rho(w-w_z)E + wP \end{bmatrix} \right)$$

Transport (Advection) Equation:

$$\frac{\partial c}{\partial t} + \frac{\partial(c(u-w_x))}{\partial x} + \frac{\partial(c(v-w_y))}{\partial y} + \frac{\partial(c(w-w_z))}{\partial z} = 0$$

- *$c=0$ a cell full of hydrogen*
- *$0<c<1$ discontinuity (hydrogen-air interface)*
- *$c=1$ a cell full of air*

Abel Nobel Real Gas Law:

$$p = (1 - b\rho)^{-1}\rho R_{mix} T, \qquad b = 0.00775\ m^3/kg$$

Discretization

- The system of Euler Equations is discretized using an **implicit finite volume** discretization scheme.

$$|V_i|\frac{\vec{U}_i^{n+1}-\vec{U}_i^{n}}{\Delta t}+\sum_{over\ \partial V_i}\vec{\vec{F}}_{\partial V_i}^{n+1}.\ \vec{n}_{\partial V_i}\ \Delta S_{\partial V_i}=0$$

Moving Mesh ⇒ **$\vec{n}_{\partial V_i}$, $\Delta S_{\partial V_i}$ and V_i are time-dependent.**

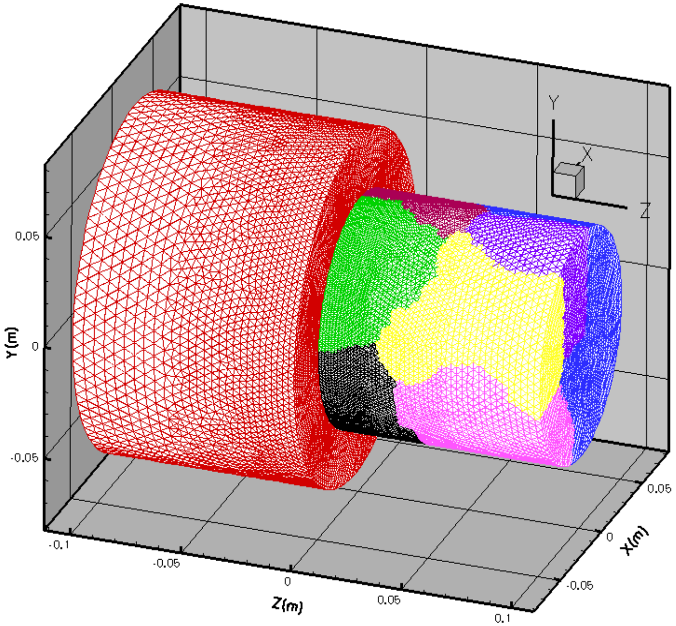
$$\left(\frac{|V_i|}{\Delta t}\vec{\vec{I}}+\sum_{over\ \partial V_i}\left(\frac{\partial\vec{\vec{F}}}{\partial\vec{U}}\right)_{\partial V_i}^{n}.\vec{n}_{\partial V_i}\ \Delta S_{\partial V_i}\right)\delta\vec{U}_i^{n+1}=-\sum_{over\ \partial V_i}\vec{\vec{F}}_{\partial V_i}^{n}.\vec{n}_{\partial V_i}\ \Delta S_{\partial V_i}$$

- **Spatial Discretization (Convection Flux)**
  - ***2^{nd} order Roe-MUSCL scheme***
- **Temporal Discretization**
  - ***1^{st} order Implicit Scheme***
- ***Linear Solver***
  - ***Iterative Method : GMRES***

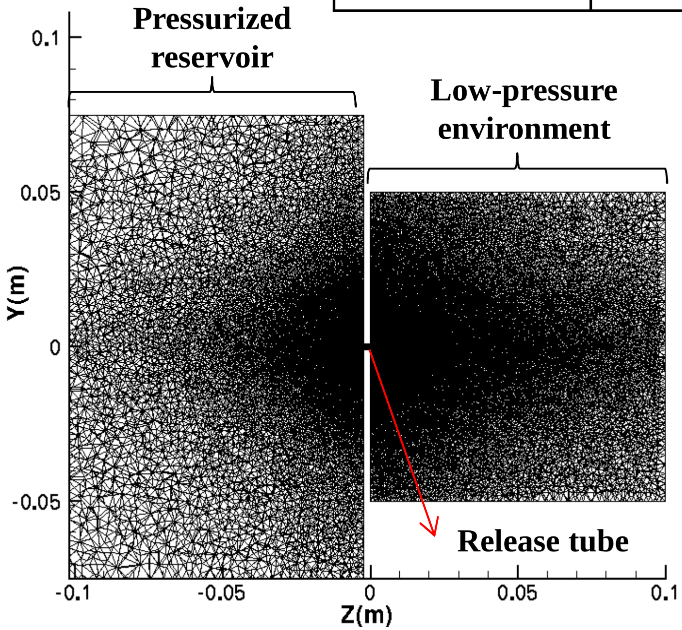
Computational Domain

- **3D unstructured tetrahedral mesh**
- **METIS** software package is used to distribute the finite element/volume mesh to the processors and partition the domain for parallel computing.

Grid Resolution		
Grid Level	**Number of Nodes**	**Number of Tetrahedrons**
Fine	$\approx 3 \times 10^6$	$\approx 17.5 \times 10^6$
Medium	$\approx 2 \times 10^6$	$\approx 12 \times 10^6$
Coarse	$\approx 1 \times 10^6$	$\approx 6 \times 10^6$



the discretized domain with decomposed zones using METIS (partially shown)

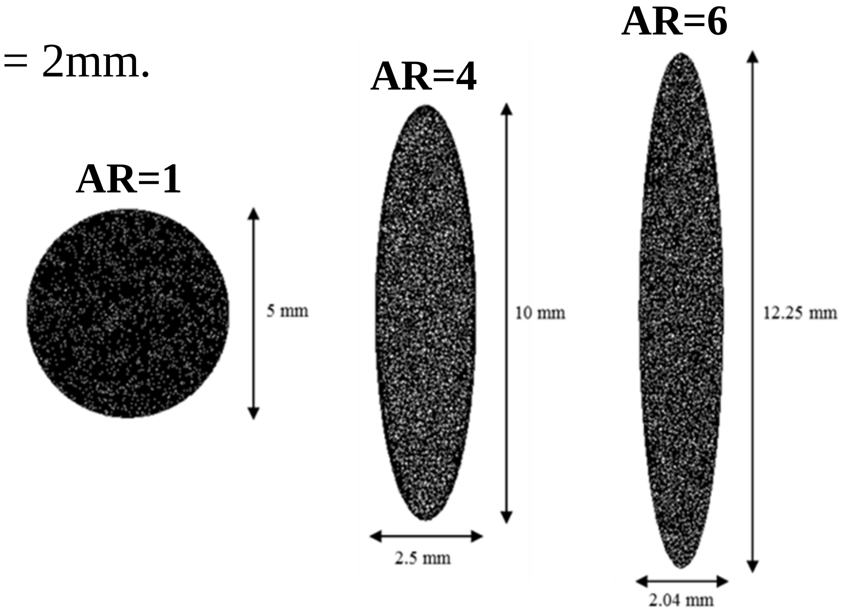


2D slice of the computational domain

Fixed (Circular & Elliptical) and Enlarging Orifices

- The parameter under consideration for comparable fixed circular and elliptical orifices is **the same exit area**.
- Expanding orifices with initial diameters of **D_i=1 mm** and **D_i=2 mm.**
- The **length of release tube** is **equal** in all cases = 2mm.

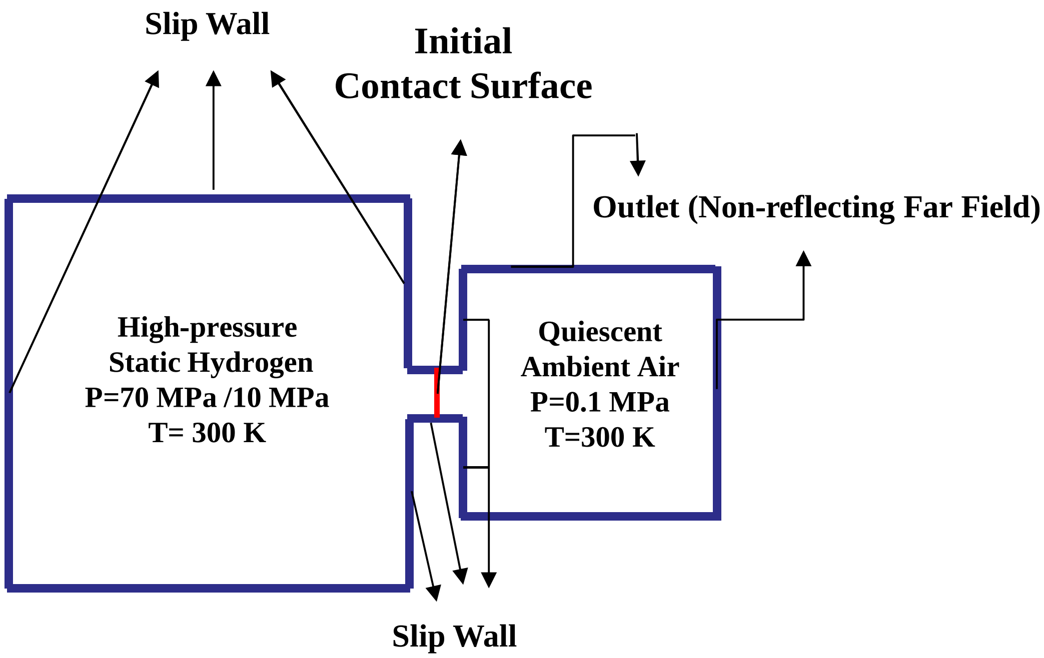
Area=0.8 (mm^2)			
Orifice Type	Major Axis, a (mm)	Minor Axis, b (mm)	Aspect Ratio, a/b
Circular	1	1	1
Elliptical 1	2	0.5	4
Elliptical 2	2.45	0.41	6
Area=3.14 (mm^2)			
Circular	2	2	1
Elliptical 1	4	1	4
Elliptical 2	5	0.82	6
Area=19.63 (mm^2)			
Circular	5	5	1
Elliptical 1	10	2.5	4
Elliptical 2	12.25	2.04	6



The cross sectional surfaces of the varying ARs of the orifices with the equal exit area (A=19.63 mm^2)

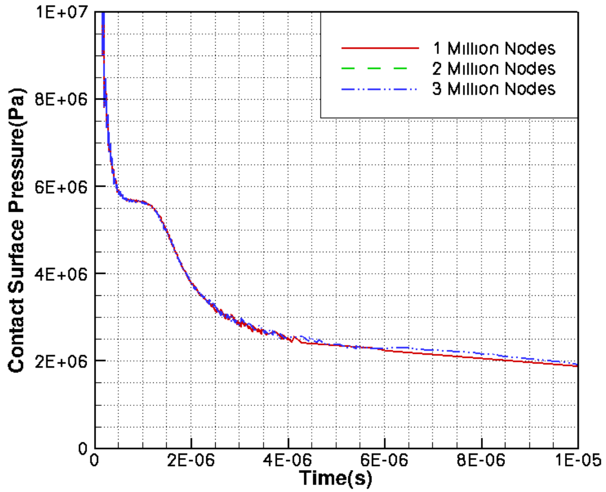
Initial and Boundary Conditions

Initial Reservoir Pressure	70MPa & 10MPa
Initial Temperature	300 K
Air mixture fraction	1
Hydrogen mixture fraction	0
Hydrogen & air isentropic exponent (γ)	1.4
Molecular mass of hydrogen (M_{H_2})	2.016 g/mol
Molecular mass of air (M_{air})	28.96 g/mol
Initial time step	10^{-10}
Initial CFL Number (Fixed cases)	0.15
Max CFL Number (Fixed cases)	0.8
Initial CFL Number (Moving cases)	0.3
Max CFL Number (Moving cases)	5.0

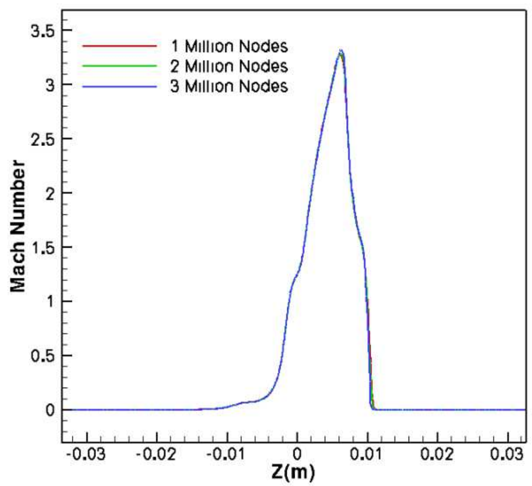


- The viscosity effect and the heat transfer are neglected.
- The effect of the gravity on the fluid is neglected.
- Free-slip and adiabatic solid walls
- Non-reflecting farfield

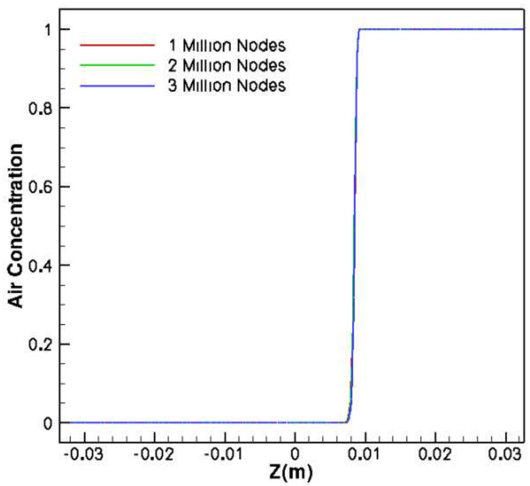
Grid Sensitivity study



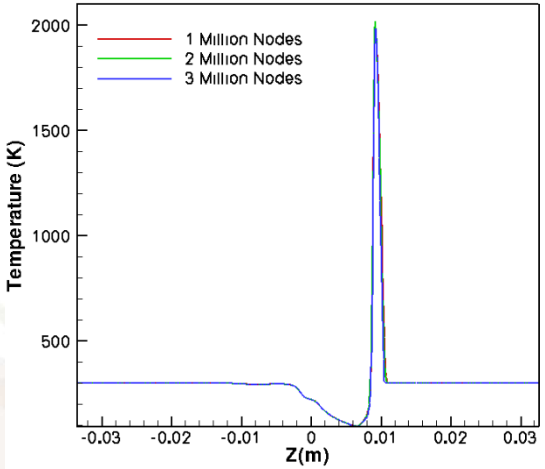
contact surface pressure along the centerline



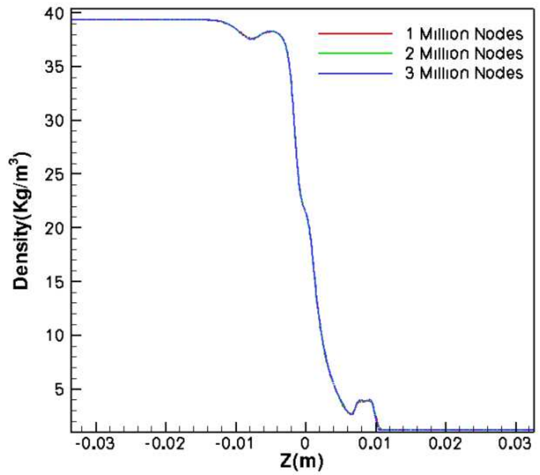
Centerline Mach Number



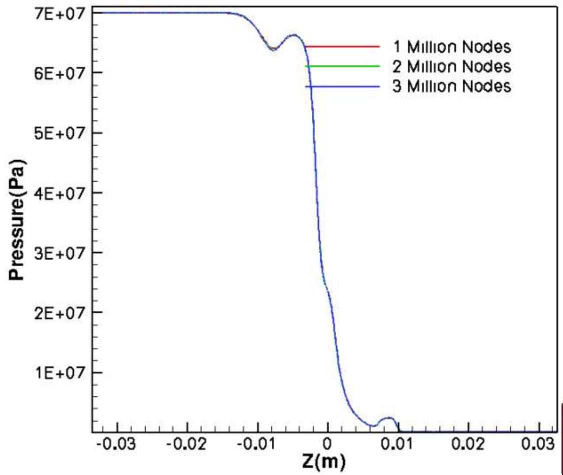
Centerline Concentration



Centerline Temperature

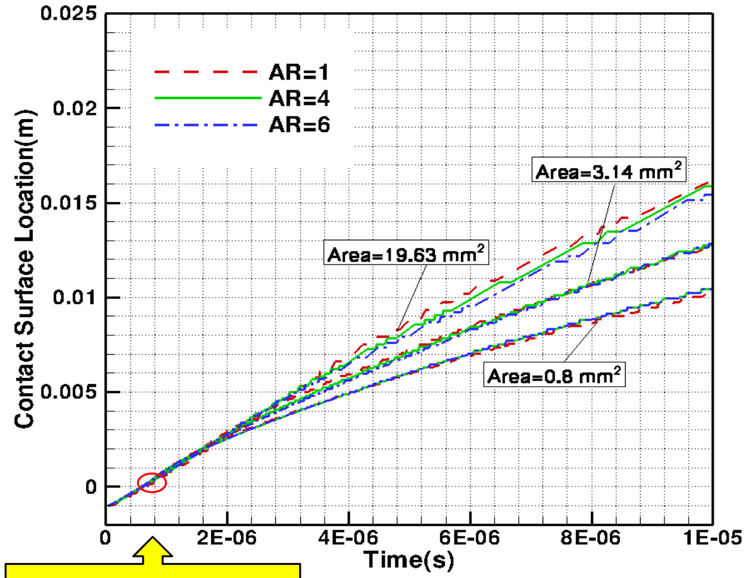


Centerline Density



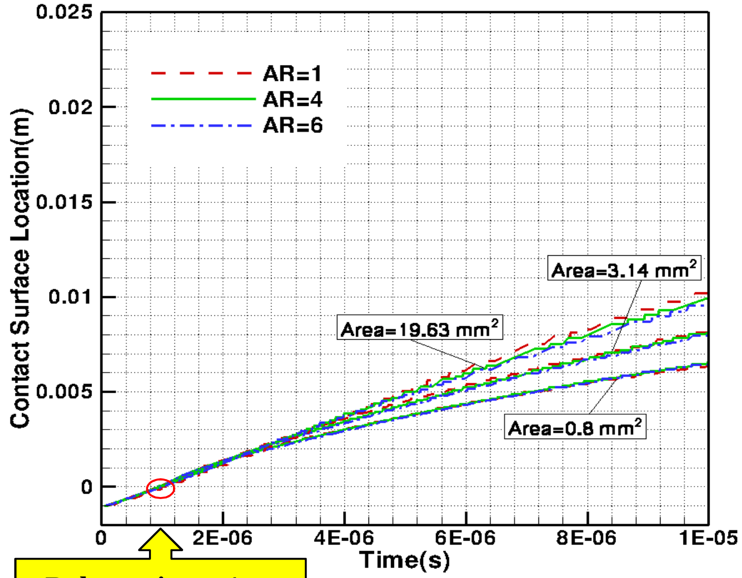
Centerline Pressure

Evaluation of the contact surface location and the release time (Fixed Circular & Elliptical Orifices)



Release time= 0.6 μs

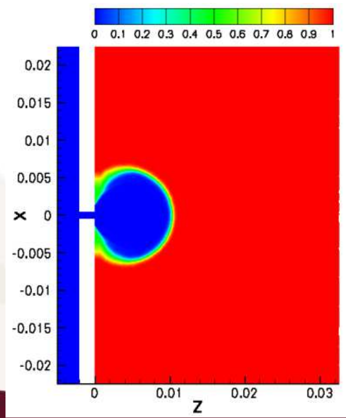
Storage Pressure =70 MPa



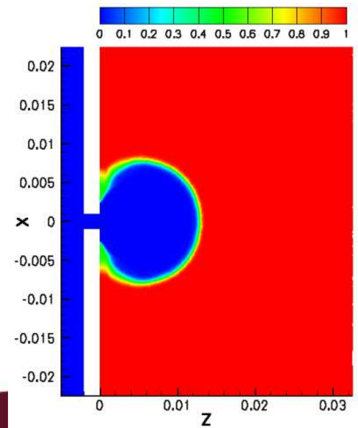
Release time= 1 μs

Storage Pressure =10 MPa

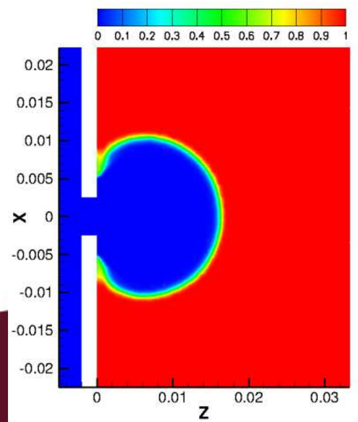
D= 1mm



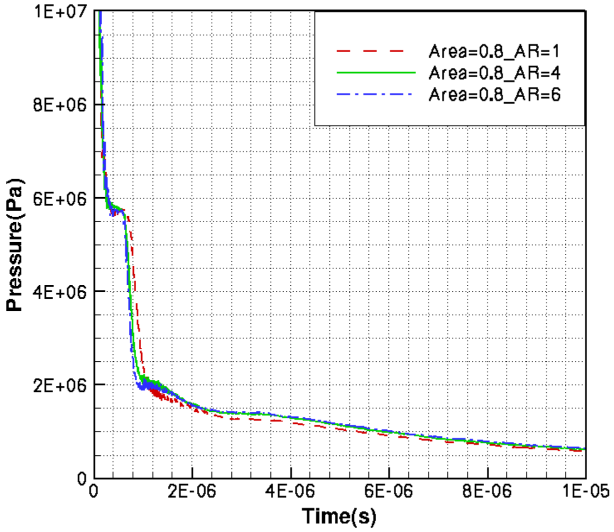
D= 2mm



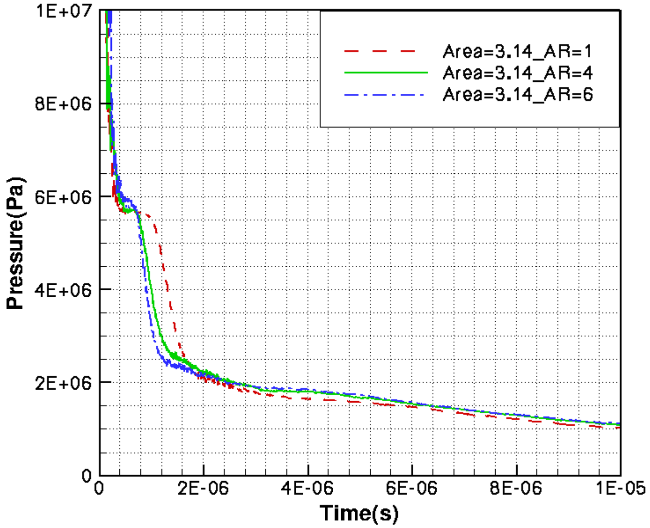
D= 5mm



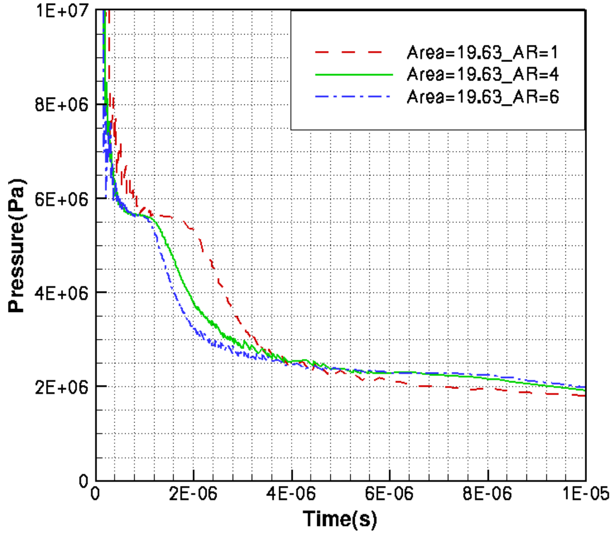
Contact Surface Pressure (Fixed Orifices), P=70 MPa



a) Area= 0.8 mm^2



b) Area= 3.14 mm^2



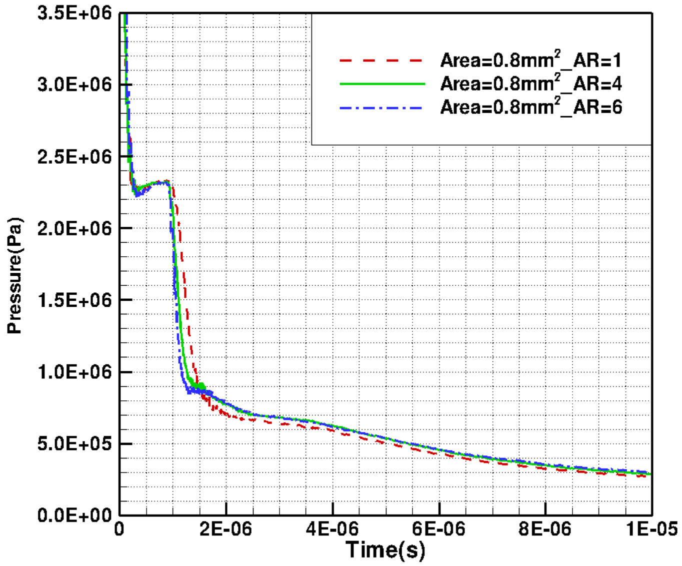
c) Area= 19.63 mm^2

The same cross sectional area ⟩ [**Higher Aspect Ratio** → **More pronounced expansion**]

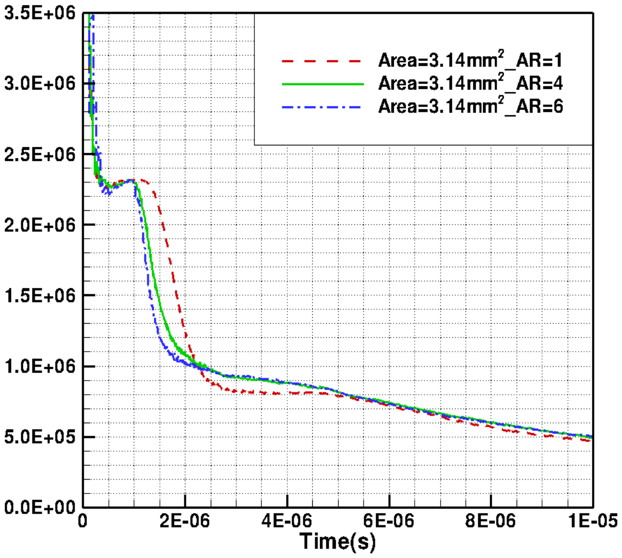
The same aspect ratio ⟩ [**Smaller release hole** → **More pronounced expansion** → **Rapid depressurization**]

Université Concordia University

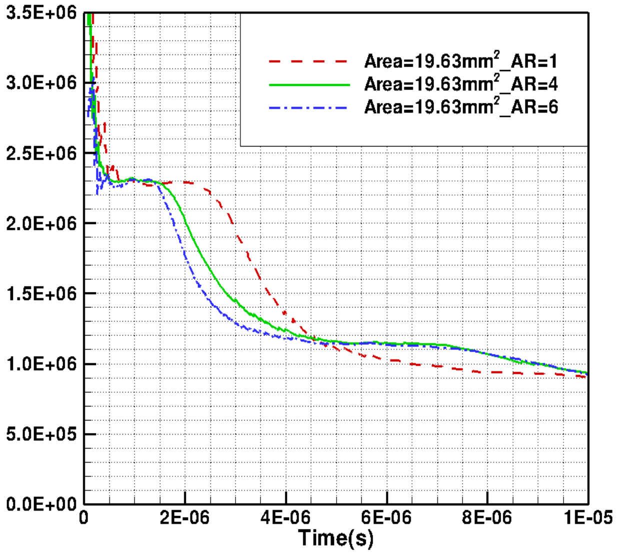
Contact Surface Pressure (Fixed Orifices), P=10 MPa



a) Area= 0.8 mm ^{2}



b) Area= 3.14 mm ^{2}



c) Area= 19.63 mm ^{2}

The same cross sectional area ⇒ [**Lower the storage pressure** → **Less pronounced expansion**]

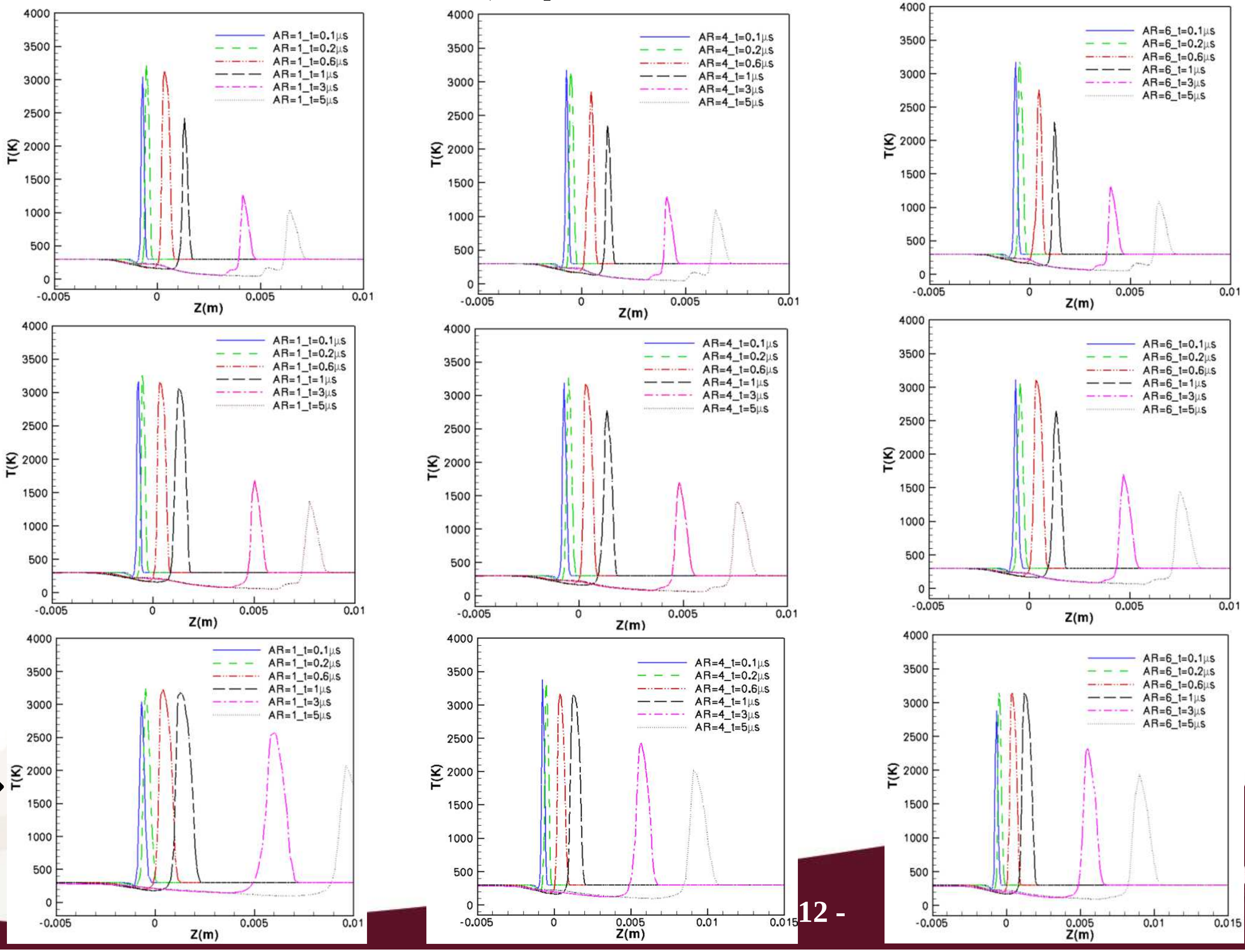
Centerline Temperature (Fixed Orifices, P=70 MPa)

a) Circular Orifice, AR=1 | **b) Elliptical Orifice, AR=4** | **c) Elliptical Orifice, AR=6**

Area= 0.8 mm ^{2}

Area= 3.14 mm ^{2}

Area= 19.63 mm ^{2}



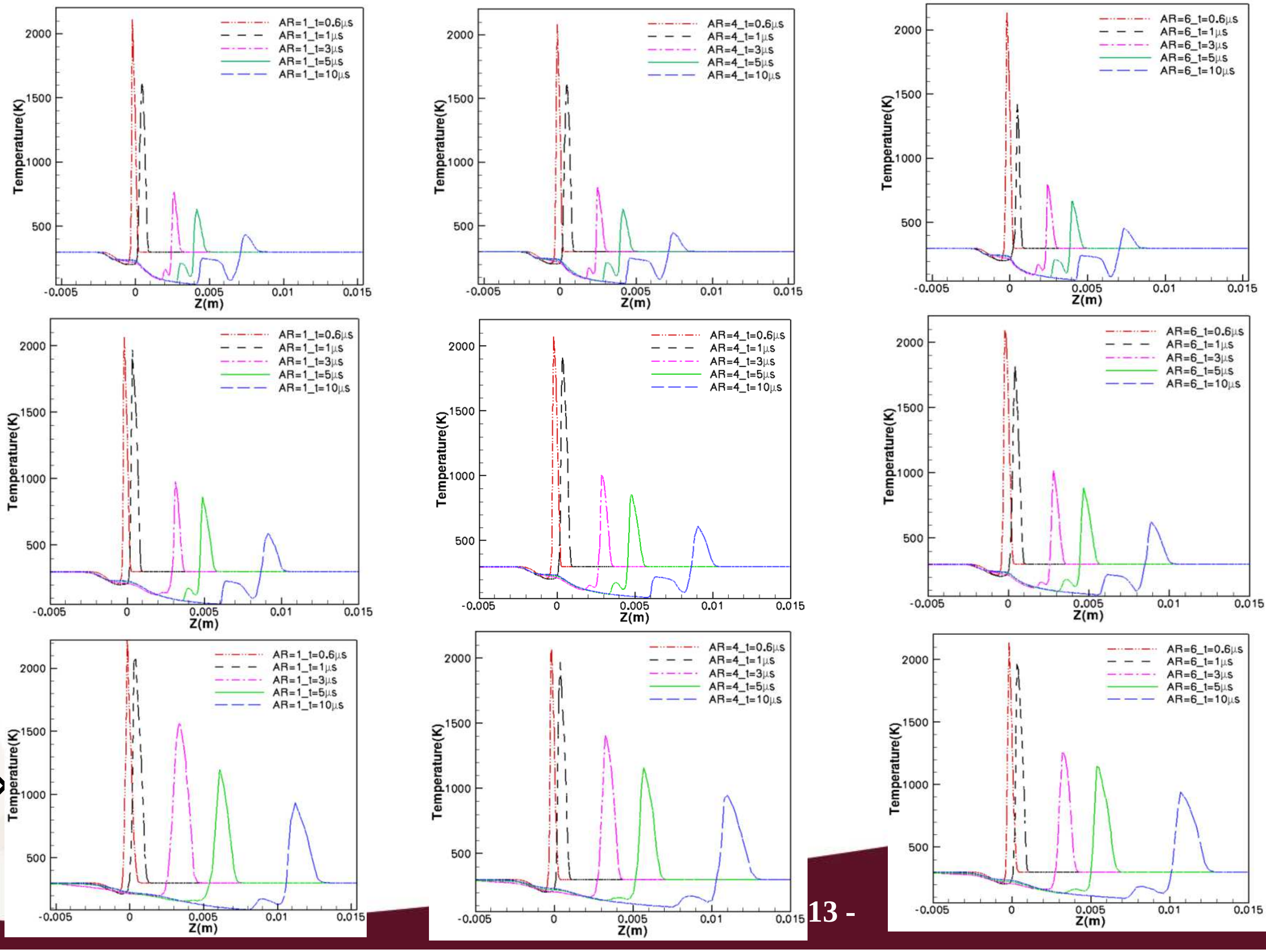
Centerline Temperature (Fixed Orifices, P=10 MPa)

a) Circular Orifice, AR=1 | b) Elliptical Orifice, AR=4 | c) Elliptical Orifice, AR=6

Area= 0.8 mm ^{2}

Area= 3.14 mm ^{2}

Area= 19.63 mm ^{2}



Centerline Temperature (Fixed Orifices, P=10 MPa)

a) Centerline Mach Number

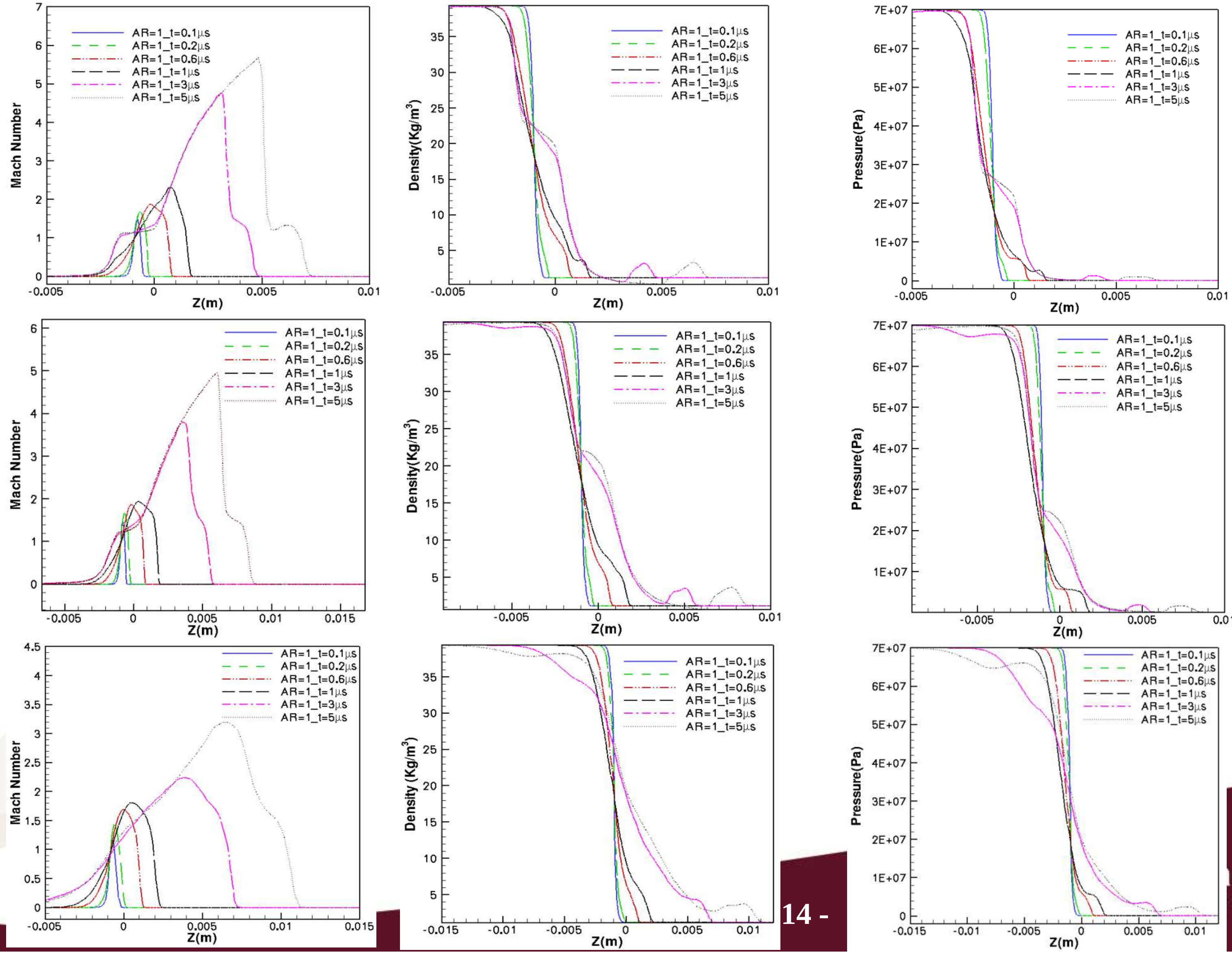
b) Centerline Density

c) Centerline Pressure

Area= 0.8 mm ^{2}

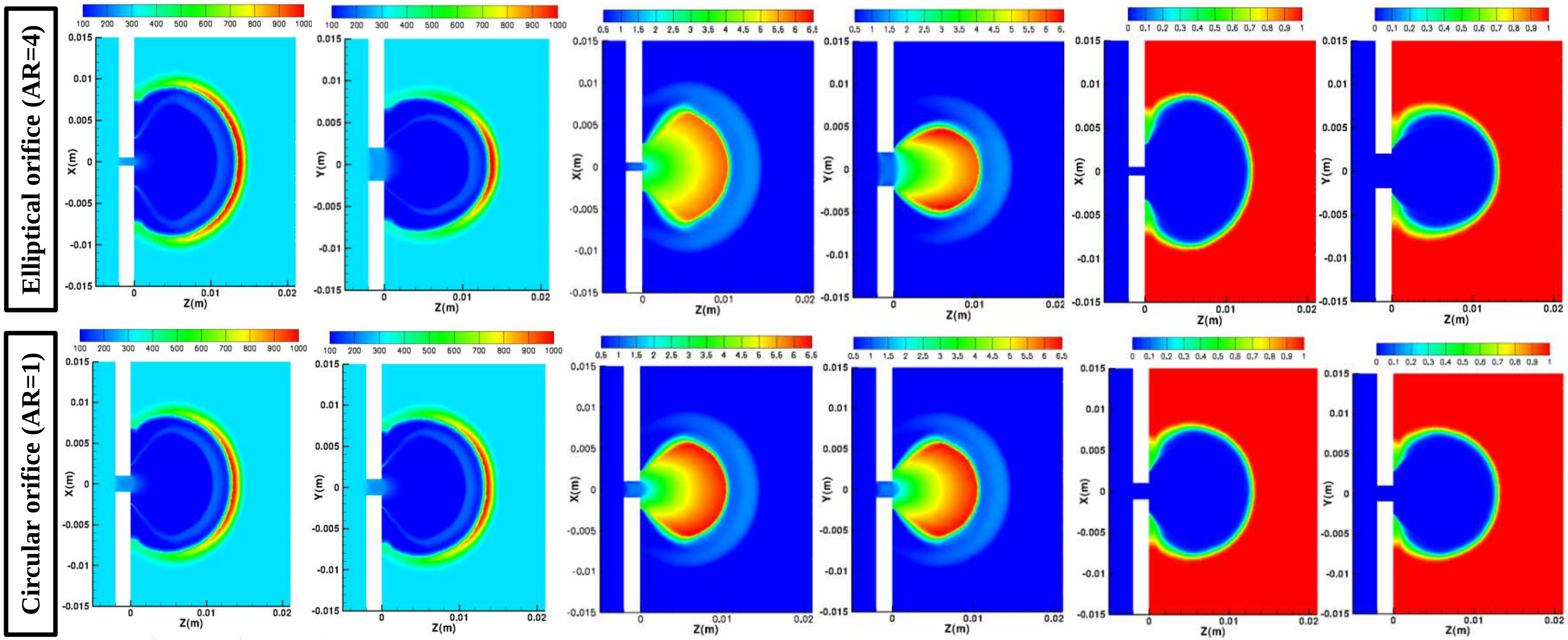
Area= 3.14 mm ^{2}

Area= 19.63 mm ^{2}



Temperature | **Mach Number** | **Concentration**

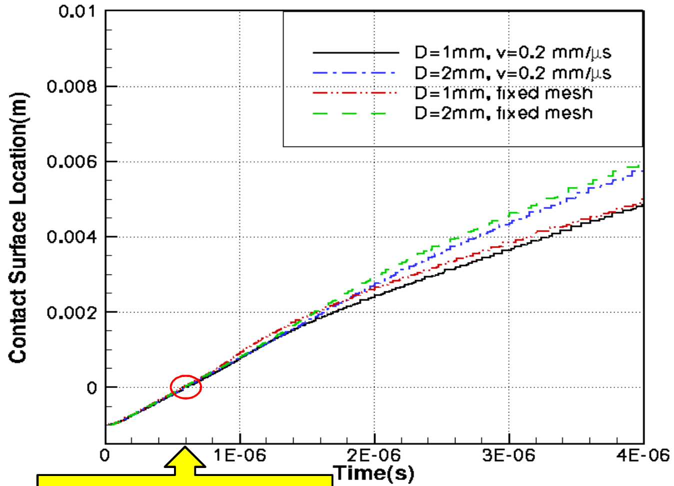
(Minor Axis) (Major Axis) (Minor Axis) (Major Axis) (Minor Axis) (Major Axis)



After 10 μs of hydrogen release into air from the circular and elliptical orifices (Area=3.14 mm^2)

Circular Expanding Orifices effective at t=0

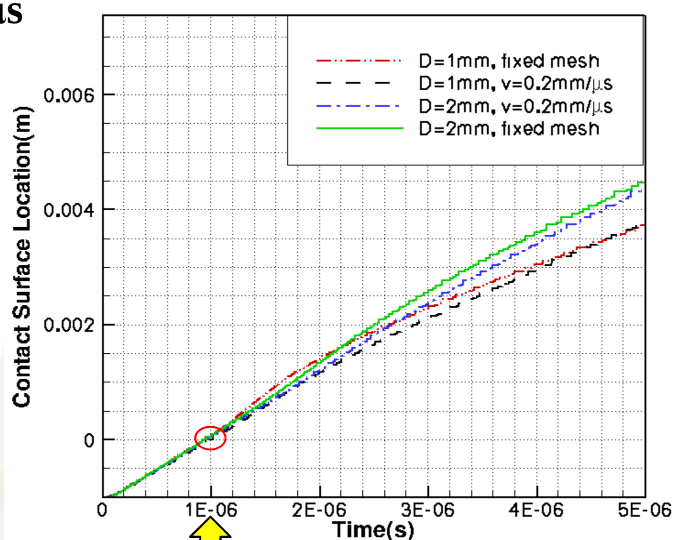
P=70 MPa



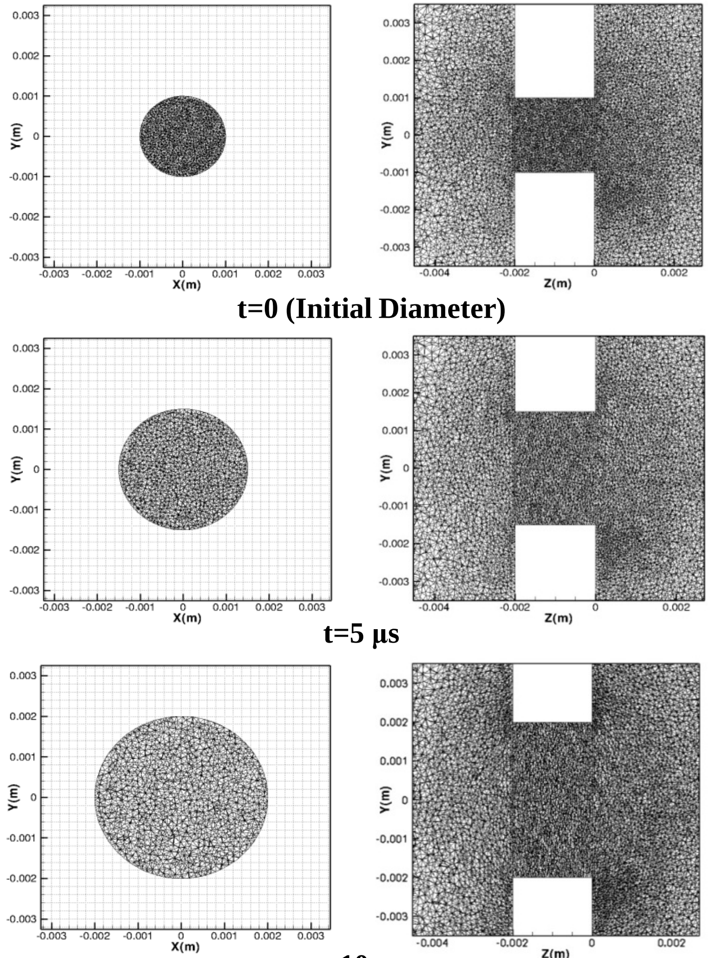
Release time= 0.6 µs

- **Growth Rate V= 0.2 mm/µs**

P=10 MPa



Release time= 1 µs



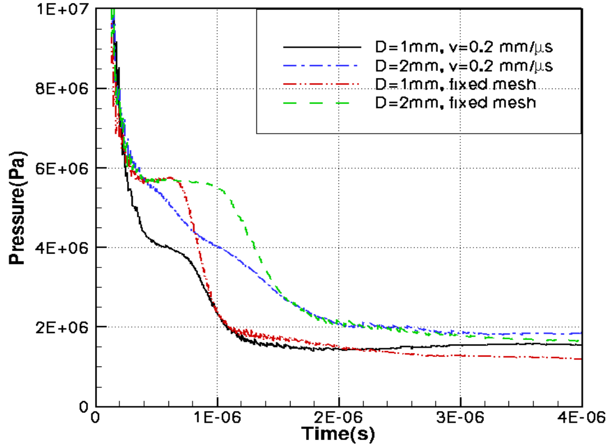
t=0 (Initial Diameter)

t=5 µs

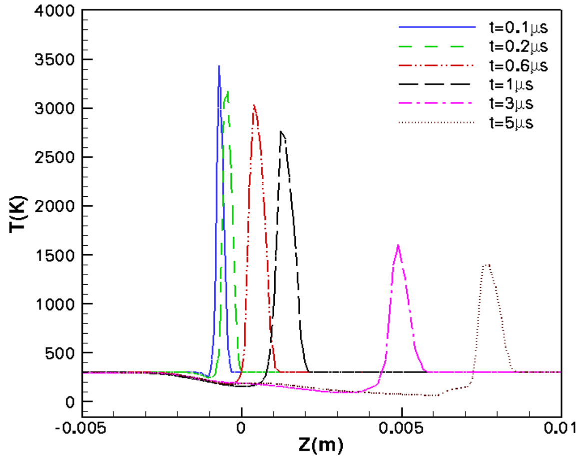
t=10 µs

Two dimensional views of the expanding release hole (D_i=2mm)

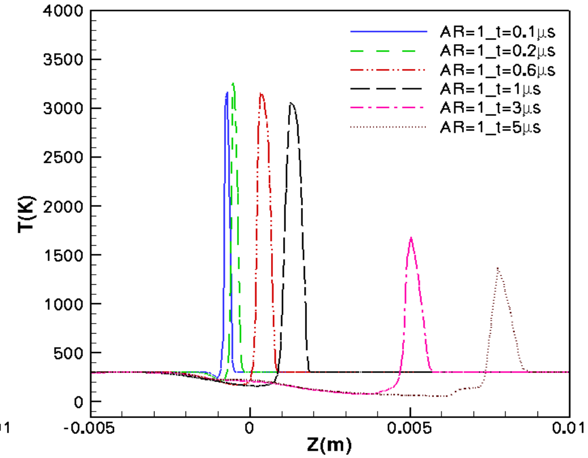
Contact Surface Pressure and Centerline Temperature (Expanding Exit)



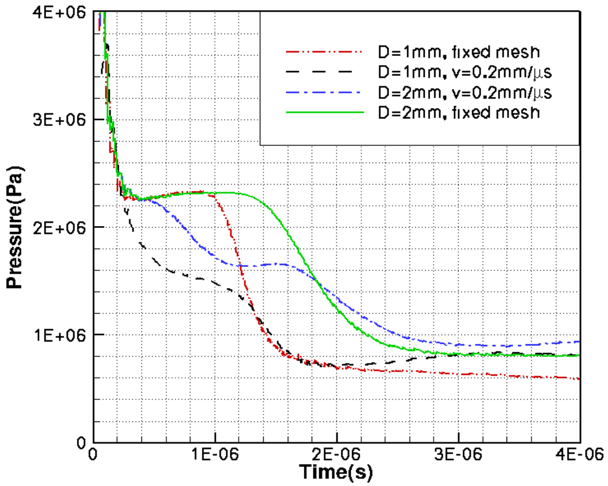
(Fixed Circular Vs. Expanding Orifices)
D_i=1 mm and D_i=2 mm



Expanding Exit Hole
(P=70 MPa), D_i =2 mm



Fixed Circular Orifice
(P=70 MPa), D =2 mm



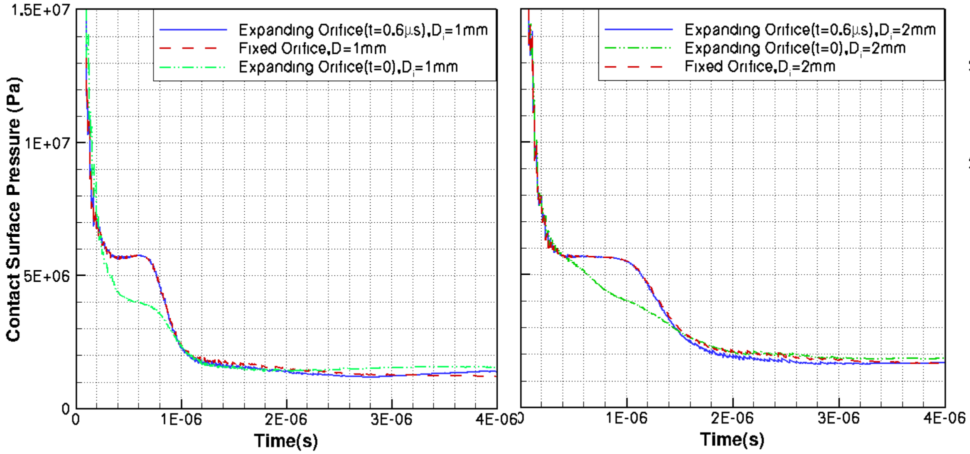
(Fixed Circular Vs. Expanding Orifices)
D_i=1 mm and D_i=2 mm, P=10 MPa

Identical Initial Diameter ⟩ [**Expanding Release Hole** → **More Pronounced Expansion**]

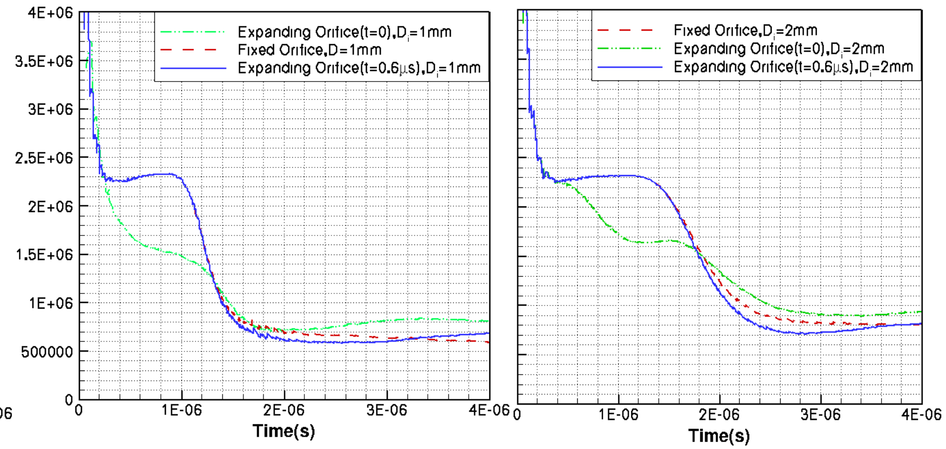
- During the expansion, the hydrogen jet issuing from the **Expanding release hole** has **lower temperature peaks** compared to the jet from the fixed circular orifice.

UNIVERSITÉ Concordia UNIVERSITY

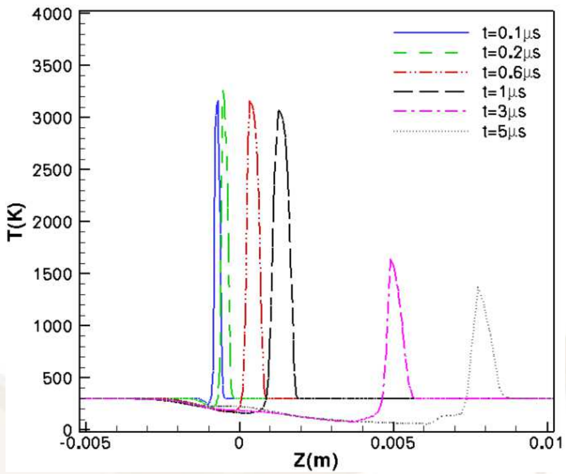
Circular expanding orifices effective after the release



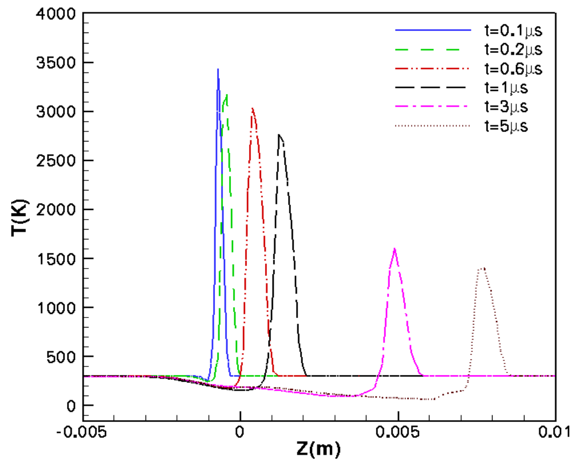
Expanding orifices (started at t=0. 6 µs & t=0) and fixed orifice, (D_i=1 mm & D_i=2 mm, P=70 MPa)



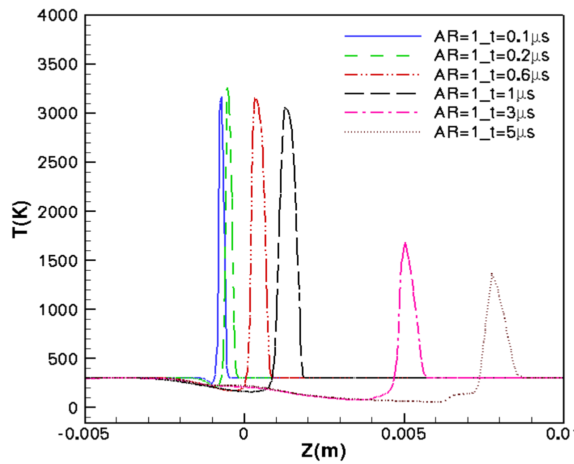
Expanding orifices (started at t=0. 6 µs & t=0) and fixed orifice, (D_i=1 mm & D_i=2 mm, P=10 MPa)



Expanding Exit Hole (t=0.6) (P=70 MPa), D_i =2 mm

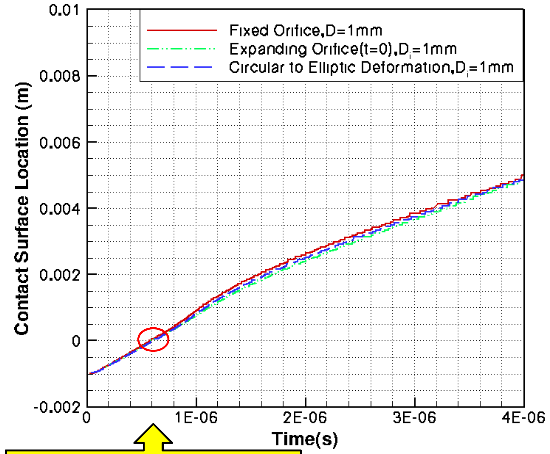


Expanding Exit Hole (t=0) (P=70 MPa), D_i =2 mm



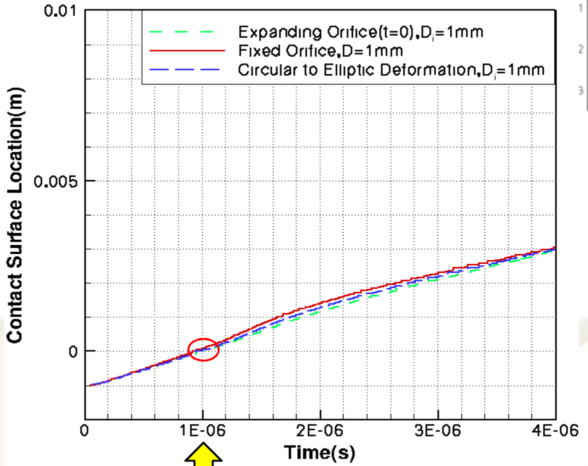
Fixed Circular Orifice (P=70 MPa), D =2 mm

Deformation of a small circular hole to an elliptical opening



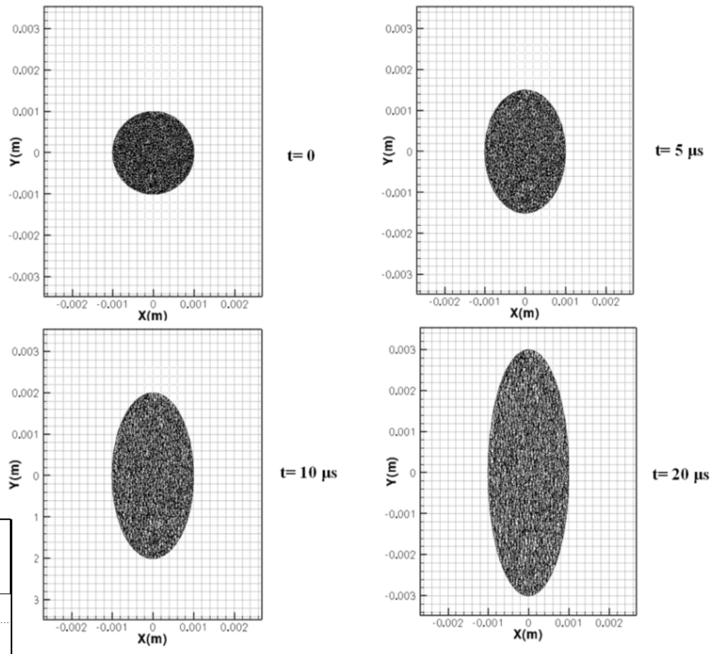
Release time= 0.6 µs

P=70 MPa

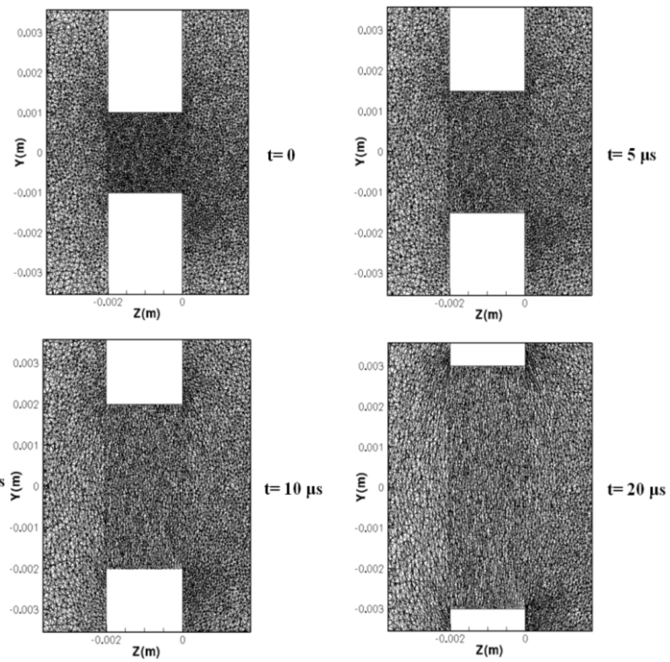


Release time= 1 µs

P=10 MPa



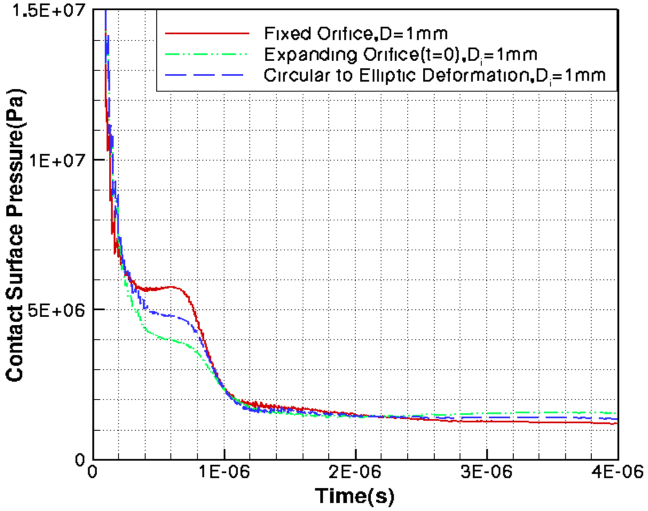
Cross sectional areas, D_i=2mm, v=0.2mm/µs

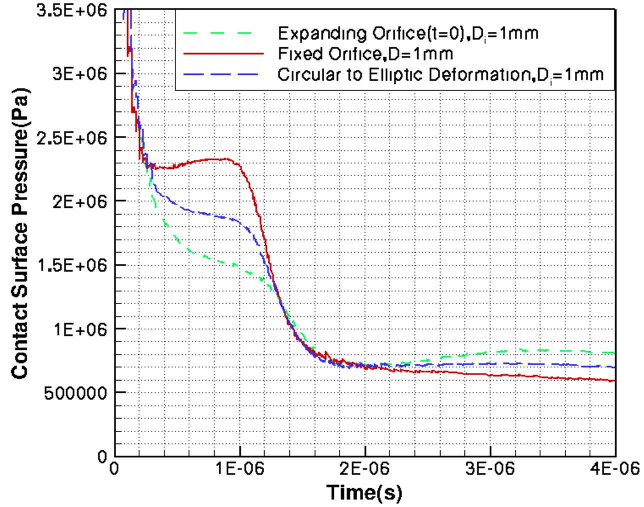


Side views, D_i=2mm, v=0.2mm/µs

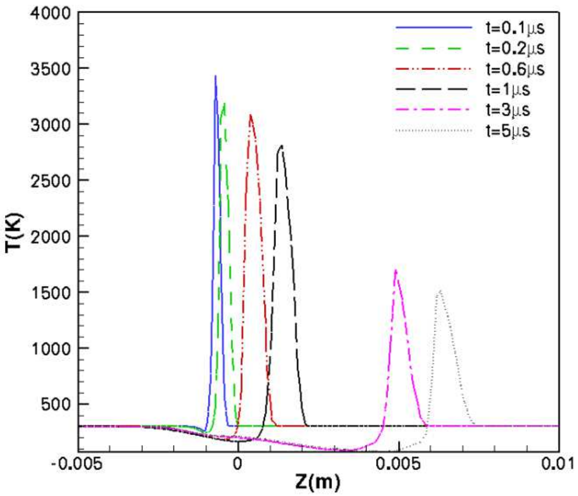
- Stretching rate = 0.2 mm/µs

Contact Surface Pressure and Centerline Temperature

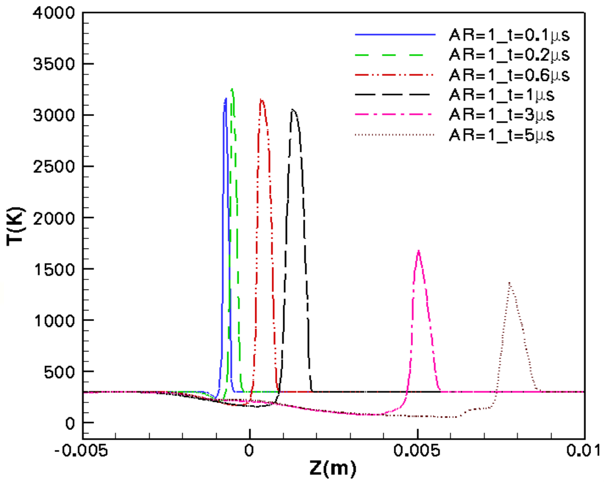




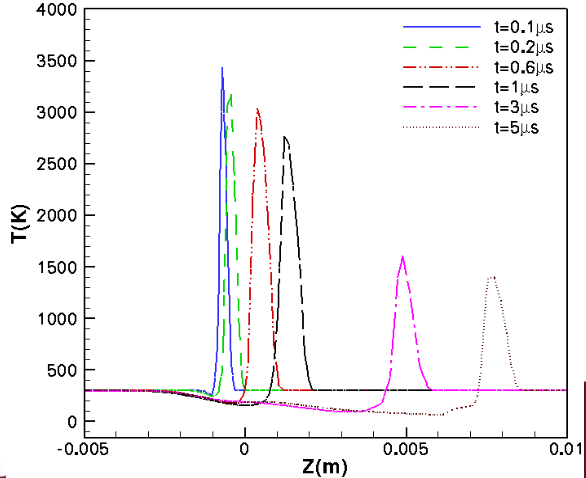
Stretching, Expanding (started at the release time) and Fixed holes, (D_i=1 mm & D_i=2 mm), P=70 MPa



Stretching Exit Hole (P=70 MPa)



Fixed Circular Orifice (P=70 MPa)



Expanding Exit Hole (P=70 MPa)

Contributions

- The effects of different geometries and configurations of the exit hole including fixed elliptical, fixed circular and expanding orifices on the dispersion of hydrogen were studied using a 3D parallel in-house code.

- The effects of the storage pressure and the size of the orifice on the dispersion and development of the hydrogen jet are dominant than the effect of the orifice shape.

- The possibility of auto-ignition may be affected by applying expanding orifices.

Thank You