Numerical Simulation of Detonative Explosion in a Hydrogen Mixture (수소 혼합 기체에서의 폭발 해석)

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- Hydrogen safety in a nuclear power plant (NPP)
- Development of OpenFOAM-based containment analysis code

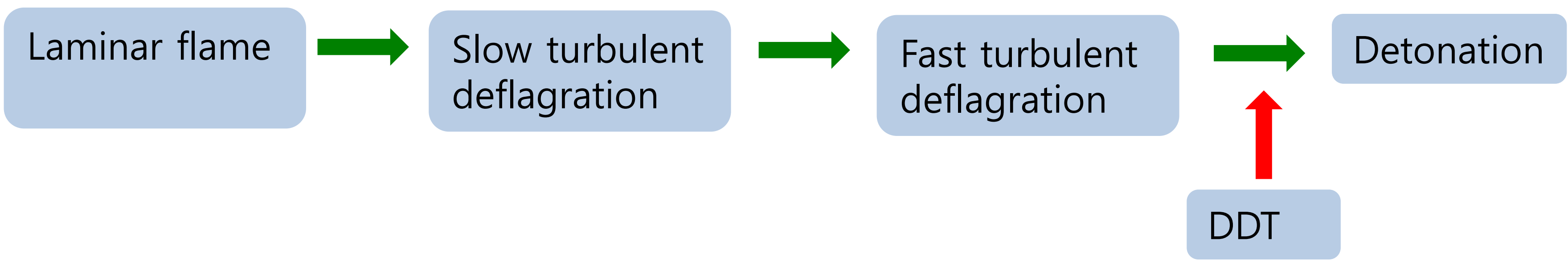
Development of a technology to simulate a detonation

- Numerical method
- Validation
- Application to a containment

Summary and Future Plan

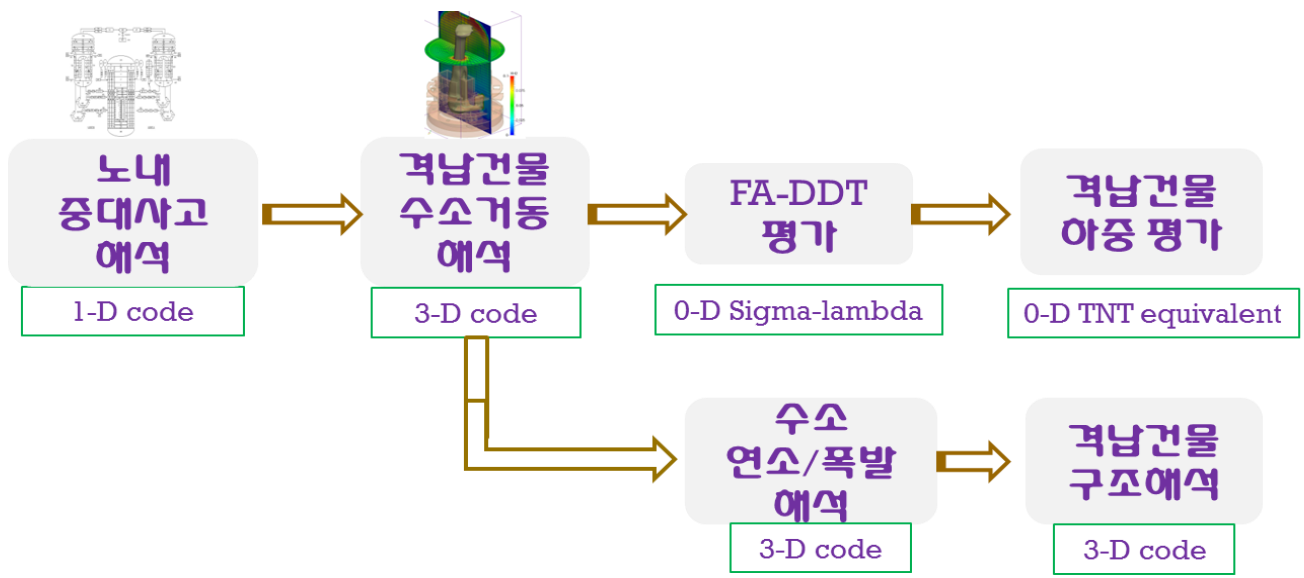
Hydrogen safety in a NPP

- **Hydrogen generation and release**
  - hydrogen is generated by oxidation of the fuel-cladding in a reactor during a severe accident and is released with a steam into the reactor containment.
  - The released hydrogen and steam are mixed with air in the containment.
- **Hydrogen safety in NPPs**
  - NPPs are required to be safe from a thermo-mechanical load generated by hydrogen explosion by adopting a hydrogen mitigation strategy.
- **Hydrogen explosion in NPPs**
  - Hydrogen flame propagation complies with the following combustion regime.



Hydrogen safety evaluation strategy

- Strategy for hydrogen safety evaluation
  - It follows a course of hydrogen behaviors along an accident progress.
  - H2 generation → distribution → combustion → FA → DDT
    - FA: flame acceleration, DDT: deflagration to detonation transition
- Methodology for hydrogen safety evaluation
  - 0-D analysis
  - Lumped-parameter system analysis
  - 3-D analysis



Containment code for hydrogen safety

- Hydrogen behaviors during a severe accident in an NPP containment are strongly dependent on thermal hydraulics in the containment.

- Important thermal and hydraulic physics in a containment
  - buoyant jet flow, turbulent mixing, gas species diffusion by concentration gradients, steam condensation, thermal radiation, structure heat transfer, condensed/sprayed droplet flow, combustion of hydrogen, and et al.

- Active or passive devices installed in a containment in order to control a containment atmosphere must also be modeled.
  - PAR, igniter, fan/cooler and passive heat removal system

- Implementation of all the models in a single code makes it complicated and heavy to run for long-term accident scenarios.

Development of OpenFOAM-based containment analysis code

- Modularized development of a containment analysis code
  - Modularization of an analysis code is a commonly used technology to keep the code manageable.
- An analysis tool for hydrogen behavior in a containment is under development based on the OpenFOAM library which supplies modularized numerical and physical models by using classes and namespaces

Turbulence module	Time-averaged (quasi-steady)	Volume-averaged (transient)		
Phasic module	Condensation	spray	aerosol	
Combustion module	Turbulent combustion	detonation		
Heat structure module	Thin wall conduction	Radiation HT	Thick wall conduction	
Component module	PAR	igniter	Fan	Cooler
Flow solver module	Buoyant solver	Euler shock-capturing solver	Two-phase drift-flux solver	Two-phase two-fluid solver

Numerical and physical models for detonation simulation

Governing equations and models for a hydrogen detonation analysis

- **Compressible Euler equations without diffusion fluxes**
- **detonation shock capturing by central upwind scheme of Kurganov-Tadmore**
- **7-step chemical reaction of Shang et al.**

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0$$

$$\frac{\partial}{\partial t}(\rho \mathbf{U}) + \nabla \cdot (\rho \mathbf{U}\mathbf{U}) + \nabla p = \mathbf{S}$$

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla \cdot (\rho Y_i \mathbf{U}) = \dot{\omega}_i$$

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho H \mathbf{U}) = \dot{Q}$$

$$F_{j+1/2} = \frac{1}{2}\left[F\left(w^{+}_{j+1/2}\right) + F\left(w^{-}_{j+1/2}\right)\right] - \frac{1}{2} a_{j+1/2}\left[w^{+}_{j+1/2} - w^{-}_{j+1/2}\right]$$

$$a_{j+1/2} = \max\left[\lambda\left(\frac{\partial F(w^{-}_{j+1/2})}{\partial w}\right), \lambda\left(\frac{\partial F(w^{+}_{j+1/2})}{\partial w}\right)\right]$$

$$H_f = \frac{a^{+}_f f\left(w^{L}_f\right) + a^{-}_f f\left(w^{R}_f\right)}{a^{+}_f + a^{-}_f} - \frac{a^{+}_f a^{-}_f}{a^{+}_f + a^{-}_f}\left(w^{R}_f - w^{L}_f\right)$$

n	reaction	A	β	$T_a = E_a/R_u$
1	$H_2 + O_2 = 2OH$	1.7×10^{10}	0	24233
2	$H + O_2 = OH + O$	1.42×10^{11}	0	8254
3	$H_2 + OH = H + H_2O$	3.16×10^{4}	1.8	1525
4	$O + H_2 = OH + H$	2.07×10^{11}	0	6920
5	$2OH = H_2O + O$	5.5×10^{10}	0	3523
6	$H + OH + M = H_2O + M$	2.21×10^{16}	-2	0
7	$2H + M = H_2 + M$	6.53×10^{11}	-1	0

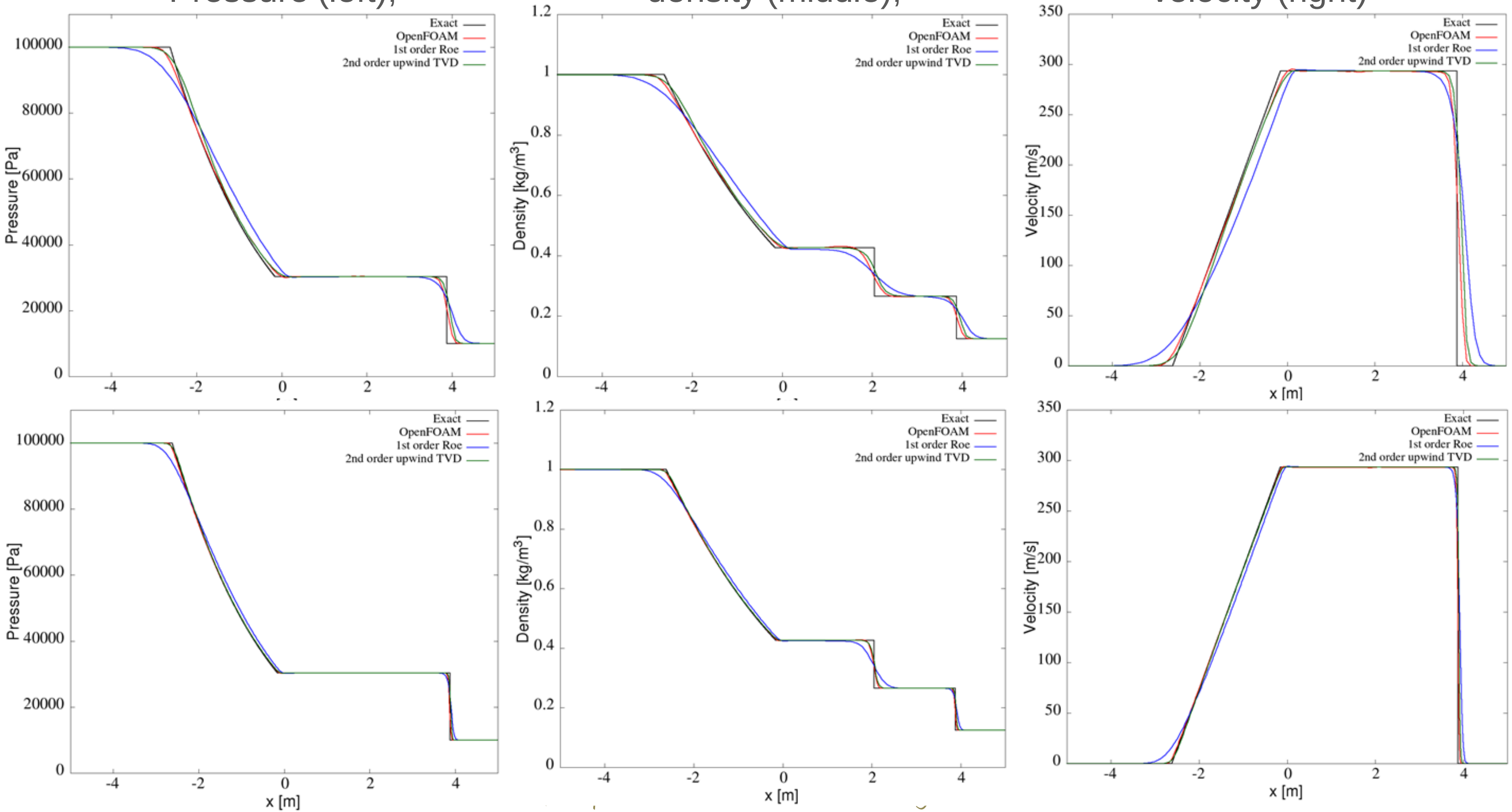
1-D shock tube problem

- Simulation of a shock tube problem
  - Calculation of shock tube to 7 ms with 100 and 400 grid points
  - Data comparison using 1st order Roe, 2nd order Upwind TVD, OpenFOAM, exact solution

< Pressure (left), density (middle), velocity (right) >

by 100 cells

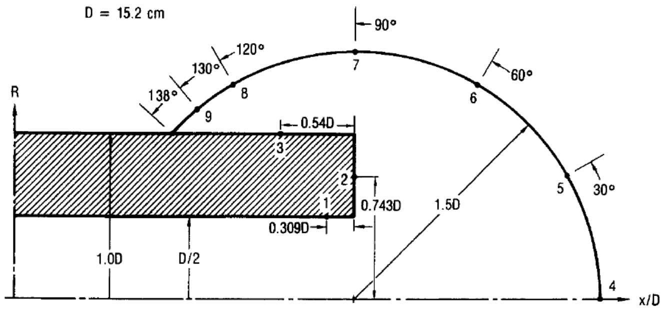
by 400 cells

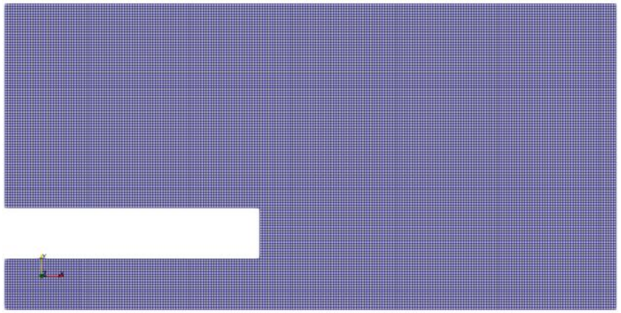


Simulation of blast wave problem

- Simulation of the blast experiment by Schmidt and Duffy
  - Computational domain is 2-D axisymmetric.
  - Mesh is composed of 26,800 hexahedral cells.
  - Shock tube inlet has fixed total pressure and temperature BCs

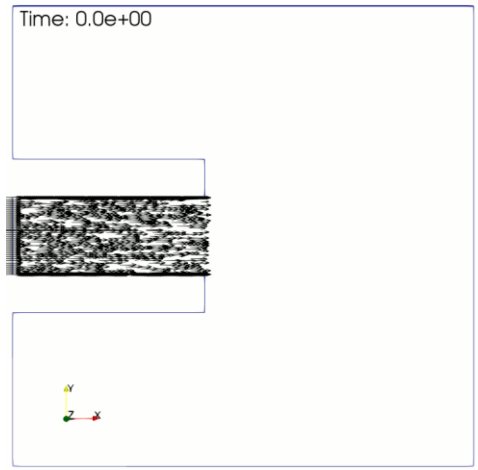
Schematic of shock tube experiment

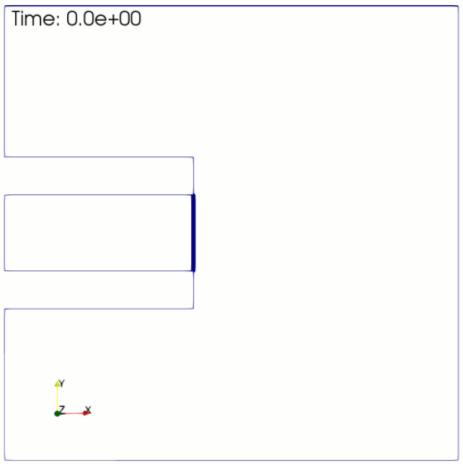




Mesh for simulation

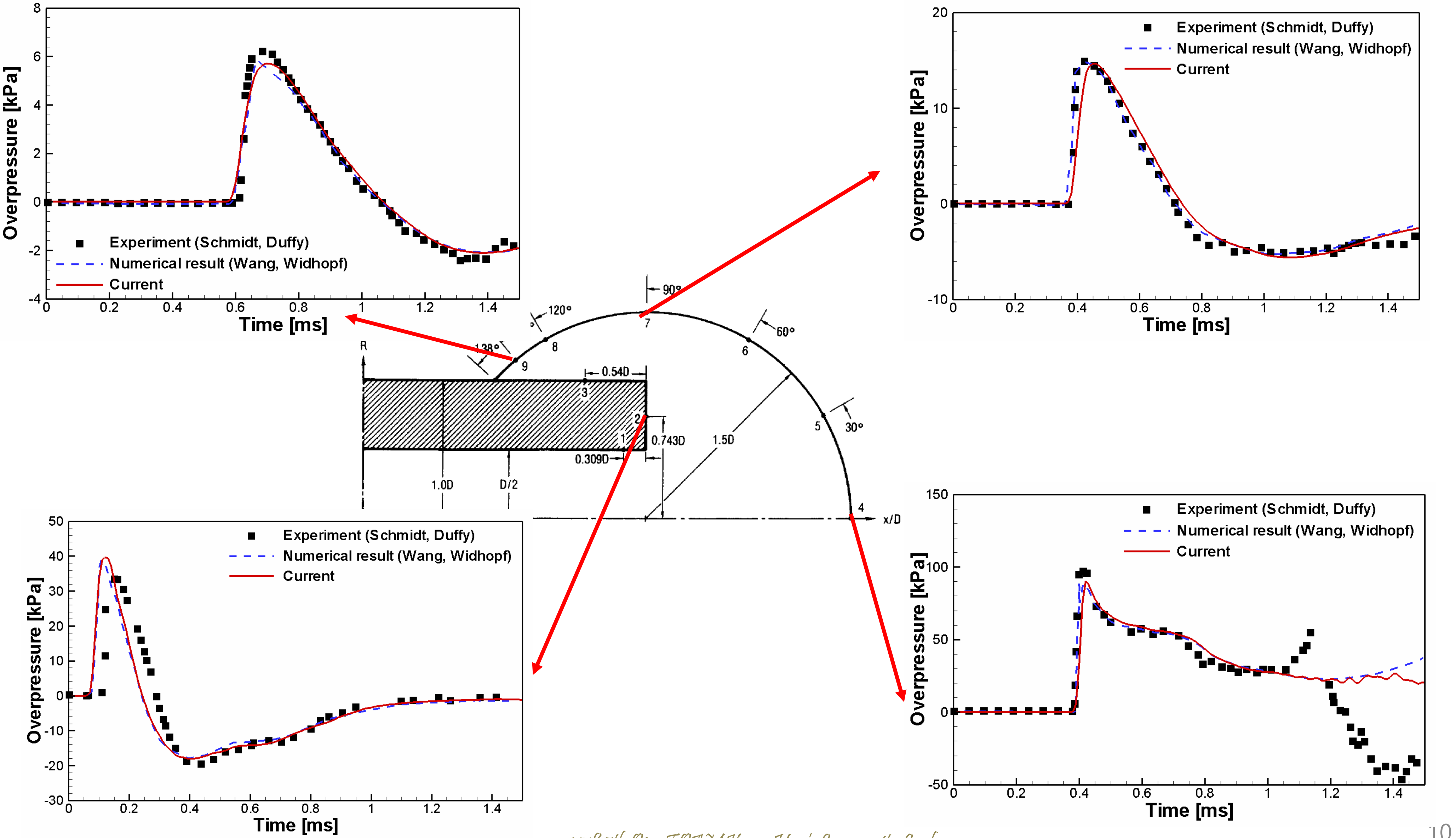
Velocity fields from simulation





Pressure field from simulation

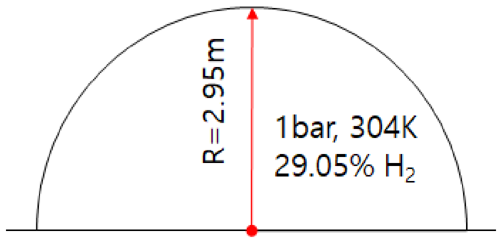
Comparison of overpressures along time

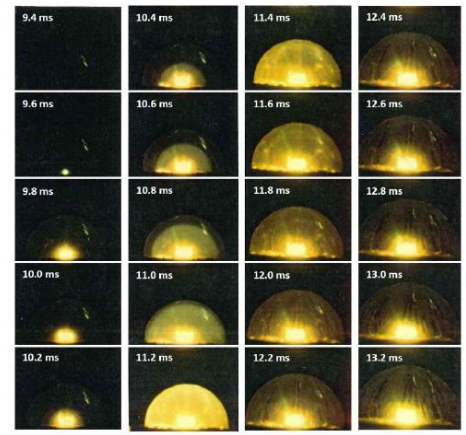


Simulation of spherical balloon test

❑ Spherical detonation experiment

- Hydrogen-air detonation experiments in hemispherical balloons were performed at Fraunhofer Institute.
- 29vol% hydrogen-air in 2.95m balloon
- Mixture was ignited centrally with 50 g of high explosive

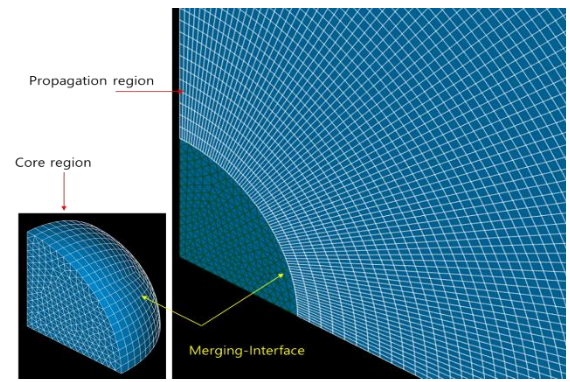




❑ Simulation of the spherical balloon test

- Simulation geometry: a quarter of the hydrogen balloon, number of cells: 731,190
- Initiation of detonation
  - blast pressure from Sadovsky equation

$$\Delta p_m = \left[1.02 + \left(4.36 + 14\frac{m^{1/3}}{r}\right)\frac{m^{1/3}}{r}\right]\frac{m^{1/3}}{r} \quad [\text{bar}]$$



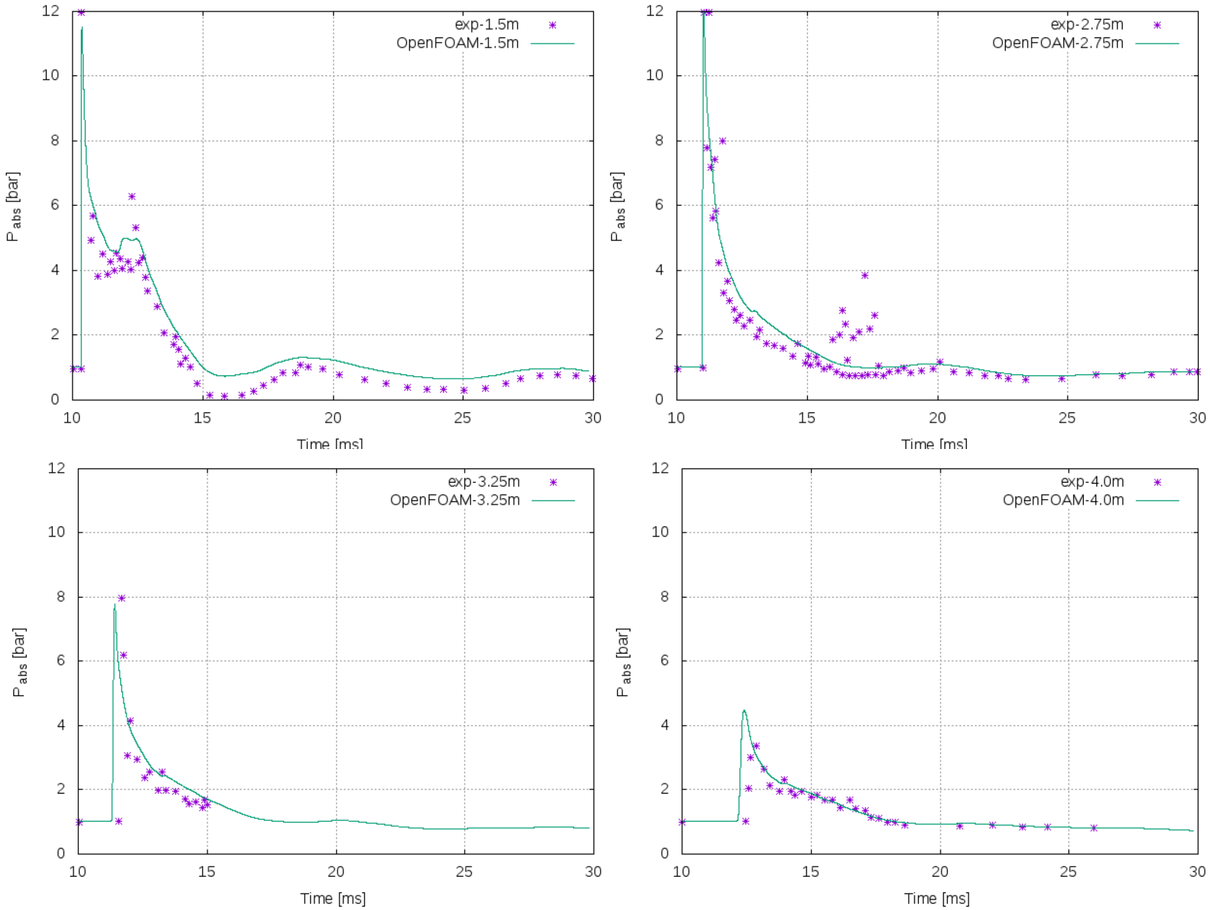
Simulation of spherical balloon test

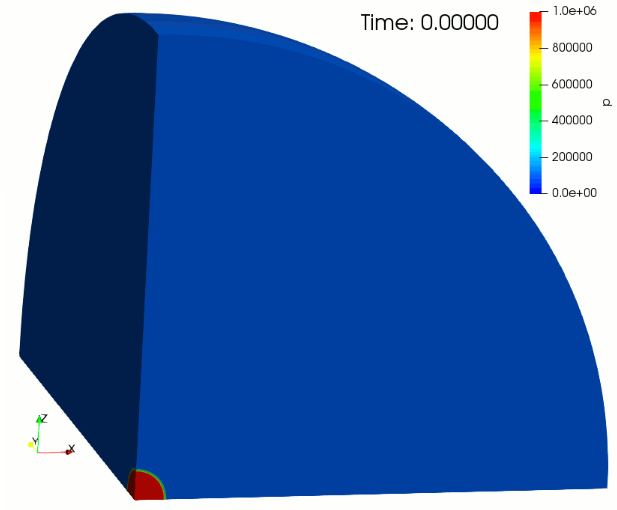
❑ Simulation results of the spherical balloon test

❍ Comparison of results from OpenFOAM and experiments

Inside balloon

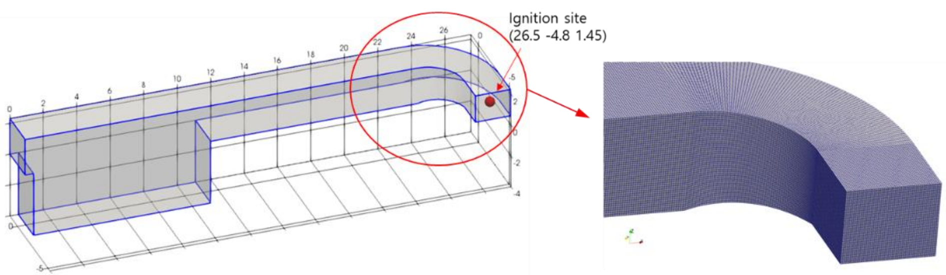
Outside balloon

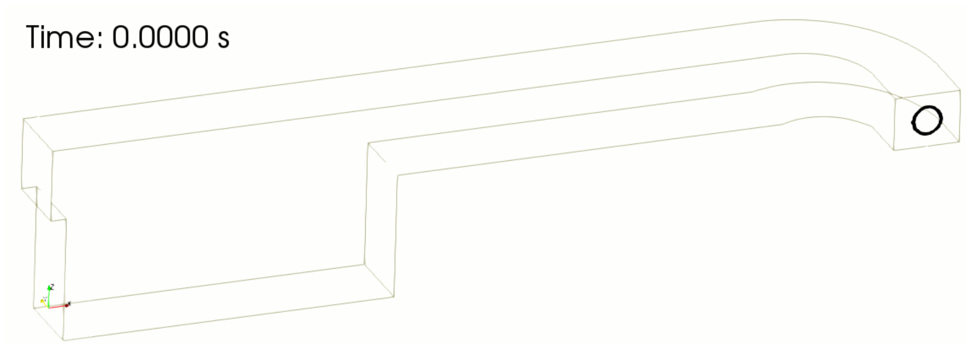




Simulation of RUT detonation experiment

- **Simulation of the KI-RUT-HYD09 test**
  - detonation initiation by 200g of TNT
    - spherical shock with radius of 0.65 m and pressure of 15.85 bar was set
  - Internal structure neglected
  - Mesh is composed of hexahedral cells of 2,211,900
- **Propagation of shock waves**
  - In the simulation result, shock waves interact very complicatedly

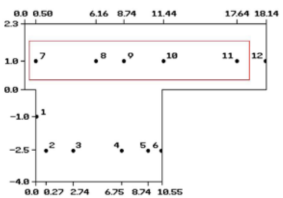


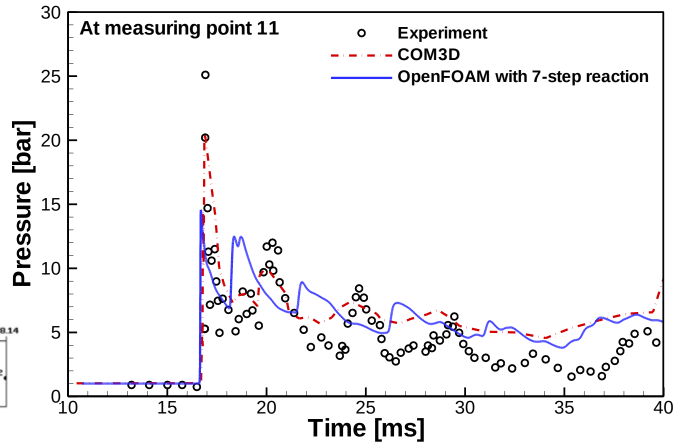


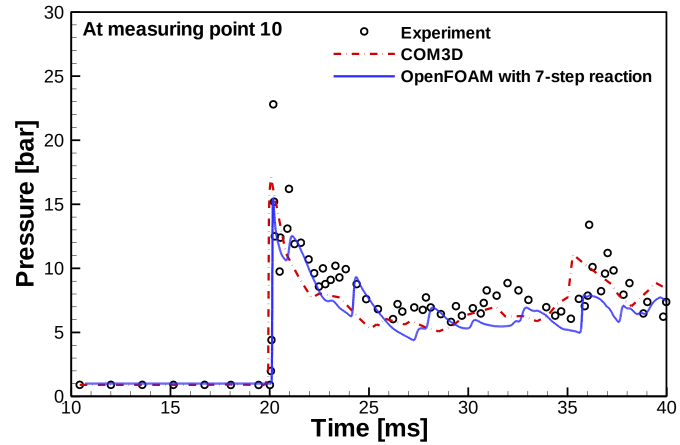
Simulation of RUT detonation experiment (2)

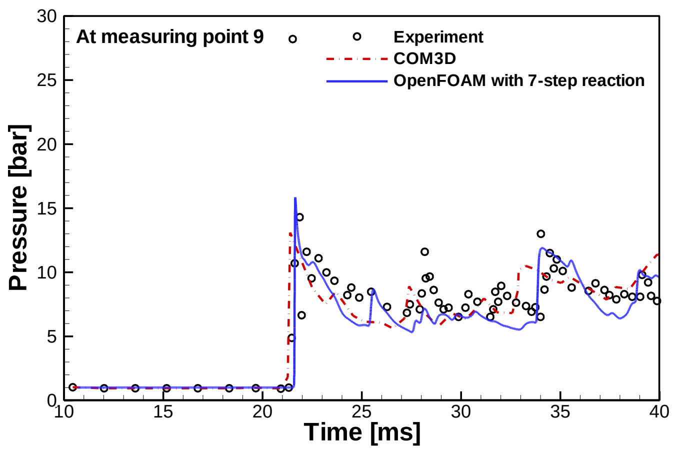
❑ Pressure variations for KI_RUT-HYD09

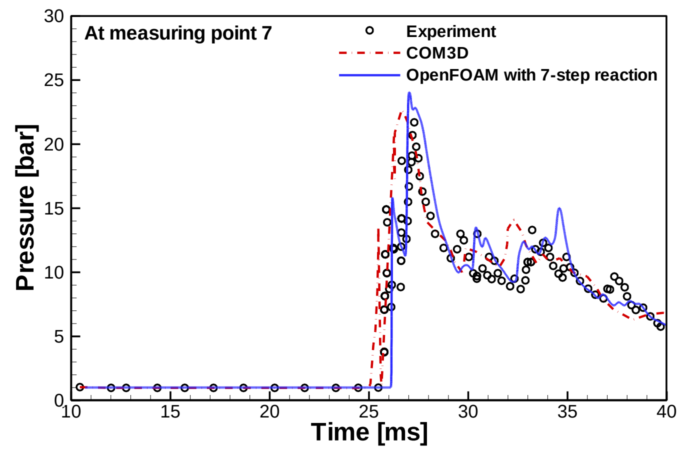
- The arrival time of the leading shock at the point 11 in the simulation was shifted in order to synchronize the pressure-time histories between the experimental and numerical data









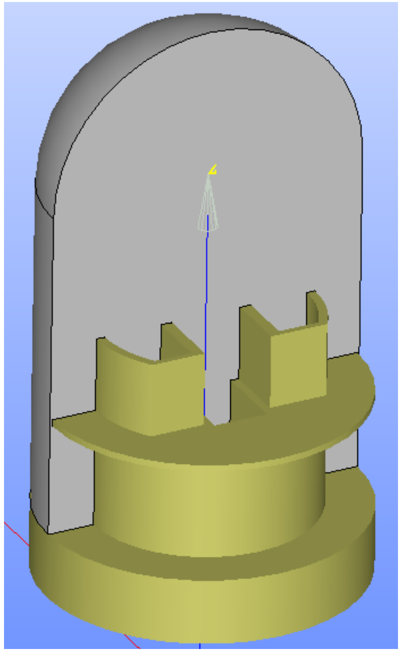


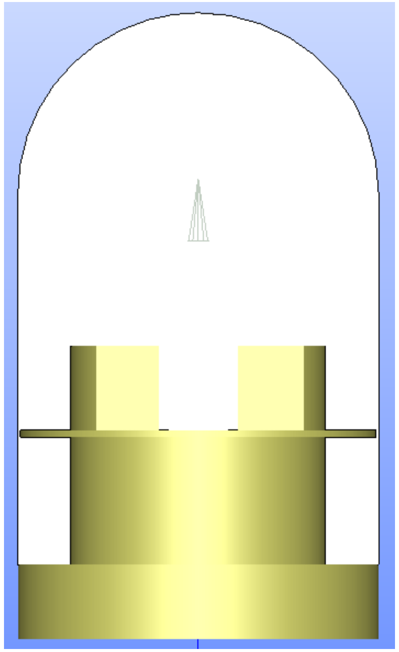
Detonation in a generic containment

❑ Generic containment

- Virtual containment for an evaluation of detonation in a dome region
- Basic shape is hemi-spherical dome on a cylinder similar to domestic LWR (light water reactor) containments
- Internal structure is simplified

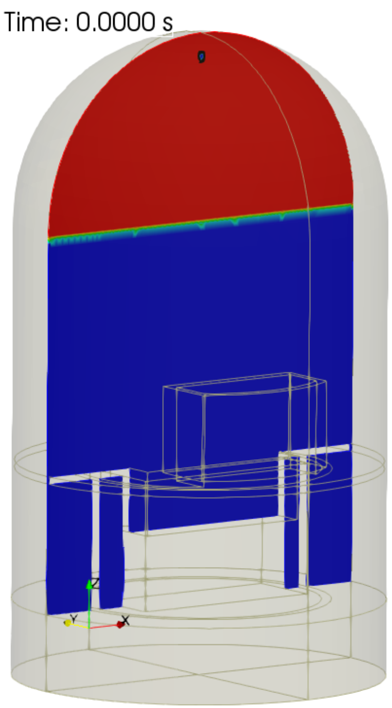
Height	79 m
Diameter	46 m
Free volume	95,400 m^3



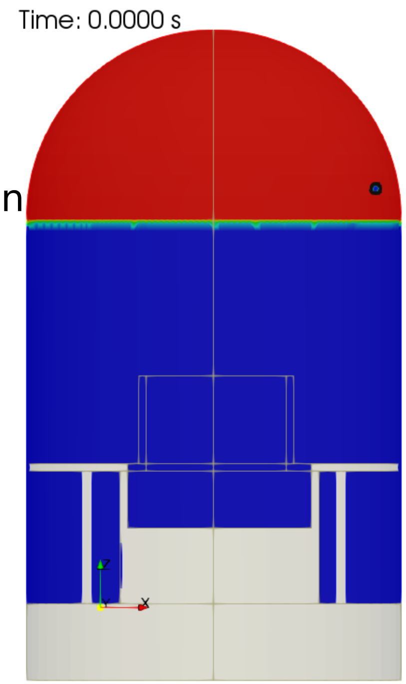


Detonation in a generic containment (2)

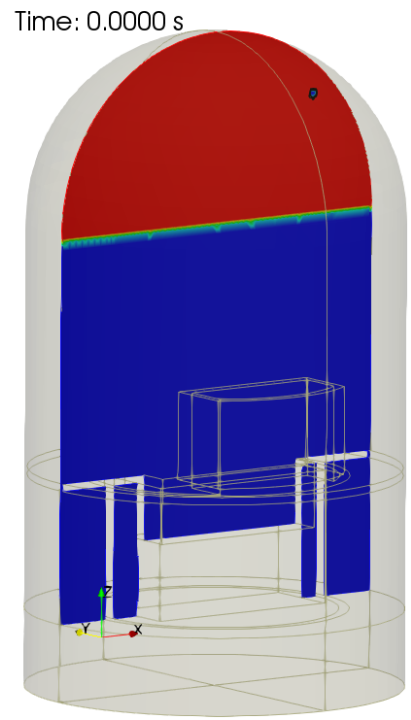
- **Hydrogen distribution**
  - **In dome region hydrogen concentration of 20 vol% ($X_{air}:X_{h2}$ = 0.8:0.2)**
- **Detonation initiation by 200g of TNT**
- **Study on detonation shock propagation dependent on initial detonation locations**



Case1: top point initiation



Case2: side point initiation

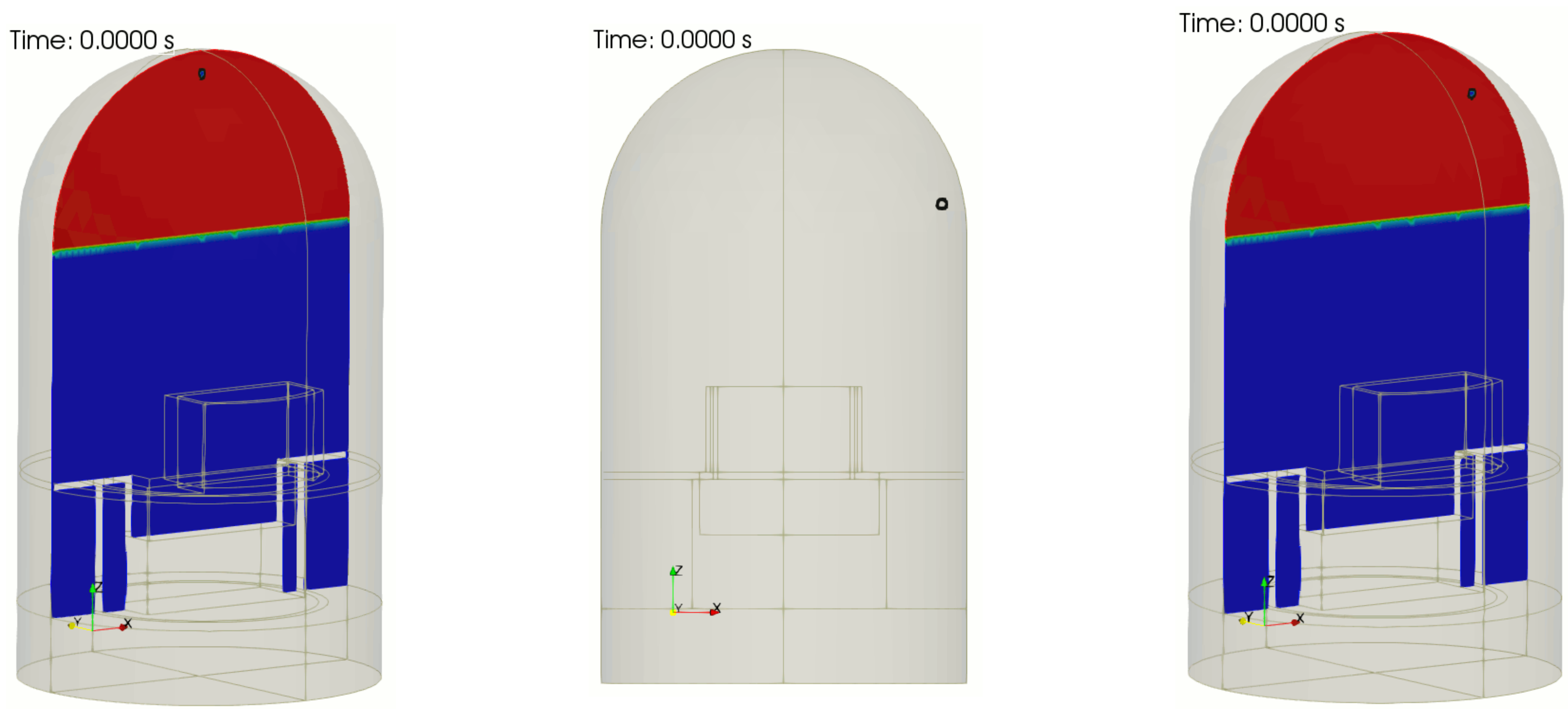


Case3: middle point initiation

Detonation in a generic containment (3)

❑ Simulation results for detonation propagation

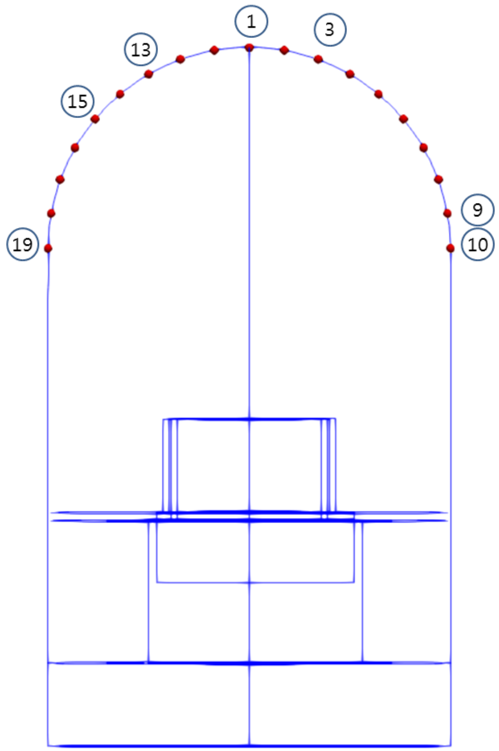
- Detonation shock propagations for three test cases
- As can be expected, the structure of the detonation shock and its propagation is dependent on the initiation location.

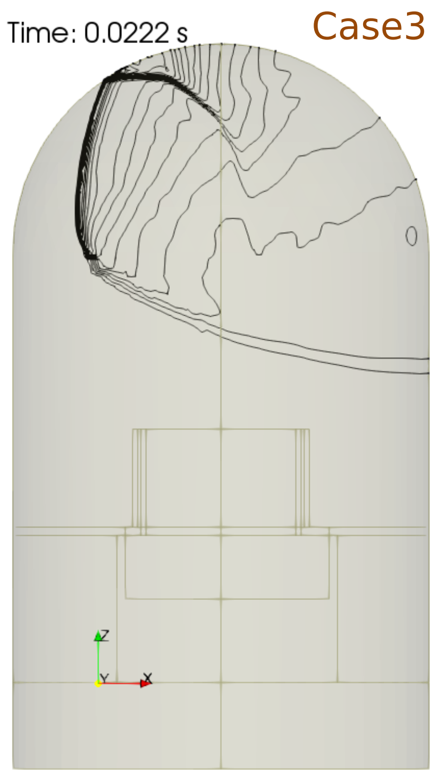


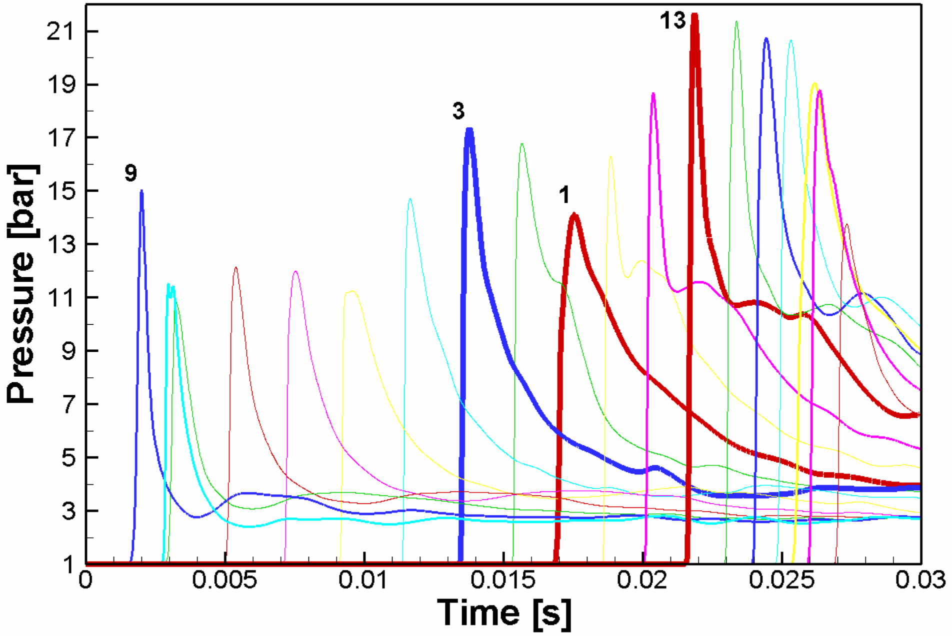
Detonation in a generic plant (4)

❑ Pressure load on the dome wall

- Pressure-time histories for the case3
- The pressure magnitude is doubled at point 13 because of a reflected shock.







Summary and future plan

- Detonation phenomena accompanying chemical reactions have been simulated with an OpenFOAM solver with a reduced 7-step chemistry model.
- It was found out that the OpenFOAM solver can resolve complicated shock structures well. The OpenFOAM solver gives similar performance to 2nd order upwind TVD scheme.
- As a future work it is considered to develop a methodology to evaluate structure integrity by coupling detonation analysis code and structural analysis code