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Modelling structural Responses in Vented lean deflagrations

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Outline

- Objective
- HyFOAM solver description
- CFD and FE
- Numerical results
- Concluding remarks

Introduction

- Explosion venting is a preventive measure used to reduce the overpressures in an enclosure and confinements, during an accidental explosion.
- The excess pressure generated as a result of explosion is channeling into atmosphere through vent opening to protect the integrity of the enclosure
- The important design parameter is the appropriate vent area necessary for effective release of overpressures to atmosphere without causing much of flow constriction

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Objective

- Container installations are being considered for hydrogen application.
  - standalone portable power generation units – Fuel cells
  - refuelling station accessories – compressor , pumps
- Developing CFD solver to model the vented lean hydrogen deflagrations. (OpenFOAM libraries)
- Non-rigid structures effect on overpressure trends.
- Aid in filling the experimental knowledge gap.
- Improving Engineering models.

Numerical method (HYFOAM)

- Large Eddy Simulations (LES) /RANS method in OpenFOAM.
- The Favre-filtered unsteady compressible Navier-Stokes equations are solved in a segregated manner, wherein each dependent variable equation is solved sequentially.
- The pressure-velocity coupling is handled using Pressure-Implicit Split Operator (PISO) solution method.
- Sub-grid turbulence kinetic energy is solved using the one equation eddy viscosity model.

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Combustion model

- The flame wrinkling combustion model of Weller et al. (1998).
- Considering a single step chemistry, **unity Lewis number** and flamelet regime, the thermo chemistry of the reacting flow is described by the unburnt zone volume fraction denoted as regress variable (b), taking values 1 and 0 in unburnt and fully burnt region. The transport equation for the regress variable:

$$\frac{\partial \bar{\rho}\tilde{b}}{\partial t} + \nabla.\left(\bar{\rho}\tilde{U}\tilde{b}\right) - \nabla.\left(\bar{\rho}D\nabla\tilde{b}\right) = -\bar{\rho}_u S_u \Xi \left|\nabla\tilde{b}\right|$$

where, Ξ is subgrid flame wrinkling, S_u is laminar flame speed

- Mixture fraction equation is also solved – inhomogeneous mixtures

WELLER, H. G., TABOR, G., GOSMAN, A. D. & FUREBY, C. (1988) Application of a flame-wrinkling les combustion model to a turbulent mixing layer. Symp. (Int.) on Combustion, 27, 899-907.

Experimental observation of vented gas explosions

Physical phenomena (McCann et al. 1985):

- Helmholtz oscillations.
- Cellular spherical flames.
- RT instabilities.
- Acoustical modes of the enclosure.
- Turbulence

McCANN, P. J., THOMAS, G. O., and EDWARDS, D. H. (1985) Geodynamics of Vented explosions Part I: Experimental studies, Combustion and Flame, 59 : 233-250.

Flame wrinkling factor

- The closure for the sub-grid wrinkling (Ξ) is provided considering the flame instabilities into three components *,

$$\Xi = \Xi_T * \Xi_{RT} * \Xi_{DL}$$

where, Ξ_T corresponds to the surface wrinkling factor due to turbulence,

Ξ_{DL} is surface wrinkling factor due to the Darrieus-Landau flame instability,

Ξ_{RT} is the surface wrinkling factor due to the Rayleigh-Taylor instability.

** BAUWENS, C. R., CHAFFEE, J. & DOROFEEV, S. B. (2011a) Vented explosion overpressures from combustion of hydrogen and hydrocarbon mixtures. International Journal of Hydrogen Energy, 36, 2329-2336.*

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Flame wrinkling due to turbulence

- The surface wrinkling factor due to turbulence (Ξ_t) is modelled as transport equation *

$$\frac{\partial \overline{\rho} \Xi_T}{\partial t} + \widehat{U}_s . \nabla \Xi_T = \overline{\rho} G \Xi_T - \overline{\rho} R (\Xi_T - 1) + \overline{\rho} \max\left[(\sigma_s - \sigma_t), 0 \right] \Xi_T$$

The modelling for the respective terms in above equation are given as,

$\sigma_t = \frac{1}{2} \left\| \nabla \widehat{U}_t + \widehat{U}_t^T \right\|$ and $\sigma_s = \frac{1}{2} \left\| \nabla \widehat{U}_s + \widehat{U}_s^T \right\|$ resolved strain rates,

$\mathrm{G} = \mathrm{R} \frac{\mathrm{E}_{eq} - 1}{\mathrm{E}_{eq}}$ and $\mathrm{R} = \frac{0.28}{\tau_\mathrm{n}} \frac{\mathrm{E}_{eq}^*}{\mathrm{E}_{eq}^* - 1}$ are subgrid turbulence generation and removal rates with $\mathrm{E}_{eq} = 1 + 2(1 - \overline{b})(\mathrm{E}_{eq}^* - 1)$, E_{eq}^*

* WELLER, H. G., TABOR, G., GOSMAN, A. D. & FUREBY, C. (1988) Application of a flame-wrinkling les combustion model to a turbulent mixing layer. Symp. (Int.) on Combustion, 27, 899-907.

Darrieus-Landau flame instability

- The surface wrinkling factor due to the Darrieus-Landau flame instability is modelled as (Ξ_{DL})

$$\Xi_{DL} = \max\left[1, \alpha_1\left(\frac{\Delta}{\lambda_c}\right)^{1/3}\right]$$

where, λ_c is cutoff wavelength of unstable scale, α_1 is a coefficient to account for the uncertainty in λ_c.

* BAUWENS, C. R., CHAO, J. & DOROFEEV, S. B. (2011) Evaluation of a multi peak explosion vent sizing methodology .

RT instability - Transport Eq.

- The surface wrinkling factor due to turbulence (Ξ_{RT}) is modelled as transport equation *.

$$\frac{\partial \bar{\rho} \Xi_{RT}}{\partial t} + \hat{U}_s . \nabla \Xi_{RT} = \bar{\rho} G_{RT} (\Xi_{RT} - 1) - \bar{\rho} R_{RT} (\Xi_{RT} - 1)$$

- generation rate of flame wrinkling due to RT instability

$$\mathrm{G} = 2\left(k_{G_{RT}} \frac{\sigma - 1}{\sigma + 1} \vec{a}.\vec{n} \right)^{1/2}$$

- removal rate of flame wrinkling due to RT instability

$$R_{RT} = \frac{8 \sigma S_L k_{R_{RT}}}{\pi}$$

* BAUWENS, C. R., CHAFFEE, J. & DOROFEEV, S. B. (2011) Vented explosion overpressures from combustion of hydrogen and hydrocarbon mixtures. International Journal of Hydrogen Energy, 36, 2329-2336.

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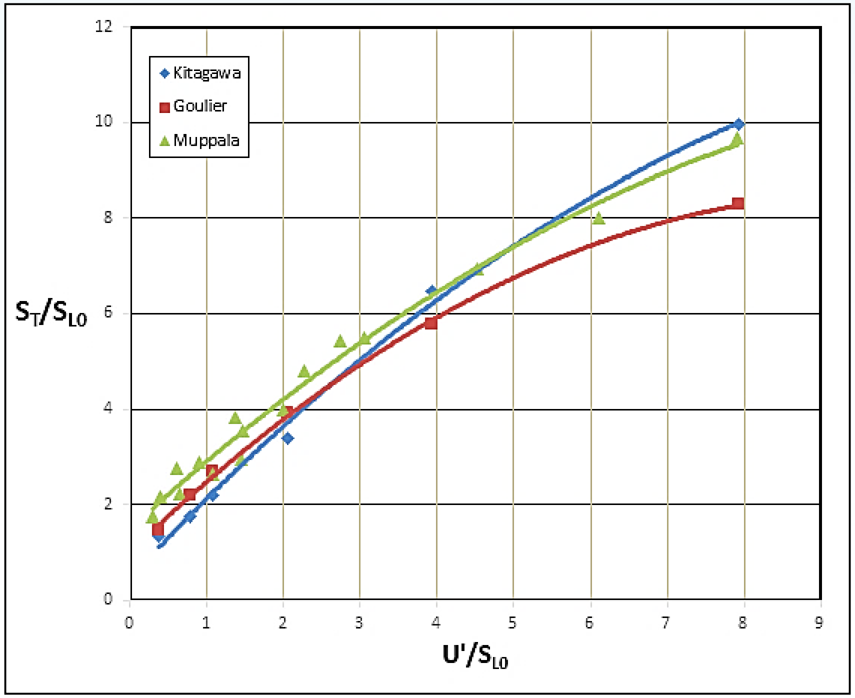
Turbulent flame speed correlation



$$\Xi_{eq}^{*} = 1 + \frac{0.46}{Le} Re_t^{0.25} \left(\frac{\hat{u}}{S_{Lo}} \right)^{0.3}$$

- Muppala Reddy, S. P., Aluri Naresh K., Dinkelacker, F., Development of an algebraic reaction rate closure for the numerical calculation of turbulent premixed methane, ethylene, and propane/air flames for pressure up to 1.0 MPa (2005), Combust. And Flame, 140
- Kitagawa, T., Nakahara, T., Maruyama, K, Kado, K., Hayakawa, A., Kobayashi, S., Turbulent burning velocity of hydrogen-air premixed propagating flames at elevated pressure (2008), Int. Jol. of hyd. Energy, 20:33.
- Goulier, J. Comandini, A., Halter, F., Chayumeix, N., experimental study on turbulent expanding flames of lean hydrogen/air mixtures (2016), Proc. Combust. Inst.

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Laminar flame speed for lean-hydrogen-air mixtures

- Power law function of elevated temperature and pressure*

$$S_L = S_{L0}(\lambda, P)\left(\frac{T_u}{T_{u0}}\right)^{\alpha(\lambda,\ P)}$$

$$S_{L0} = 499.63 - 308.60\lambda + 48.887\lambda^2 - 76.238P + 4.825P^2 + 45.813\lambda P - 2.926\lambda P^2 - 7.163\lambda^2 P + 0.436\lambda^2 P^2$$

$$\alpha(\lambda, P) = 1.85175 - 0.70875\lambda + 0.50171\lambda^2 - 0.19366P + 0.0067834P^2 + 0.27495\lambda P - 0.0088924\lambda P^2 - 0.052058\lambda^2 P + 0.00146015\lambda^2 P^2$$

- S_L in cm/s , P is pressure in bar and unburnt gas temperature in K.
- Correlation is valid for the equivalence ratios between 0.33 and 0.47 (lean mixtures), pressures range of 1 bar to 8.5 bar and temperature range of 300 K to 800 K.

* Verhelst, S, Sierens , R., A laminar burning velocity correlation for hydrogen-air mixture valid at the spark ignition engine conditioned, ASME spring engine technology conference, 2003, Austria.

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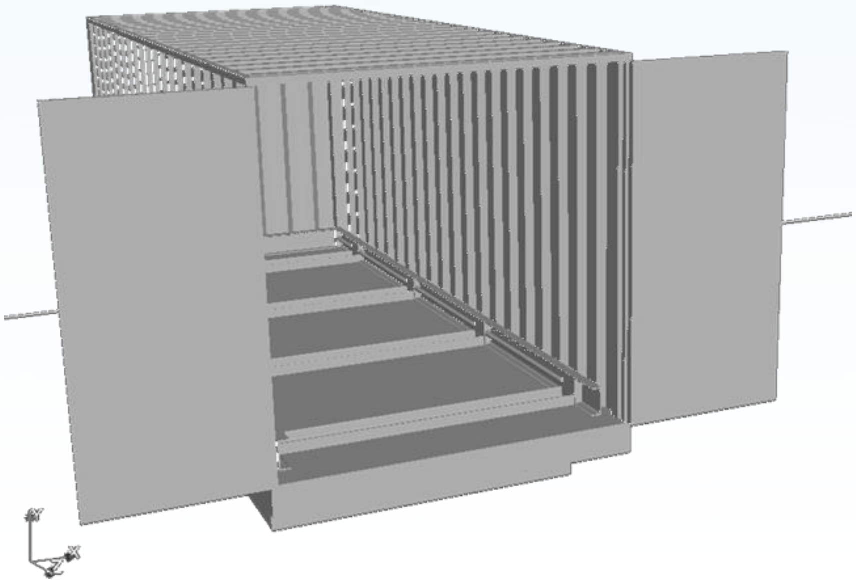
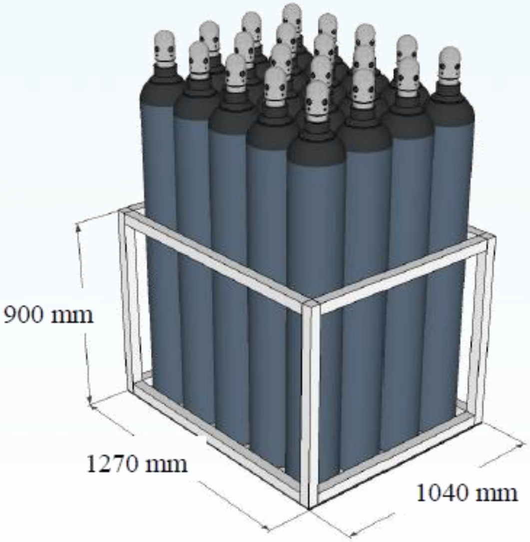
Geometry



A typical standard 20 ft. ISO container used in the experiments at GEXCON

Congestion

(a) Container corrugation



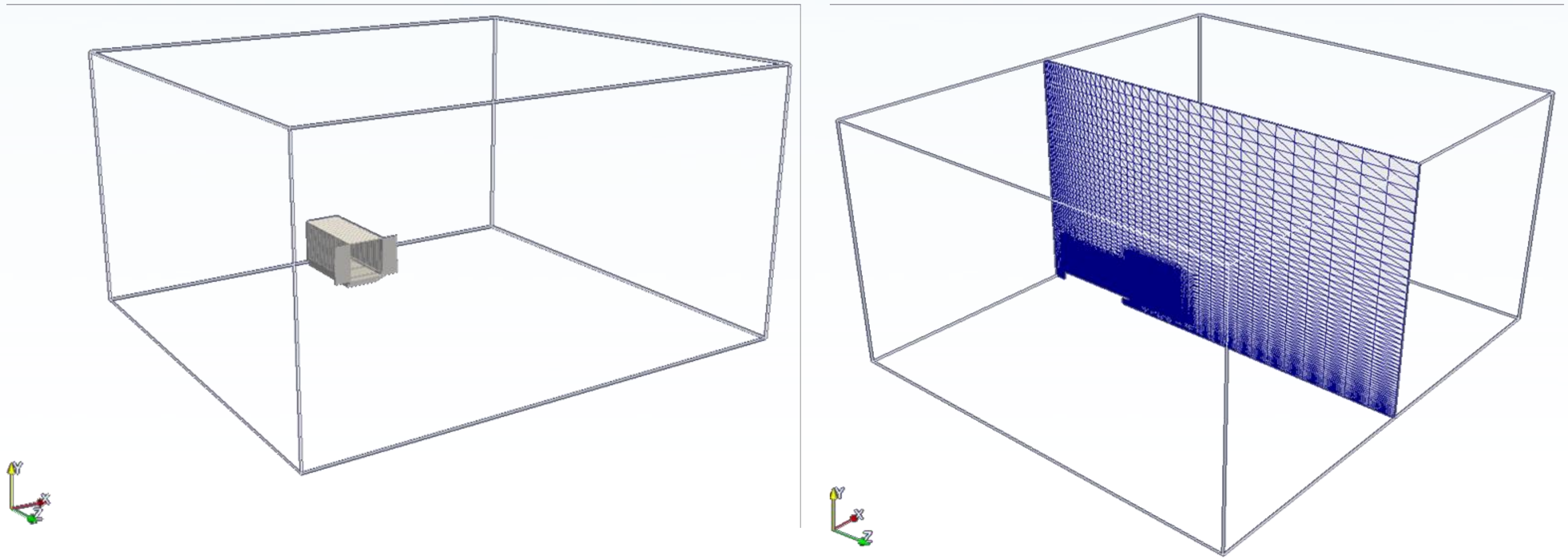
(c) Bottle stack

(b) Obstacle holding frame

(d) Pipe rack

Computational domain

The vented chamber is enclosed by 30.0 x 10.0 x 30 m mesh volume to capture the venting of burned gas, the external explosions and to reduce the effect of boundary conditions on the numerical results



Computation domain and the mesh distribution in the vertical and horizontal plan.

Total domain discretized into (5-8) x 10^6 hybrid cells (hex, tet, prisms)

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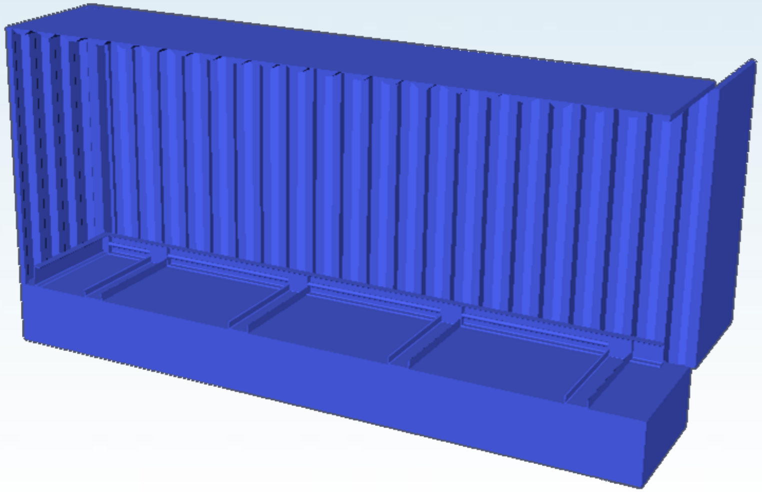
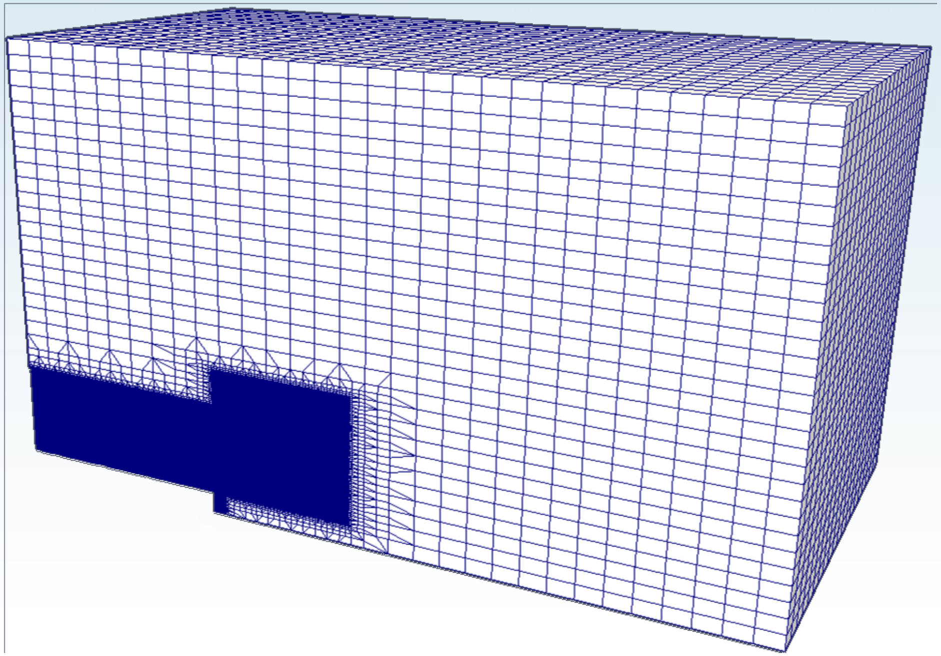
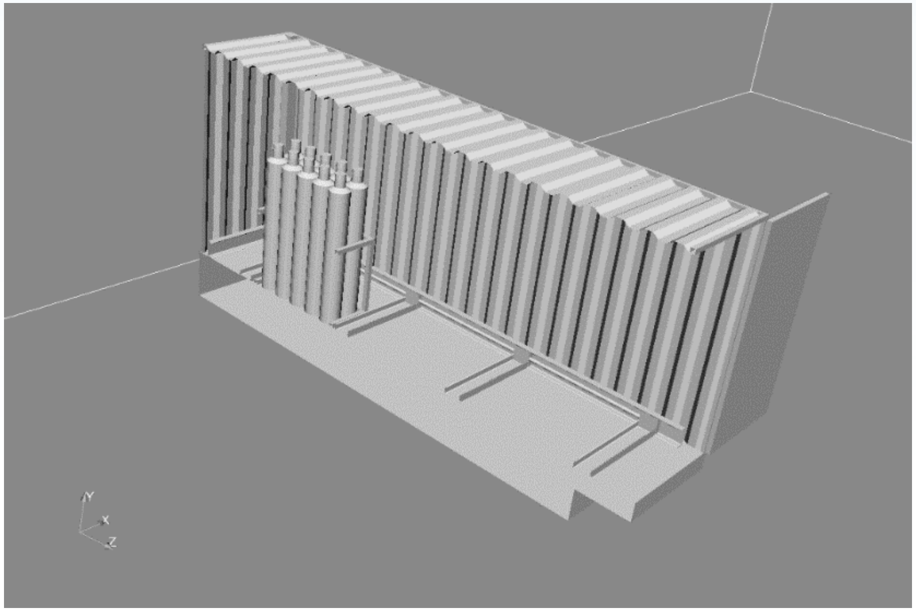
Geometry



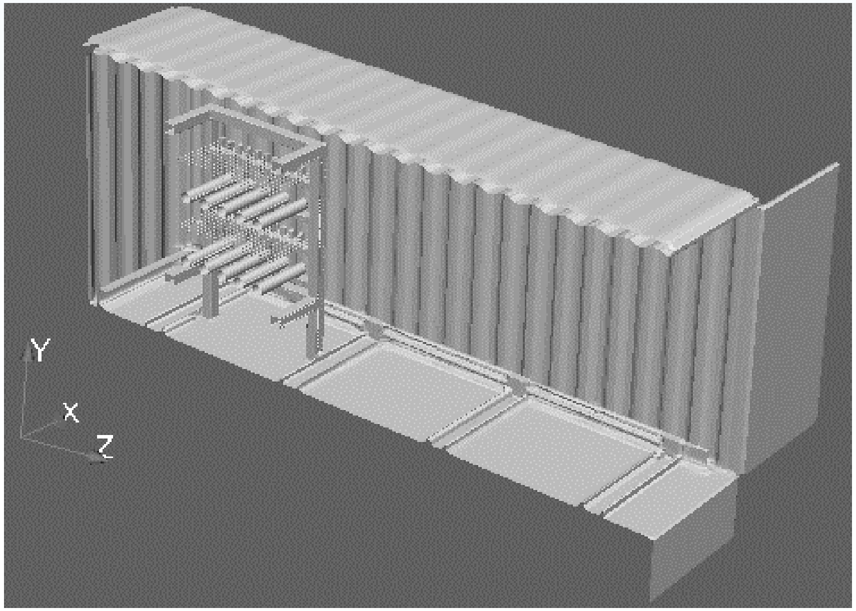


Geometry and Meshing

Computational domain



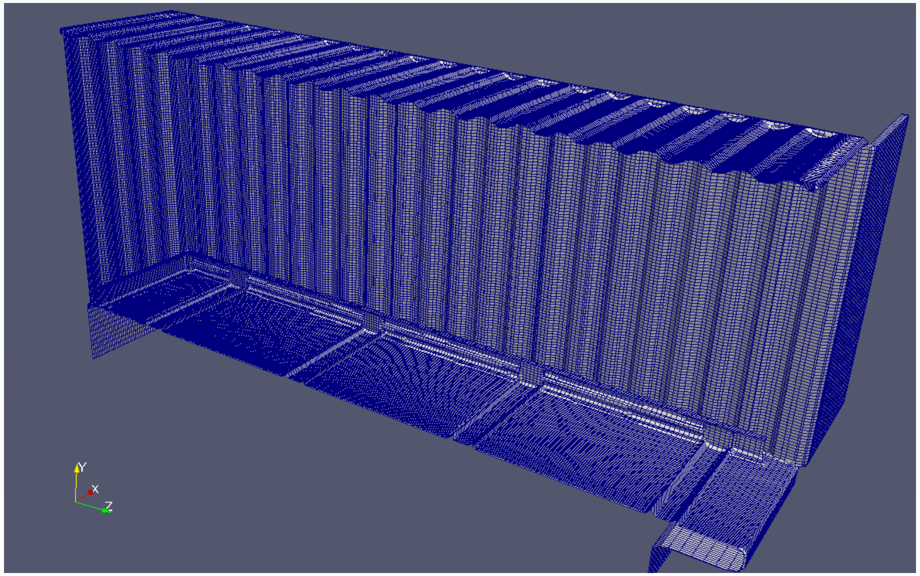
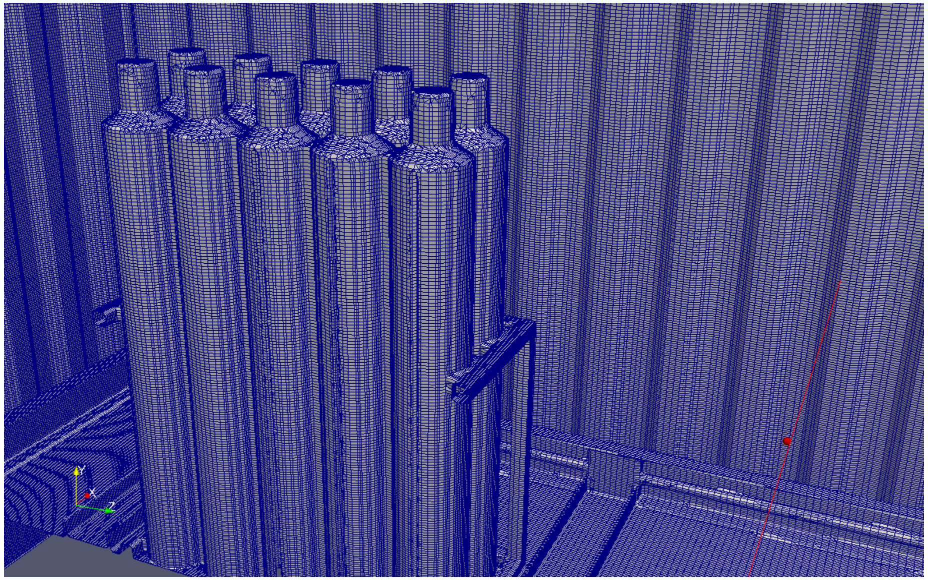
(a) With bottle basket obstacle



(b) With pipe rack obstacle

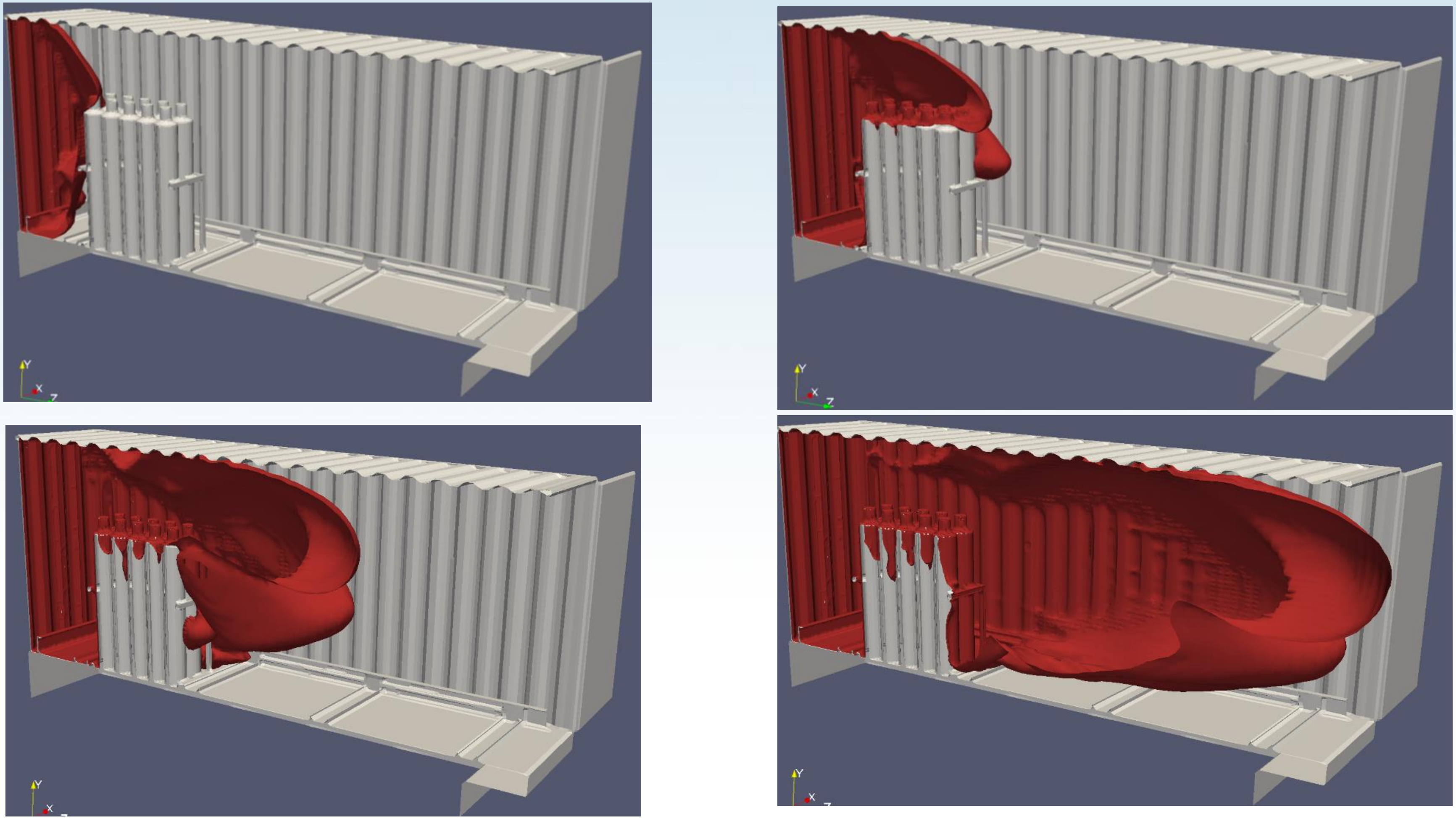
The standard 20-ft ISO container with model obstacles

Mesh resolution

The mesh distribution on the obstacles (sample)

Flame contours



Numerical Setup

- Boundary conditions

Variable	boundary	condition
velocity	Opening	totalpressure
	Wall	No-Slip
Pressure	Opening	Pressurevelocityinlet outlet
	Wall	Zero Gradient
Temperature	Opening	inletOutlet
	Wall	FixedValue

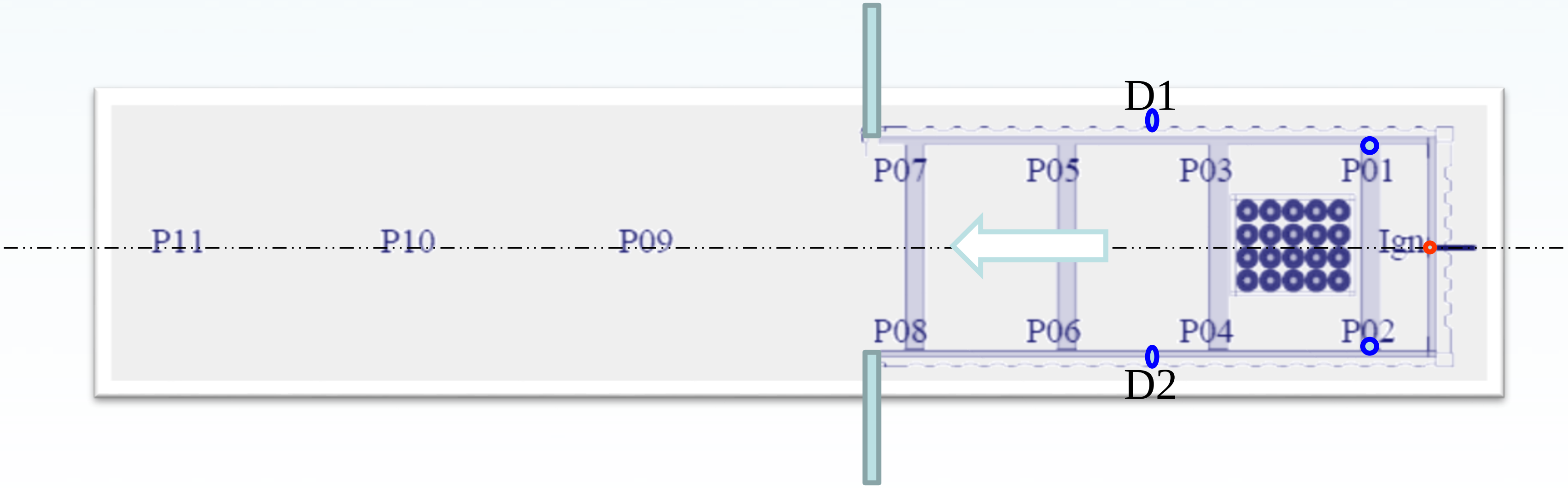
- The flow field is initialized with zero mean and u' = 0.1 m/s rms velocity.
- The mixture faction value of 0.0122 was initialized inside the venting chamber volume for 15 % hydrogen volume concentration.

Venting scenarios

Through Door

Container Roof

Probe locations



Top view

Vented explosion Experiment (empty) at Gexcon

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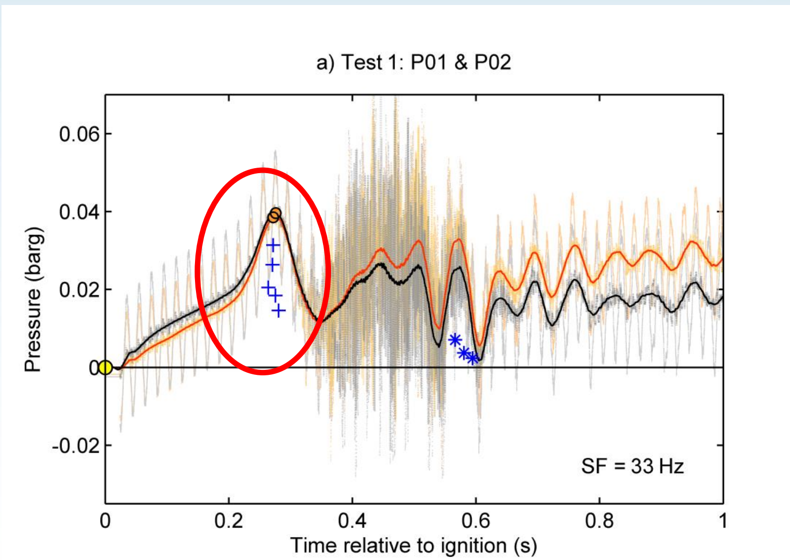
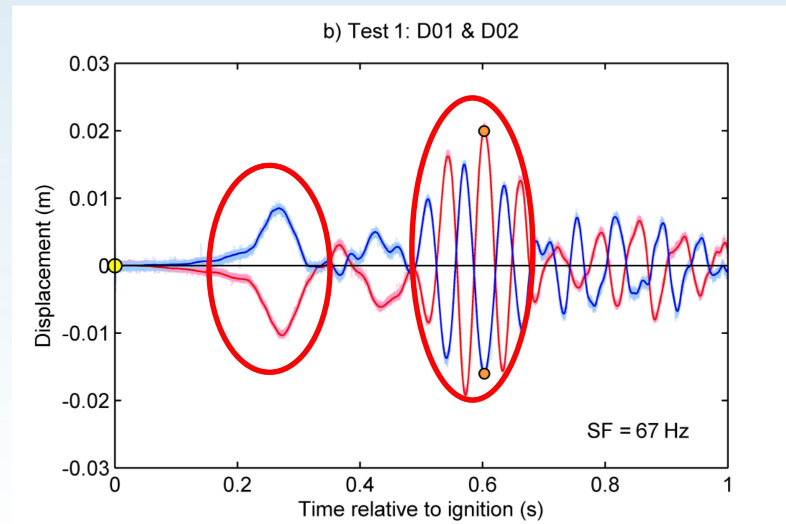
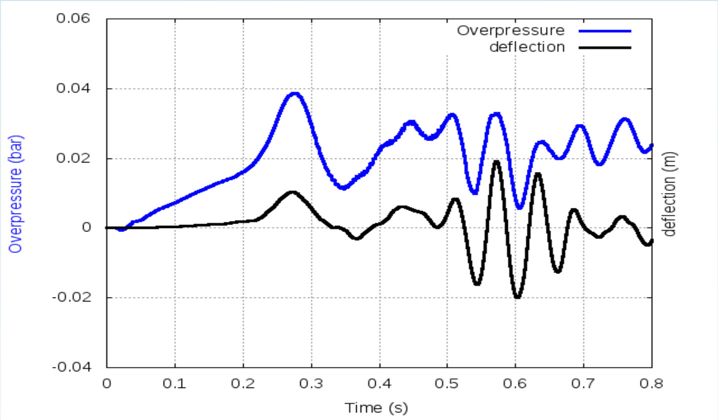
Pressure vs wall deflections

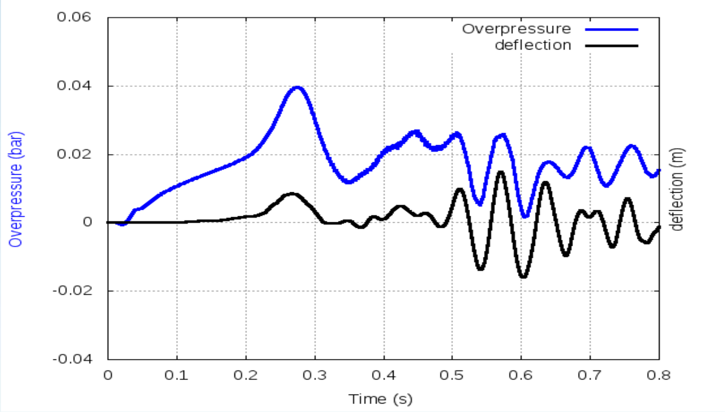




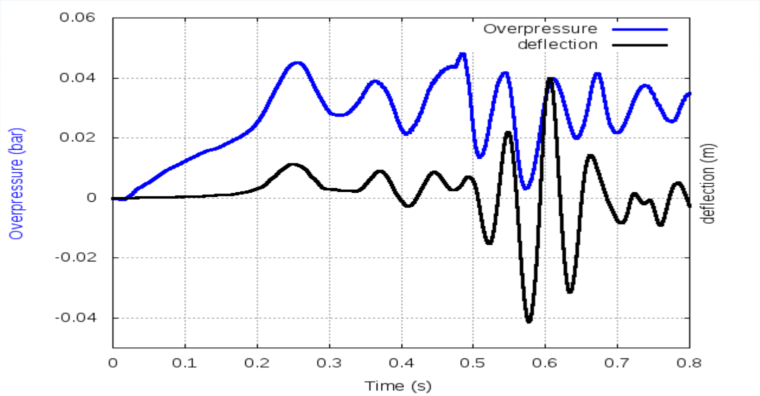
Test - 1: 15% H_2, Empty Container, overpressure and deflection trace curves (done at Gexcon)

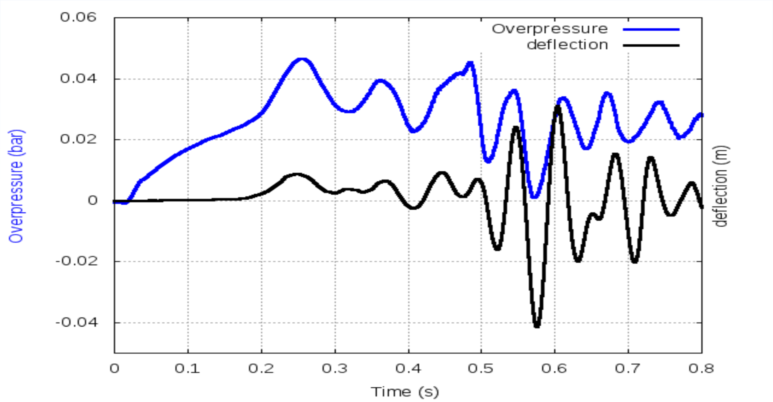
Quasi-equilibrium





Test-1 : 15% H_2, Empty, overpressure and deflection trace curves





Test-2 : 15% H_2, Empty, overpressure and deflection trace curves (done at Gexcon)

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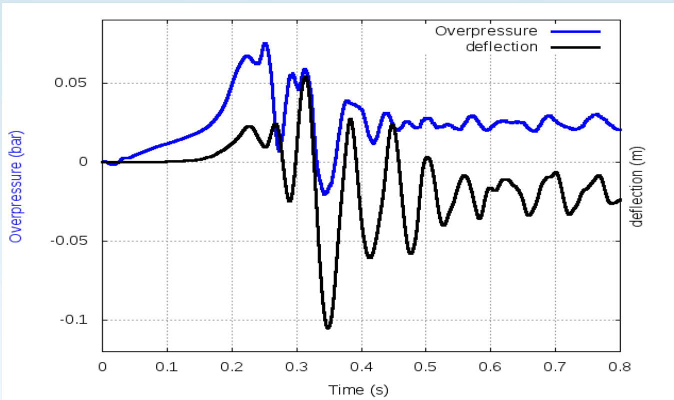
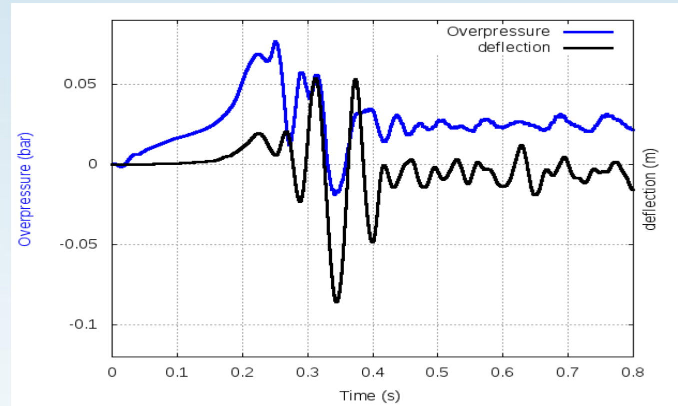
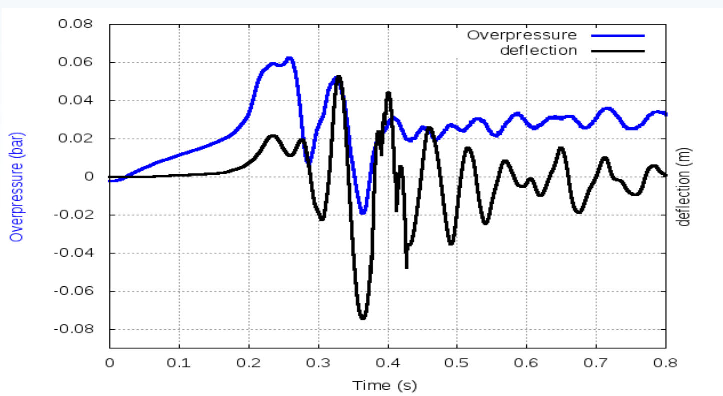
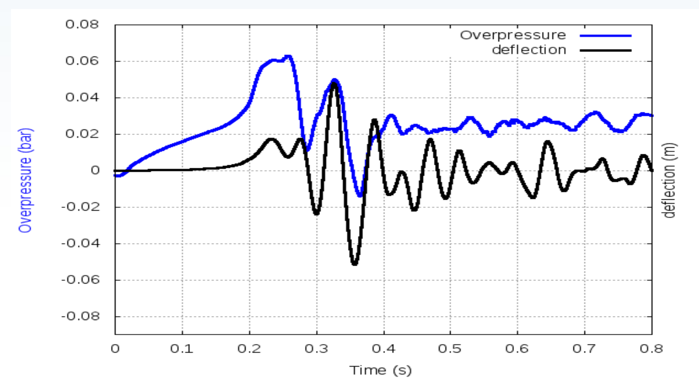
Quasi-equilibrium (2)





Test-3 : 15% H_2, Cylinder , overpressure and deflection trace curves





Test-4 : 15% H_2, Cylinder , overpressure and deflection trace curves (done at Gexcon)

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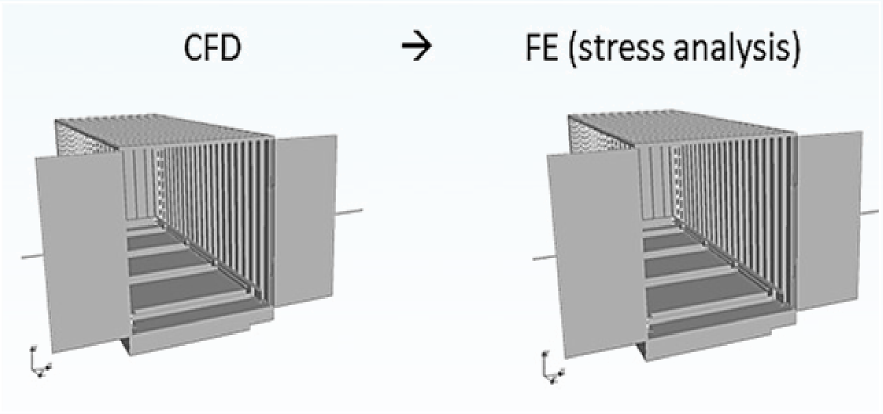
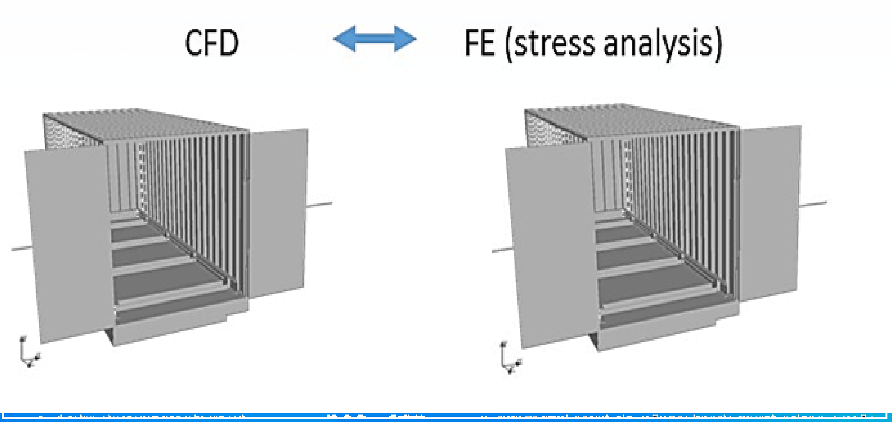
Fluid Structure Interactions



One-way : flow and structural variable coupling

Pressure fields affect the structural deformations only.



Two-way : flow and structural variable coupling

The fluid flow and pressure fields affect the structural deformations, and the structural deformations affect the flow and pressure.

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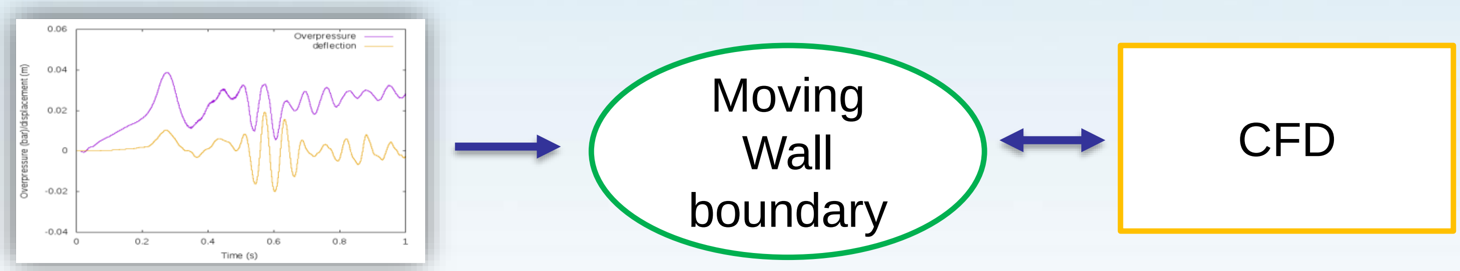
Two-way pseudo coupling

Structural response

Interface

Numerical simulations



FEA or Experiments

The structural displacements are read at the container boundaries and scaled according to the generated peak overpressures values at probe location P1, during the explosion process.

Pseudo two-way coupling

- Using experimental pressure vs deflection curves
- Using spring mass analogy - SDOF
- Using the experimental static pressure vs defection curves

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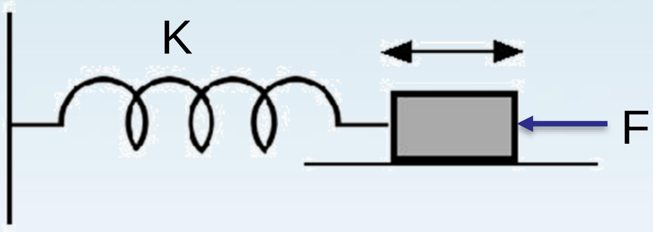
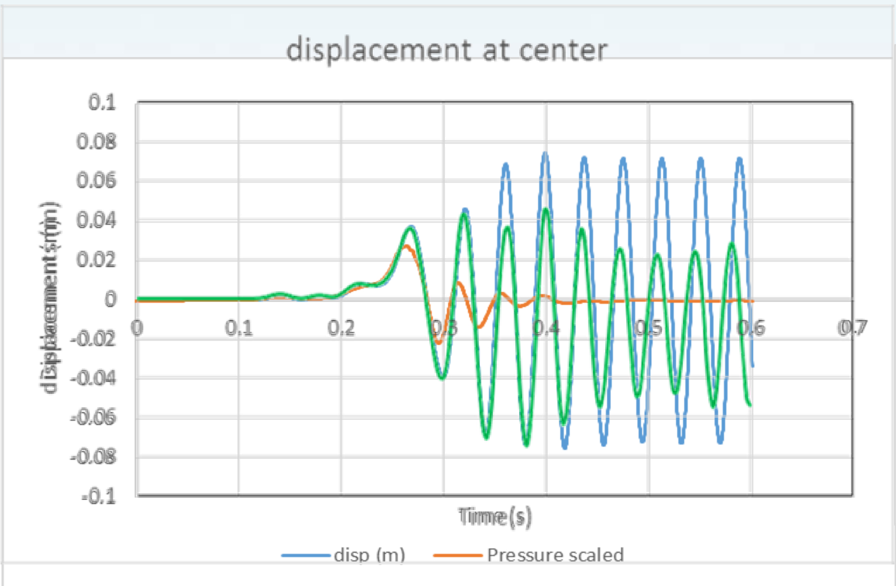
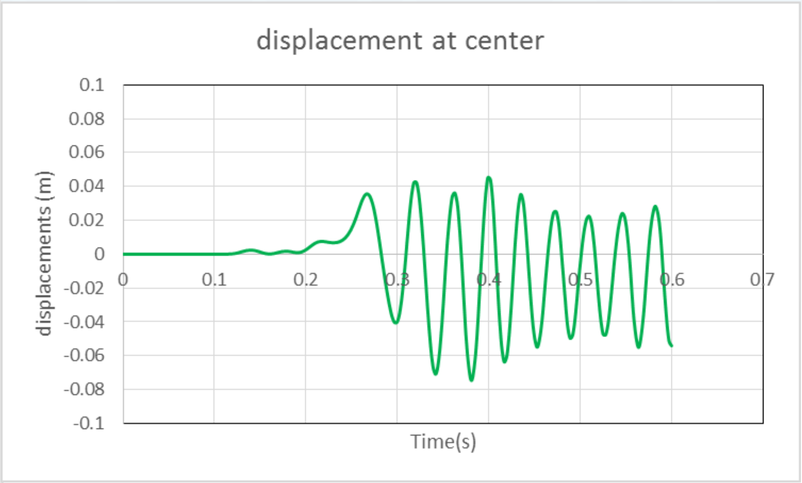
Using spring mass analogy



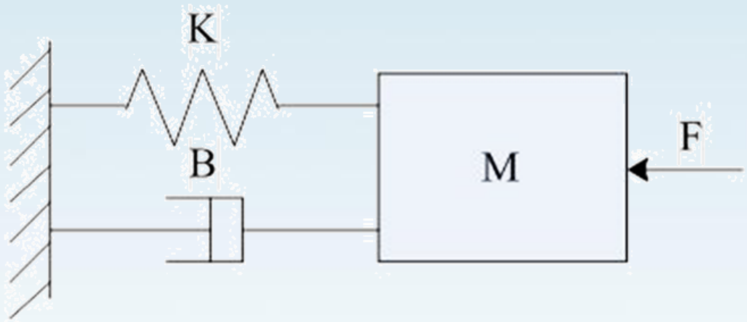
$$F(t) = m\frac{d^2x(t)}{dt^2} + kx(t)$$

$$m\frac{d^2x(t)}{dt^2} = F(t) - kx(t)$$



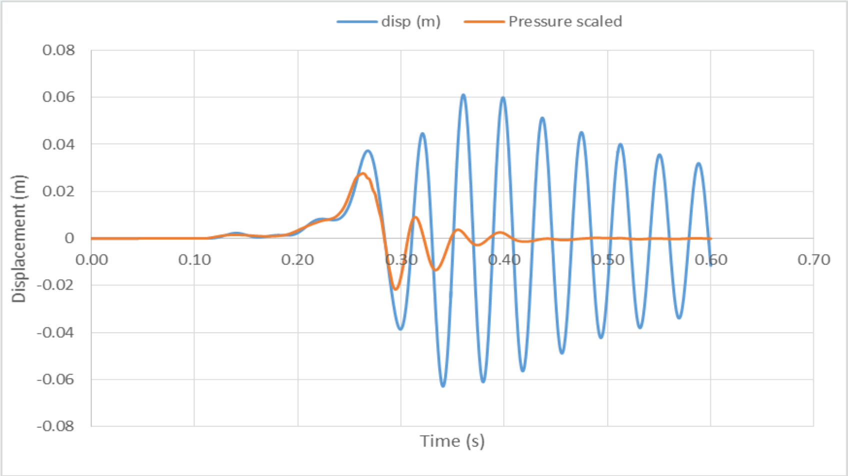


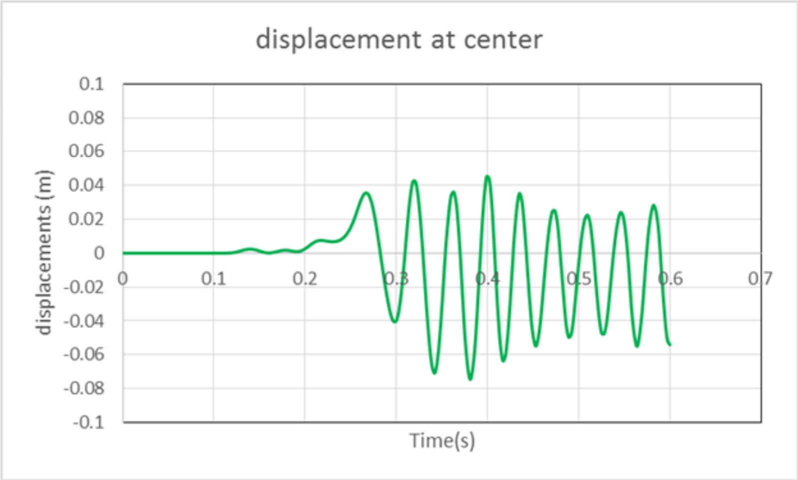
Using spring mass analogy



Applied Force
Spring Force
Inertial force
Damping force

$$F(t) = kx(t) + M\frac{d^2x(t)}{dt^2} + k_d \cdot \frac{dx(t)}{dt}$$





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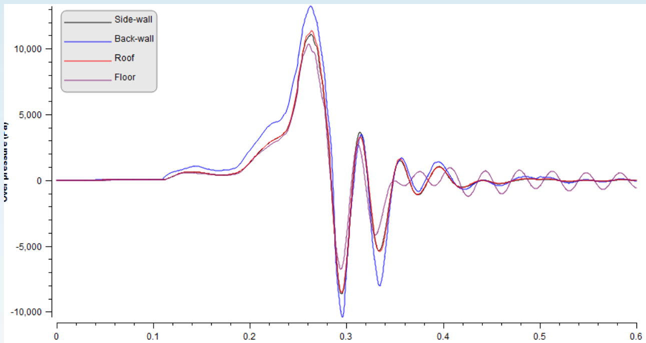
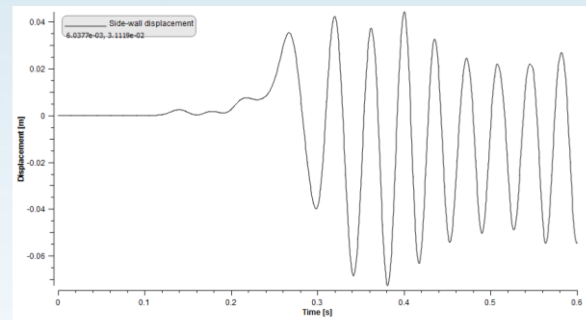
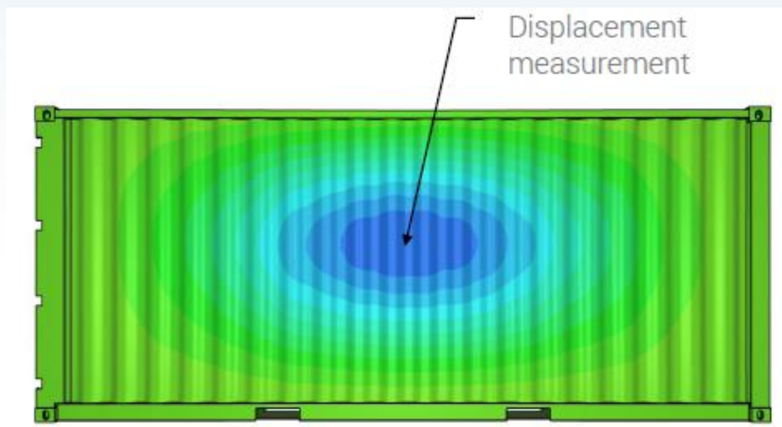
One-way : Flow and structural variable coupling

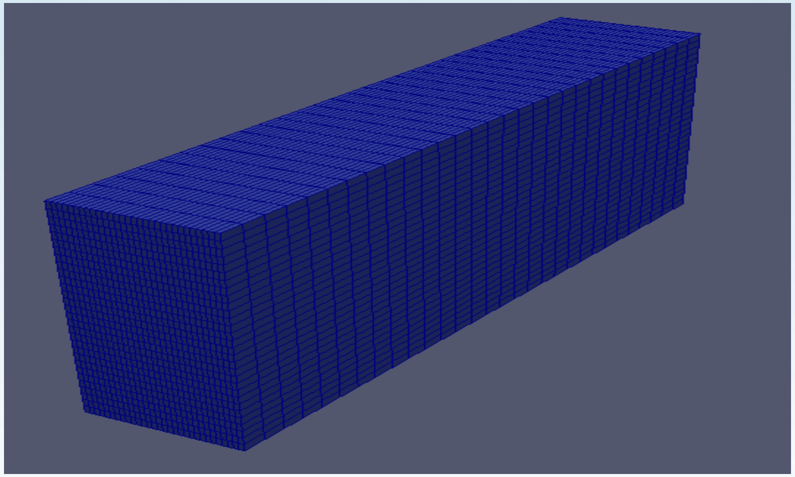


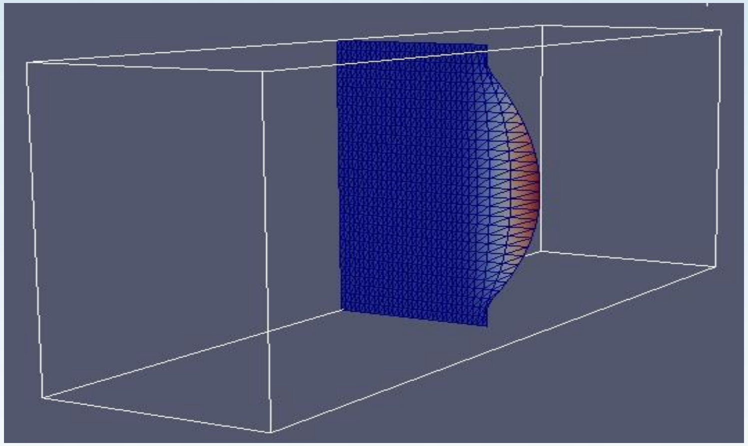


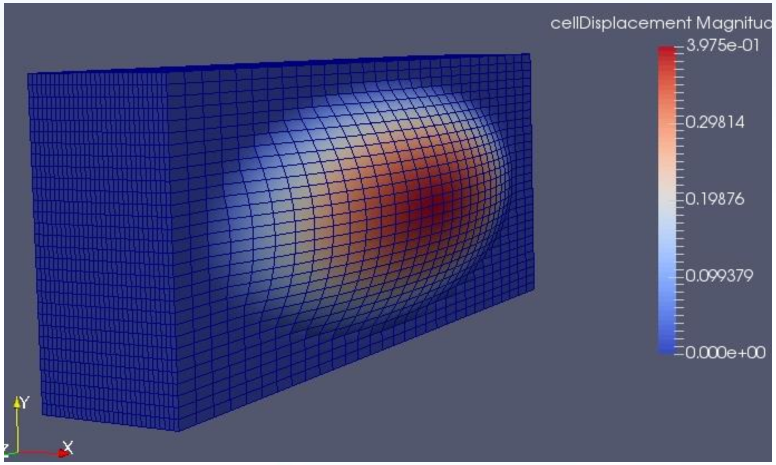


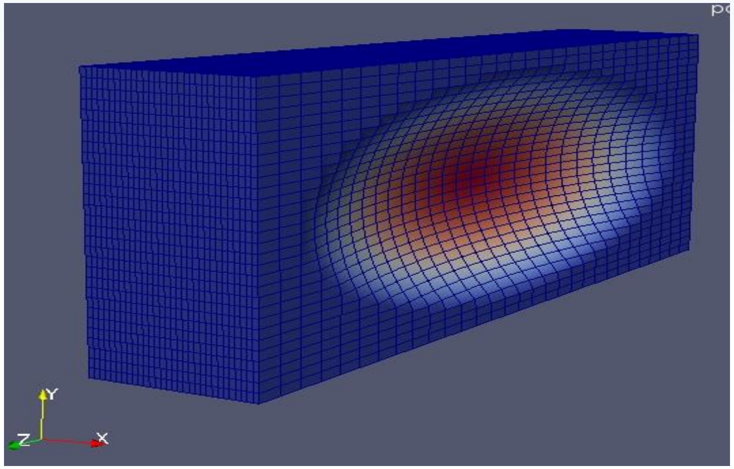
Atanga, Gordon, Lakshmipathy, Sunil, Skjold, Trygve, Hisken, Helene, & Hanssen. (2017), "Structural response for vented hydrogen deflagrations: coupling CFD and FE tools". Zenodo. http://doi.org/10.5281/zenodo.1165356

Wall Patch displacement

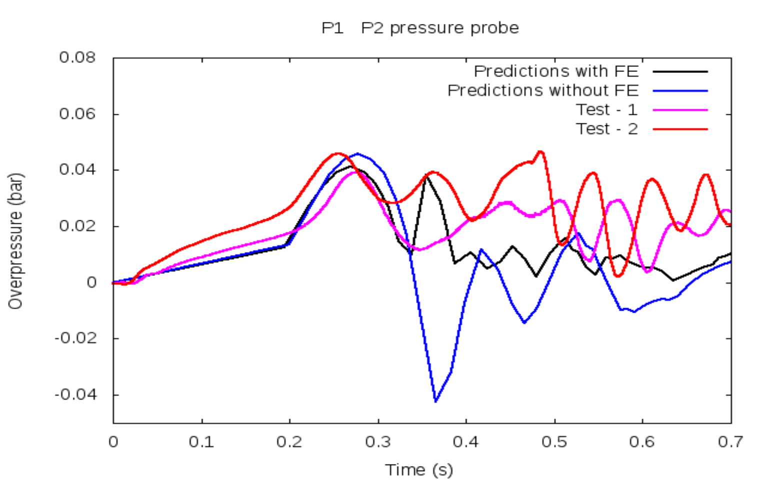


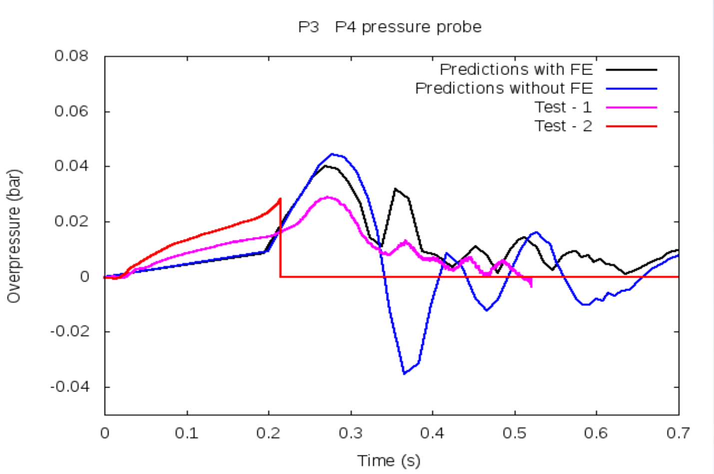


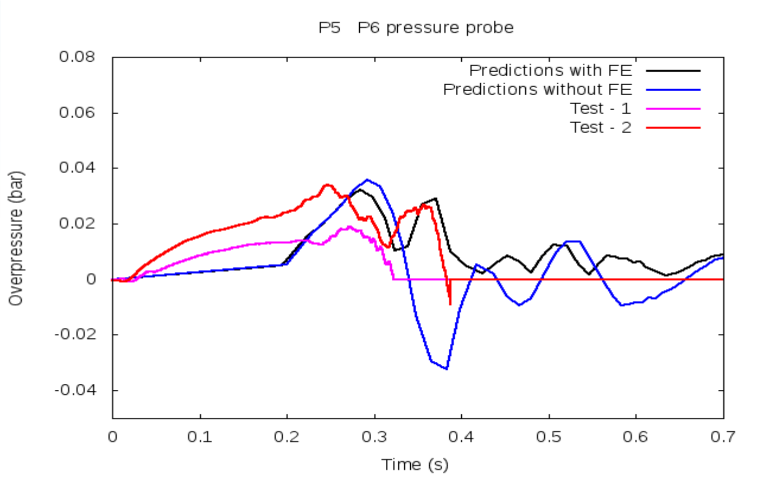


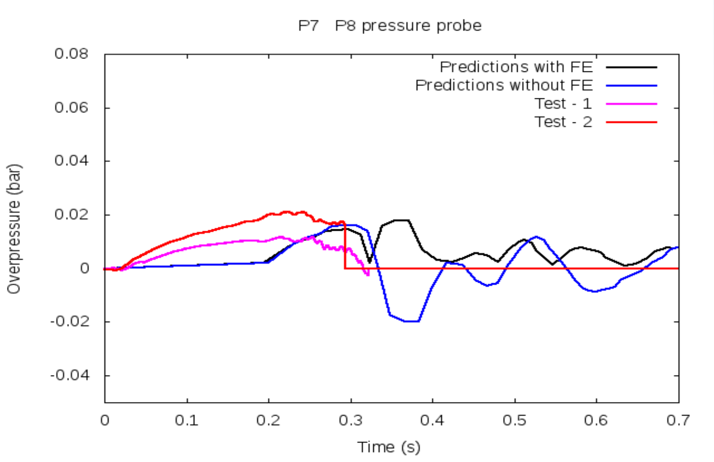


15% H_2 concentration









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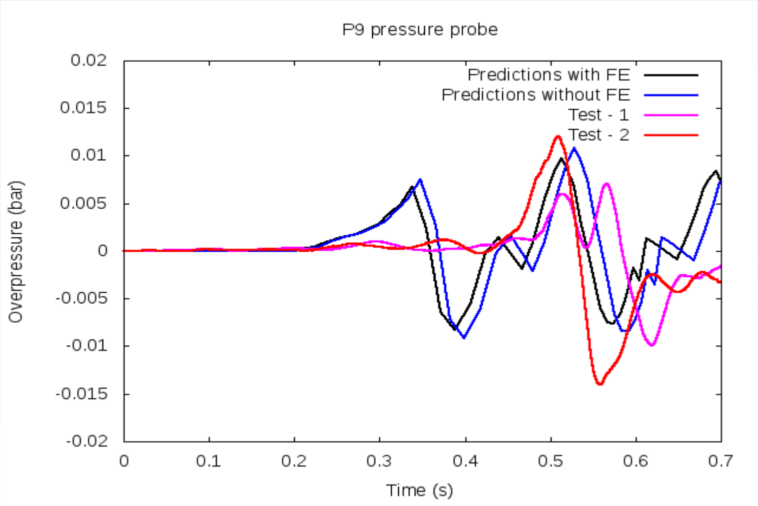
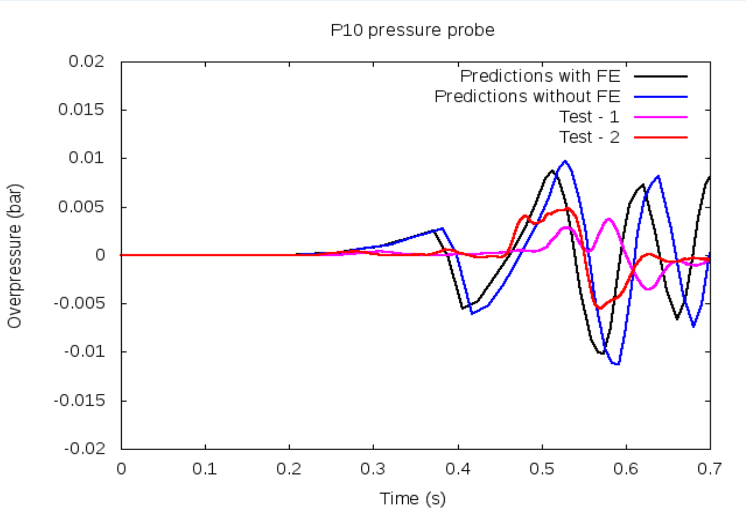
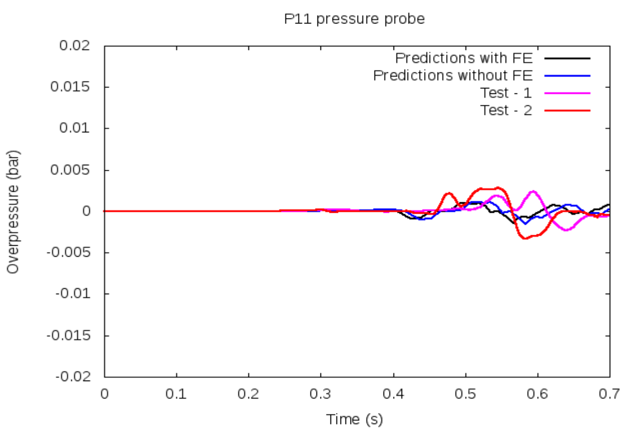
15% H_2 concentration







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Conclusions remarks

- Vented explosion modelling in RANS/LES method - HyFOAM solver development.
- Dominant Combustion instabilities in vented explosion process are included.
- Non-rigid structures effect the overpressures, Acoustics , oscillations/vibrations, resonance
- CFD and FE integration are considered in two-way pseudo coupling.
- CFD and FE coupling improved the overpressure trace curves in ISO containers.
- Peak negative is reduced when structure non-rigid.

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