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CFD Analysis of Vented Lean Hydrogen Deflagrations in an ISO Container

Vendra C. Madhav Rao & Jennifer X. Wen

Warwick FIRE, School of Engineering
University of Warwick, UK

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Outline

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

Numerical method

- 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.*

* MENON S., YEUNG P. K., and KIM W. W., Effect of Subgrid Models on the Computed Interscale Energy Transfer in Isotropic Turbulence," Computer and Fluids (1996), Vol. 25, No. 2, pp. 165-180

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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:

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

  where, Ξ is sub grid flame wrinkling, S_u is laminar flame speed

- Mixture fraction equation is also solved.

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.

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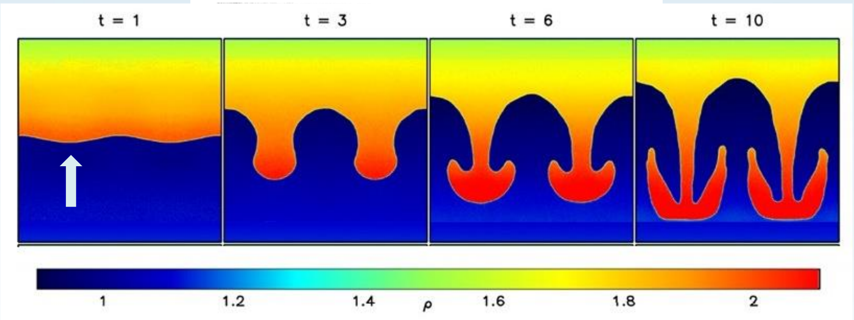
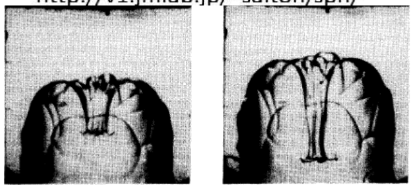
Experimental observation of vented gas explosions

Physical phenomena (McCann et al. 1985):

- Helmholtz oscillations.
- Cellular spherical flames (DL).
- RT instabilities.
- Acoustical modes of the enclosure.
- Turbulence
- External explosion
- Structural response



http://v1.jmlab.jp/~saitoh/sph/



t = 32.3 ms   t = 34.3 ms

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.

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Flame wrinkling factor

- The closure for the sub-grid wrinkling (Ξ) is provided considering the flame instabilities into three components, (Bauwens, C. R (2011)a),

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

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,

$G = R\frac{E_{eq} - 1}{E_{eq}}$ and $R = \frac{0.28}{\tau_n}\frac{E_{eq}^{*}}{E_{eq}^{*} - 1}$ are subgrid turbulence

generation and removal rates with $E_{eq} = 1 + 2(1 - \overline{b})(E_{eq}^{*} - 1)$, 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.*

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Darrieus-Landau flame instability

- The surface wrinkling factor due to the Darrieus-Landau flame instability (Ξ_{DL}) is modelled as (Bauwens, C. R (2011)),

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

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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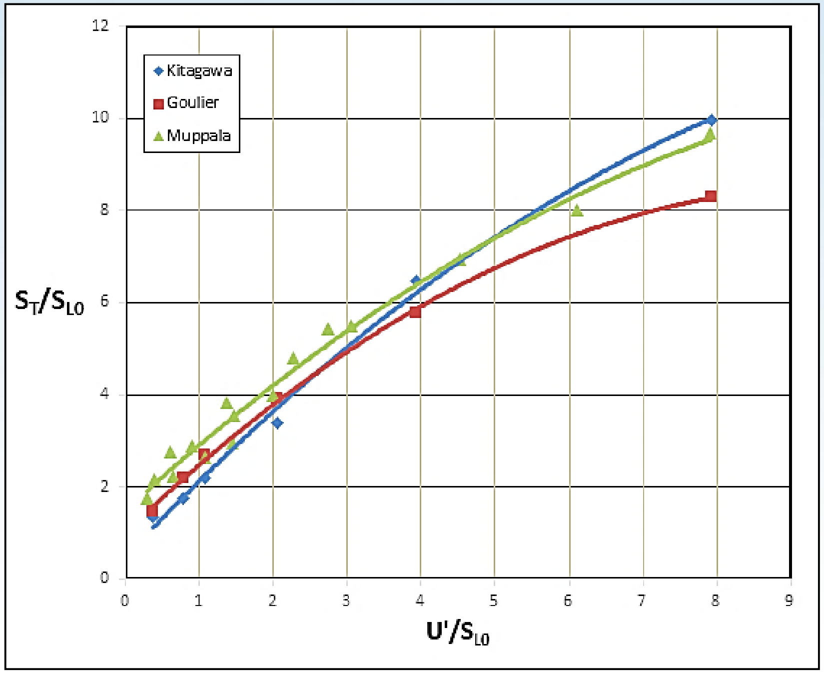
Turbulent flame speed correlation



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

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 1bar 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 :555.

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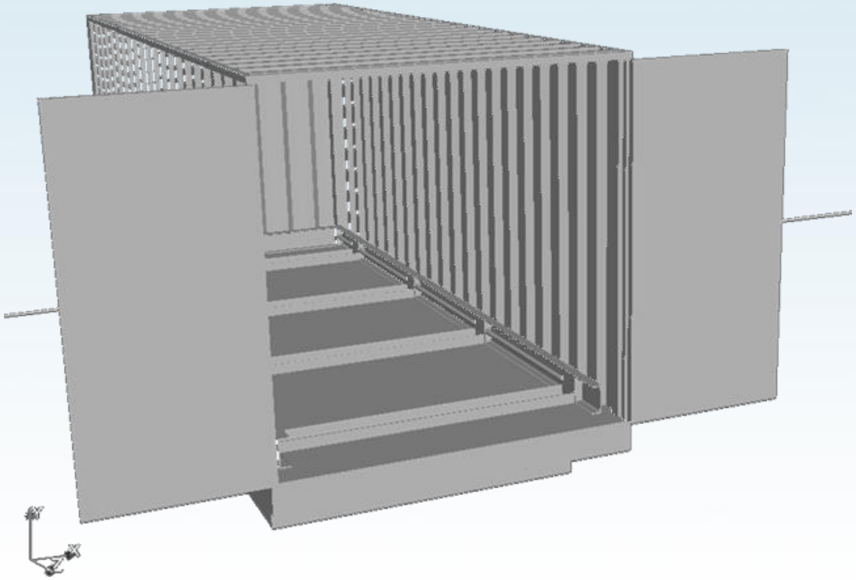
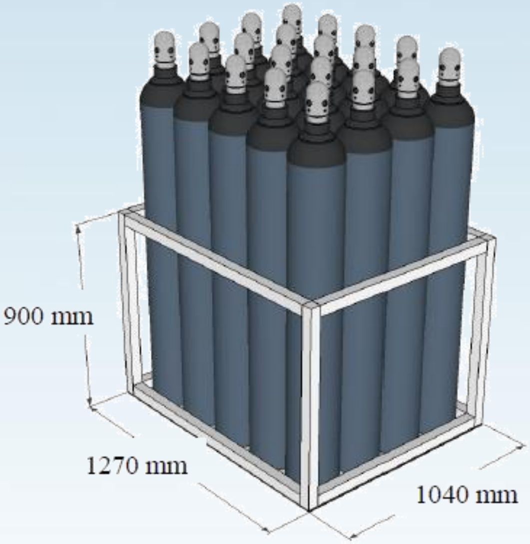
Geometry



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

Congestion

(a) Container corrugation



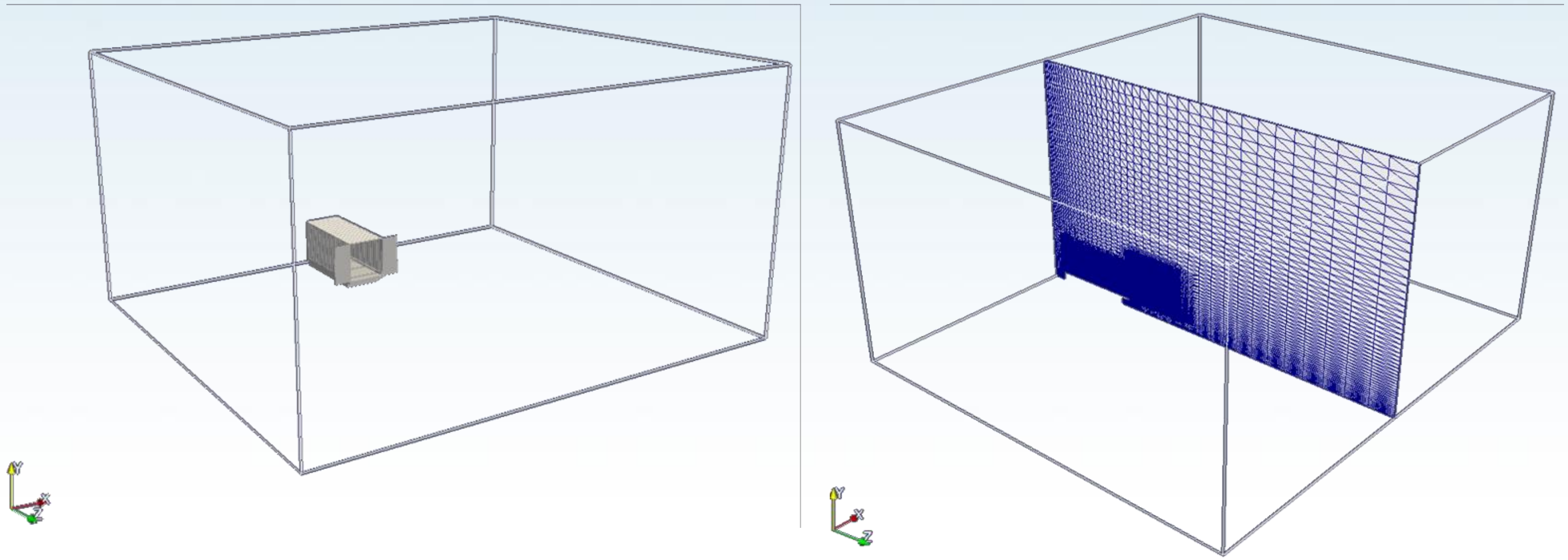
(c) Bottle stack

(b) Obstacle holding frame

(d) Pipe rack

Computational domain

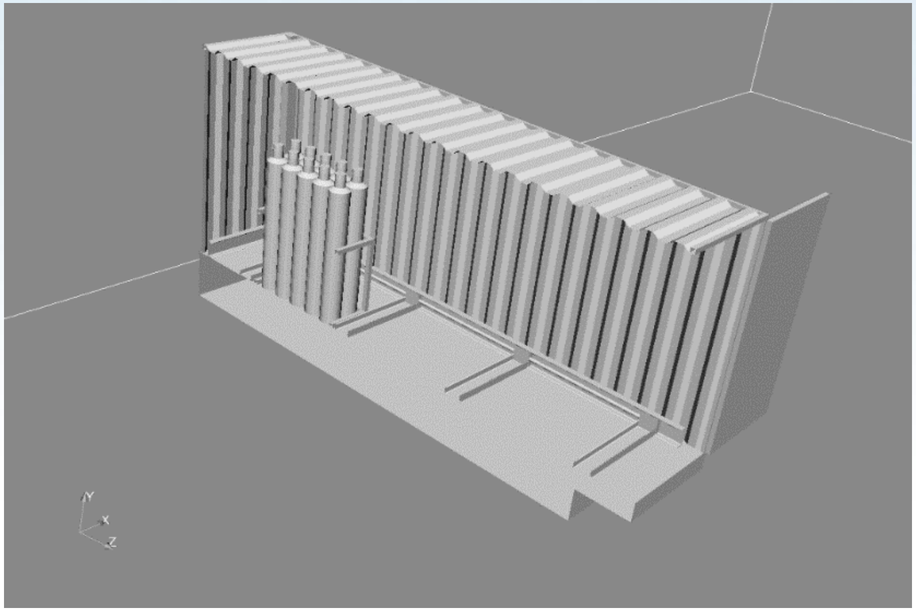
The vented chamber is enclosed by 30.0 x 10.0 x 30 m mesh volume to capture the venting of burned gas, the external explosions and to reduce the effect of boundary conditions on the numerical results



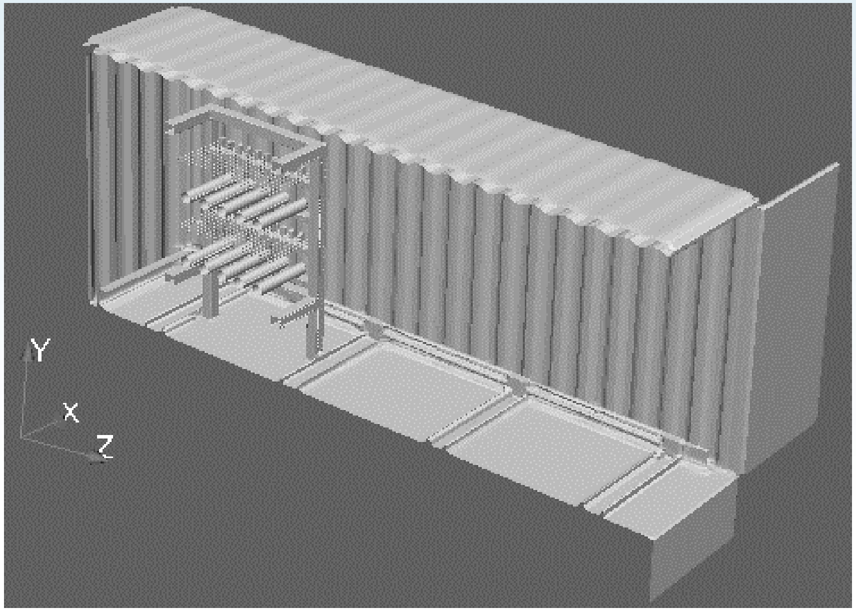
Computation domain and the mesh distribution in the vertical and horizontal plan.

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

Computational domain (2)



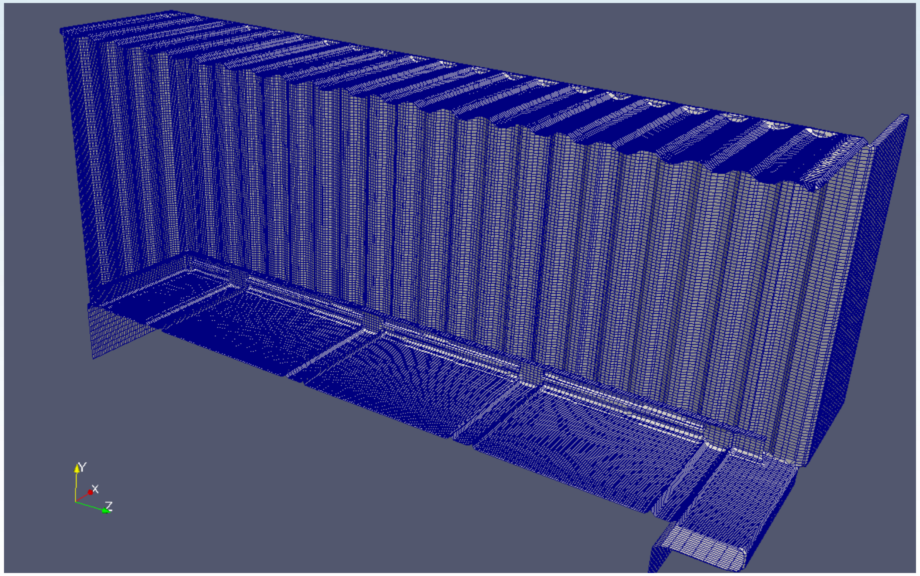
(a) With bottle basket obstacle

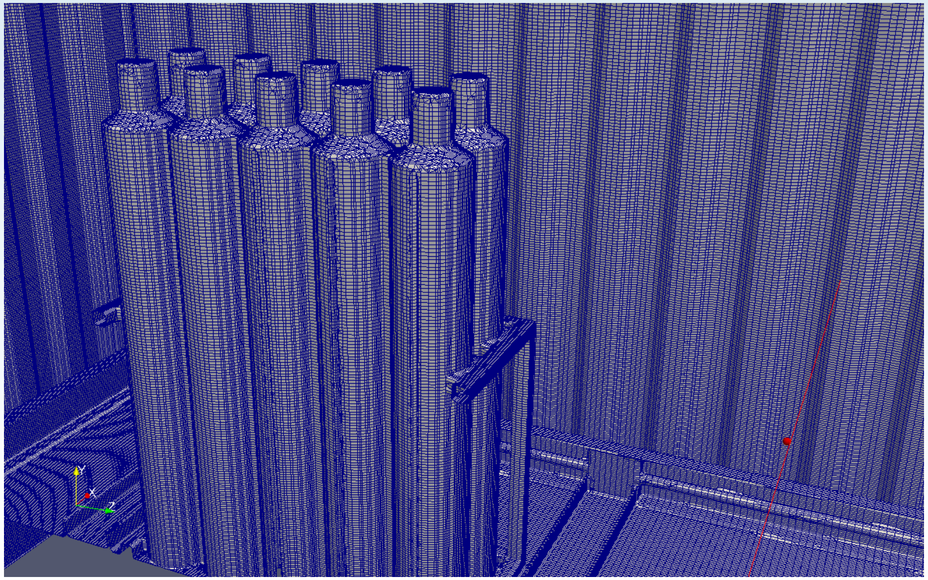


(b) With pipe rack obstacle

The standard 20-ft ISO container with model obstacles

Mesh resolution





The mesh distribution on the obstacles (sample)

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 : Door

20 feet ISO container Base test case scenarios

Configuration			
Vent	Obstructions	Hydrogen concentration	Ignition position
Door open	Empty frame	15% (+/- 0.2%)	Mid back wall
Door open	Cylinder bundle	15% (+/- 0.2%)	Mid back wall
Door open	Pipe rack	15% (+/- 0.2%)	Mid back wall

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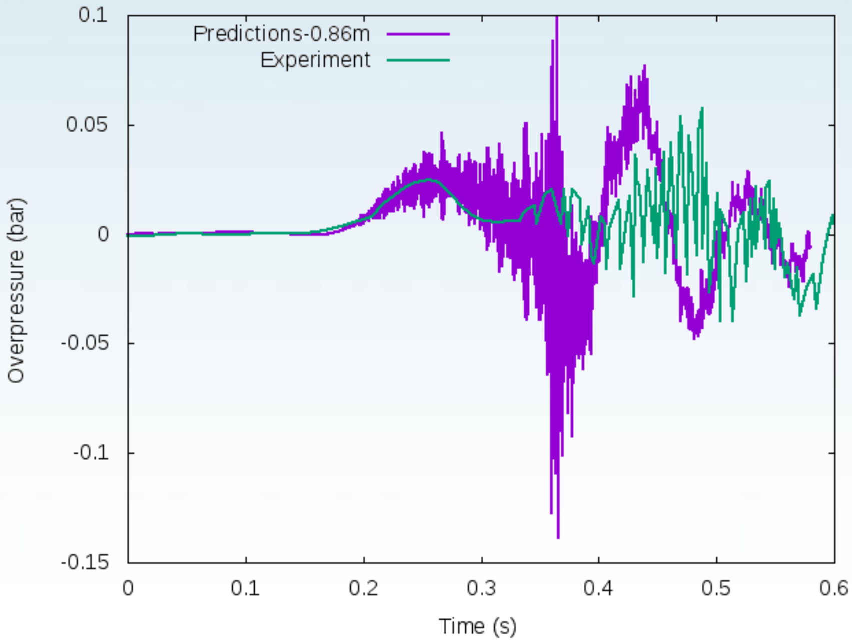
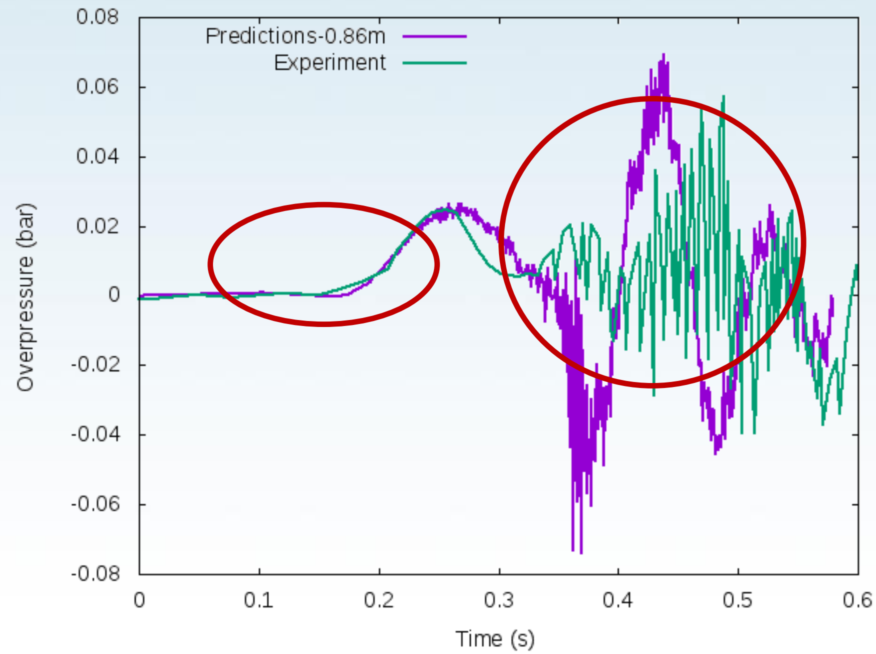
15 % Hydrogen concentrations (Empty)



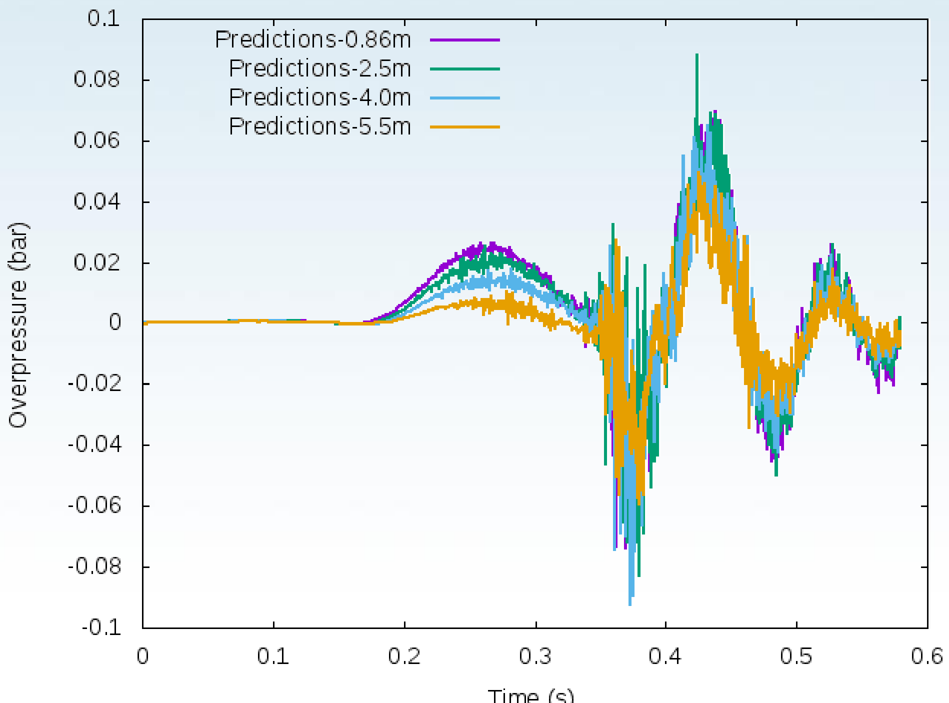
(a) Instantaneous pressure profile



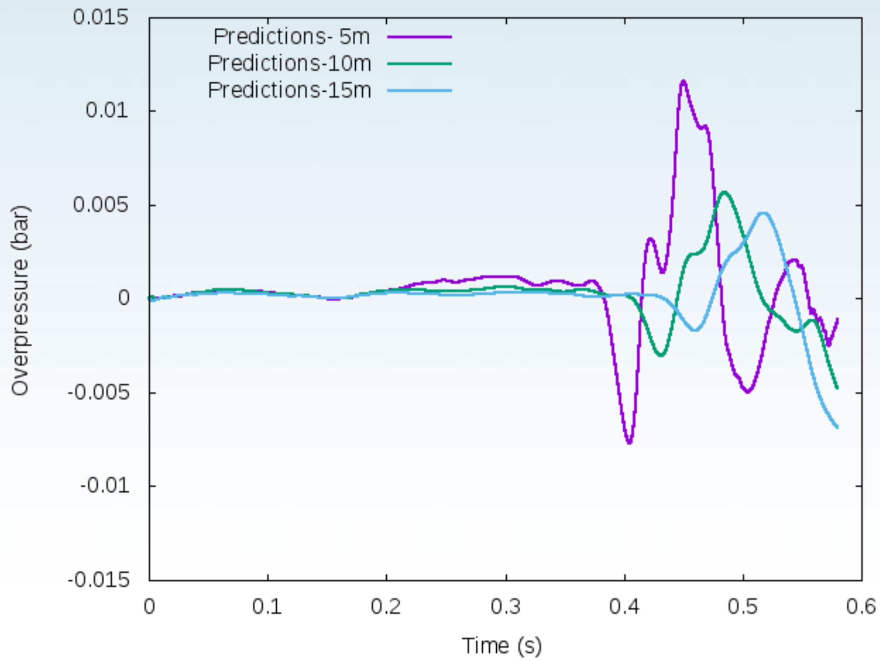
(b) Time averaged profile for 5 ms

Pressure trace curve for P1 pressure probe location along with experiment measurements

15 % Hydrogen concentrations (Empty)



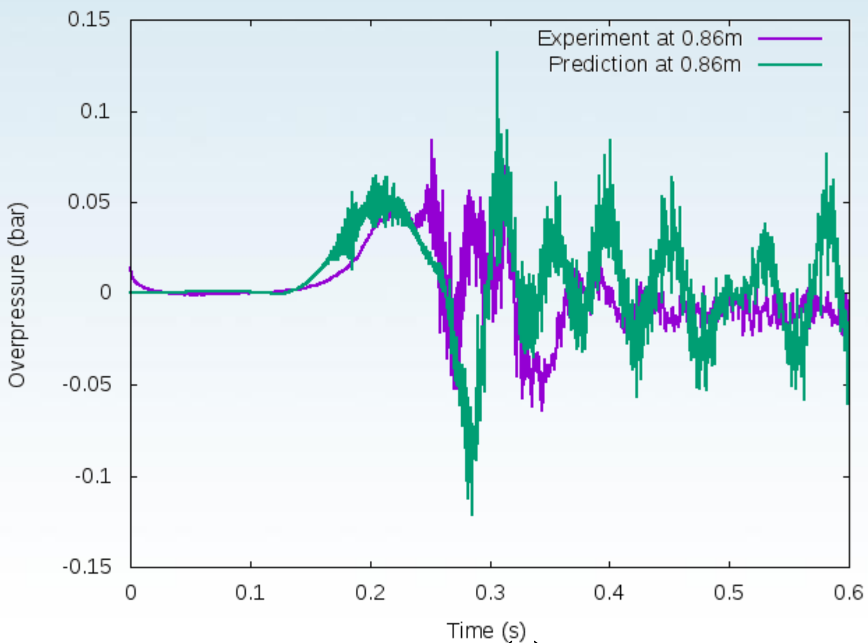
(a)



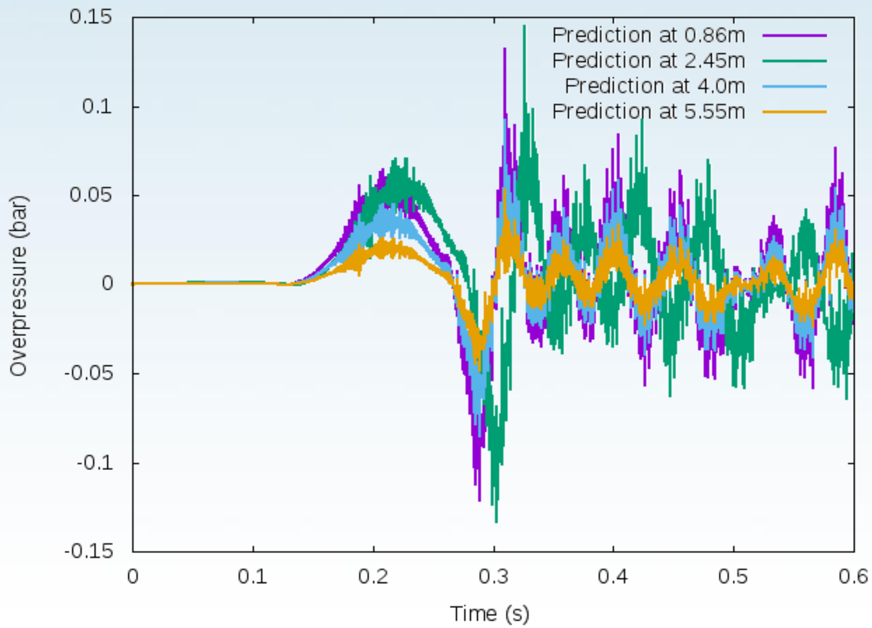
(b)

Numerical predicted of pressure trace curve for pressure probes (time averaged 5 ms), (a) inside the container, (b) outside and in front of the open container door

15 % hydrogen concentration with bottles



(a)



(b)

Numerical predicted of pressure trace curve for pressure probes inside container

(a) time averaged 5 ms

(c) time averaged curves for probes inside the container

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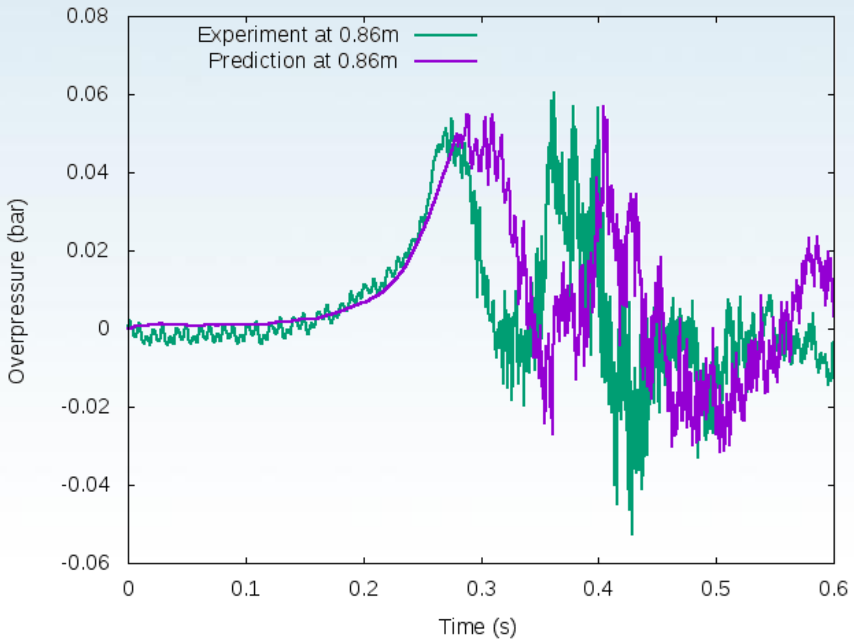
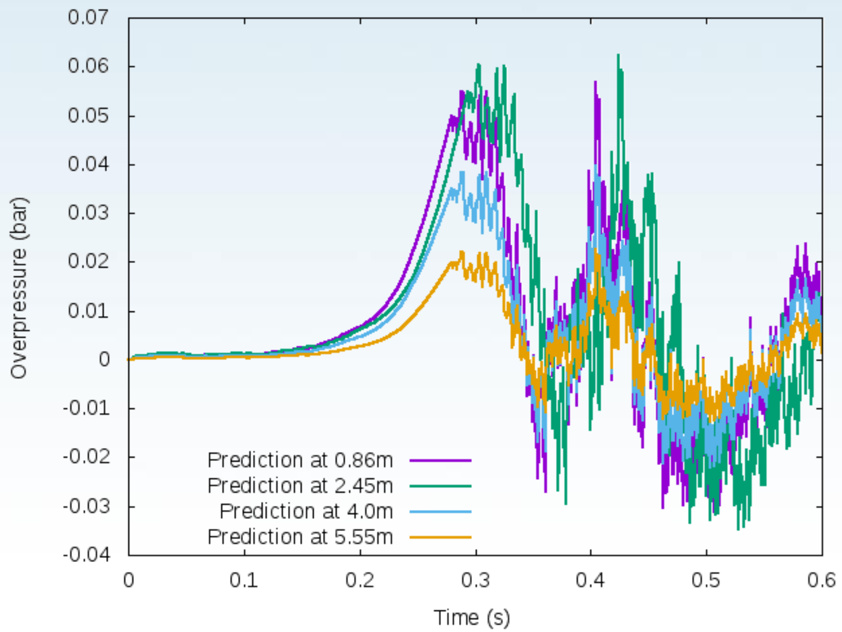
15% Hydrogen Concentration with pipe rig





Pressure trace curve for P1 pressure probe location along with experiment measurements with pipe rack as obstacle

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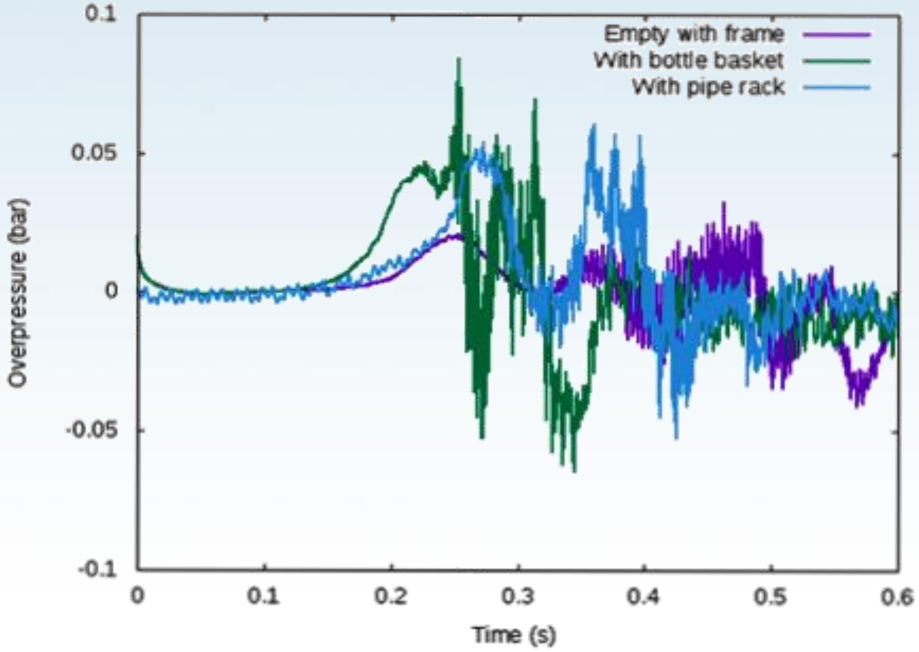
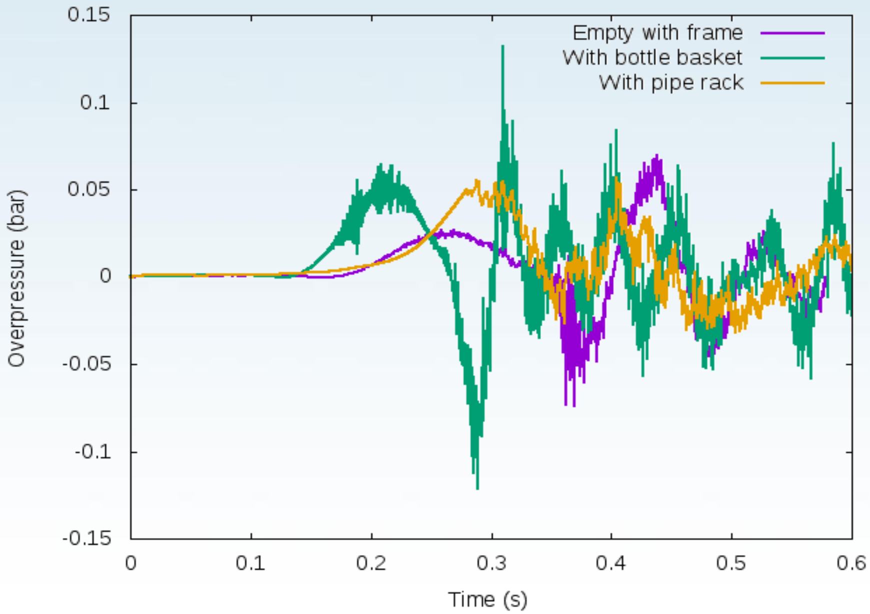
Overall Overpressures trends



(a) Experiments results



(b) Numerical predictions

Pressure trace curve for P1 pressure probe location for three scenarios

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CFD & FE

Vented explosion Experiment (empty) at Gexcon

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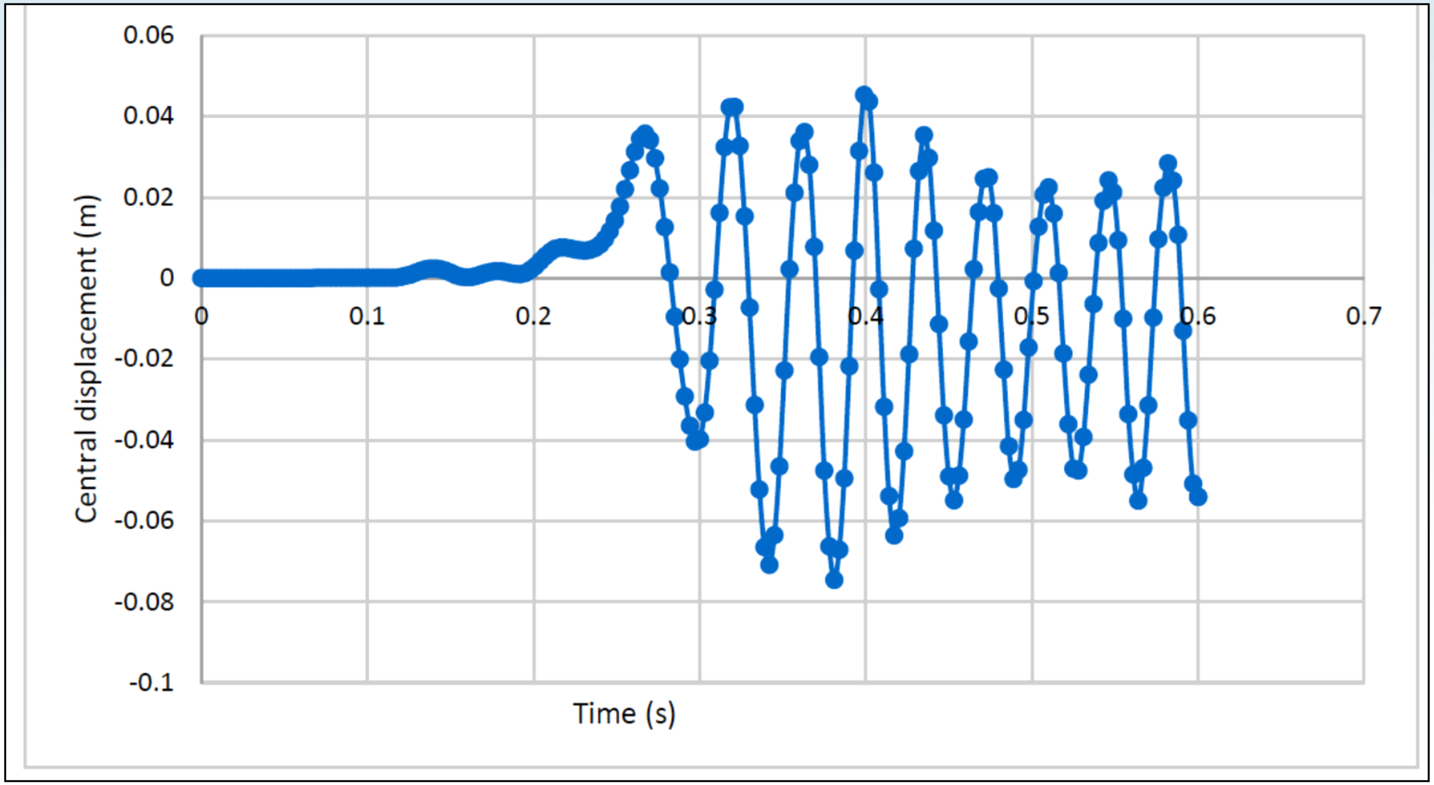
Container wall displacement



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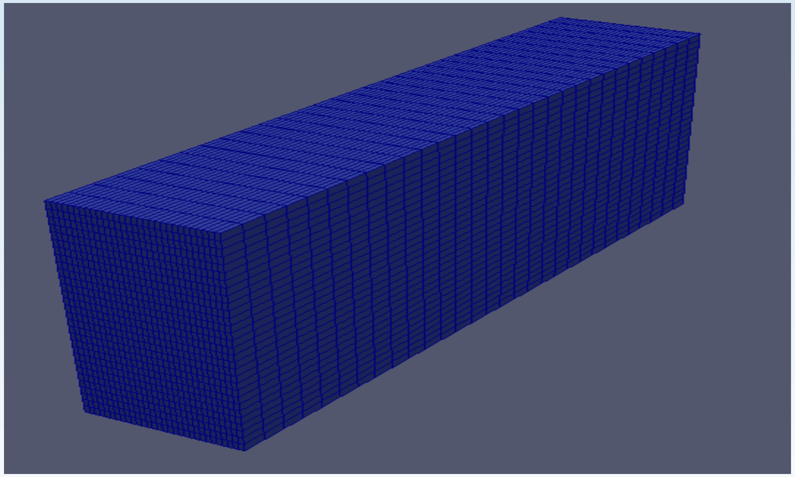
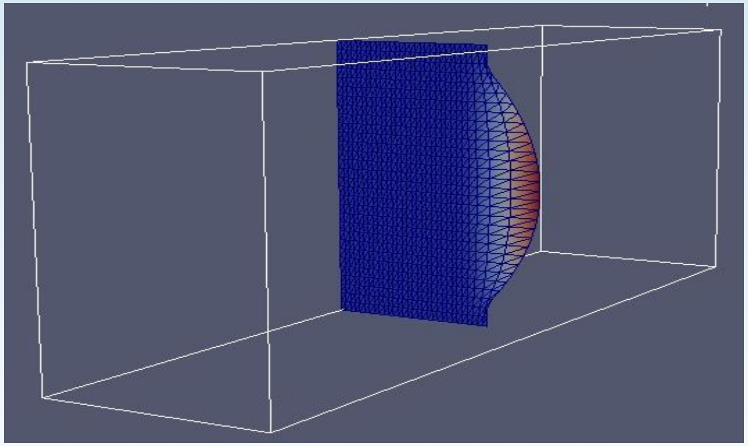
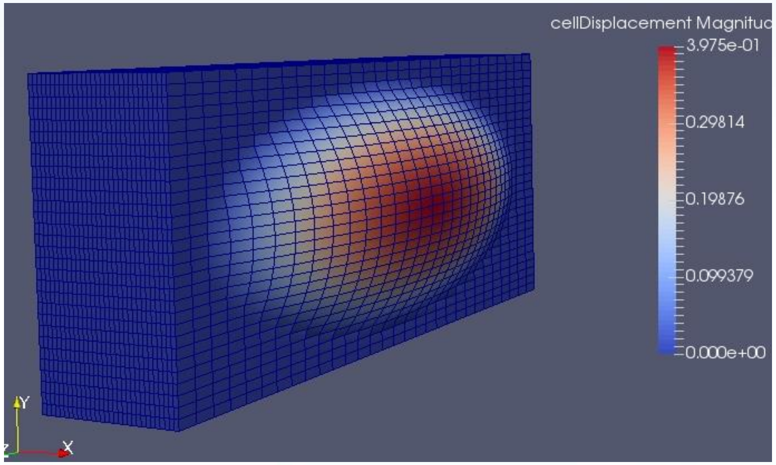
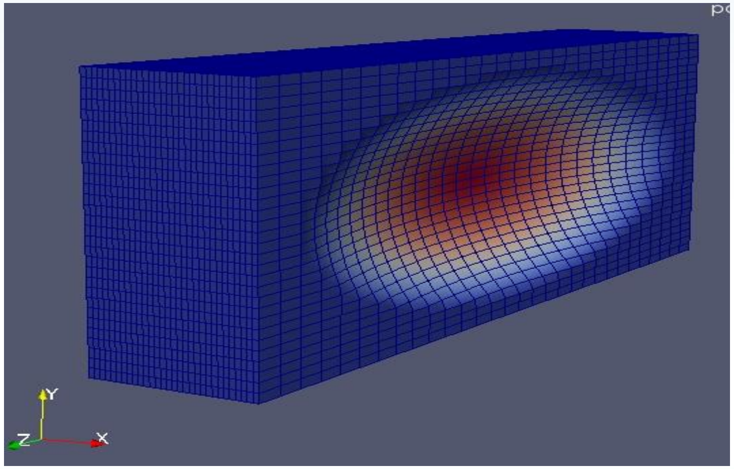
Wall Patch displacement









Conclusions remarks

- Vented explosion modelling in RANS/LES method using HyFOAM solver.
- Dominant Combustion instabilities in vented explosion process are modelled.
- The modelled equations are validated for the container experiments available results.
- Experiments geometry details are included in modelling.
- CFD and FE integration are considered in one-way coupling (to start with).

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Thank you

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