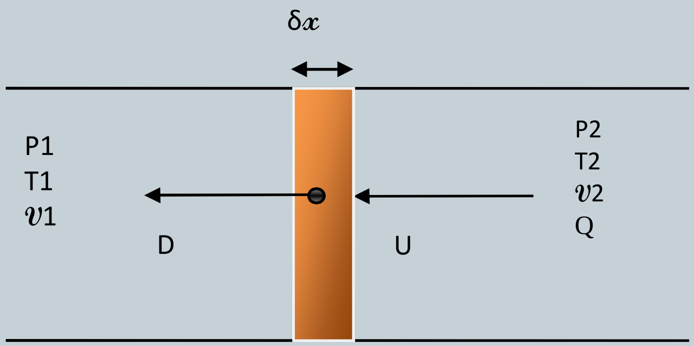
Numerical simulation of large scale hydrogen detonation

A HEIDARI, S FERRARIS, J X WEN AND V H Y TAM

CENTRE FOR FIRE AND EXPLOSION STUDIES,
KINGSTON UNIVERSITY LONDON

Detonation wave

- Detonation is a supersonic combustion wave



- Mechanism of detonation propagation

- The shock and combustion region are coupled

Governing equations

$$\partial\rho/\partial t = -\nabla(\rho\mathbf{v})$$

Mass conservation

$$\partial\rho\mathbf{v}/\partial t = -\nabla(\rho\mathbf{v}\mathbf{v}) - \nabla P$$

Momentum Conservation

$$\partial\rho E/\partial t = -\nabla(\rho E\mathbf{v}) - \nabla(\mathbf{v}P)$$

Energy conservation

$$\partial\rho\alpha/\partial t = -\nabla(\rho\alpha\mathbf{v}) + \rho W$$

Reaction progress

$$E = -\alpha Q + P/[\rho(\gamma - 1)] + \mathrm{v}^2/2$$

Energy equation

Chemistry

$$H_2 + \frac{1}{2}(O_2 + 3.76N_2) \rightarrow H_2O \ + \ 1.88N_2$$

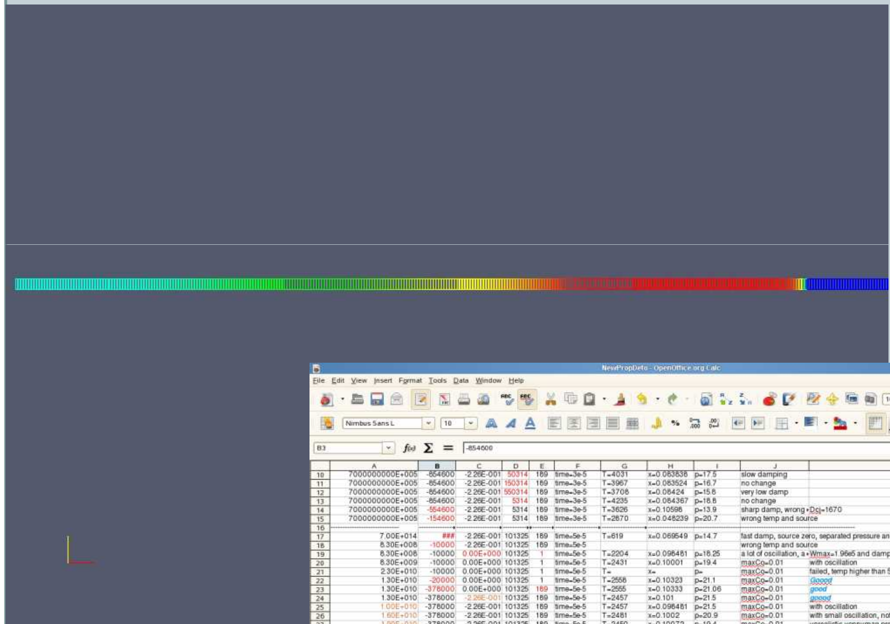
$$Reactants \rightarrow products$$

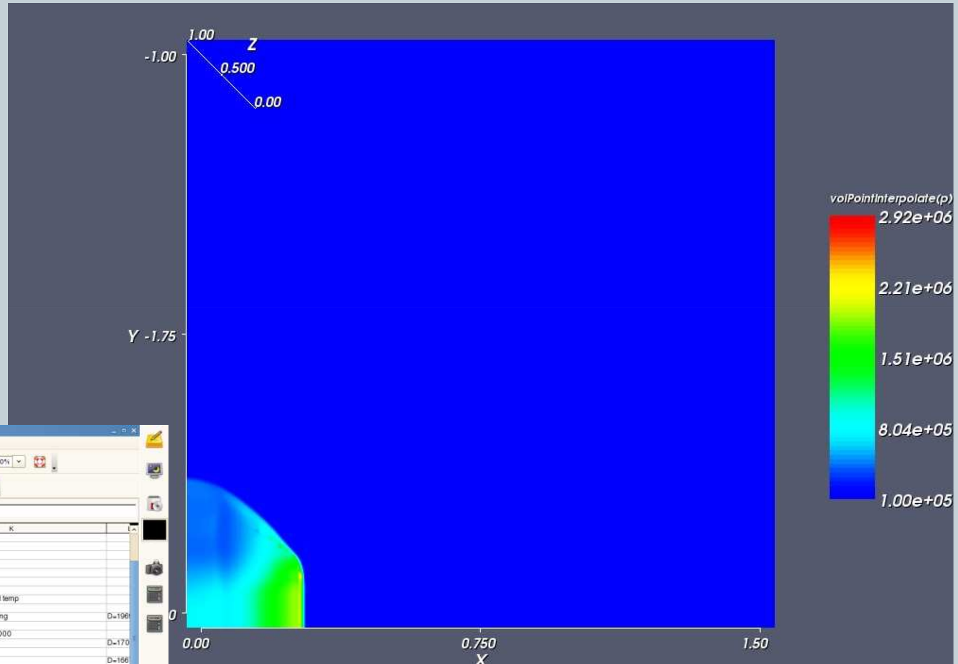
$$W = A(1 - \alpha)\exp(-E_a/RT)$$

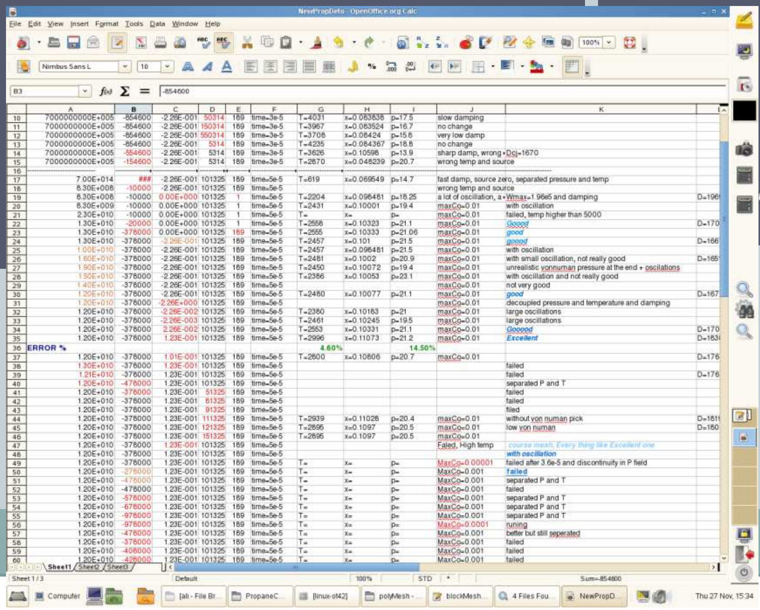
CJ Pressure	Temperature	Shock Velocity	Products Velocity
17 atm	3364 K	2090 m/s	890 m/s

Tuning the chemistry parameters

- The reaction parameters are tuned in 1D and 2D test cases with different grid resolutions







Numerical schemes

- Discretization: Gaussian finite volume integration
- Time derivatives: Explicit Euler scheme
- Upwind interpolation for $(U.\varphi)$ convection
- Van Leer (TVD) interpolation for the rest of divergence (convection) derivative terms
- Linear interpolation for gradient derivative terms

Two test cases

- CASE 1 – Hydrogen detonation in the RUT tunnel facility (Laboratory of Induced Chemical Reactions, Russian Research Center "Kurchatov Institute")
- CASE 2 – A planar hydrogen-air cloud

CASE 1 - Hydrogen detonation in the RUT tunnel facility

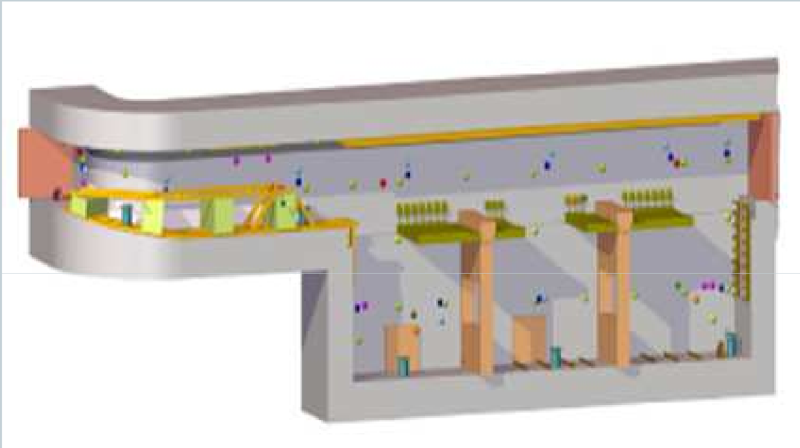
- RUT tunnel facilities in Russia, (standard test cases selected for HYSAFE)
  - Hydrogen air mixture
  - volume = 263 m^3
  - 5 cm uniform grid

Boundaries

- Wall for all boundaries

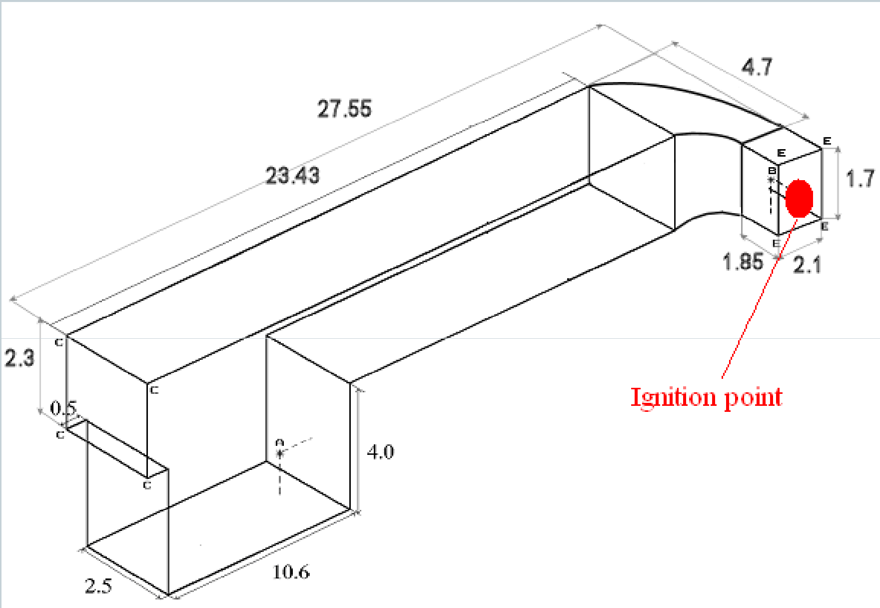
Initial ignition

- a region of high temperature and pressure (3000 K, 15atm)

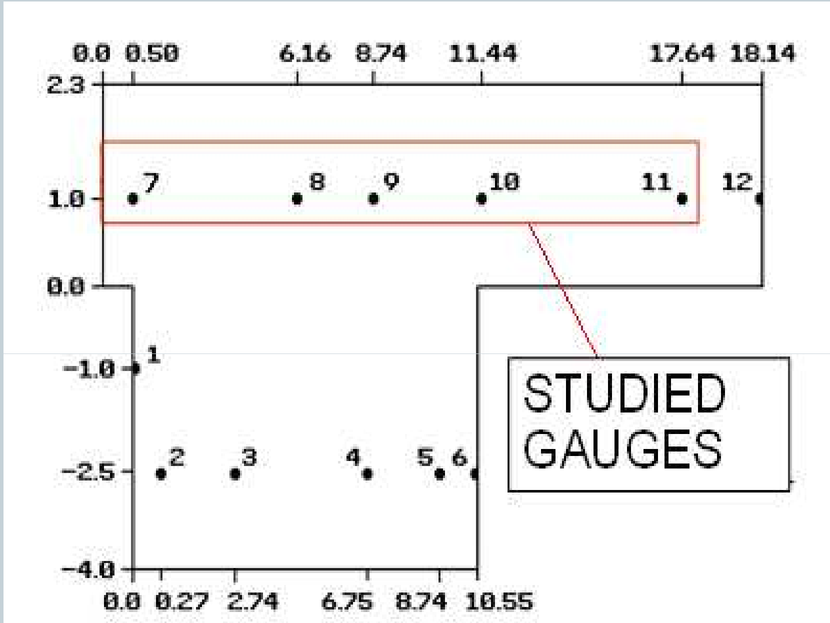


The experiment channel (reproduced from [1]), Laboratory of Induced Chemical Reactions, Russian Research Center "Kurchatov Institute”

CASE 1 - Hydrogen detonation in the RUT tunnel facility

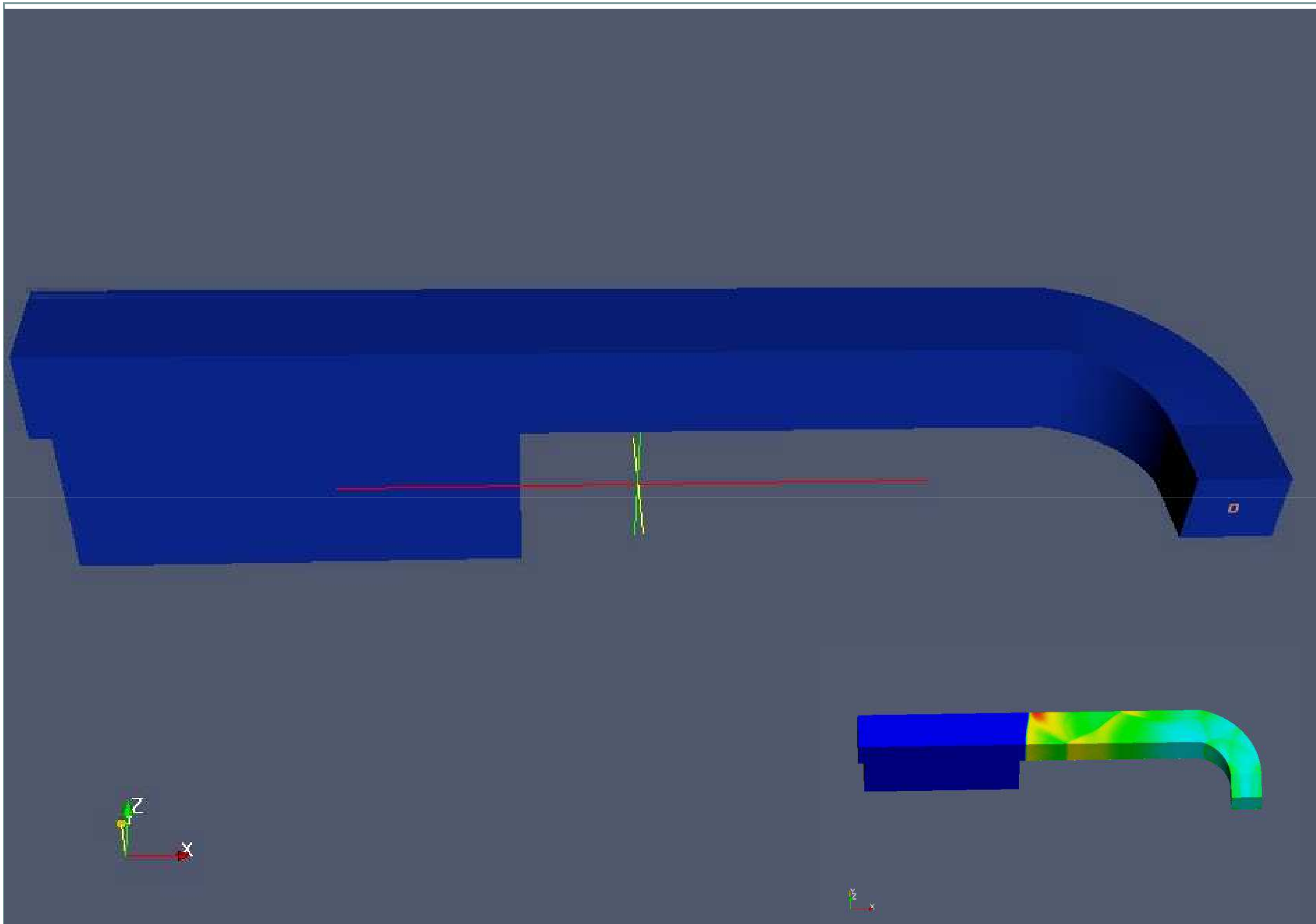


The tunnel dimensions (reproduced from [1])



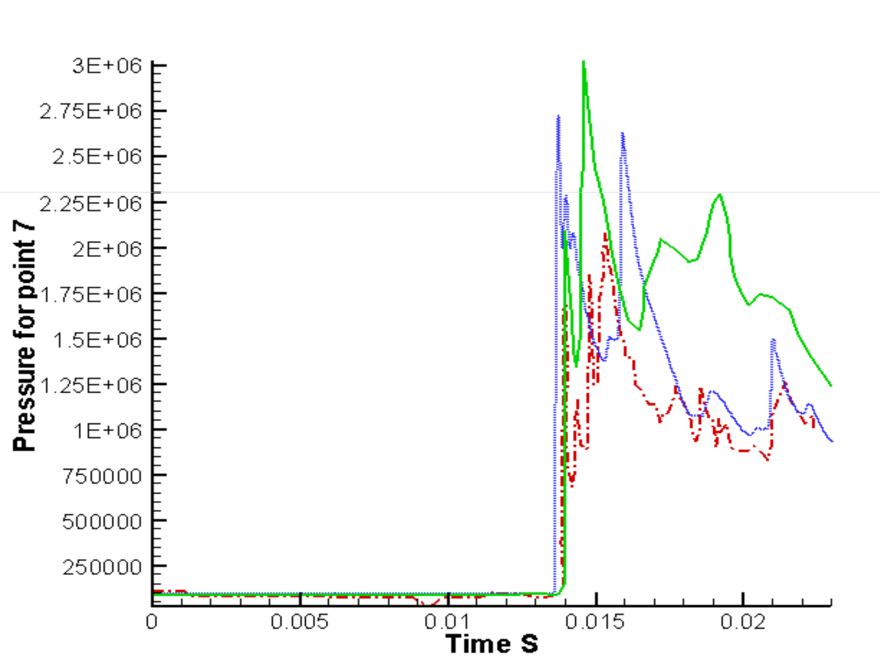
Locations of the monitoring gauges (reproduced from [1])

[1] Kotchourko, "Safety of hydrogen as an Energy carrier", compilation report on SBEPs results of the 4th period, HYSAFE, 2007.

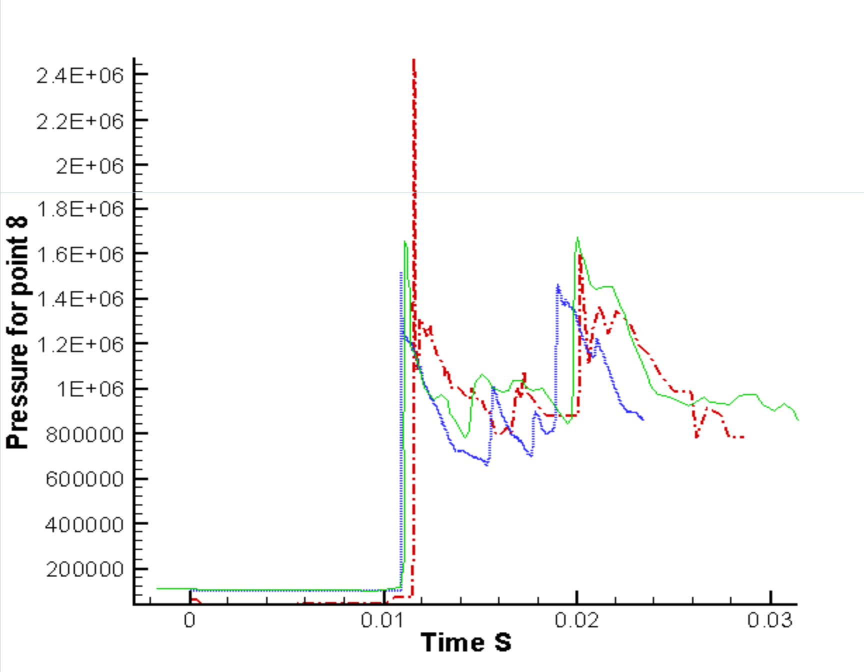

Z
X

CASE 1 - Hydrogen detonation in the RUT tunnel facility

Red - Experimental results of RUT [1]
Blue - Present predictions
Green - RUT predictions [1]



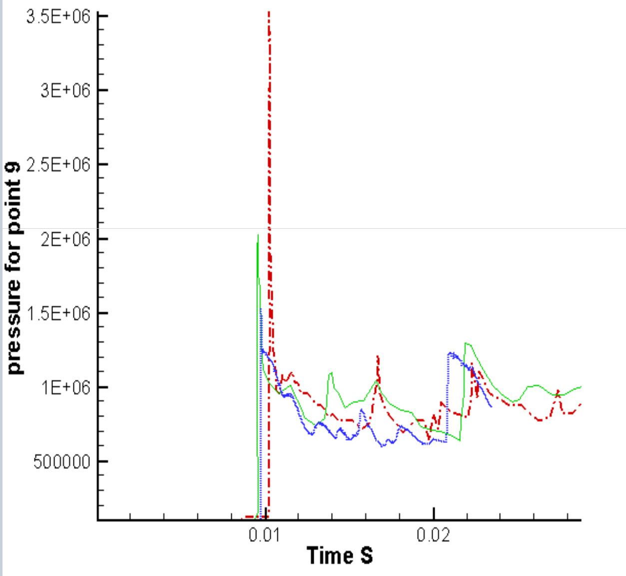
The predicted pressure (in Pascal) *vs* time for point 7.



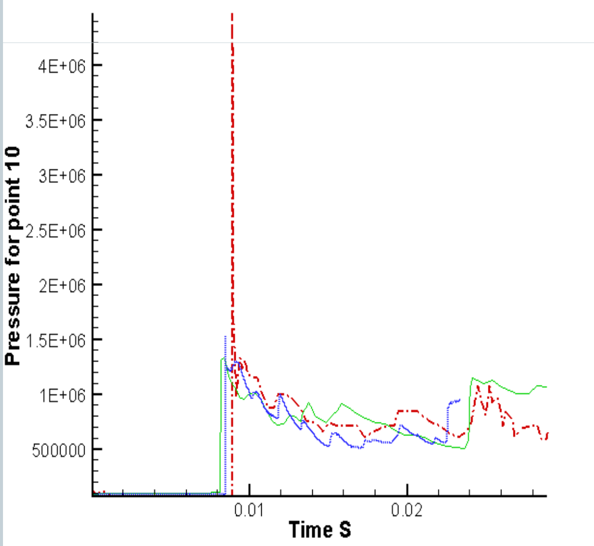
The predicted pressure (in Pascal) *vs* time for point 8

CASE 1 - Hydrogen detonation in the RUT tunnel facility

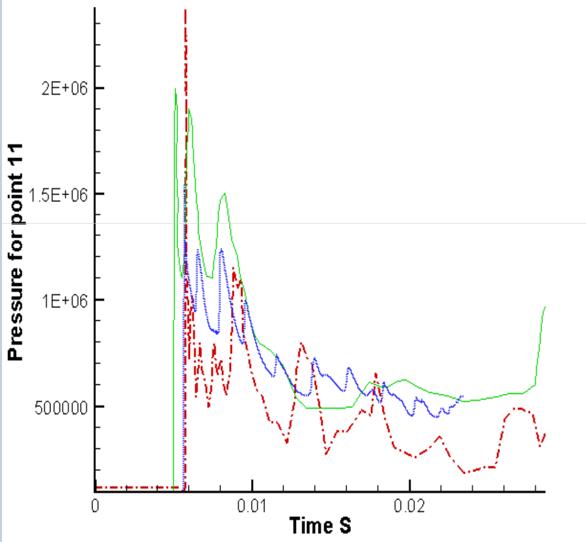
Red - Experimental results of RUT [1]
Blue - Present predictions
Green - RUT predictions [1]



The predicted pressure (in Pascal) *vs* time for point 9

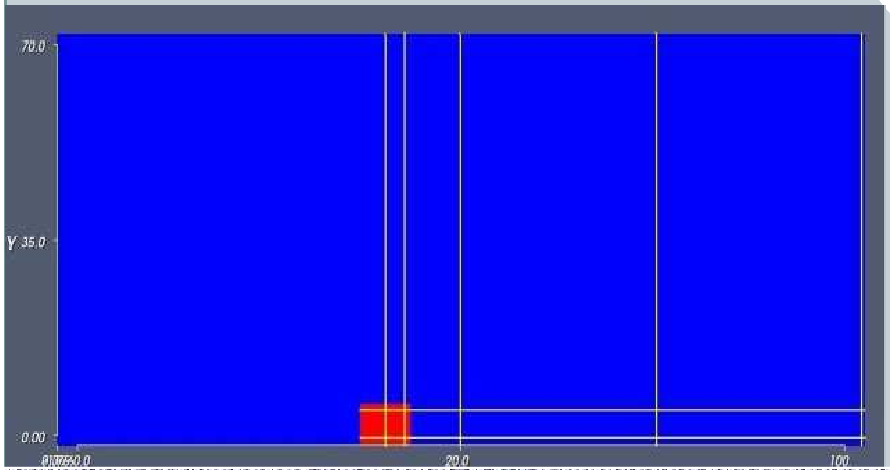


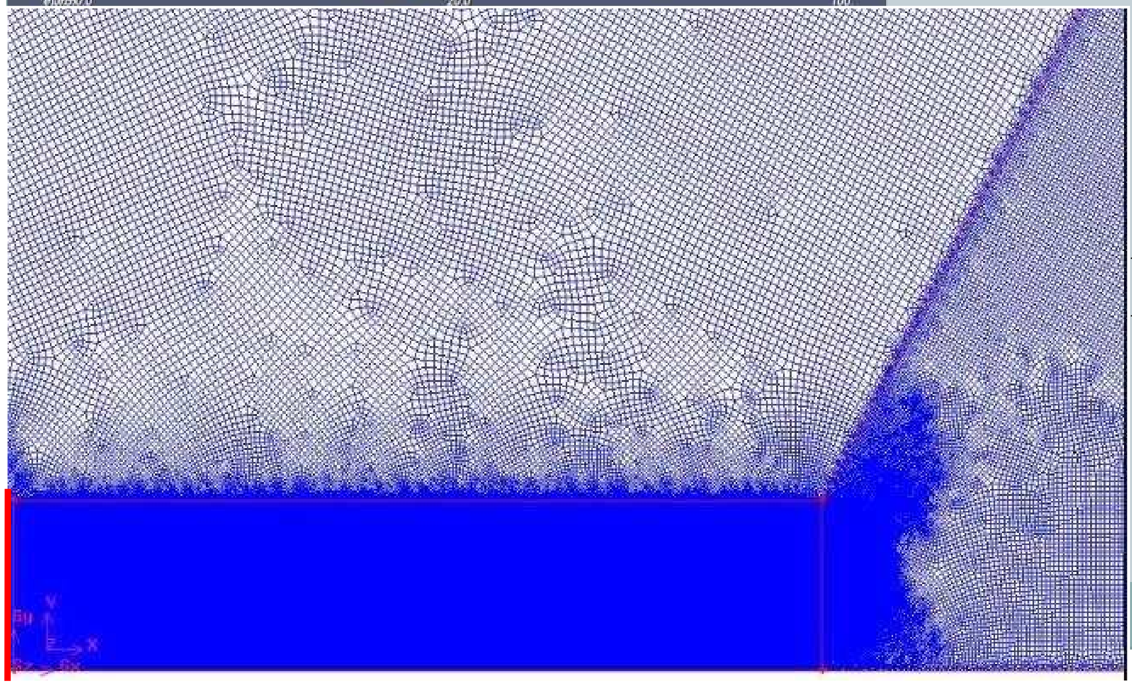
The predicted pressure (in Pascal) *vs* time for point 10



The predicted pressure (in Pascal) *vs* time for point 11

CASE 2 - planar hydrogen-air cloud





- **Case 2: The planar hydrogen-air cloud (2D)**
  - ➢vapour cloud of stoichiometric Hydrogen air mixture
  - ➢Domain size =70 ×160 m
  - ➢Cloud size = 7 ×10 m
  - ➢1 cm uniform mesh inside the cloud
  - ➢Non-uniform extending mesh outside the cloud

Wall (ground) and pressure transmissive (for top and sides of the domain) boundaries

Initial ignition

- ➢a region of high temperature and pressure (3000 K, 15atm)

CASE 2 - planar hydrogen-air cloud

- Pressure and is monitored on 5 vertical and 2 horizontal Monitoring lines

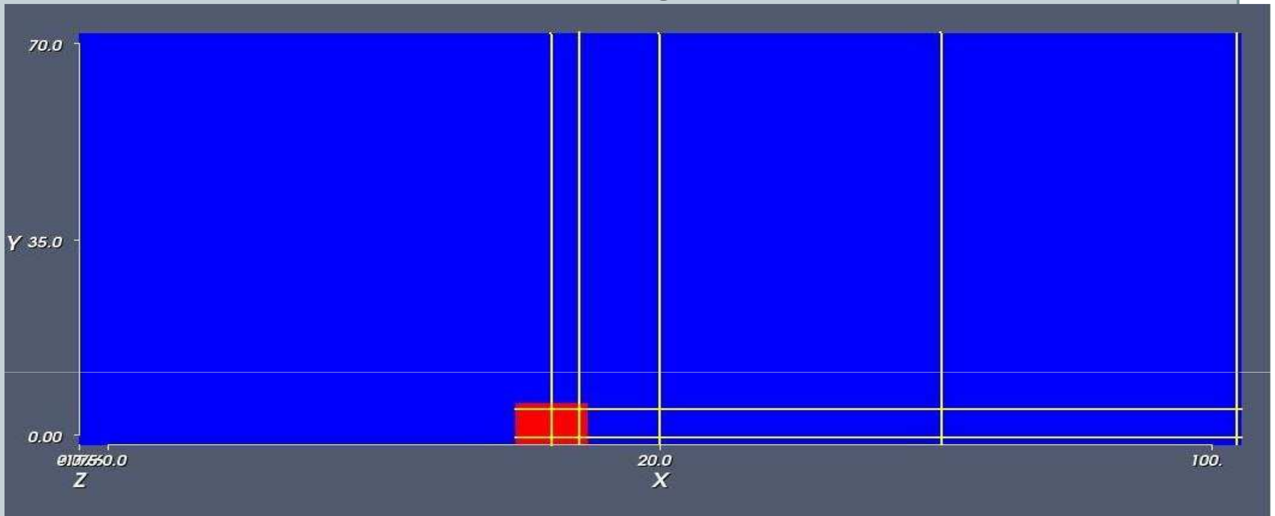
Vertical:

X = 5, 9, 20, 60 and 100 m

Horizontal:

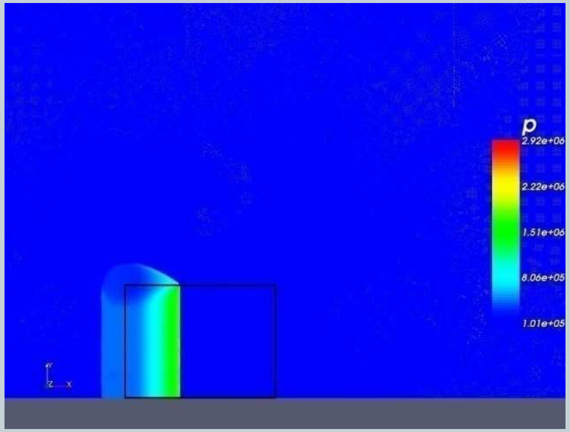
Y = 1 m

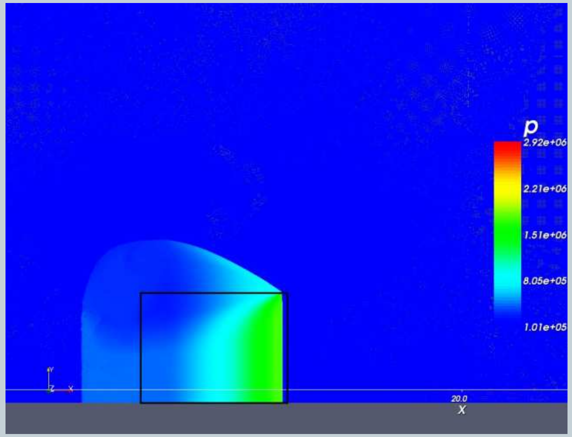
Y = 6 m



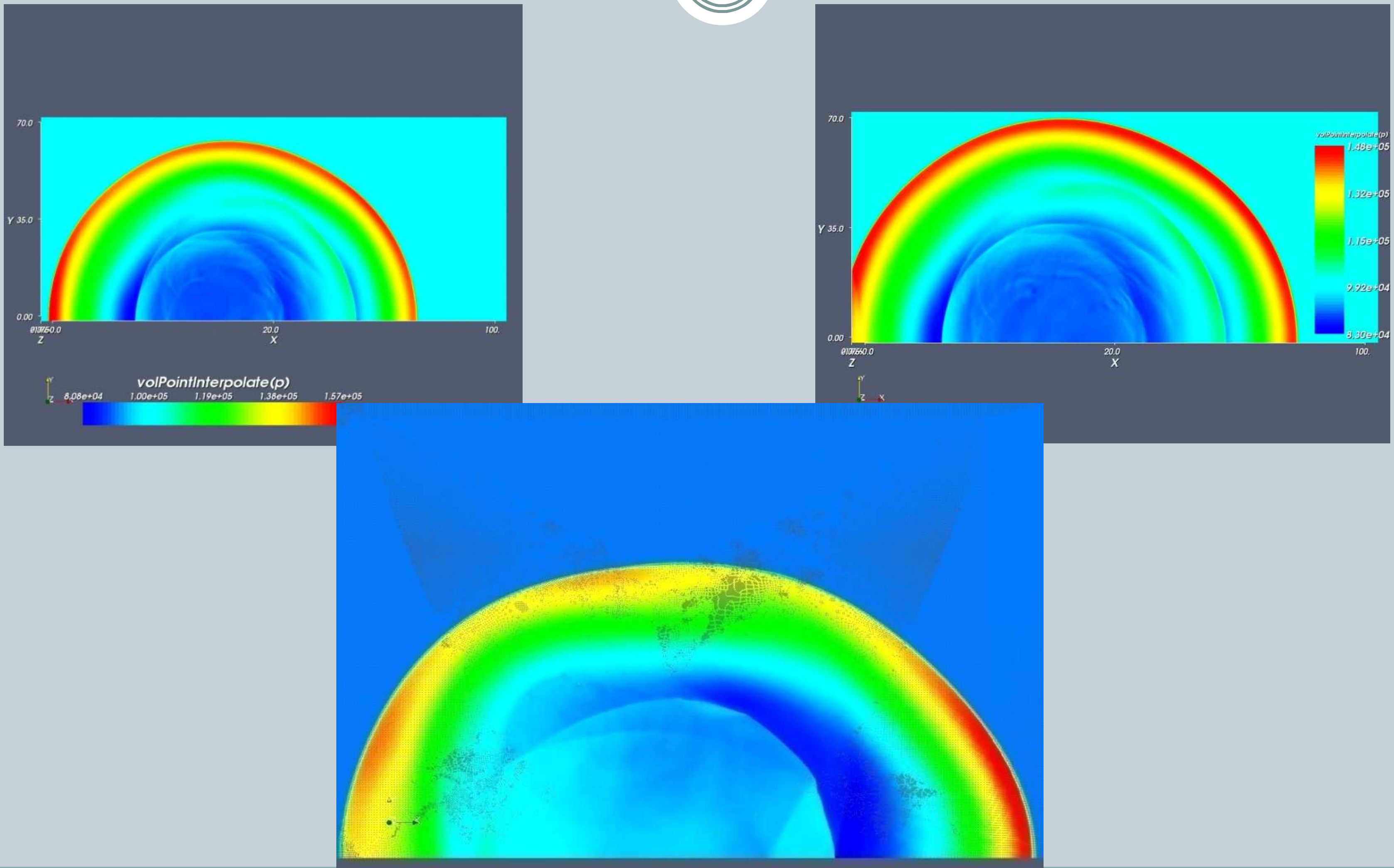
Monitoring points	Coordinates
1	(0.2 1.0)
2	(5.0 1.0)
3	(10 1.0)
4	(12 1.0)
5	(19 1.0)

Coordinates of the monitoring points





CASE 2 – Blast wave in the planar hydrogen-air cloud
Blast wave



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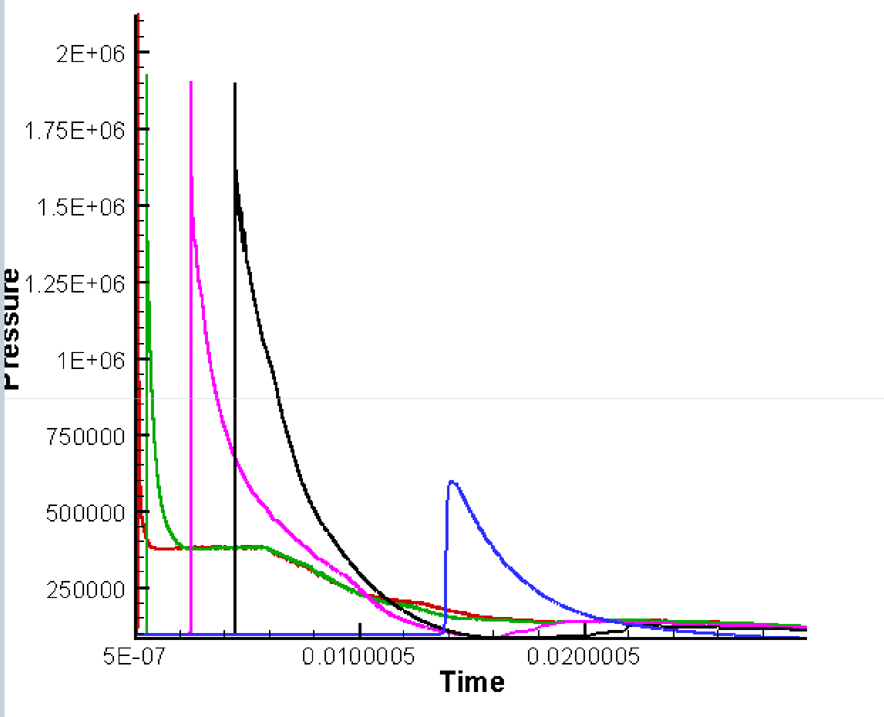
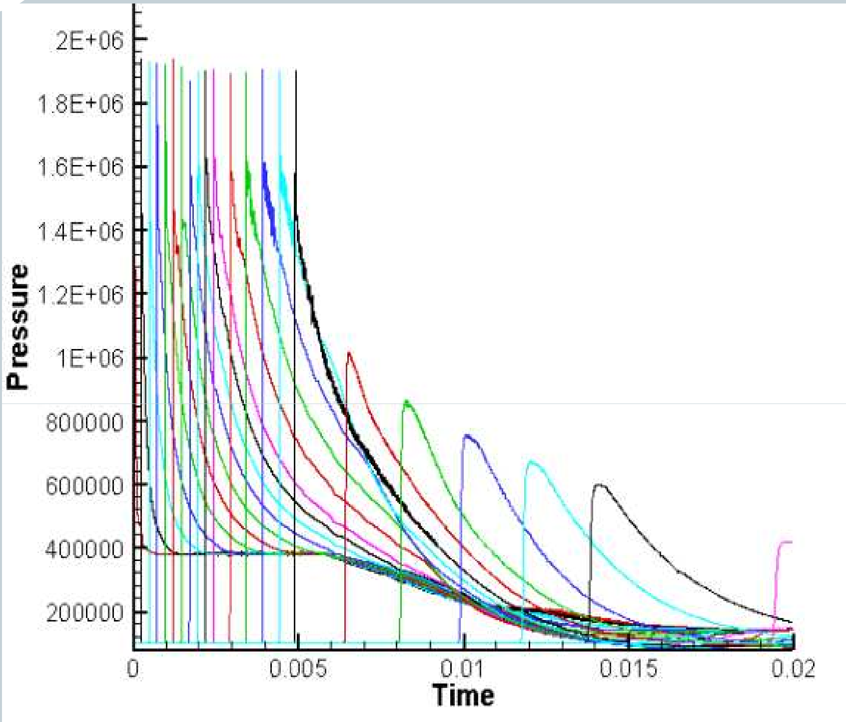
CASE 2 - planar hydrogen-air cloud

Pressure diagram



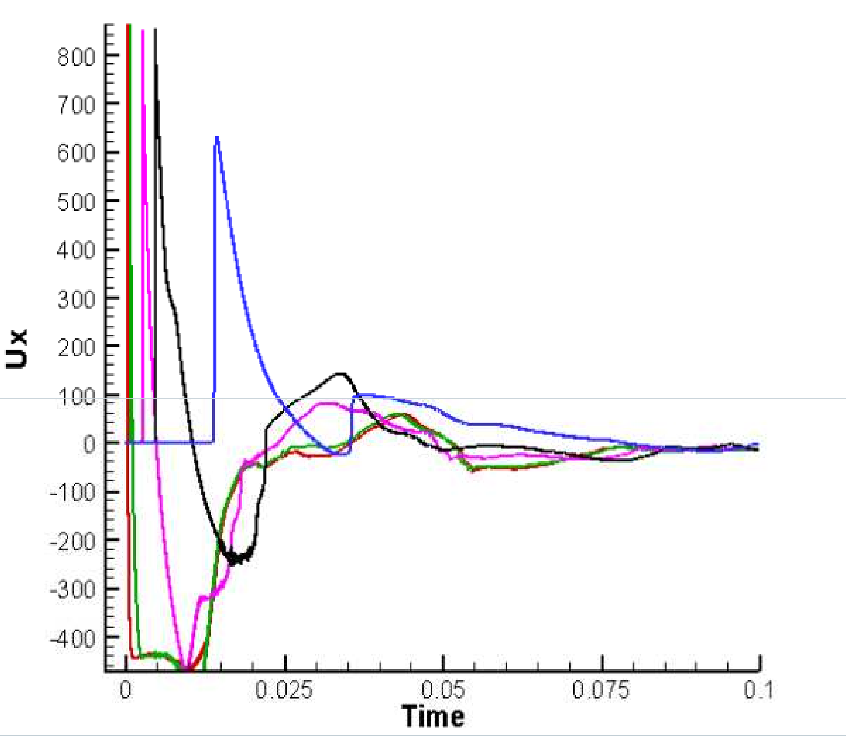
The pressure-time diagram the line 1 m above the ground (P unit is Pascal)

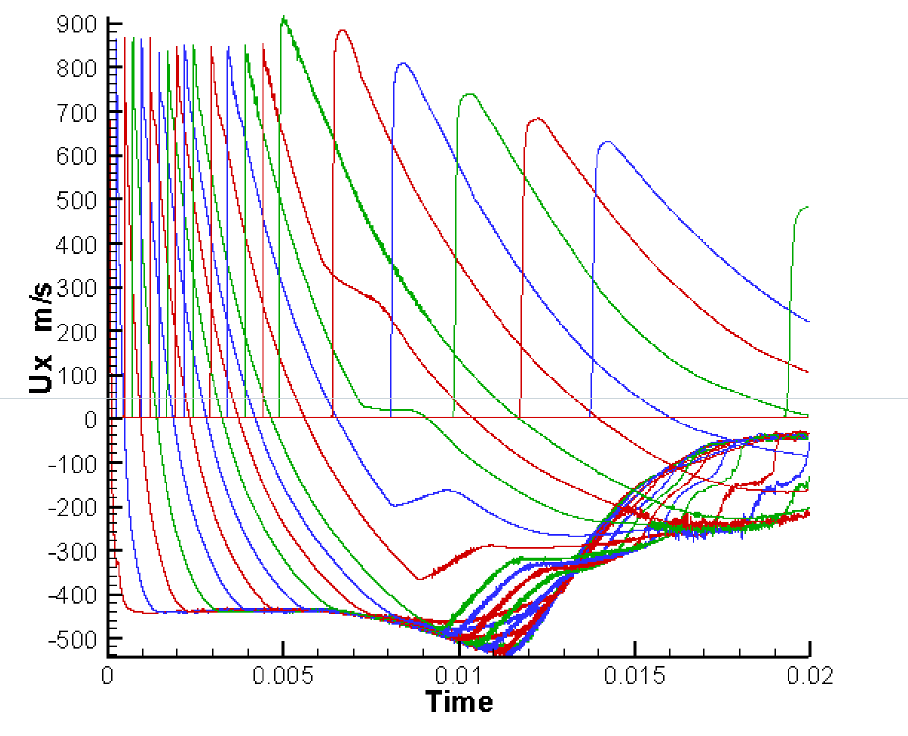


The velocity-time diagram at selected points 1m above the ground (U unit is meter per second)

CASE 2 - planar hydrogen-air cloud

Pressure and Velocity diagram (horizontal line, y=1m)



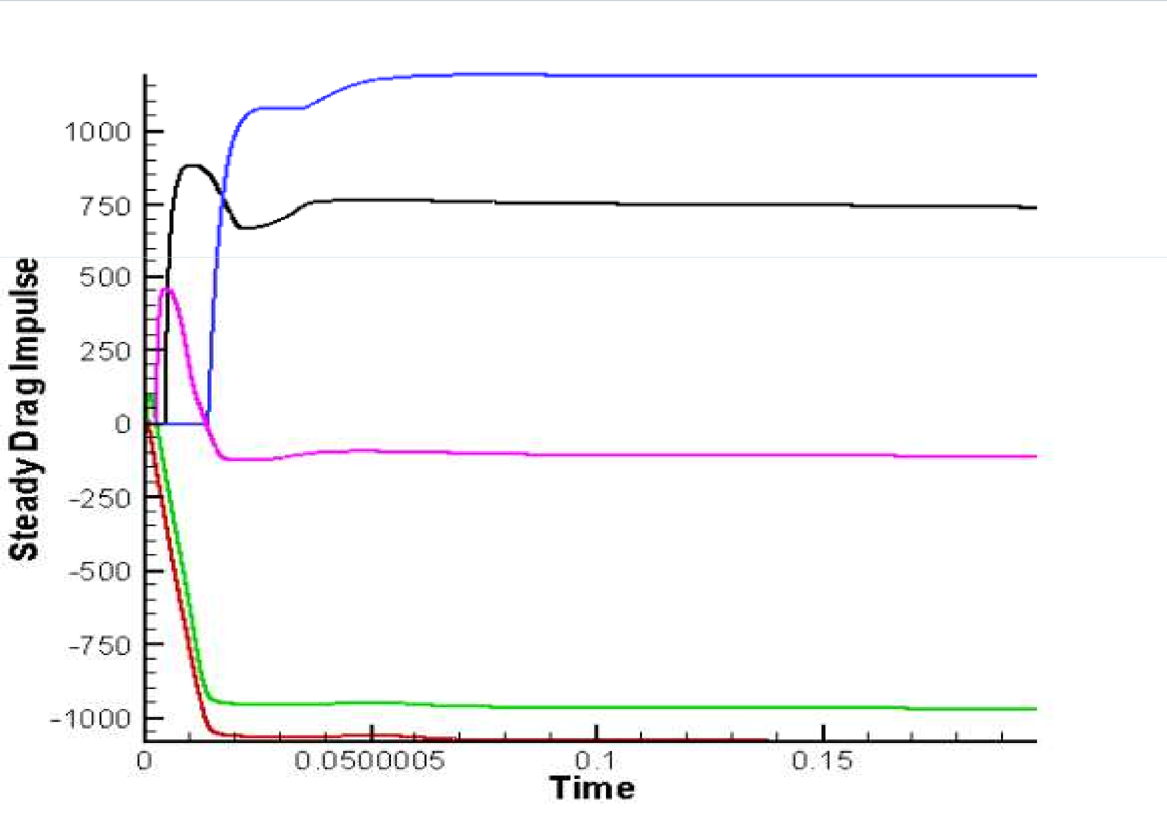


The pressure-time diagram the line 1 m above the ground (P unit is Pascal)

CASE 2 - planar hydrogen-air cloud

Drag Impulse diagram

$$I = \int f_D dt = \int_0^{t_i} \left\{ \left(\frac{1}{2} C_d \times \rho \times A \times Ux \times |Ux| \right) + \rho \frac{dU_x}{dt} \right\} dt$$



The drag impulse *vs* time at selected points 1 m above the ground

Conclusion

- A numerical approach for the simulation of large scale detonation has been developed.
- Predictions of the detonation tests in the RUT tunnel facility are in reasonably good agreement with the data in terms of the time of detonation arrival at different monitoring point. The general trend of the pressure wave has also been captured.
- For the planar cloud case, the blast wave was found to damp very quickly from the edge of the cloud. This shows the importance of coupling between combustion and shock in order to sustain the shock strength.
- In planar cloud case, due to pressure gradient behind the shock passage, a long duration of negative velocity was predicted, resulting in negative drag impulse. This phenomena is of important relevance in explaining damages following some large scale industrial accident.