

# Numerical simulation of large scale hydrogen detonation



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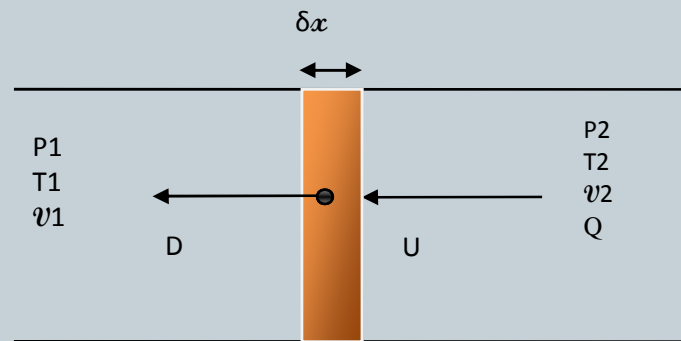
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# Detonation wave



- 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

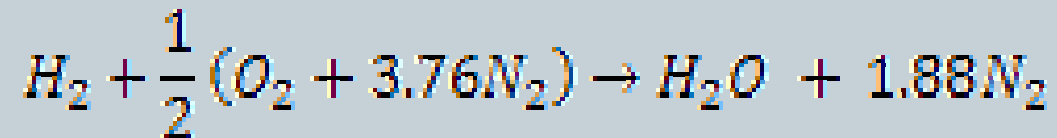
$$\partial\rho\alpha/\partial t = -\nabla(\rho\alpha\mathbf{v}) + \rho W$$

Reaction progress

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

Energy equation

# Chemistry



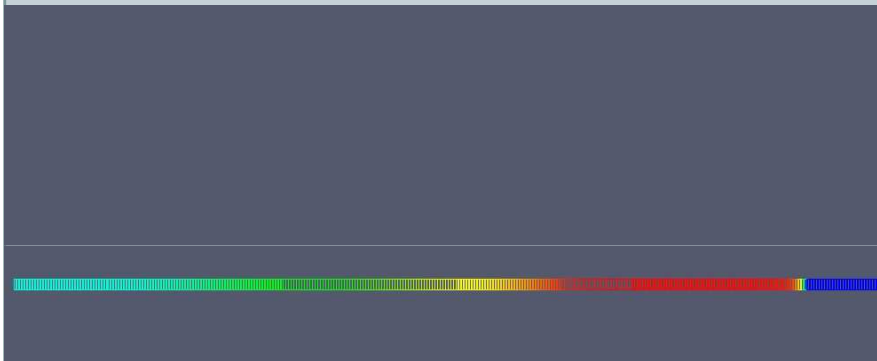
*Reactants* → *products*

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

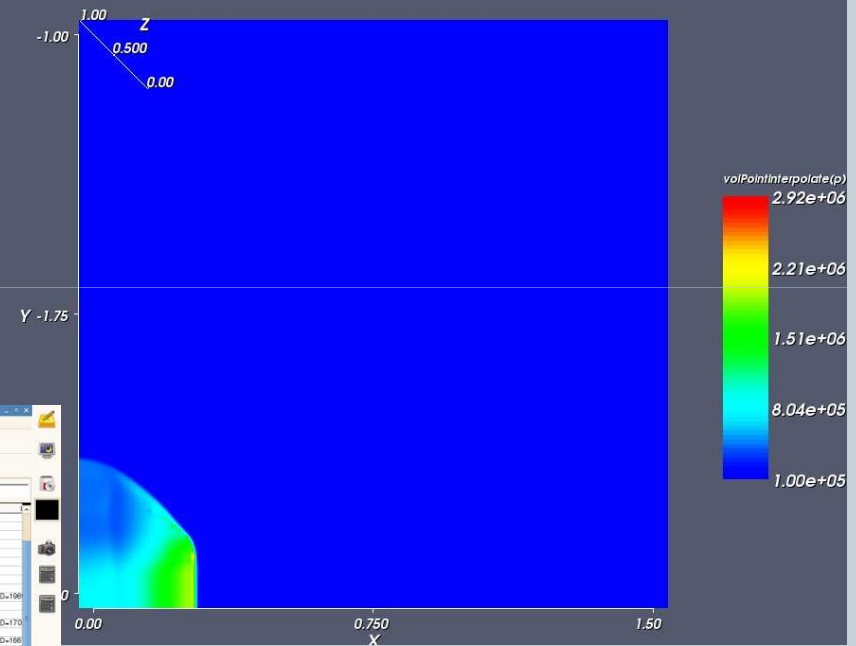
CJ Pressure	Temperature	Shock Velocity	Products Velocity
17 atm	3364 K	2090 m/s	890 m/s

# Tuning the chemistry parameters

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



	A	B	C	D	E	F	G	H	I	J	K
19	7.00000000E+005	-564600	-2.29E-001	5314	189	time-5e5	T=4031	$\mu=0.03838$	$\mu=17.3$	slow damping	
11	7.00000000E+005	-564600	-2.29E-001	5314	189	time-3e5	T=3967	$\mu=0.03804$	$\mu=16.7$	no change	
12	7.00000000E+005	-564600	-2.29E-001	5314	189	time-3e5	T=3768	$\mu=0.04424$	$\mu=15.5$	very low damp	
13	7.00000000E+005	-564600	-2.29E-001	5314	189	time-3e5	T=4226	$\mu=0.04467$	$\mu=15.8$	no change	
14	7.00000000E+005	-564600	-2.29E-001	5314	189	time-3e5	T=3625	$\mu=0.10566$	$\mu=13.9$	sharp damp, wrong DCo=1670	
15	7.00000000E+005	-154600	-2.29E-001	5314	189	time-3e5	T=2870	$\mu=0.048239$	$\mu=20.7$	wrong temp and source	
16											
17	7.00E+014	###	-2.29E-001	101325	189	time-5e5	T=619	$\mu=0.06949$	$\mu=14.7$	fast damp, source zero, separated pressure and temp	
18	8.30E+008	-10000	0.00E+000	101325	189	time-5e5	T=2304	$\mu=0.09481$	$\mu=18.25$	slow temp and source	
19	8.30E+008	-10000	0.00E+000	101325	1	time-5e5	T=2437	$\mu=0.10001$	$\mu=19.4$	a lot of oscillation, +10max, 1.06e5 and damping	D=109
20	8.30E+008	-10000	0.00E+000	101325	1	time-5e5	T=	$\mu=$	$\mu=$	with oscillation	
21	2.30E+010	-10000	0.00E+000	101325	1	time-5e5	T=	$\mu=$	$\mu=$	failed, temp higher than 5000	
22	1.30E+010	-20000	0.00E+000	101325	1	time-5e5	T=2668	$\mu=0.10323$	$\mu=21.1$	good	D=170
23	1.30E+010	-378000	0.00E+000	101325	189	time-5e5	T=2565	$\mu=0.10333$	$\mu=21.06$	good	
24	1.30E+010	-378000	-1.29E-001	101325	189	time-5e5	T=2457	$\mu=0.101$	$\mu=21.5$	good	D=166
25	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2457	$\mu=0.09481$	$\mu=21.5$	with oscillation	
26	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2481	$\mu=0.1002$	$\mu=20.9$	with small oscillation, not really good	D=168
27	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2440	$\mu=0.10072$	$\mu=19.4$	unrealistic (system) pressure at the end + oscillations	
28	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2336	$\mu=0.10053$	$\mu=23.1$	with oscillation and not really good	
29	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	not very good	
30	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2480	$\mu=0.10077$	$\mu=21.1$	good	D=167
31	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	decoupled pressure and temperature and damping	
32	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2390	$\mu=0.10183$	$\mu=21$	large oscillations	
33	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2461	$\mu=0.10245$	$\mu=19.5$	large oscillations	
34	1.00E+010	-378000	-2.29E-001	101325	189	time-5e5	T=2503	$\mu=0.10311$	$\mu=21.1$	Good	D=170
35	1.00E+010	-378000	-1.29E-001	101325	189	time-5e5	T=2996	$\mu=0.11073$	$\mu=21.2$	Excellent	D=163
36											
37	1.00E+010	-378000	1.01E-001	101325	189	time-5e5	T=2800	$\mu=0.10866$	$\mu=20.7$	maxCo=0.01	D=176
38	1.00E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
39	1.21E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	D=176
40	1.20E+010	-476000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	separated P and T	
41	1.20E+010	-378000	1.29E-001	61325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
42	1.20E+010	-378000	1.29E-001	61325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
43	1.20E+010	-378000	1.29E-001	61325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
44	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=2939	$\mu=0.11028$	$\mu=20.4$	maxCo=0.01	D=161
45	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=2895	$\mu=0.1097$	$\mu=20.5$	low rho number	D=160
46	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=2896	$\mu=0.1097$	$\mu=20.5$	maxCo=0.01	
47	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	Flapp, High temp	
48	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	with oscillation	
49	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed after 3 de-5 and discontinuity in P field	
50	1.20E+010	-476000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
51	1.20E+010	-476000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	separated P and T	
52	1.20E+010	-476000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
53	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	separated P and T	
54	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	separated P and T	
55	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	separated P and T	
56	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	flapping	
57	1.20E+010	-476000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	better but still separated	
58	1.20E+010	-378000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
59	1.20E+010	-400000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	
60	1.20E+010	-400000	1.29E-001	101325	189	time-5e5	T=	$\mu=$	$\mu=$	failed	



# 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

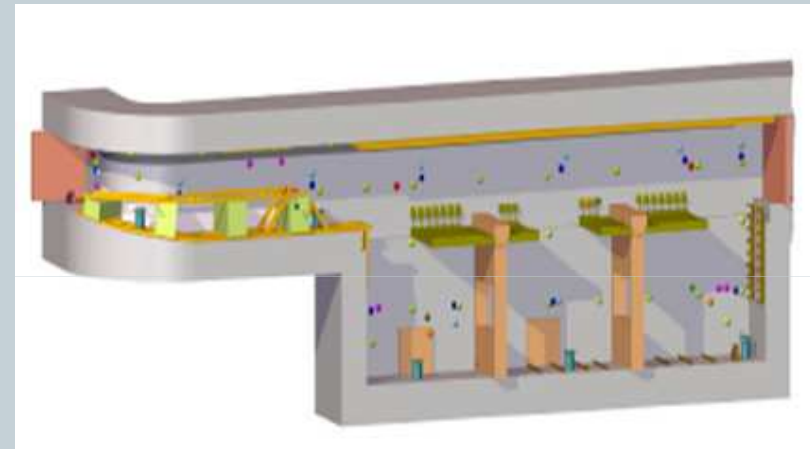
- RUT tunnel facilities in Russia, (standard test cases selected for HYSAFE)
  - Hydrogen air mixture
  - volume = 263 m<sup>3</sup>
  - 5 cm uniform grid

## Boundaries

- Wall for all boundaries

## Initial ignition

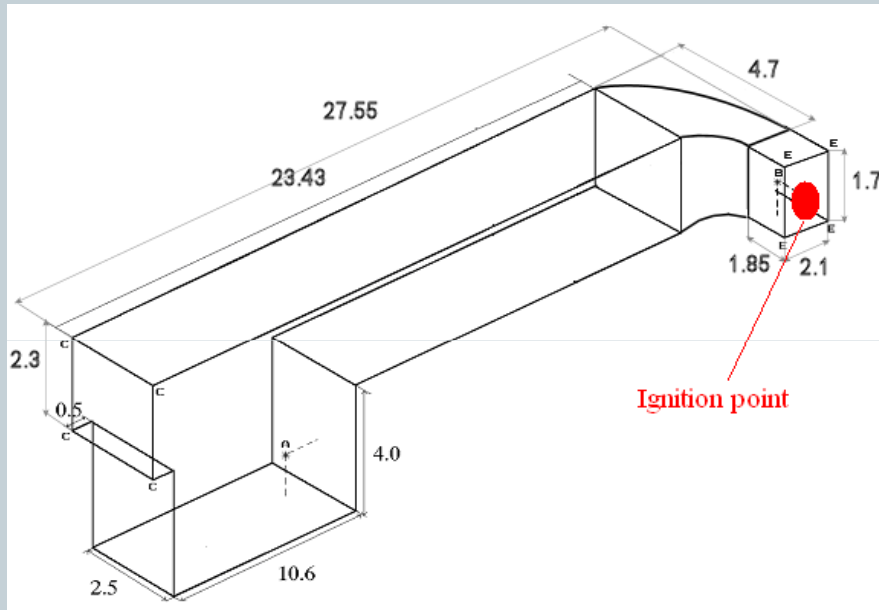
- a region of high temperature and pressure (3000 K, 15atm)



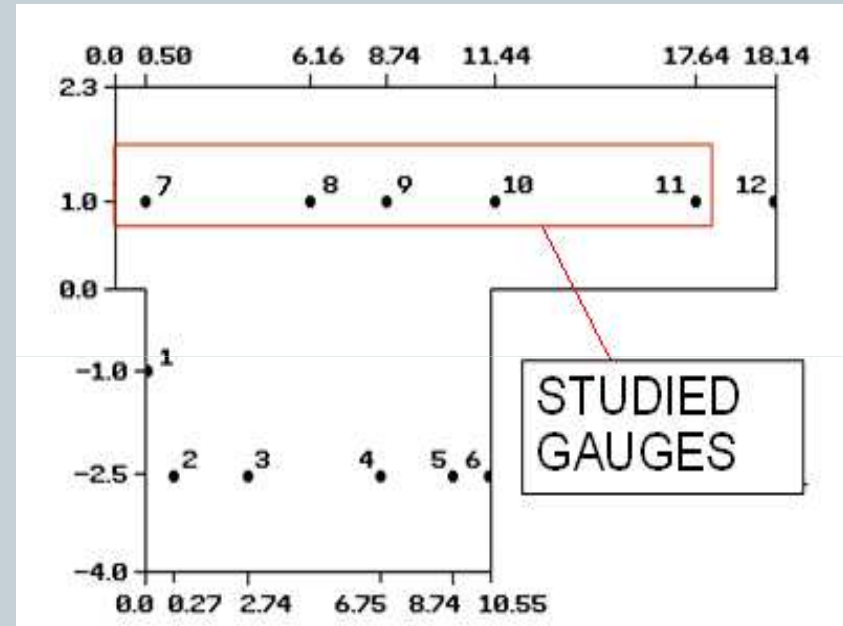
The experiment channel (reproduced from [1]),  
Laboratory of Induced Chemical Reactions,  
Russian Research Center "Kurchatov Institute"



# CASE 1 - Hydrogen detonation in the RUT tunnel facility

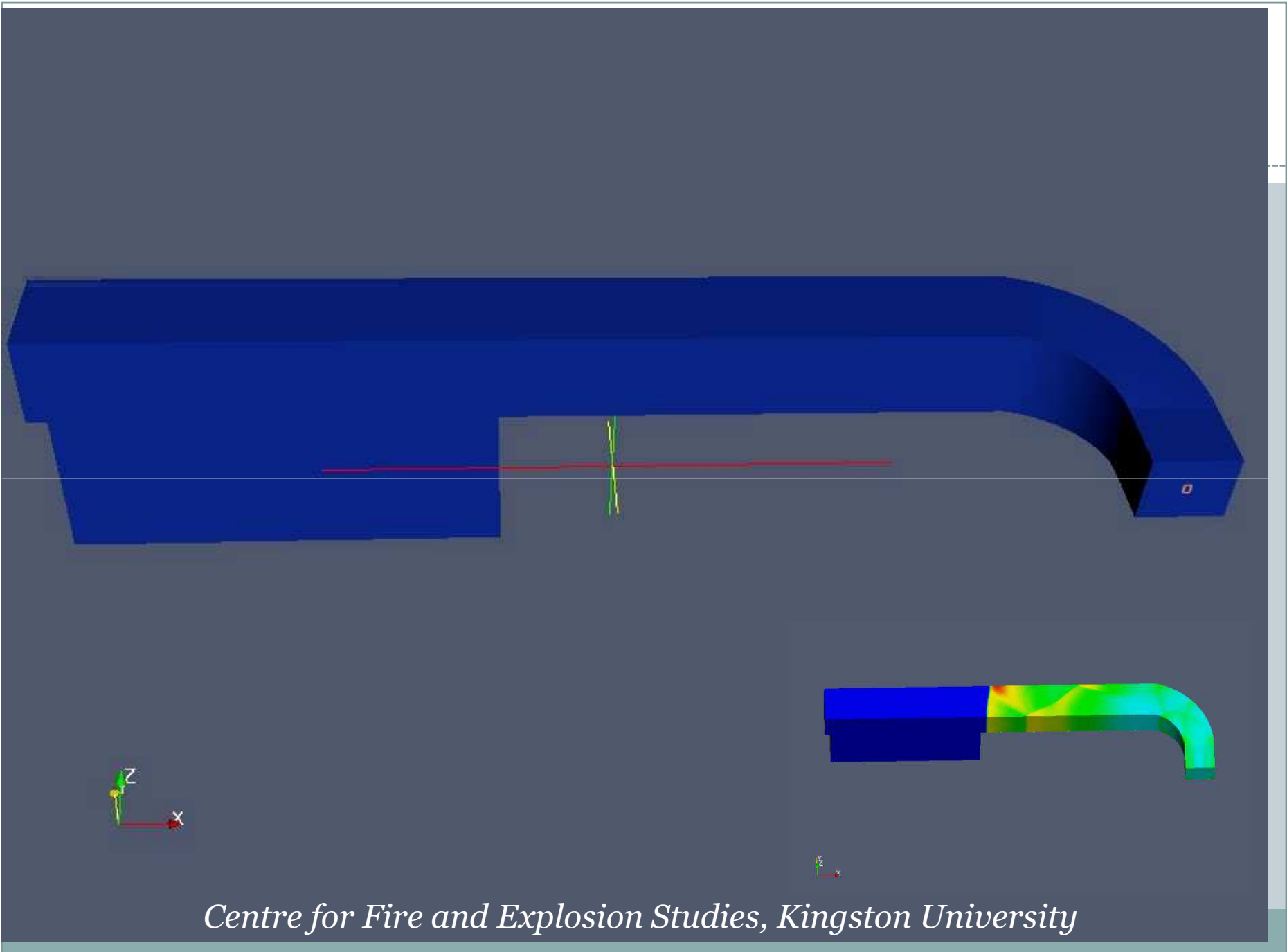


The tunnel dimensions (reproduced from [1])



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

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

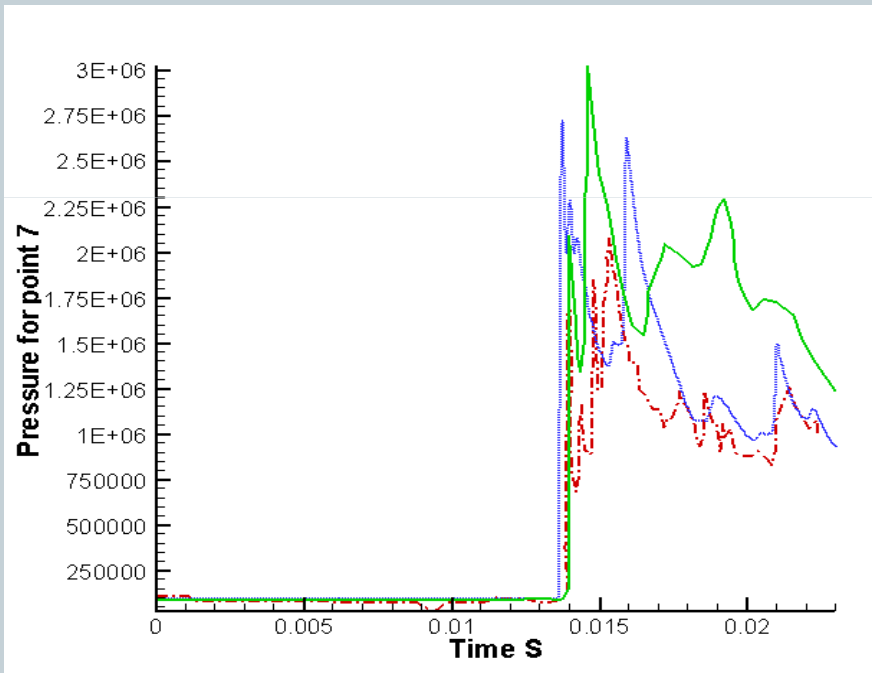


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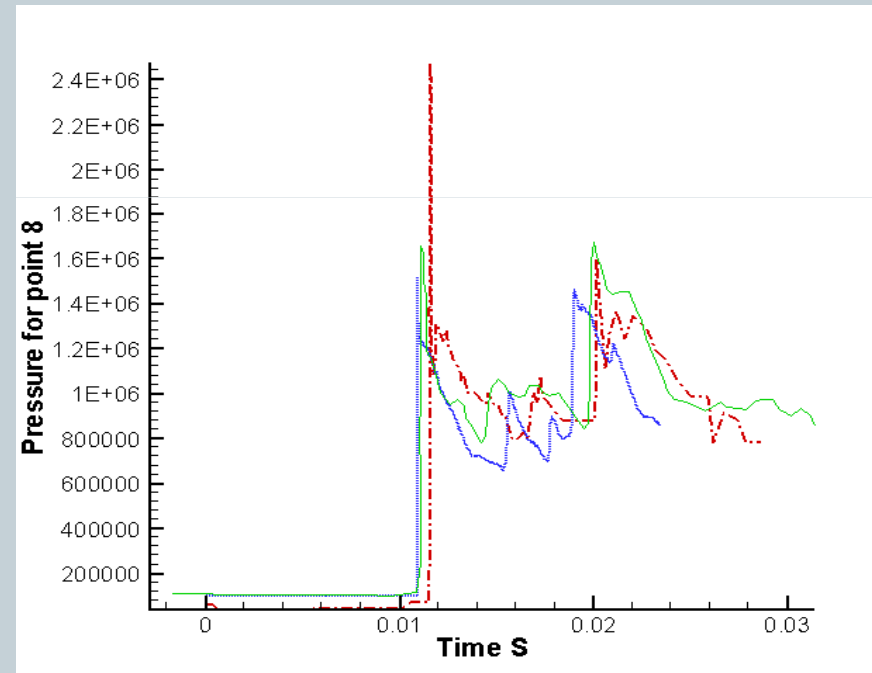
# CASE 1 - Hydrogen detonation in the RUT tunnel facility



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



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

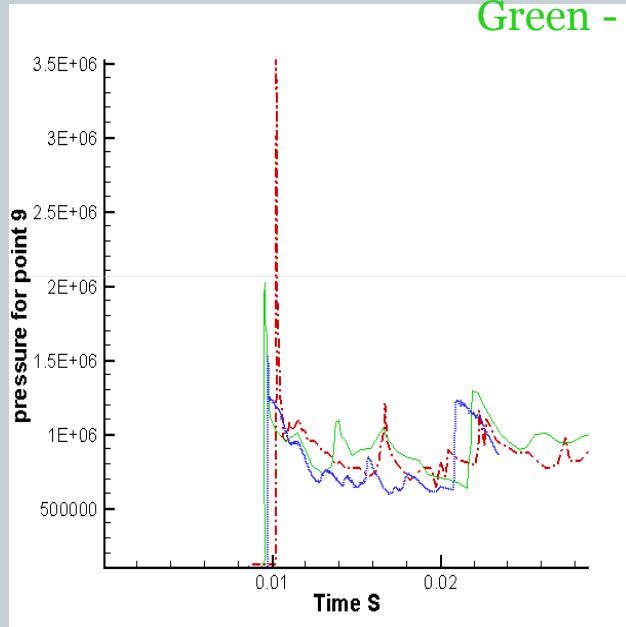


The predicted pressure (in Pascal) vs time for point 8

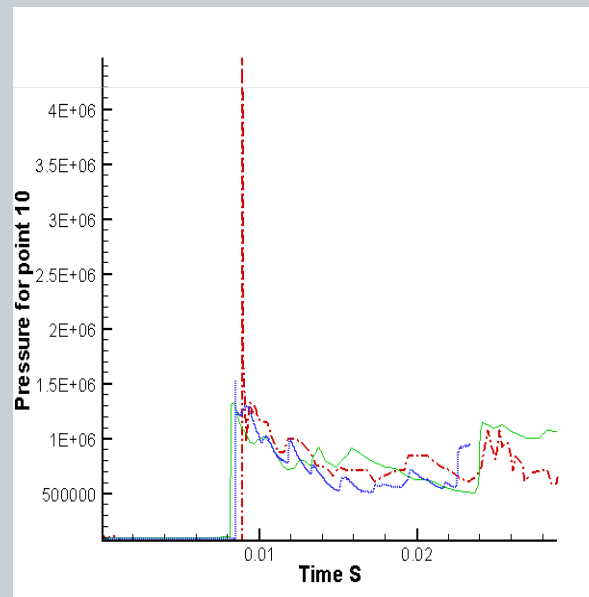
# CASE 1 - Hydrogen detonation in the RUT tunnel facility



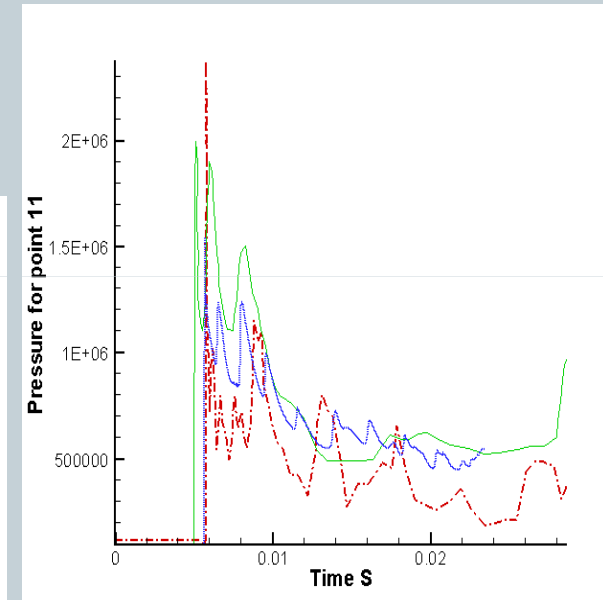
Red - Experimental results of RUT [1]  
Blue - Present predictions  
Green - RUT predictions [1]



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

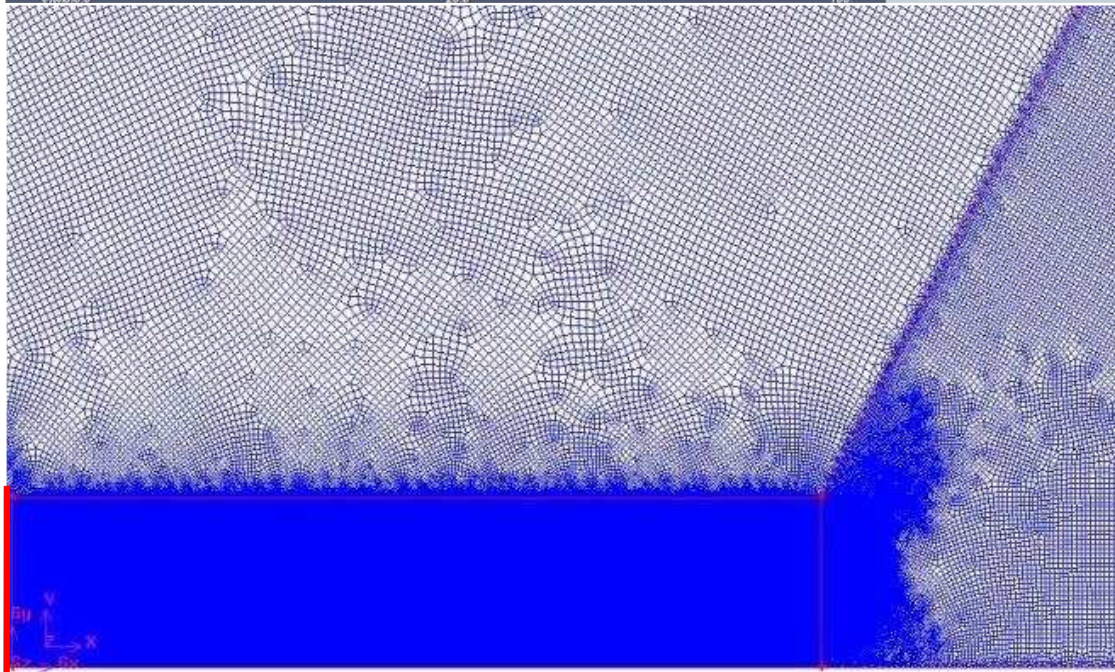
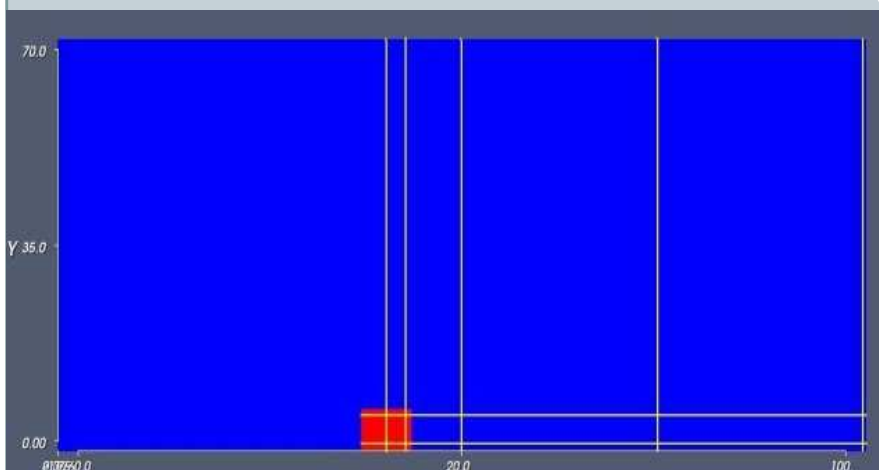


The predicted pressure (in Pascal) vs time for point 10



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 =  $70 \times 160$  m
- Cloud size =  $7 \times 10$  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

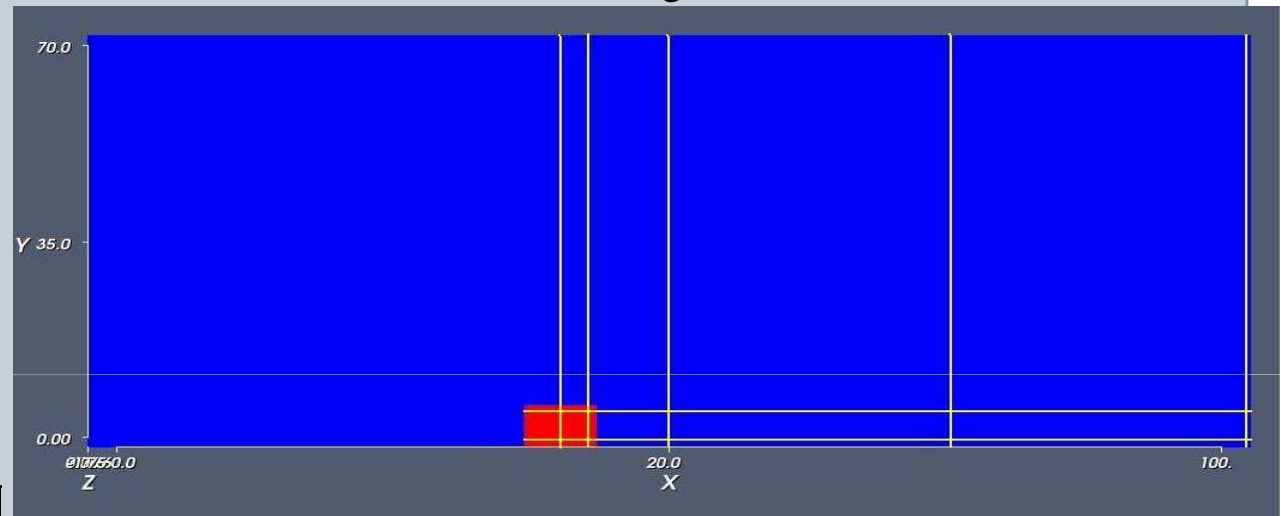
Vertical:

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

Horizontal:

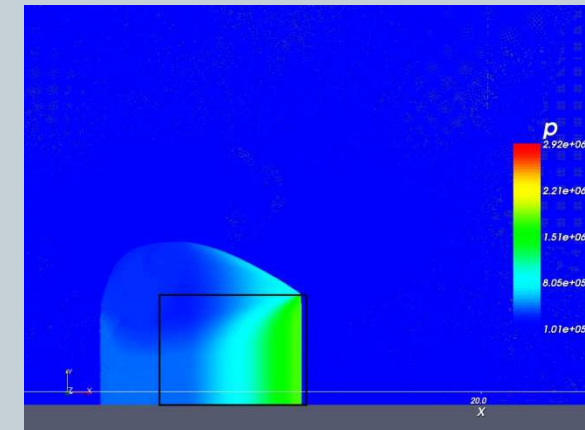
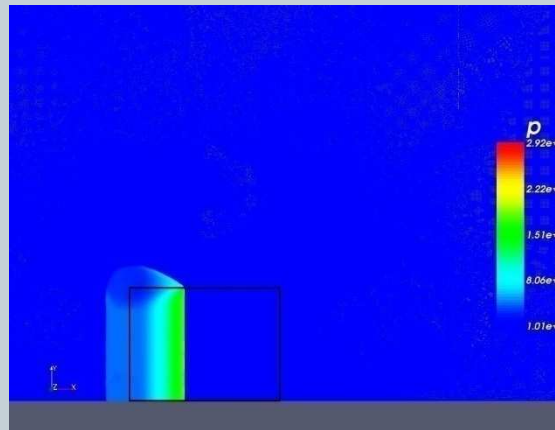
Y = 1 m

Y = 6 m



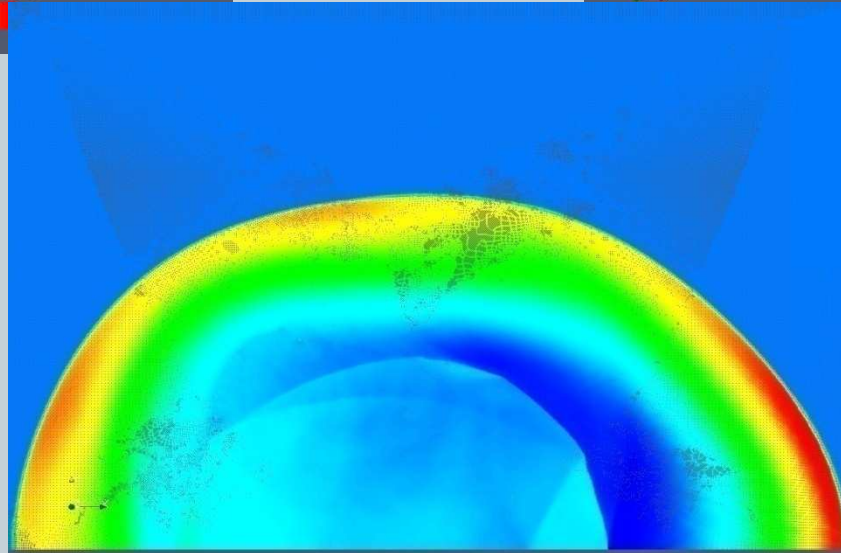
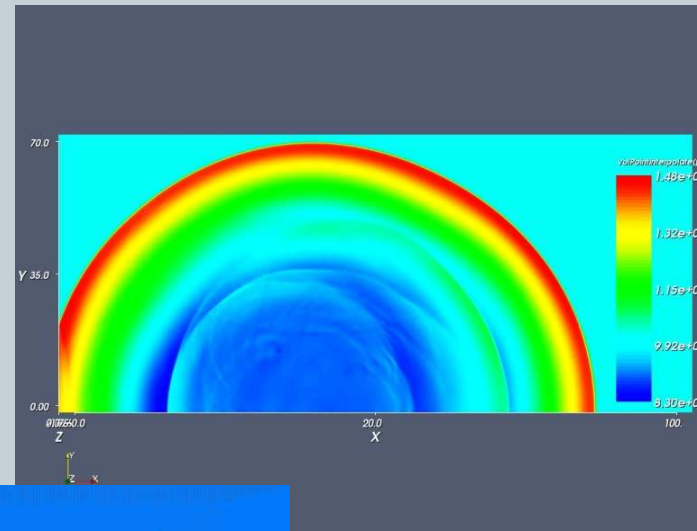
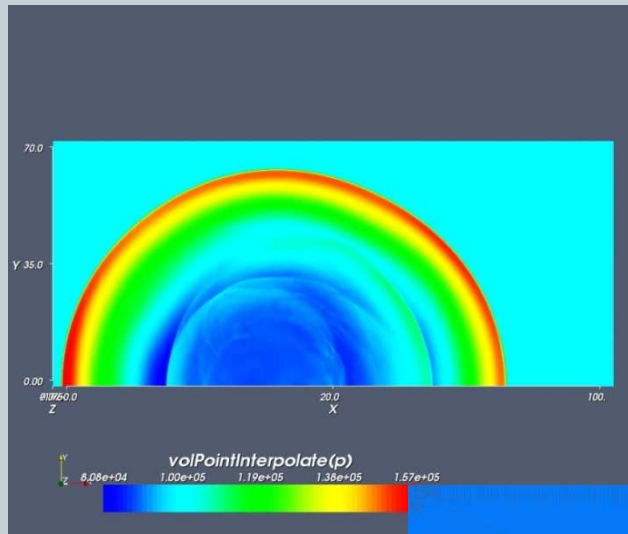
Monitoring points	Coordinates
1	(0.2 1.0)
2	(5.0 1.0)
3	(10 1.0)
4	(12 1.0)
5	(19 1.0)

Coordinates of the monitoring points

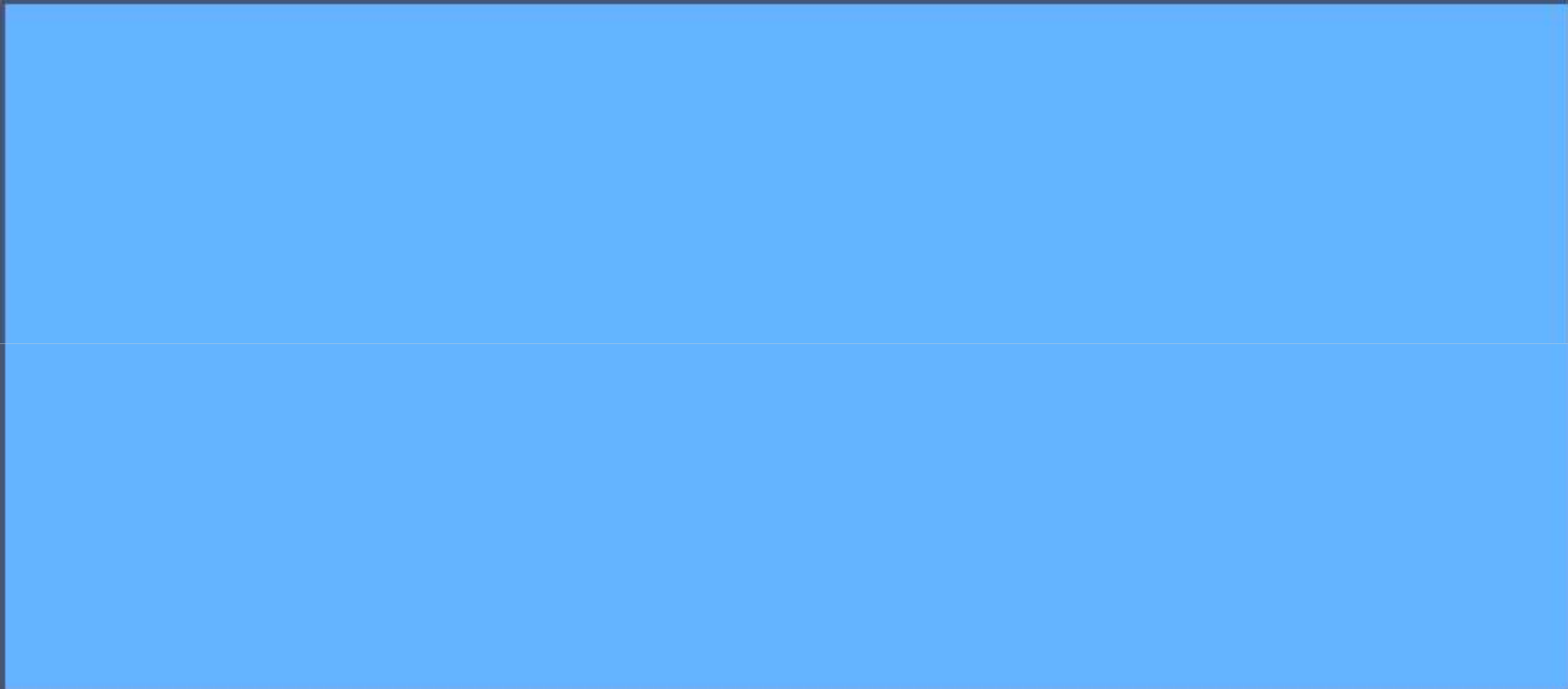


# CASE 2 – Blast wave in the planar hydrogen-air cloud

## Blast wave



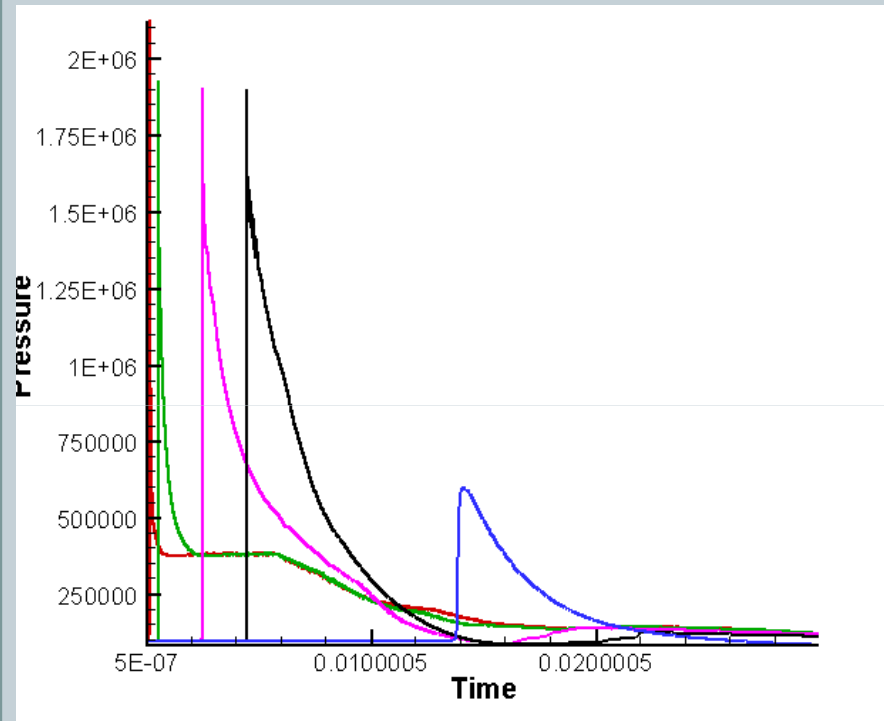
$p$   
8.0e+04 9.8e+04 1.2e+05 1.3e+05 1.5e+05



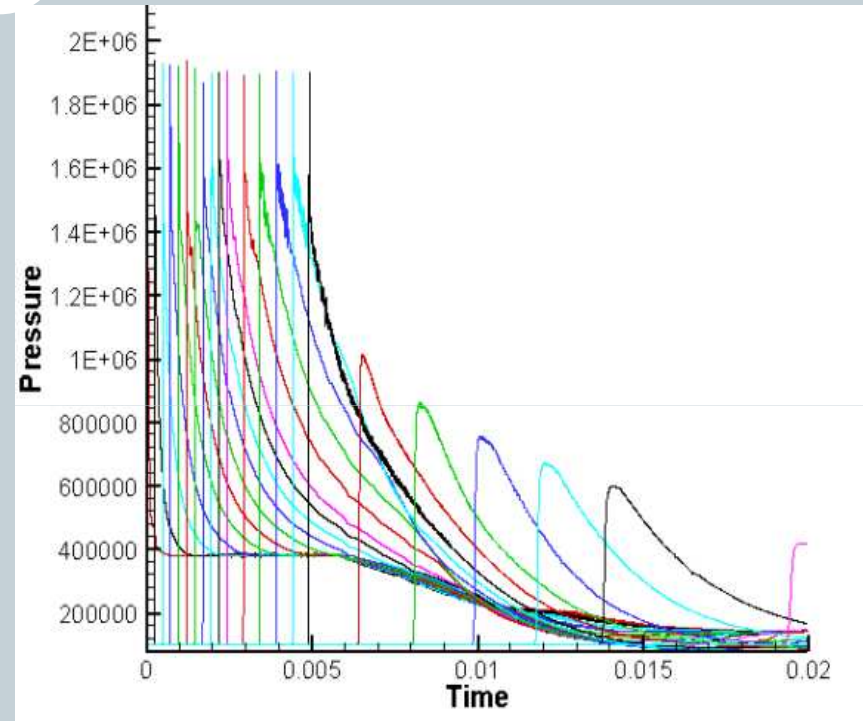


# CASE 2 - planar hydrogen-air cloud

## Pressure diagram



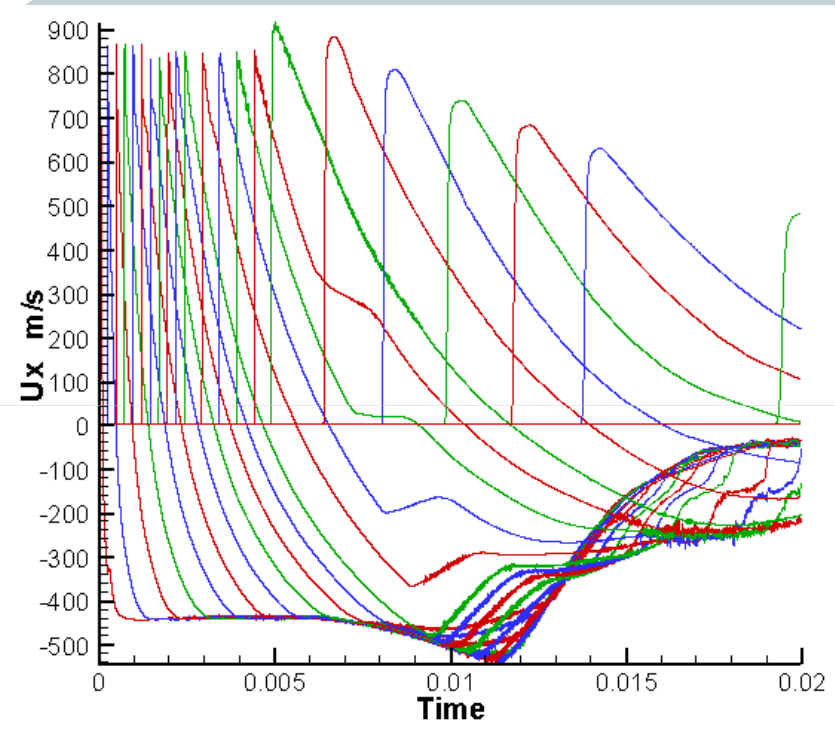
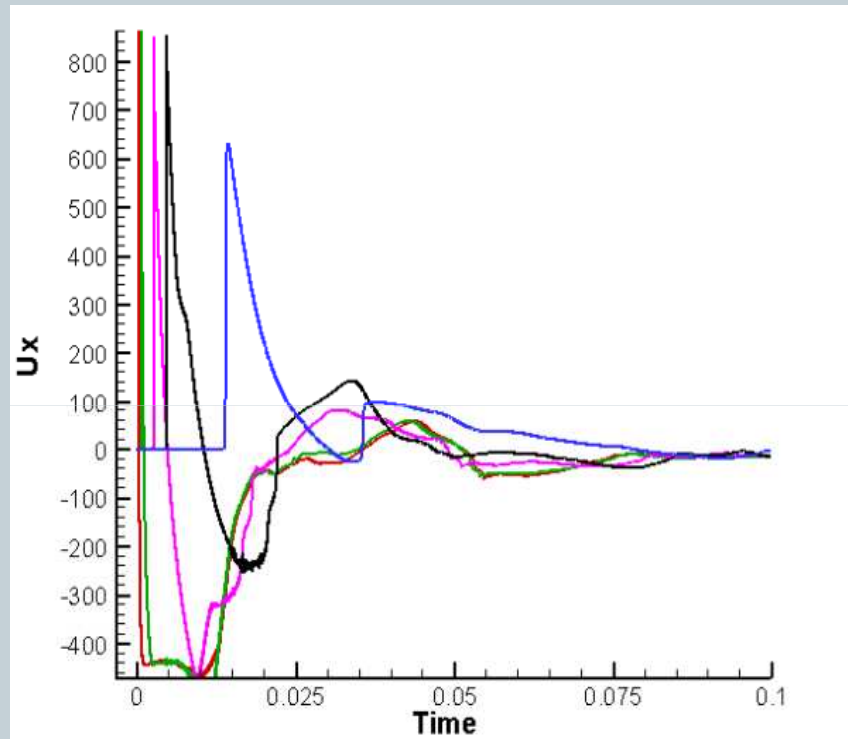
The pressure-time diagram the line 1 m above the ground (P unit is Pascal)



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,  $y=1\text{m}$ )

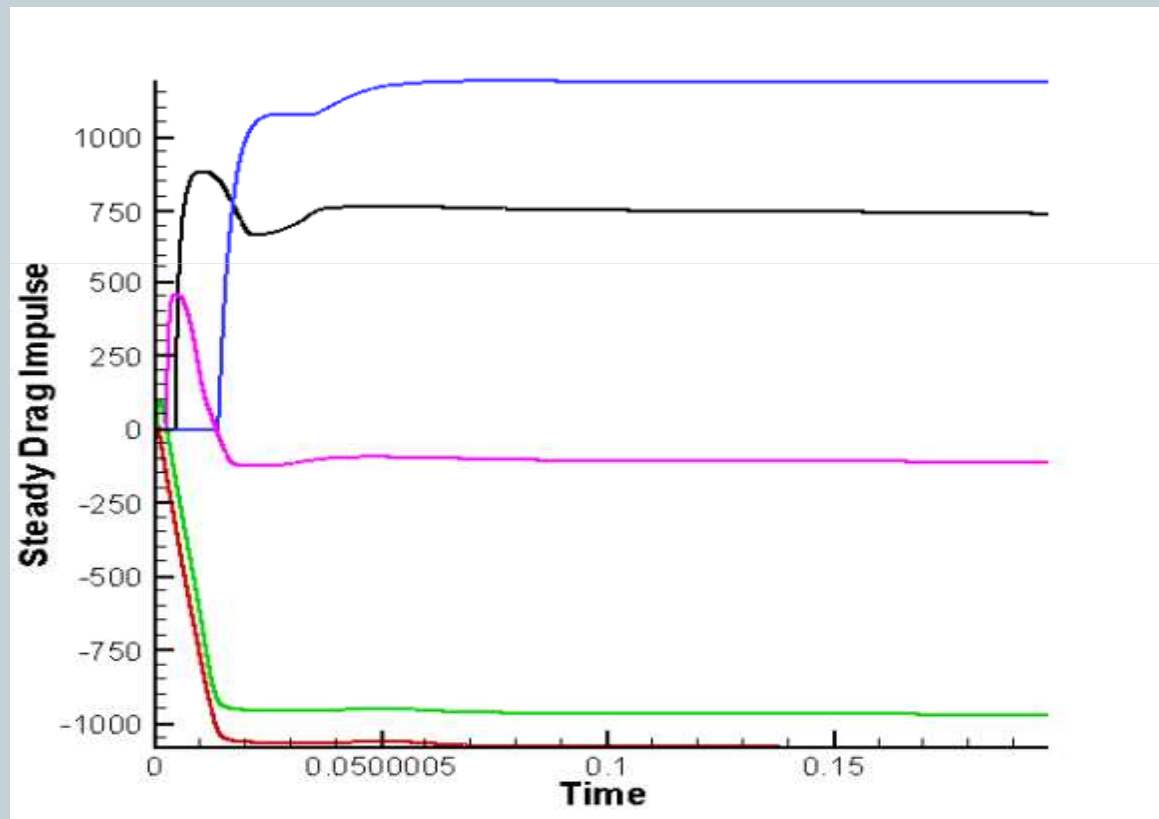


The pressure-time diagram the line 1 m above the ground (P unit is Pascal)

# CASE 2 - planar hydrogen-air cloud

## Drag Impulse diagram

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



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.