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Pressure limit of hydrogen spontaneous ignition in a T-shaped channel

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Outline

- Background
- Aim and objectives
- Experiment in T-shape channel (Golub et al., 2010)
- LES EDC model
- Modelling of membrane opening
  - Instant versus finite membrane opening
- Simulation results
  - Dynamics of spontaneous ignition at different storage pressure
- Conclusions

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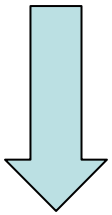
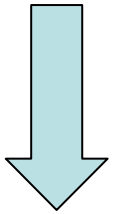
Background

Pressure relief device (PRD) activation



Sudden release of hydrogen into air



What is the lower pressure limit for spontaneous ignition in T-shape channel (PRD mock-up)?

Aim and objectives

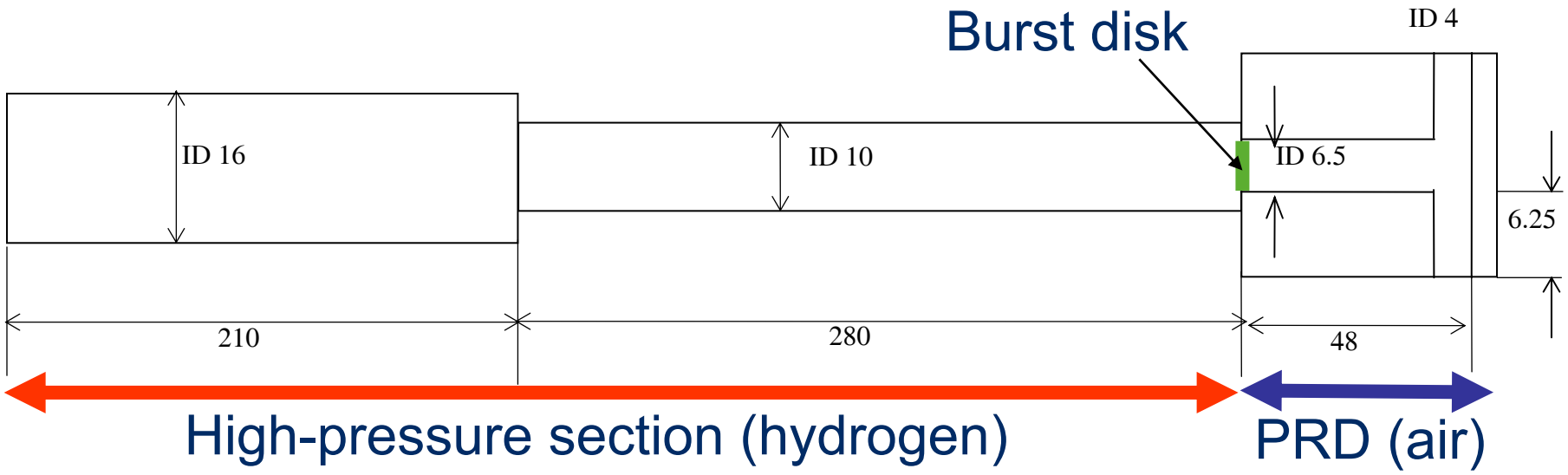
Aim: Develop contemporary model for predictive simulation of the phenomenon of hydrogen spontaneous ignition during sudden release from pressure relief devices (to be applied as a tool for hydrogen safety engineering)

Objectives:

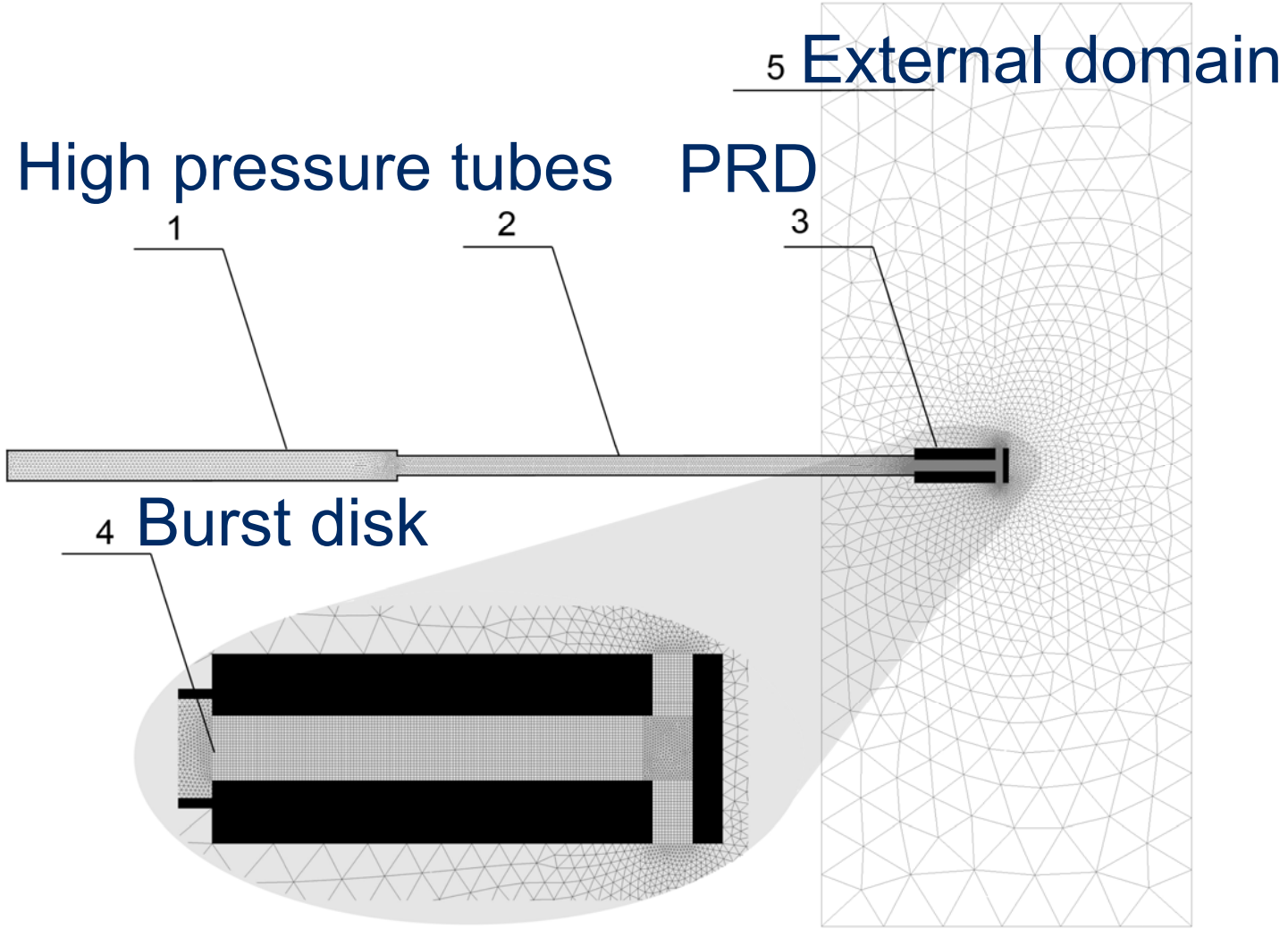
- Develop Large Eddy Simulation (LES) model based on the Eddy Dissipation Concept (EDC), full chemistry, and modelling of a burst disk opening in a finite time
- Validate the LES EDC model and simulations against experimental data by Golub et al. (2010) on spontaneous ignition in T-shape channel (mock-up PRD)
- Understand dynamics of the ignition process and explain scattering in reported experimental data (Golub et al., 2010)
- Establish the lower pressure limit for spontaneous ignition in T-shape channel

Experiment (Golub et al., 2010)

Burst disk rupture at storage pressures from 13.5 to 29 bar. Reported: **no ignition at 13.5 bar**, and **spontaneous ignition at 29 bar** (private communication – ignition at **24.3 bar**)



Computational domain



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LES equations

Continuity equation:

$$\frac{\partial \bar{\rho}}{\partial t}+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\right)=0$$

Momentum conservation equation:

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{u}_i\right)=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}-\frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right)+\bar{\rho}g_i$$

Energy conservation equation:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{E}\right)+\frac{\partial}{\partial x_j}\left(\tilde{u}_j\left(\bar{\rho}\tilde{E}+\bar{p}\right)\right)=\frac{\partial}{\partial x_j}\left[\frac{\mu_{eff}c_p}{\mathrm{Pr}_{eff}}\frac{\partial \tilde{T}}{\partial x_j}-\sum_m \tilde{h}_m\left(-\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \tilde{Y}_m}{\partial x_j}\right)+\right.$$

$$\left.+\tilde{u}_i\mu_{eff}\left(\frac{\partial \tilde{u}_i}{\partial x_j}+\frac{\partial \tilde{u}_j}{\partial x_i}-\frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right)\right]+\sum_m R_m H_C$$

Species conservation equation:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{Y}_H\right)+\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j\tilde{Y}_m\right)=\frac{\partial}{\partial x_j}\left(\frac{\mu_{eff}}{Sc_{eff}}\frac{\partial \tilde{Y}_m}{\partial x_j}\right)+R_m$$

RNG turbulence model

- The effective viscosity in RNG SGS model is calculated as

$$\mu_{eff} = \mu\left[1 + H\left(\frac{\mu_s^2}{\mu^3}\frac{\mu_{eff}}{} - 100\right)\right]^{1/3}$$, where

$$\mu_s = \overline{\rho}\left(0.157 V_{CV}^{1/3}\right)^2 \sqrt{2\widetilde{S}_{ij}\widetilde{S}_{ij}}$$

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

- In highly turbulent flows, $\mu_{eff} \approx \mu_s$ and the RNG model reduces to Smagorinsky model in laminar flow regions the argument of Heaviside function becomes negative and the model recovers molecular viscosity, $\mu_{eff} = \mu$.

- The effective Prandtl and Schmidt numbers are calculated following the RNG theory by Yakhot purely from the theoretical equation

$$\left|\frac{1/N_{eff} - 1.3929}{1/N - 1.3929}\right|^{0.6321} \left|\frac{1/N_{eff} + 2.3929}{1/N + 2.3929}\right|^{0.3679} = \frac{\mu}{\mu_{eff}}$$

EDC combustion model 1/2

- Eddy Dissipation Concept (EDC) gives an expression for a combustion rate based on an assumption that chemical reactions occur in **so-called fine structures** of Kolmogorov's scale, where the dissipation of turbulence energy takes place.
- In EDC model a source term in species transport equation is modelled as:

$$R_m = \frac{\rho(\xi^*)^2}{\tau^*\left[1-(\xi^*)^3\right]}\left(Y_m^* - Y_m\right)$$

R_m is a net rate of production of specie *m* by chemical reactions,

ξ^* is the length fraction of the fine scale turbulent structures where the reaction occurs,

Y_m^* is the fine scale species mass fraction (specie *m*) after reacting over the time τ^* ,

Y_m is a species mass fraction for specie *m* in the surrounding fine scales state.

EDC combustion model 2/2

- The length fraction of fine structures: $\xi^* = 2.1317 u_\eta / u_{SGS}$

  where $u_{SGS} = \mu_t / (\rho \cdot L_{SGS})$ and $L_{SGS} = 0.157 V^{1/3}$

  and the Kolmogorov's velocity $u_\eta = \left(\frac{\mu \cdot u_{SGS}^3}{\rho \cdot L_{SGS}} \right)^{1/4}$

- Characteristic sub-grid eddy and Kolmogorov timescales are:

  $\tau_{SGS} = L_{SGS} / u_{SGS}$ and $\tau_\eta = \left(\frac{\mu \cdot L_{SGS}}{\rho \cdot u_{SGS}^3} \right)^{1/2}$

- The volume fraction of the fine scales is calculated as ξ^{*3}

  and species are assumed to react in the fine structures over a time scale $\tau^* = 0.4082 \tau_\eta$.

  It is assumes that all the fine scales in the cell are perfectly stirred reactors with a residence time τ^*

Chemistry mechanism

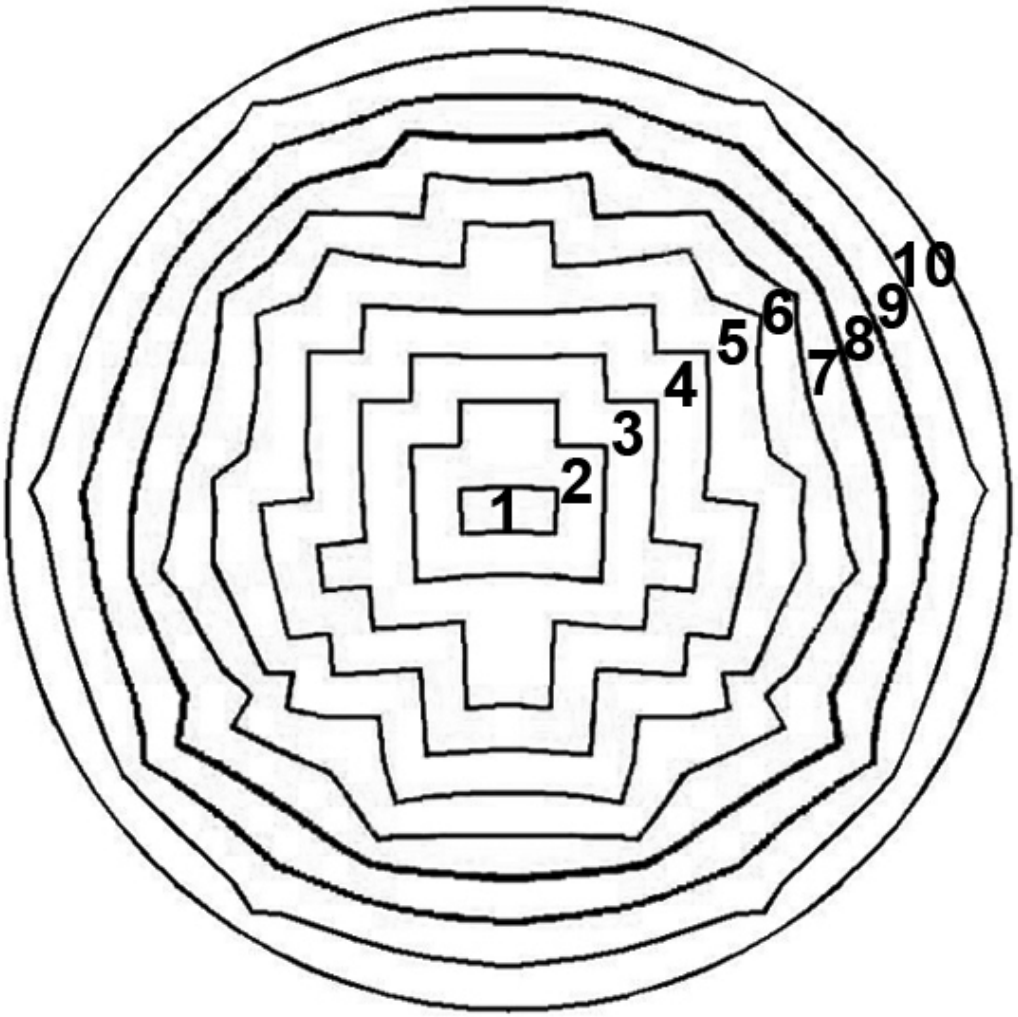
Mechanism for H2 combustion (with NOx), 13 species and 37 reactions

Units are cm3, mol, s, KJ and K			
H+O2=OH+O	2.E+14	0.00	70.30
H2+O=OH+H	1.8E+10	1.00	36.93
H2O+O=OH+OH	5.9E+09	1.30	71.25
H2+OH=H2O+H	1.17E+09	1.30	15.17
H+O2+M=HO2+M	2.3E+18	-0.8	0.00
H2/1./ H2O/6.5/ O2/0.4/ N2/0.4/			
H+HO2=OH+OH	1.5E+14	0.00	4.20
H+HO2=H2+O2	2.5E+13	0.00	2.93
OH+HO2=H2O+O2	2.E+13	0.00	4.18
H+H+M=H2+M	1.8E+18	-1.00	0.00
H2/1./ H2O/6.5/ O2/0.4/ N2/0.4/			
H+OH+M=H2O+M	2.2E+22	-2.00	0.00
H2/1./ H2O/6.5/ O2/0.4/ N2/0.4/			
HO2+HO2=H2O2+O2	2.E+12	0.00	0.00
H2O2+M=OH+OH+M	1.3E+17	0.00	190.38
H2O2+OH=H2O+HO2	1.E+13	0.00	7.53
O+HO2=OH+O2	2.E+13	0.00	0.00
H+HO2=O+H2O	5.E+12	0.00	5.90
H+O+M=OH+M	6.2E+16	-0.60	0.00

O+O+M=O2+M	6.17E+15	-0.50	0.00
H2O2+H=H2O+OH	1.E+13	0.00	15.02
H2O2+H=HO2+H2	4.79E+13	0.00	33.26
O+OH+M=HO2+M	1.E+16	0.00	0.00
H2+O2=OH+OH	1.7E+13	0.00	200.0
O+N2=N+NO	1.82E+14	0.00	319.02
O+NO=N+O2	3.8E+09	1.00	173.11
H+NO=N+OH	2.63E+14	0.00	210.94
NO+M=N+O+M	3.98E+20	-1.50	627.65
N2+M=N+N+M	3.72E+21	-1.60	941.19
N2O+O=NO+NO	6.92E+13	0.00	111.41
N2O+O=N2+O2	1.E+14	0.00	117.23
N2O+N=N2+NO	1.E+13	0.00	83.14
N+HO2=NO+OH	1.E+13	0.00	8.31
N2O+H=N2+OH	7.6E+13	0.00	63.19
HNO+O=NO+OH	5.01E+11	0.50	8.31
HNO+OH=NO+H2O	1.26E+12	0.50	8.31
NO+HO2=HNO+O2	2.E+11	0.00	8.31
HNO+HO2=NO+H2O2	3.16E+11	0.50	8.31
HNO+H=NO+H2	1.26E+13	0.00	16.63
HNO+M=H+NO+M	1.78E+16	0.00	203.7

GUTHEIL, E., BALAKRISHNAN, G. & WILLIAMS, F. A. (1993) Structure and extinction of hydrogen-air diffusion flames. IN PETERS, N. & ROGG, B. (Eds.) *Reduced kinetic mechanisms for applications in combustion systems.* New York, Springer-Verlag

Burst disk opening sections



Burst disk opening process was approximated by a 10 step process.

Sections were open from 1 to 10 at times calculated according to the table in the next slide.

Burst disk opening time

Following Spence & Woods (1964), the following formula was used to obtain the rupture time of a burst disk:

$$t = k\left(\frac{\rho b d}{p}\right)^{1/2}$$

where ρ – the density of the diaphragm material (annealed copper),
b and d are the thickness and the diameter of the diaphragm,
k – constant, 0.92
p – driving pressure

Opening times of sections for each of the simulations are listed below:

Section	1	2	3	4	5	6	7	8	9	10
Opening time, μs [1.35 MPa case]	0	4.7	9.4	14.2	18.9	23.6	28.4	33.1	37.8	42.6
Opening time, μs [1.65 MPa case]	0	4.3	8.6	12.8	17.1	21.4	25.6	29.9	34.3	38.5
Opening time, μs [2.43 MPa case]	0	3.5	7.1	10.6	14.2	17.7	21.3	24.8	28.3	31.9
Opening time, μs [2.9 MPa case]	0	3.2	6.5	9.7	12.9	16.2	19.4	22.6	25.9	29.1

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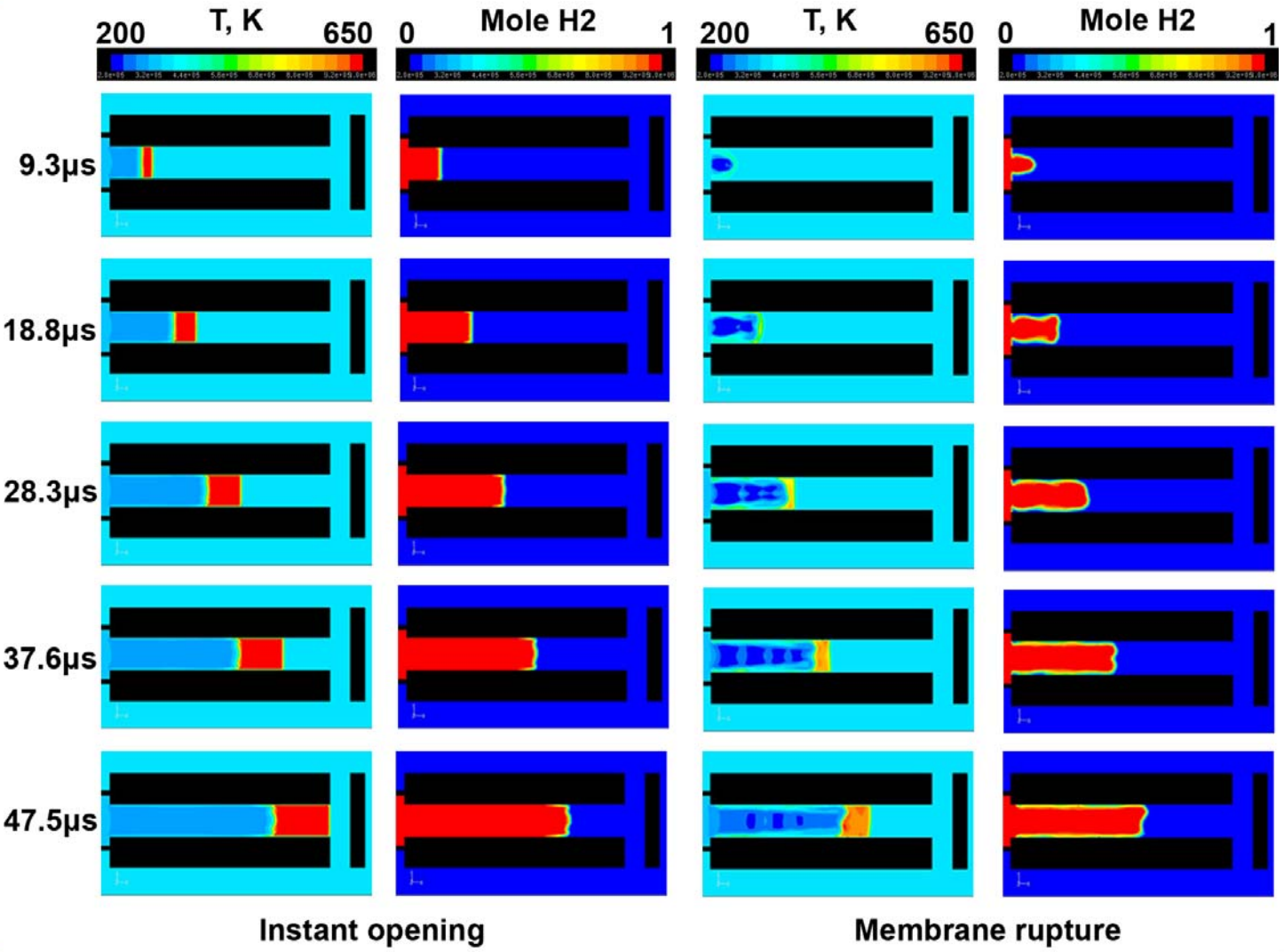
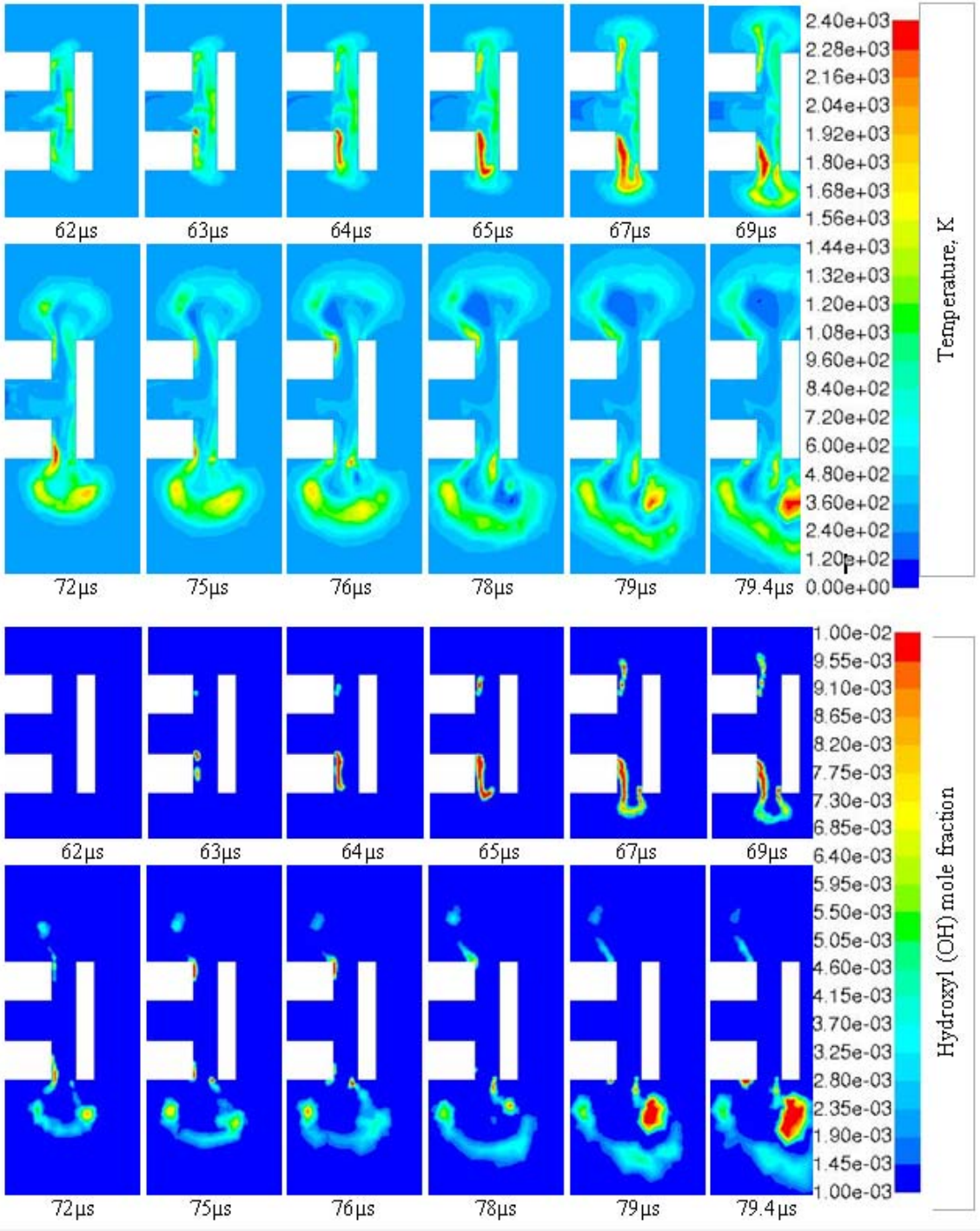
Instant vs finite opening time



Simulation results

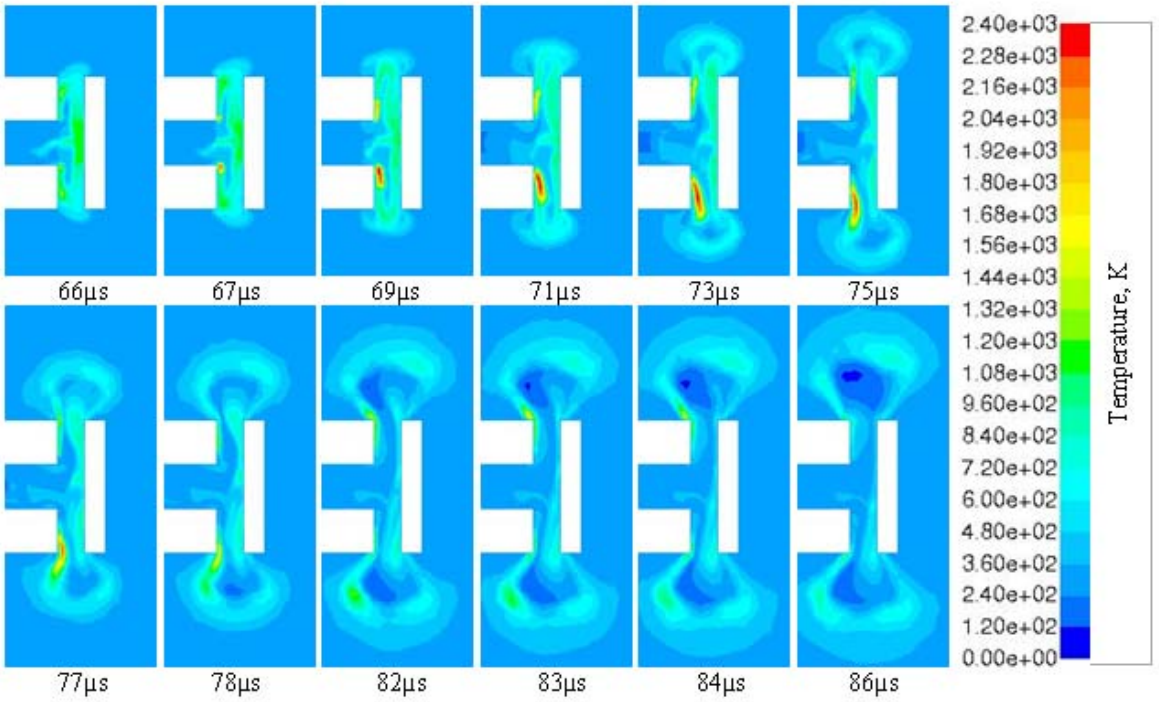
P=29 bar

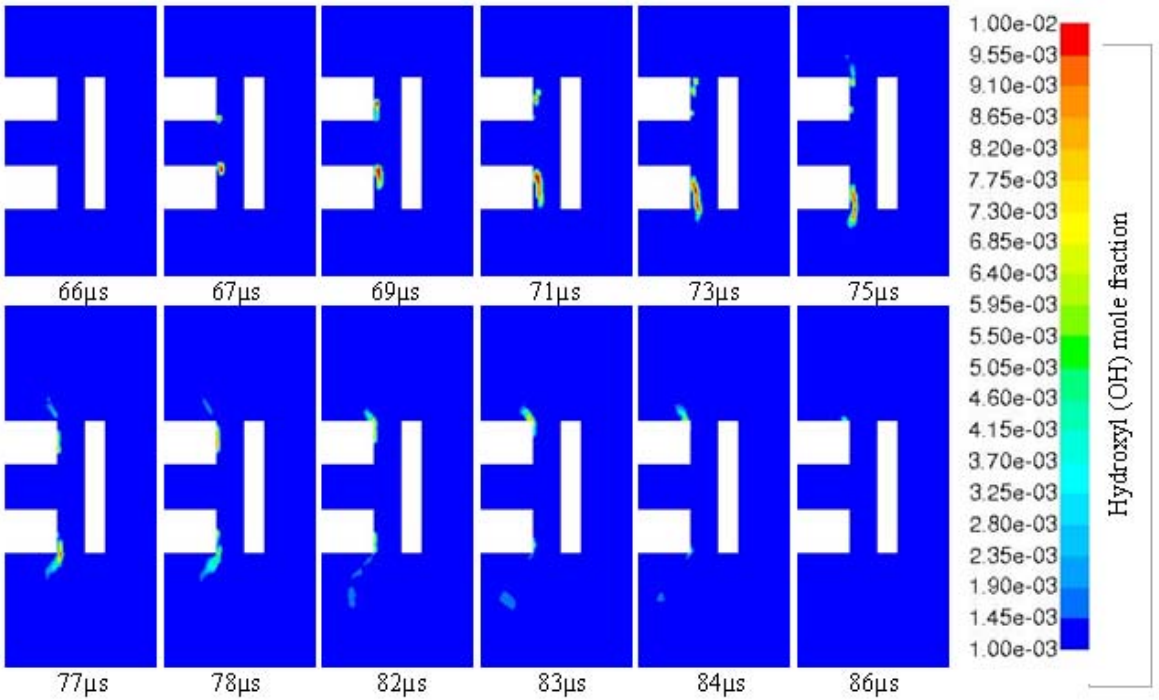


Ignition initiated in the radial vent channel and extinguished.

Combustion is reinitiated in a number of spots outside the PRD.

Concentration of hydrogen in these spots just before the ignition is in the range 29-36% by vol.



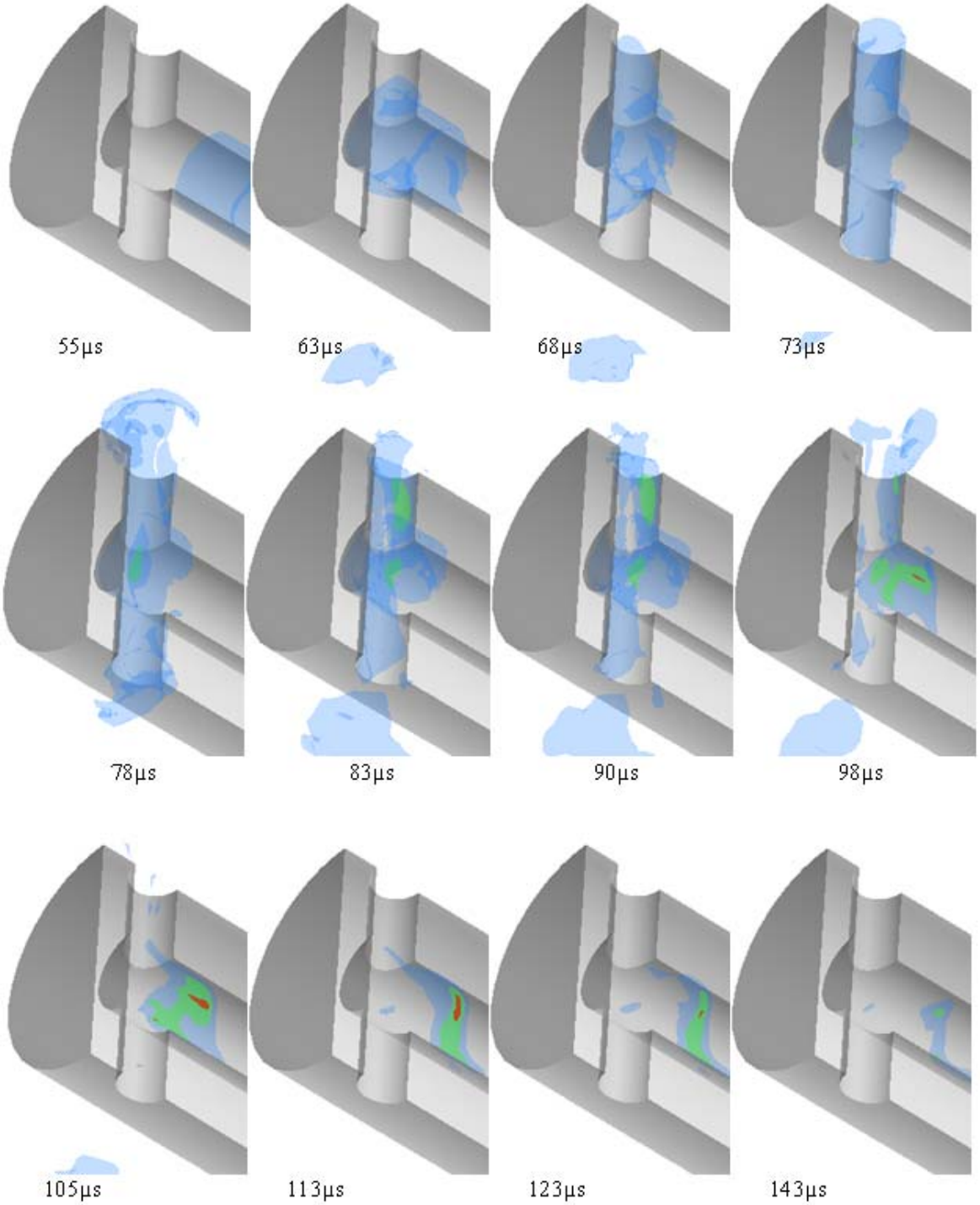


P=24.3 bar

Ignition is initiated in the radial channel (closer to the upstream wall – second shock reflection) similar to 29 bar case

Reignition outside is not observed.

Process took 10μs and was experimentally registered (“ignition” in private communication)

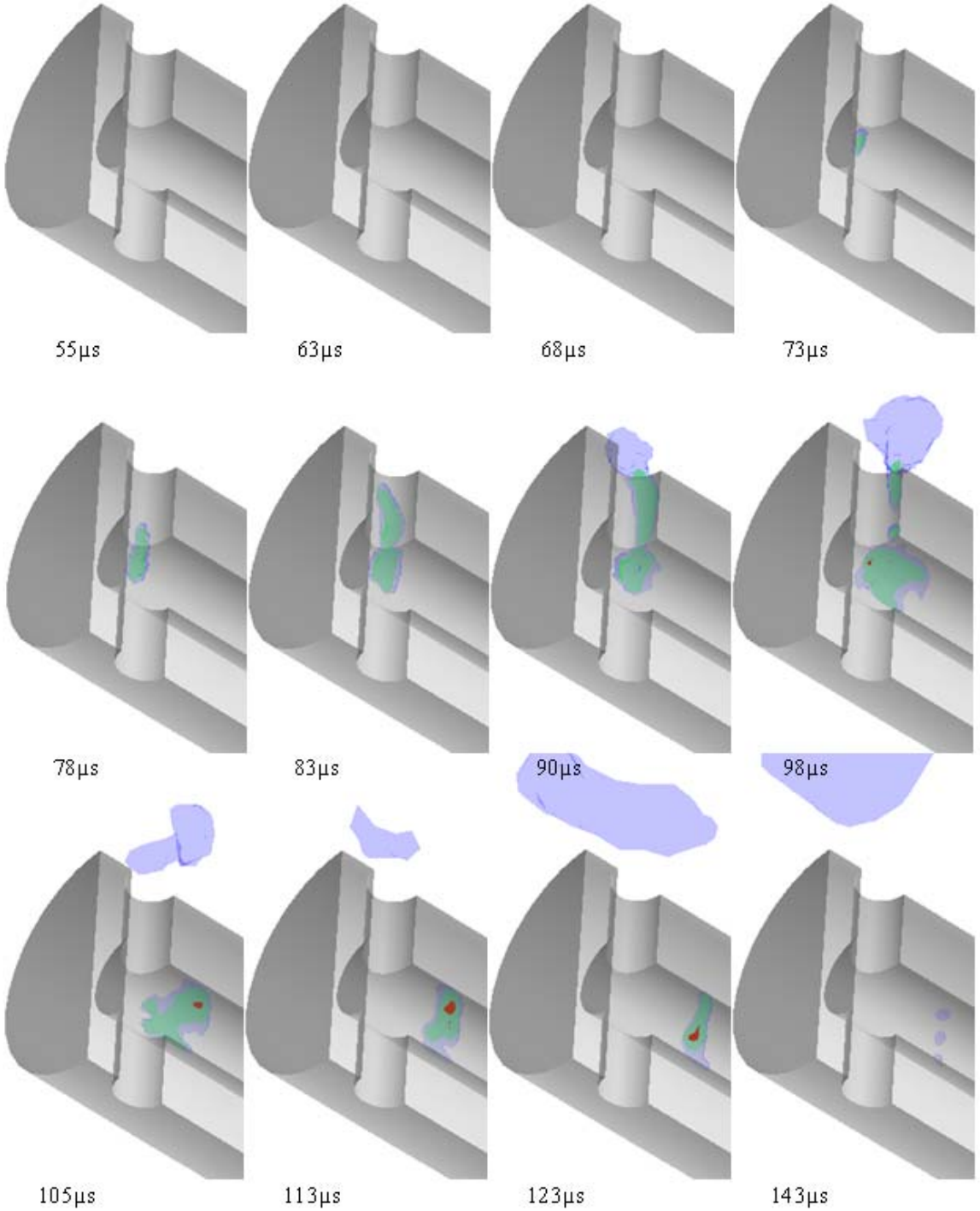


P=16.5 bar

Temperature

Ignition spot is located in the axial channel (not in a symmetry plane). The combustion propagates upstream (until oxygen is consumed)!

Iso-surfaces are:
Blue – 550 K,
Green – 1500 K,
Red – 2400 K



P=16.5 bar

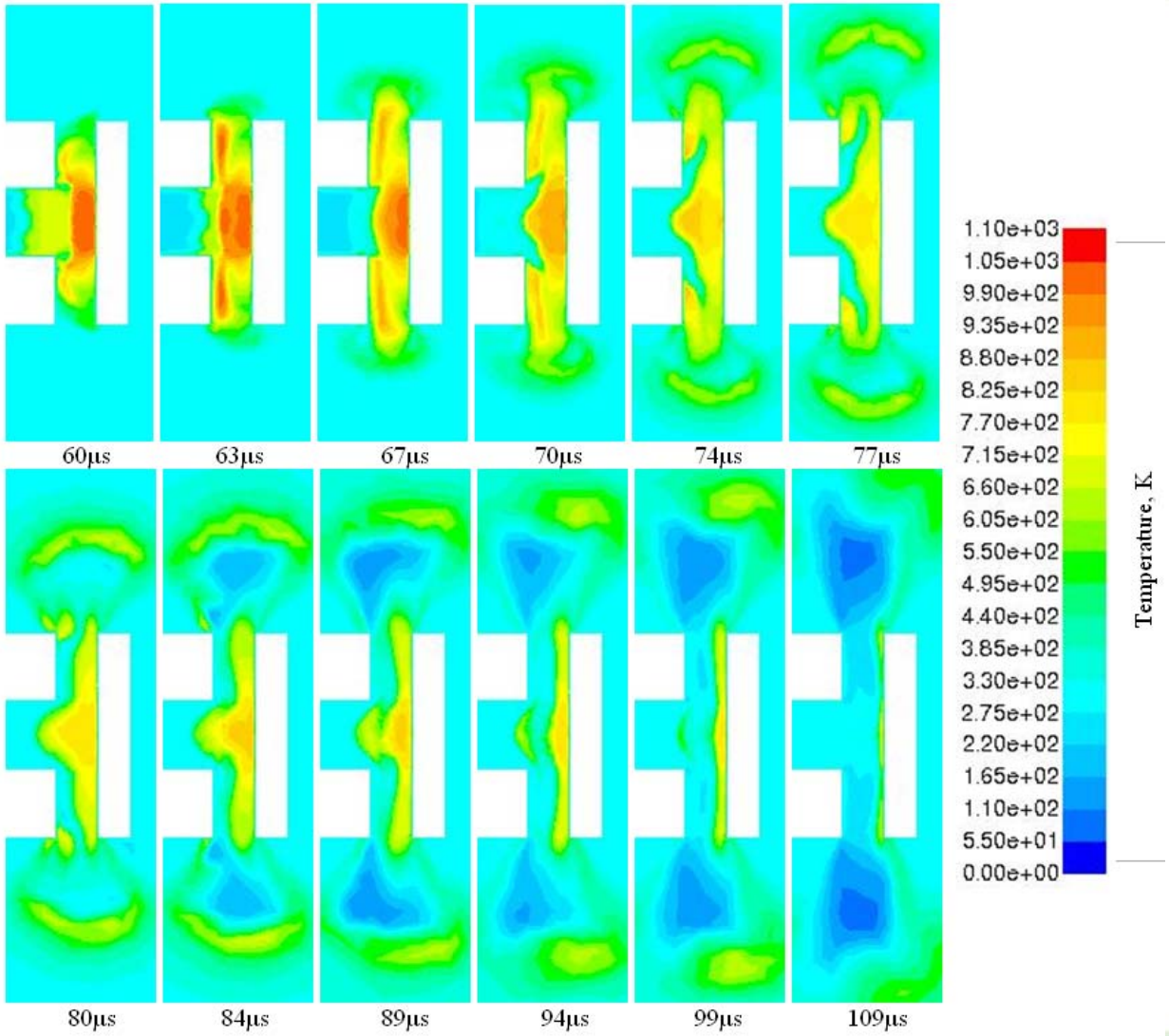
OH mole fraction

Ignition is confirmed by a hydroxyl mole fraction distribution.

Light sensor in experiments was located outside and could not have registered ignition.

Iso-surfaces are:
Blue – 0.0002,
Green – 0.002,
Red – 0.02

P=13.5 bar – no ignition



Hydroxyl mole fraction is ~10^{-9}-10^{-10} (not shown).

Note: temperature scale is different in this picture.

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Conclusions

- The LES model based on EDC with detailed kinetics and inertial burst disk was successfully applied to reproduce and explain experimental observations in T-shape channel (PRD mock-up).
- The lower pressure limit for spontaneous ignition in a T-shaped PRD is established: there is no ignition at storage pressure 13.5 bar; there is ignition followed by self-extinction at pressures 16.5 and 24.3 bar; and there is "sustainable" ignition (reignition outside the channel) for storage pressure 29 bar.
- The ignition is located in the are of the second reflection of initial shock and where the concentration of hydrogen in air is in the range 29-36% vol.
- The model can be used as a contemporary tool for design of innovative pressure relief devices.

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MSc in Hydrogen Safety Engineering (distance learning course):
http://campusone.ulster.ac.uk/potential/postgraduate.php?ppid=24