Turbulent combustion and localized preflame autoignition of hydrogen-air mixture in an enclosure

Sergey M. Frolov
Semenov Institute of Chemical Physics
Moscow, Russia

Outline

- Introduction
- Flame tracking – particle method
- Validation
- Hydrogen – air combustion in cylindrical enclosure
- Hydrogen – air combustion in square enclosure
- Hydrogen – air combustion in square enclosure with "room"
- Conclusions

Objective:

The objective of this study is to develop a CFD approach for quantitative simulations of hydrogen – air explosions in enclosures of complex geometries with due regard for possible preflame autoignition

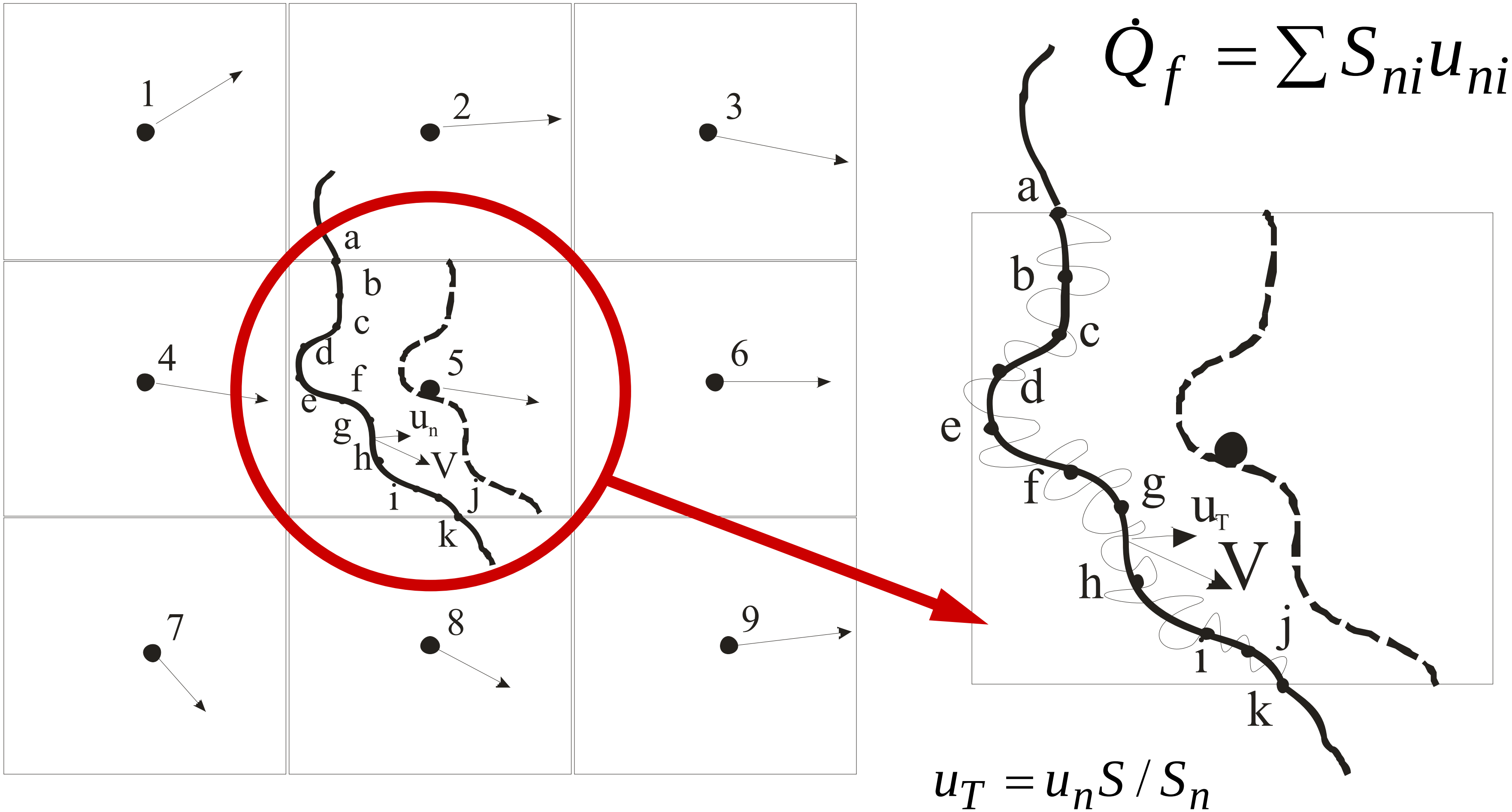
Introduction

- The objective of any combustion model in the CFD code is to provide correct values of **mean reaction rates** in each computational cell
- There exist **many combustion models** both for laminar and turbulent flows.
- If the chemistry is fast as compared to mixing, the **Spalding Eddy Break-Up model** can be used. It is simple but has a limited range of validity.
- There is a whole class of statistical combustion models with **probabilistic representation of turbulence** and its interaction with chemistry. However this approach is not capable of operating with complex chemistry due to inadequate CPU requirements.

Coupled Flame-Tracking – Particle method

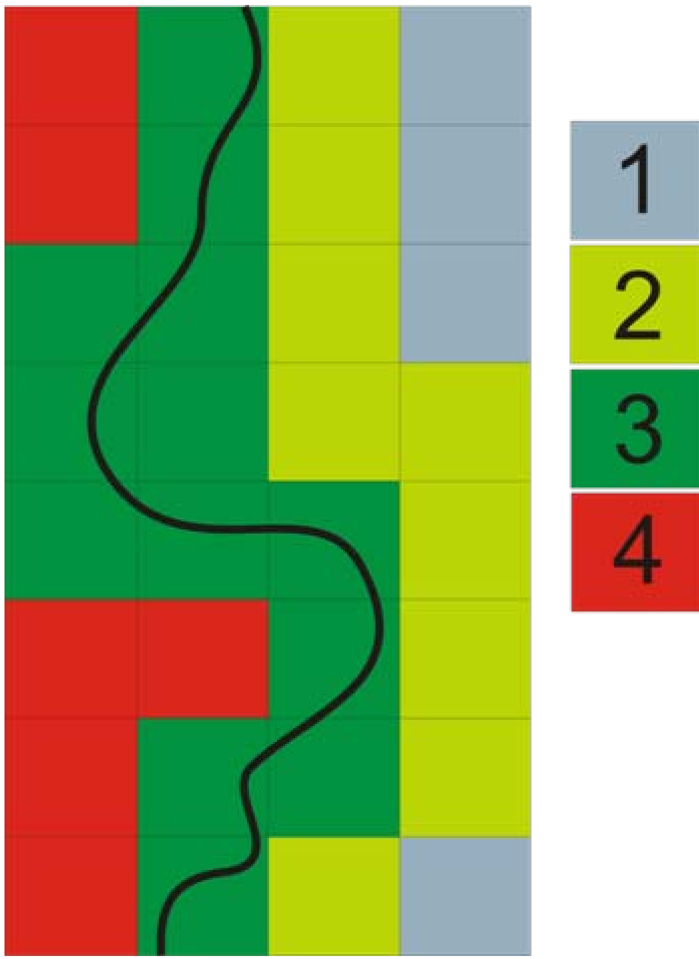
- Flame front is represented as **set of elementary portions**, lines in 2D case and triangles in 3D case.
- Each elementary portion of the flame surface displaces in time due to **burning** of the fresh mixture at local velocity u_n (normal to the flame surface) and due to **convective motion** of the mixture at local flow velocity.
- The preflame zone contains a set of Monte – Carlo particles (**Joint Velocity-Scalar PDF Method, Pope (1985)**). Each particle has its own history. These particles simulate preflame autoignition.
- **RANS + turbulence model** equations for gas dynamics.

Flame Tracking method



Any combustion model, e.g., Shchelkin (1949): $u_T = u_n (1 + u'^2 / u_n^2)^{0.5}$

Parameters from cells and reaction rate

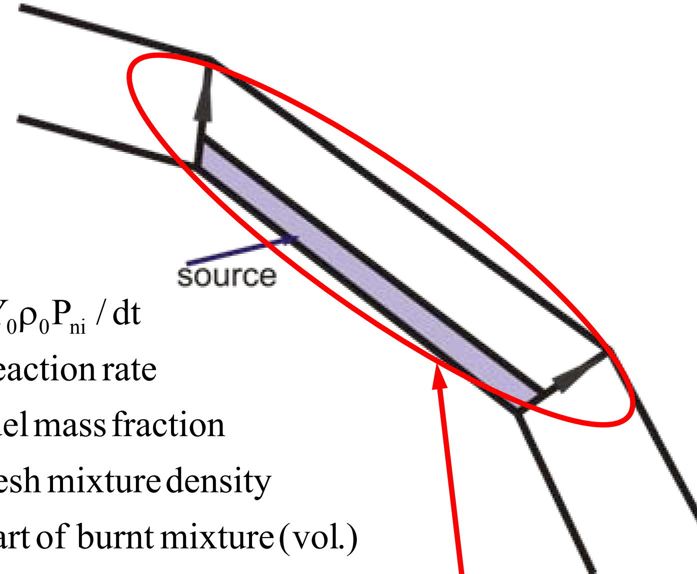


1 – cells with fresh mixture

2 – nearest to flame cells with fresh mixture

3 – mixed cells with flame front

4 – nearest to flame cells with products



$$R_n = Y_0 \rho_0 P_{ni} / dt$$

R_n – reaction rate

Y_0 – fuel mass fraction

ρ_0 – fresh mixture density

P_{ni} – part of burnt mixture (vol.)

$$P_{ni} = \frac{V_p}{V_{cell}} \frac{U_n}{U_n + U_{flow}}$$

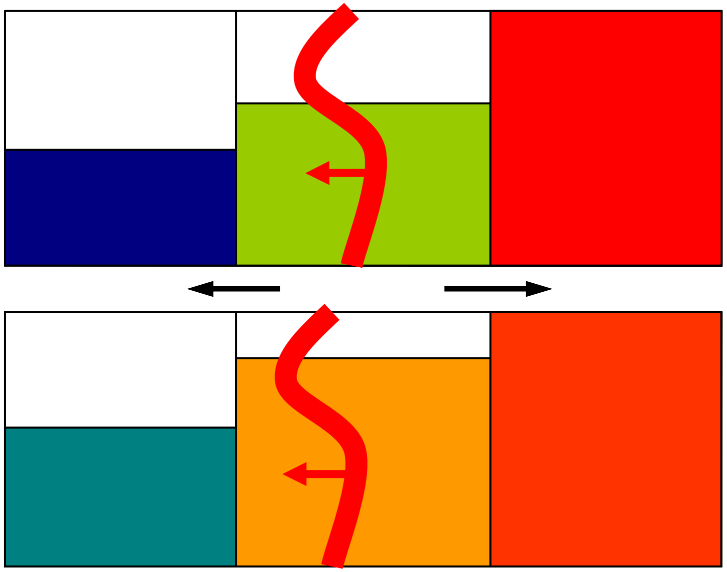
V_p calculation:

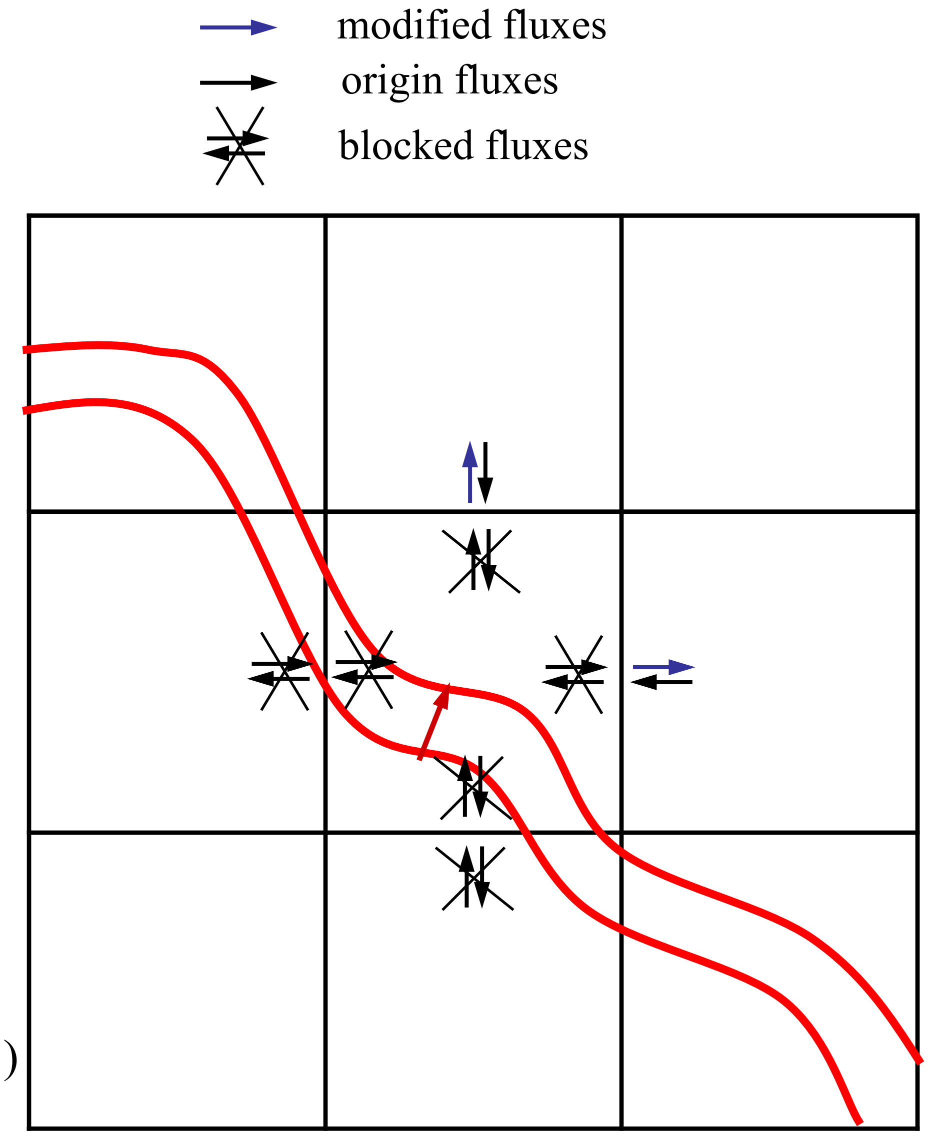
-Analytical solution

or

-Numerical integration

Modification of fluxes





SIMPLE algorithm

$$\left(\sum_{j=1}^{N_{face}} a_j + a_t\right)\phi_P = \sum_{j=1}^{N_{face}} a_j \phi_{P_j} + S_{\phi P}$$

Cell with flame

$$a_t \phi_P = S_{\phi P} + S_{flux}$$

Modified flux

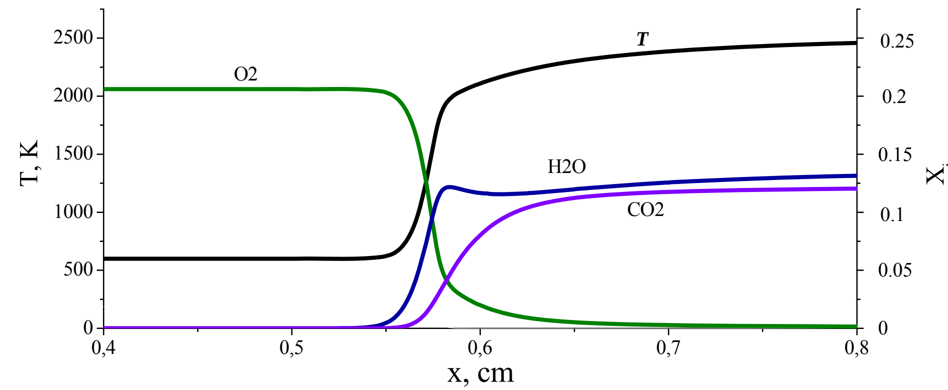
$$\left(\sum_{j=1}^{N_{face}} a_j + a_t\right)\phi_P = \sum_{j=1}^{N_{face}} a_j \phi_{P_j} + S_{\phi P} + \sum_{j=1}^{N_{flame}} a_j (\phi_P - \phi_{P_j})$$

Look-up tables for laminar flame velocity

Governing equations

$$\begin{cases} \dfrac{\partial}{\partial x}\left(\lambda \dfrac{\partial T}{\partial x}\right) - c\rho_0 u_n \dfrac{\partial T}{\partial x} + \Phi = 0 \\ \dfrac{\partial}{\partial x}\left(\rho D_j \dfrac{\partial Y_j}{\partial x}\right) - \rho_0 u_n \dfrac{\partial Y_j}{\partial x} + w_j = 0 \\ w_j = G_j \sum_{i=1}^{M} \left(v'_{ij} - v_{ij}\right) A_i T^{n_i} \exp\left(-E_i / R^o T\right) \prod_{k=1}^{N} \left(\dfrac{\rho Y_k}{G_k}\right)^{v_{ik}}, (j = 1,2,\ldots,N) \\ p = \rho R^0 T \sum_{j=1}^{M} \dfrac{Y_j}{G_j}\ _{j=1,2,\ldots,N} \end{cases}$$

Detailed or overall kinetic mechanism



Boundary conditions

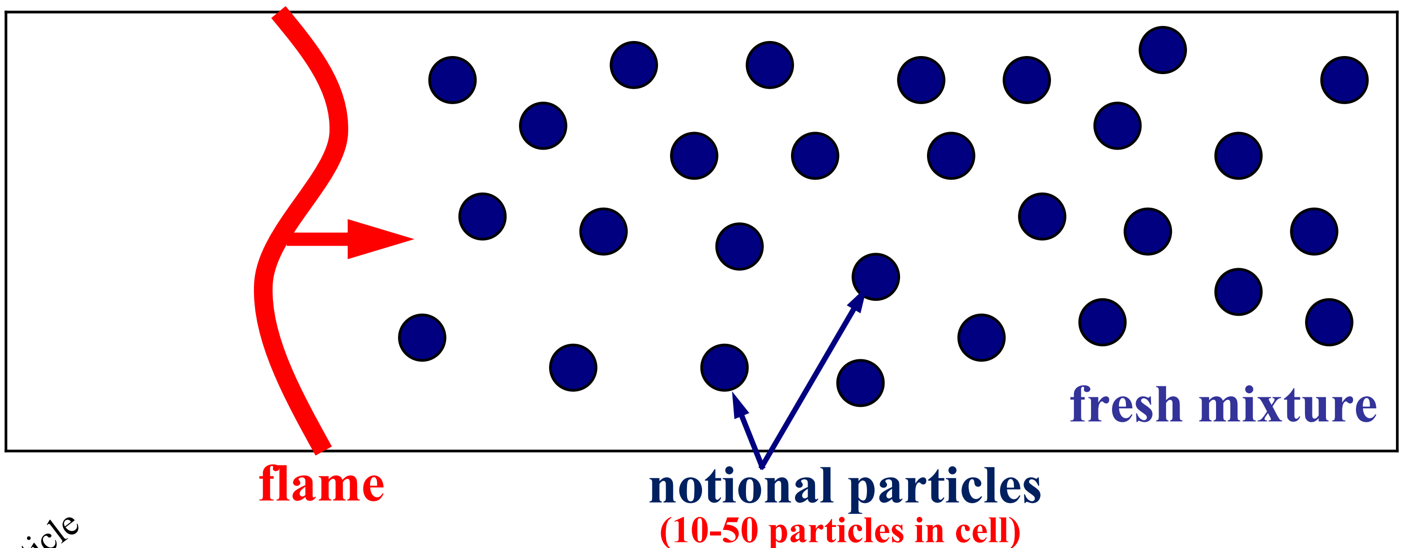
$$x \to -\infty;\ T = T_0,\ Y_j = Y_{j0}\ (j = 1,2,\ldots,N)$$

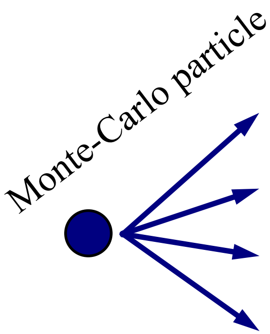
$$x \to \infty;\ \frac{dT}{dx} = 0,\ \frac{dY_j}{dx} = 0\ (j = 1,2,\ldots,N)$$

Fragment of look-up tables

T	P =100atm									
300K	Φ	0.60	0.64	0.65	0.80	1.00	1.20	1.55	7.00	12.0
	u_n	-	-	3.1	4.8	6.0	5.4	2.6	0.7	-

Particle method





Trajectory equation (particle displacement in space and time)

Mass conservation equation (molecular diffusion, **chemistry**)

Momentum conservation equation (**stochastic pressure force,** viscosity)

Energy conservation equation (molecular conductivity, **chemical energy release**)

Each particle has its own composition, velocity, and temperature

Particle represents a state realization in turbulent flow field

Governing equations

- Trajectory

$$\frac{dx_k^i}{dt} = u_k^i$$

- Mass

$$\frac{d(\rho_l^i V^i)}{dt} = \nabla \cdot J_l^i$$

- Momentum

$$\rho^i \frac{du_k^i}{dt} = \frac{\partial P}{\partial x_k} - \nabla(pE - \tau)$$

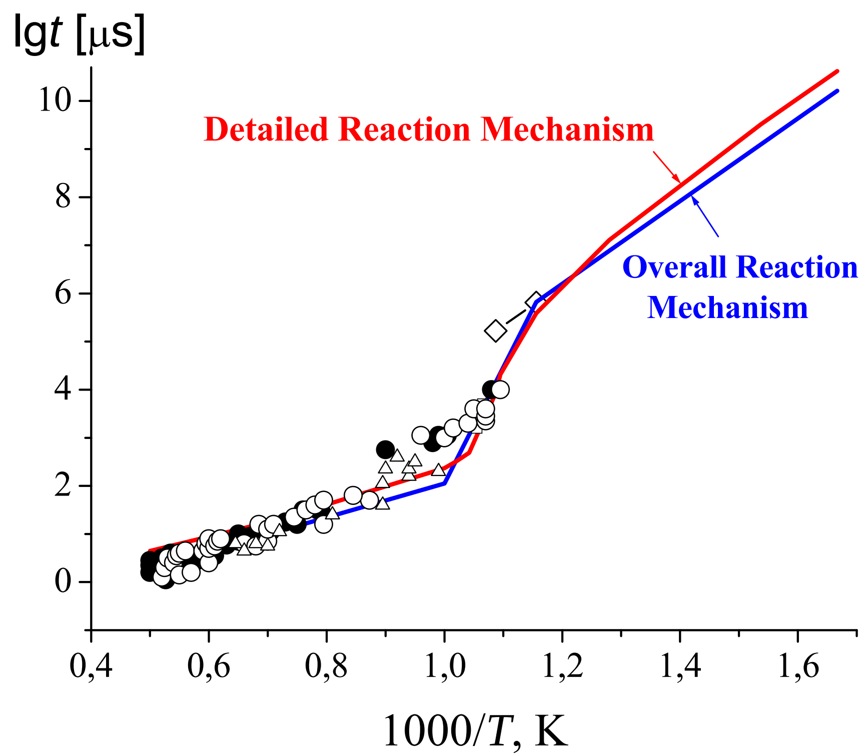
- Energy

$$\rho^i \frac{dh^i}{dt} = -\nabla q^i + h_{\mathrm{hom}}^i$$

Fuel oxidation (single-stage mechanism)

$$H_2 + H_2 + O_2 \rightarrow H_2O + H_2O$$

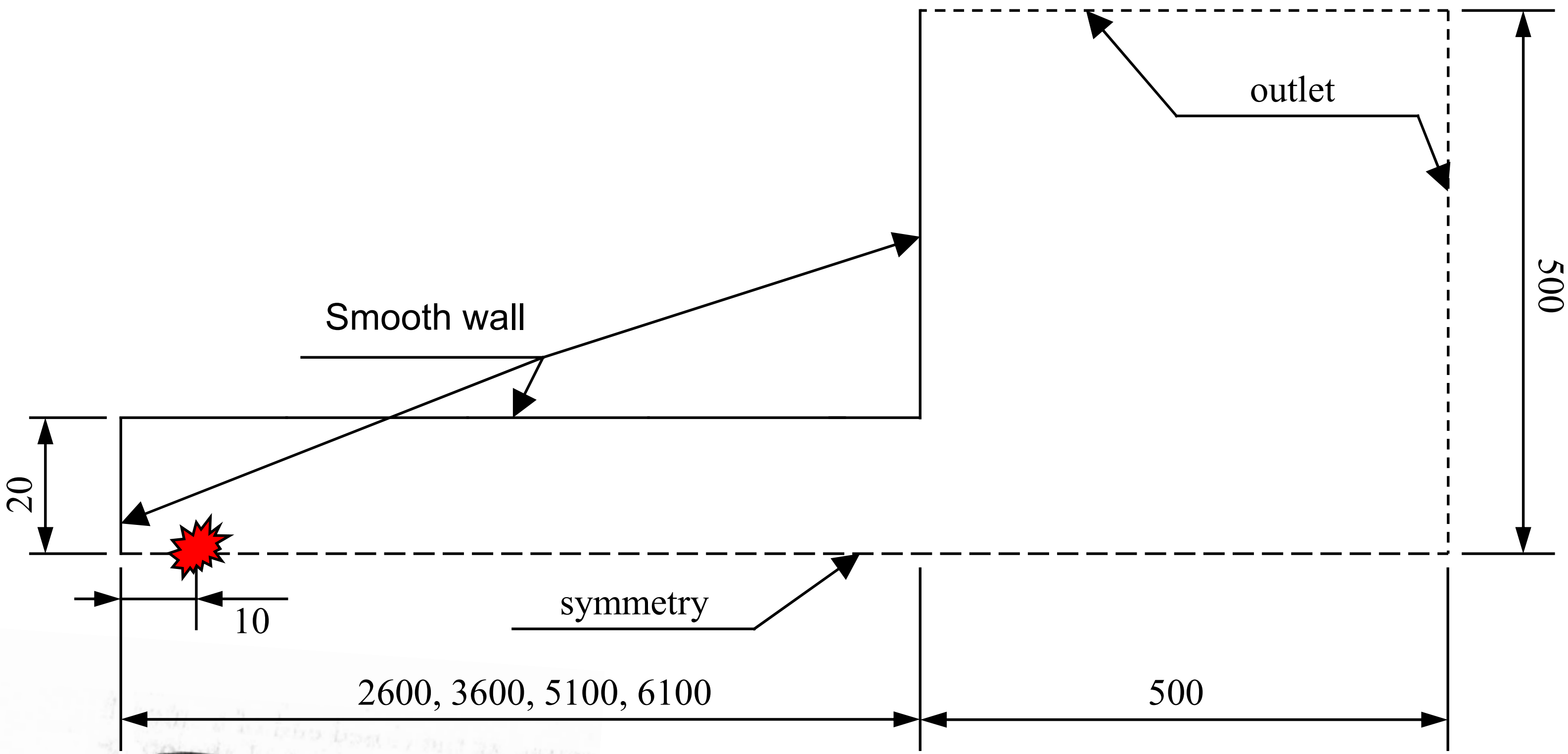
$$w = -2.25 \cdot 10^{15} p^{-1.15} [H_2]^2 [O_2] e^{-\frac{24000}{T}}$$

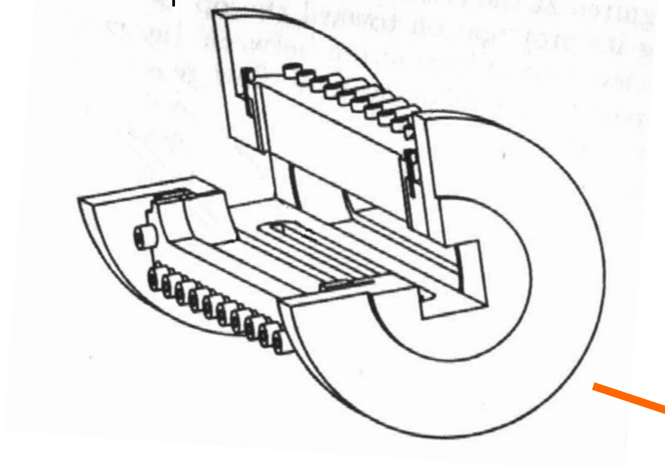


Validation:

Flame acceleration
in straight smooth-walled tubes
(propane – air)

Computational domain





Propane – air (st.) mixture at normal initial conditions

Laminar burning velocity – from look-up tables

$$u_t=u_n(1+u'^2/u_n^2)^{0.5}$$

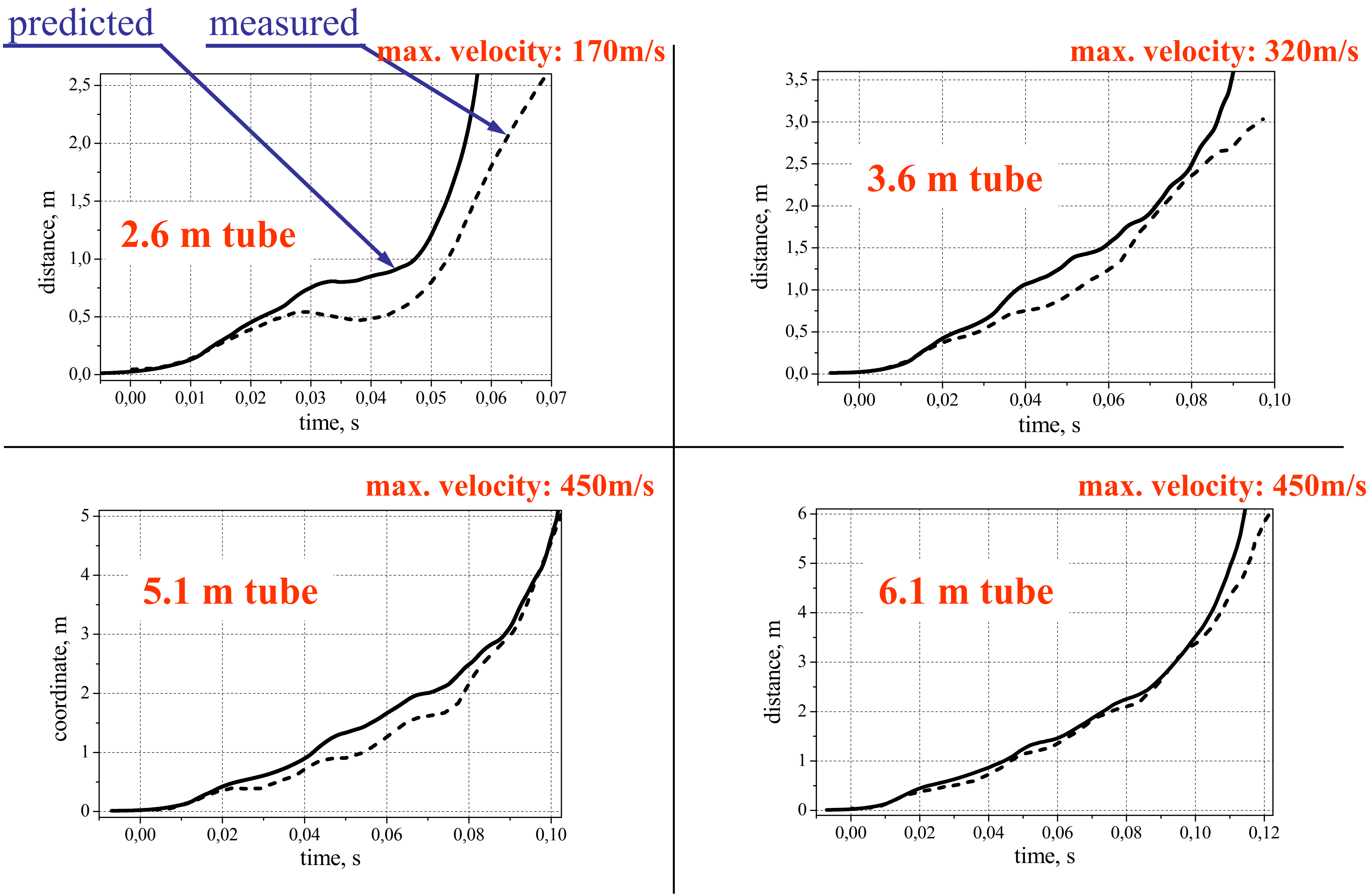
k-ε model was used

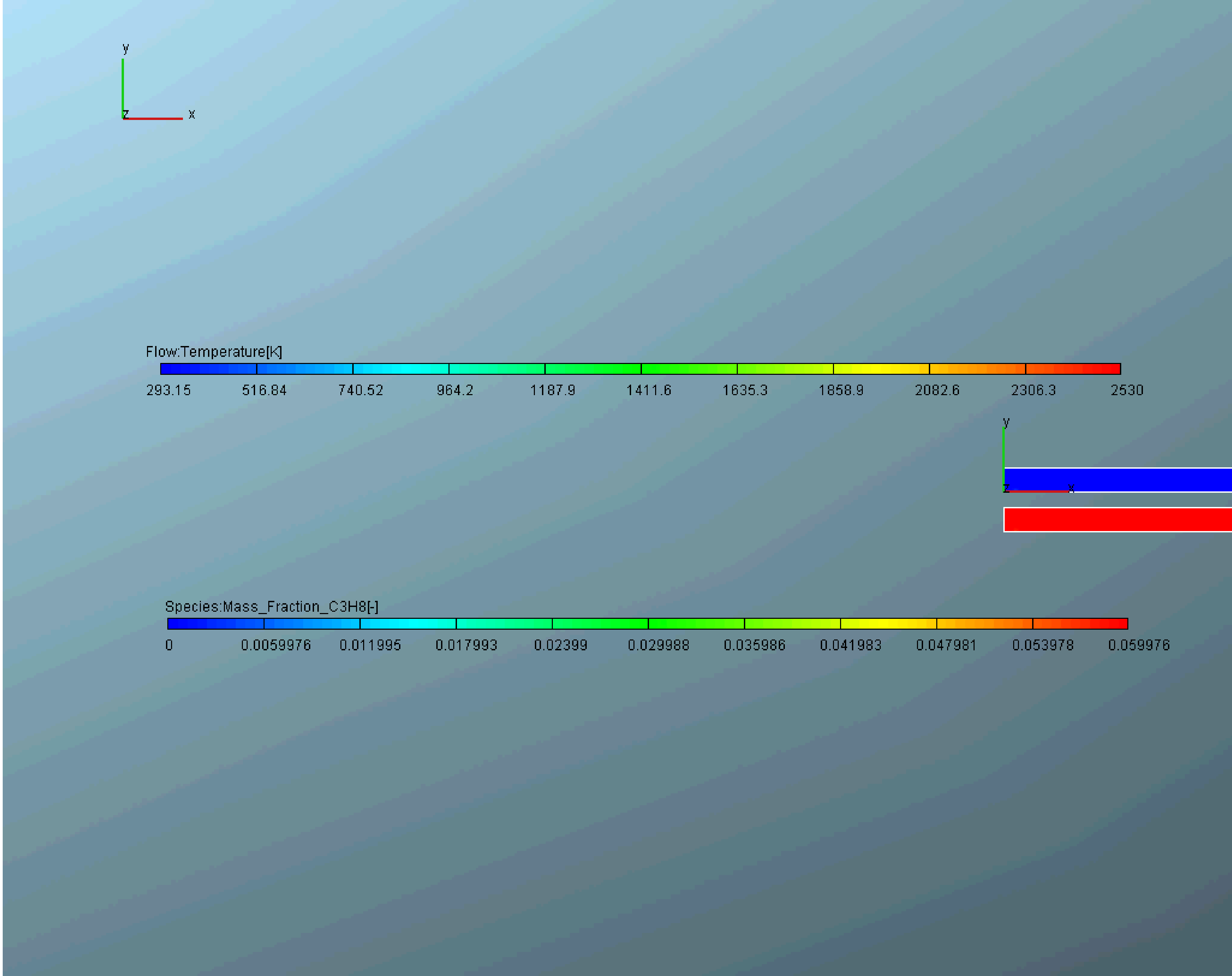
EXPEREMENTAL SETUP (Veyssiere et al. (2004))

Tube of square cross section 40x40 mm

Length: 2.6, 3.6, 5.1, 6.1 m

Comparison between predicted and measured results

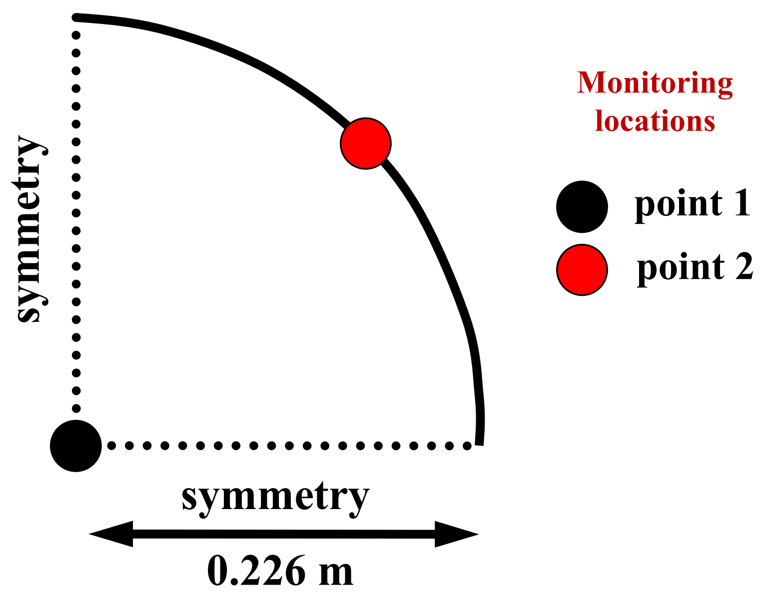


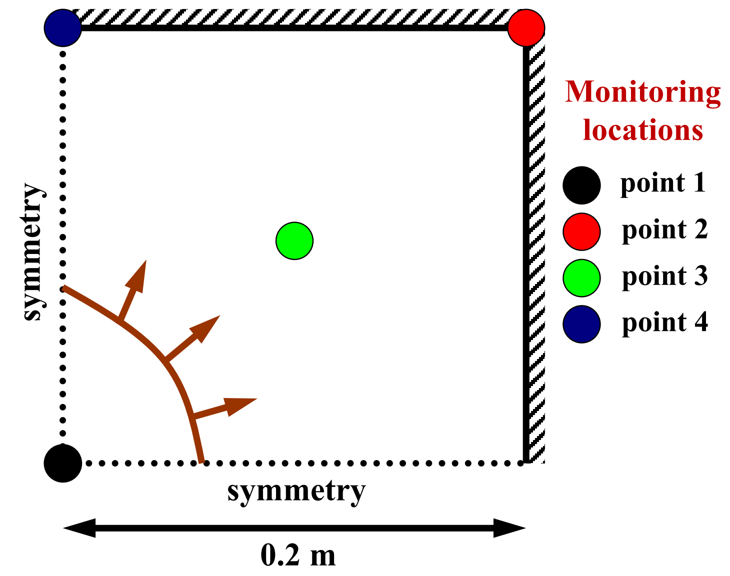


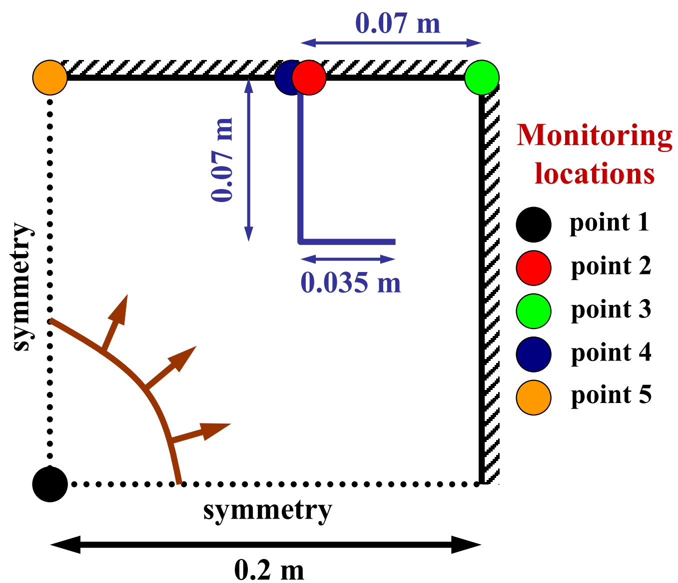
y
z
x
Flow:Temperature[K]
293.15
516.84
740.52
964.2
1187.9
1411.6
1635.3
1858.9
2082.6
2306.3
2530
Species:Mass_Fraction_C3H8[-]
0
0.0059976
0.011995
0.017993
0.02399
0.029988
0.035986
0.041983
0.047981
0.053978
0.059976

Hydrogen combustion
in enclosures

Computational domains





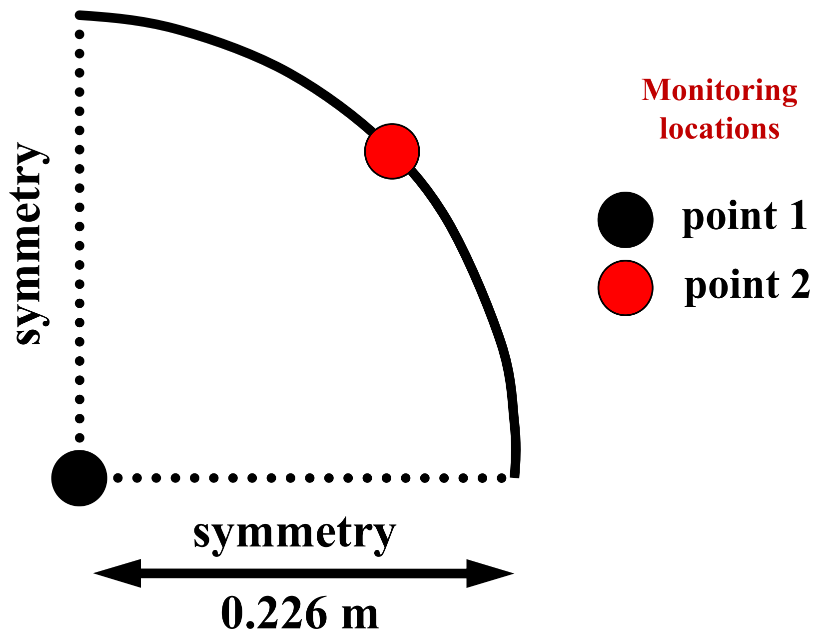


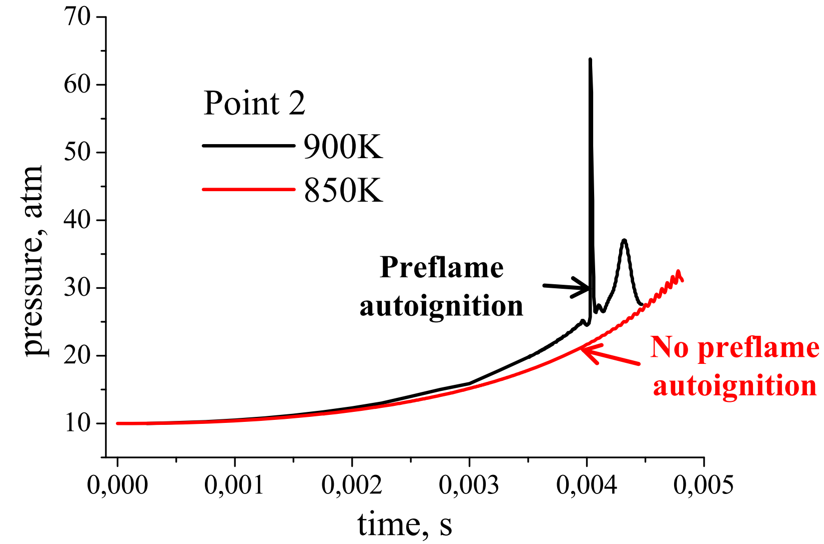
H_2 – air (st.) mixture

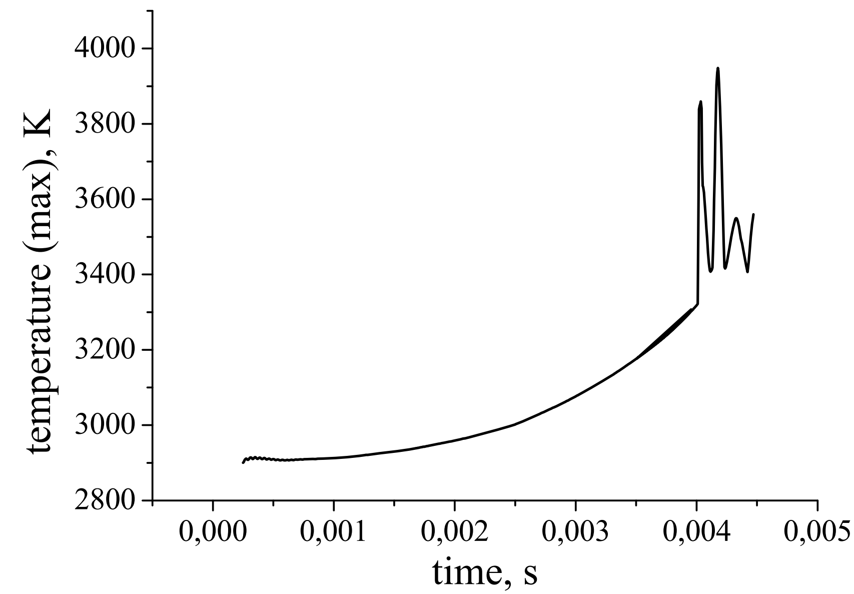
P = 10 atm

T = 850 or 900K

Results: Cylindrical domain







H_2 – air (st.) mixture
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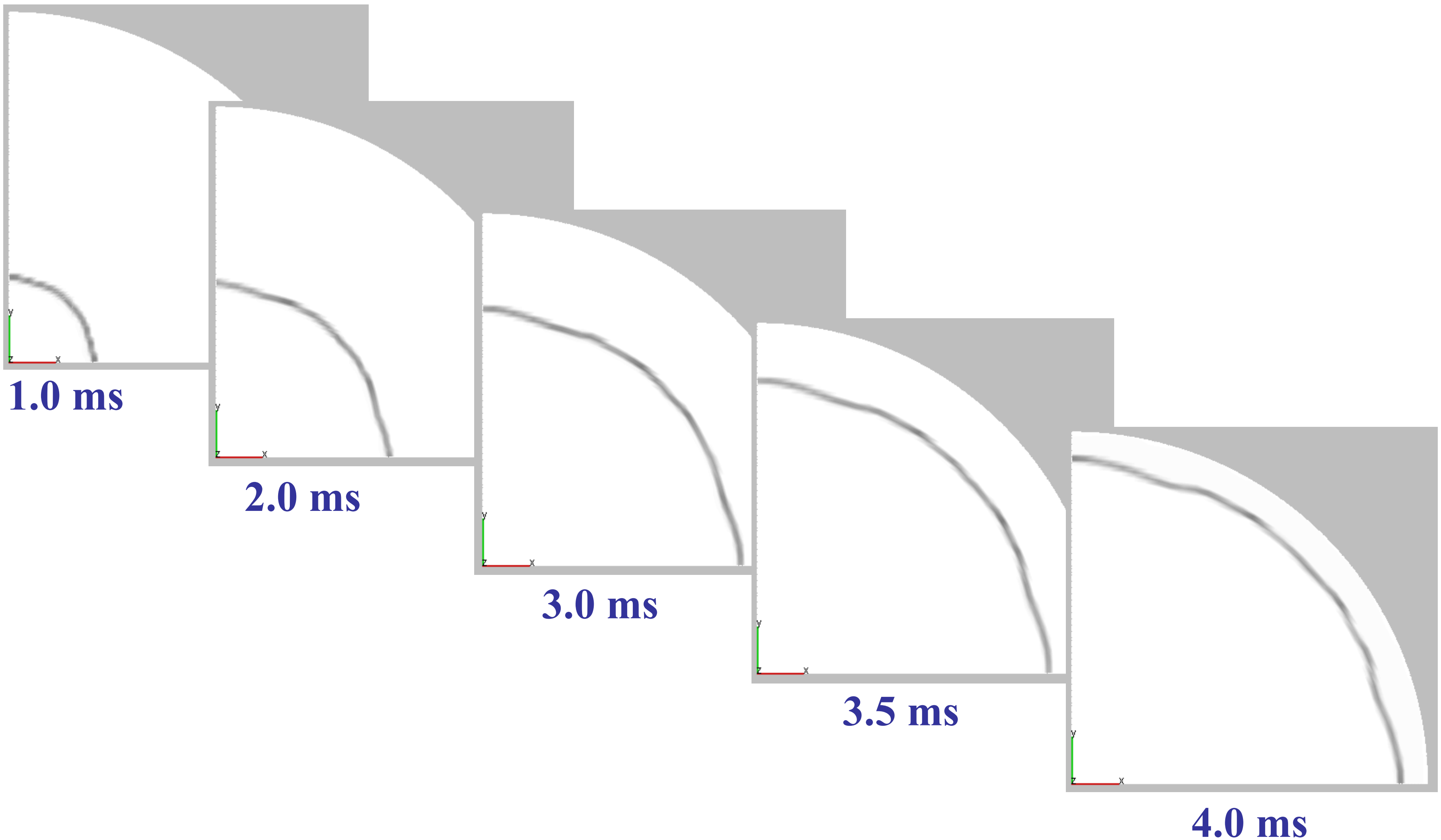
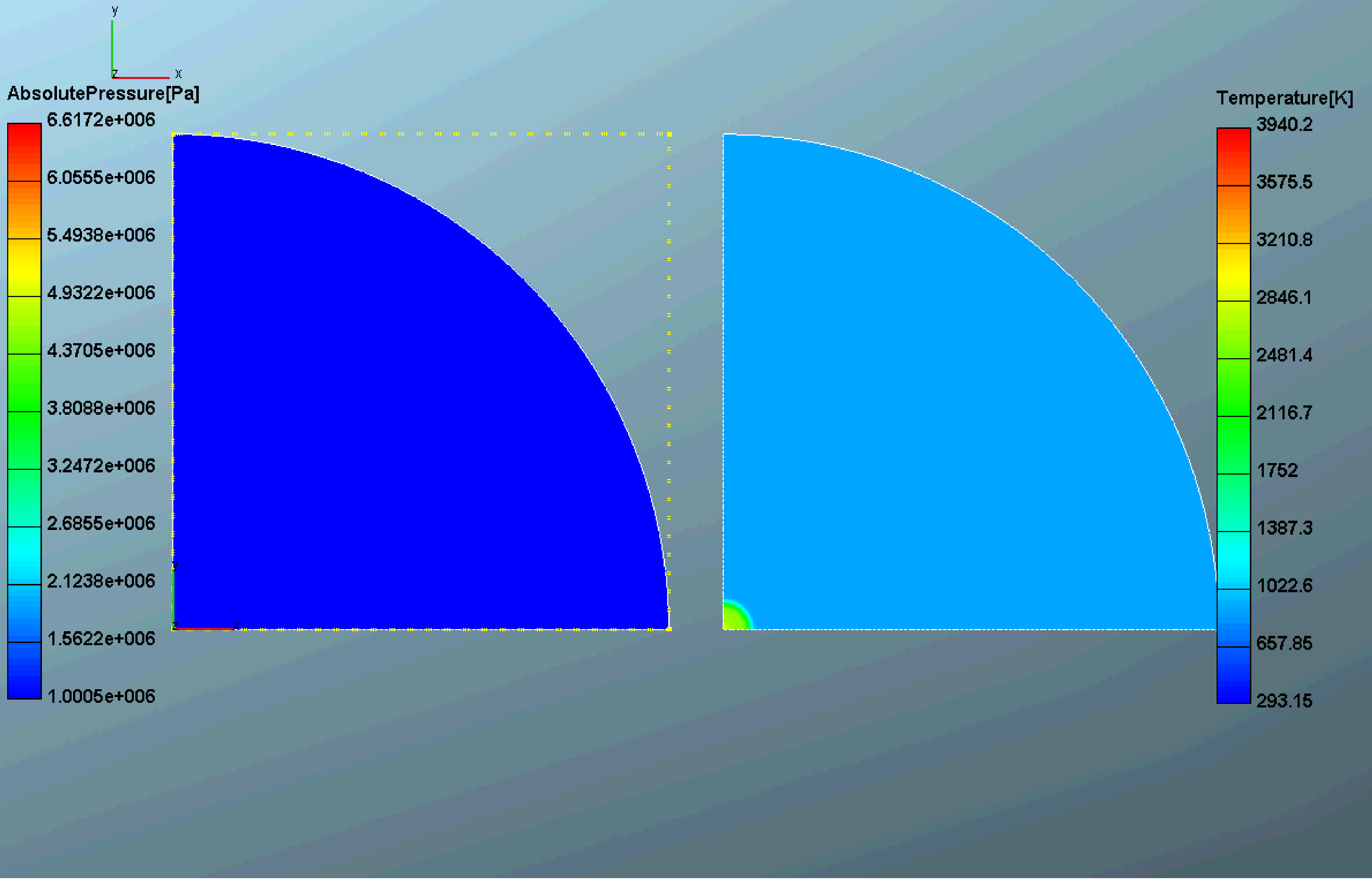
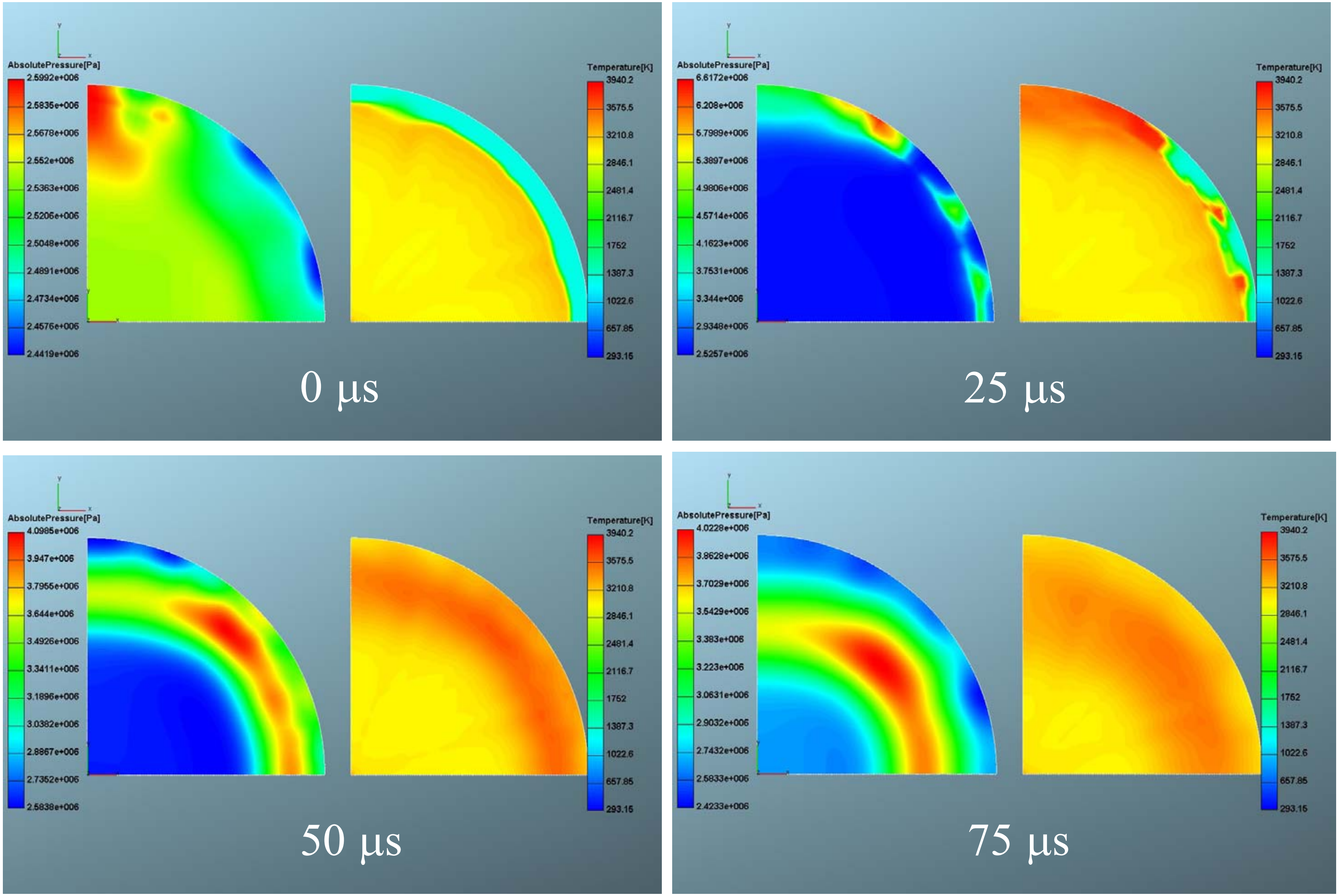
Flame propagation



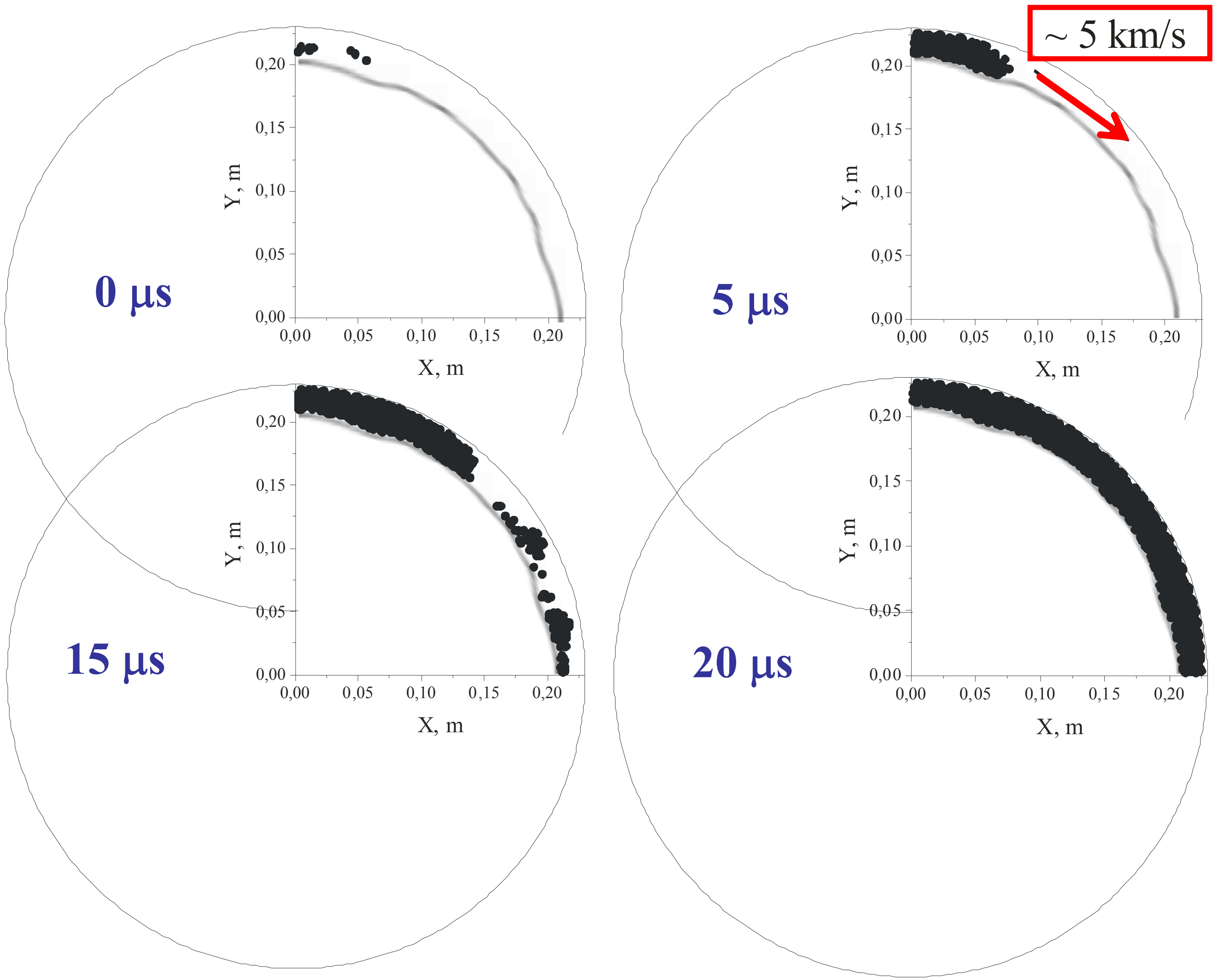


Pressure **Temperature**

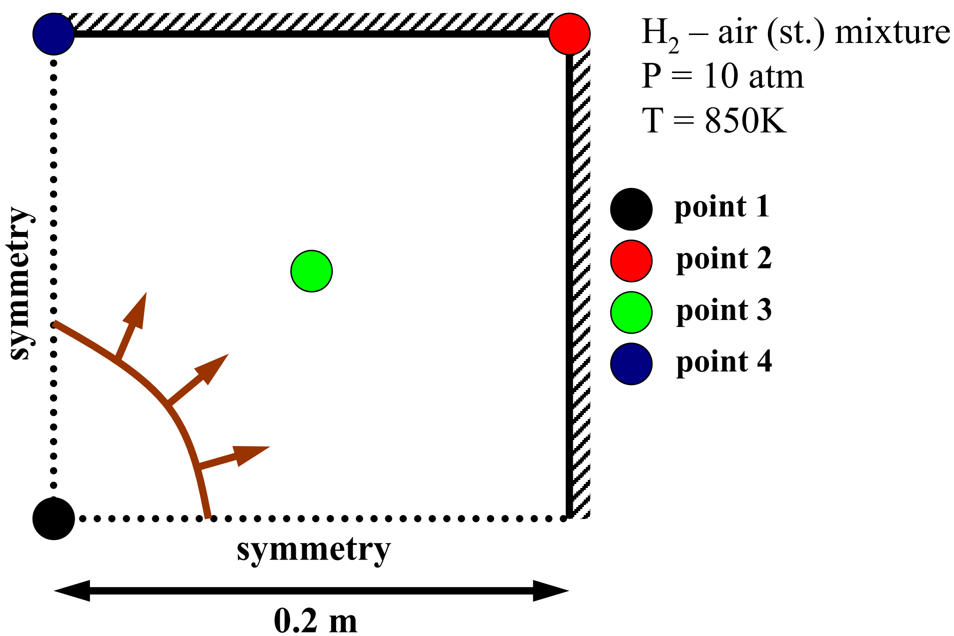
Snapshots of preflame autoignition

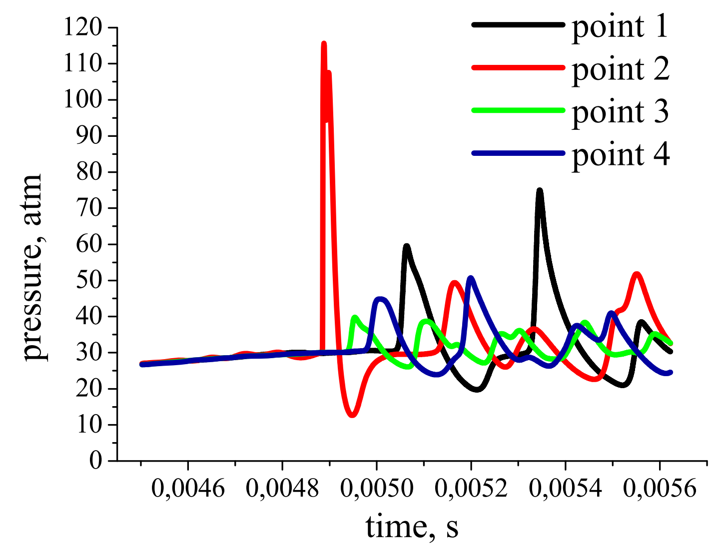


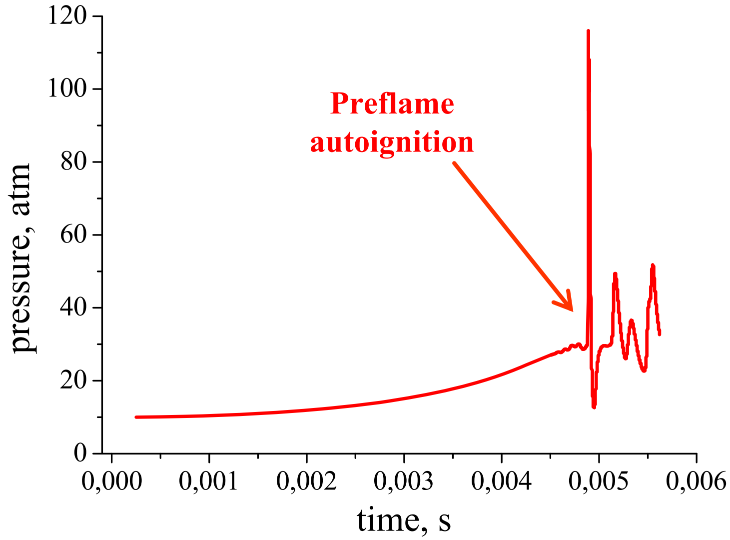
Localized autoignition dynamics

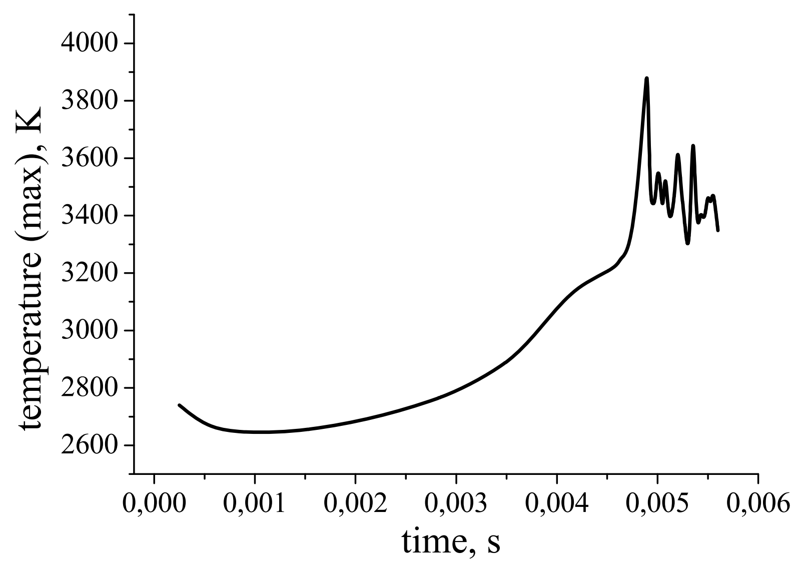


Results: Square domain

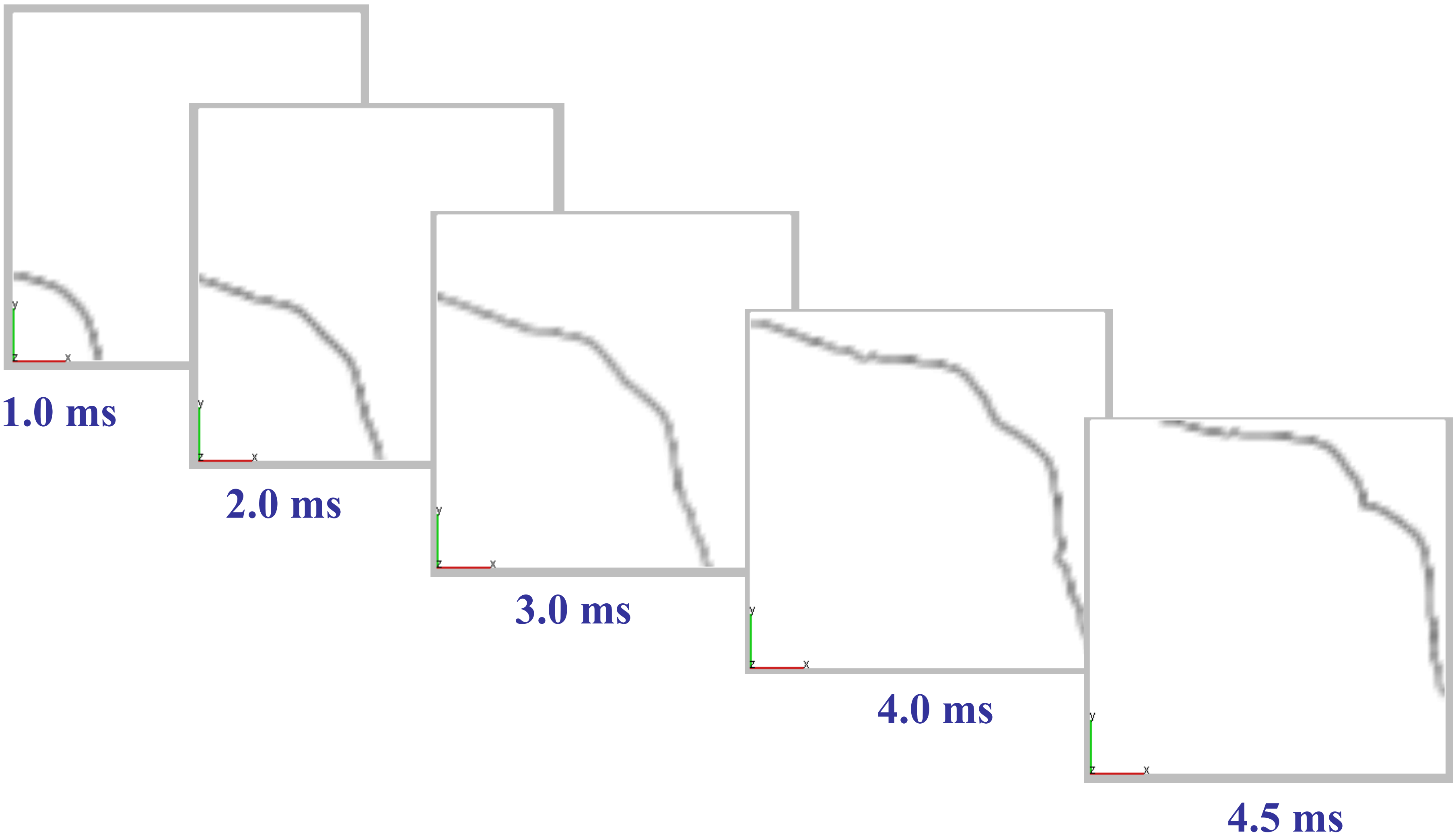


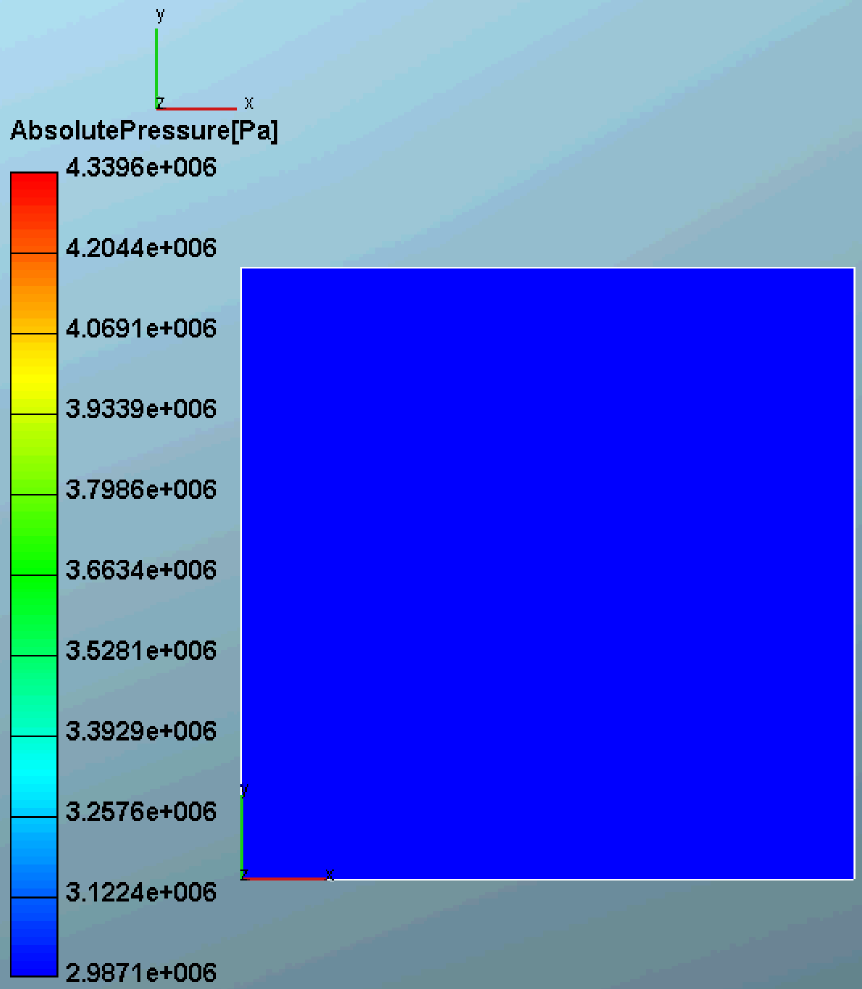


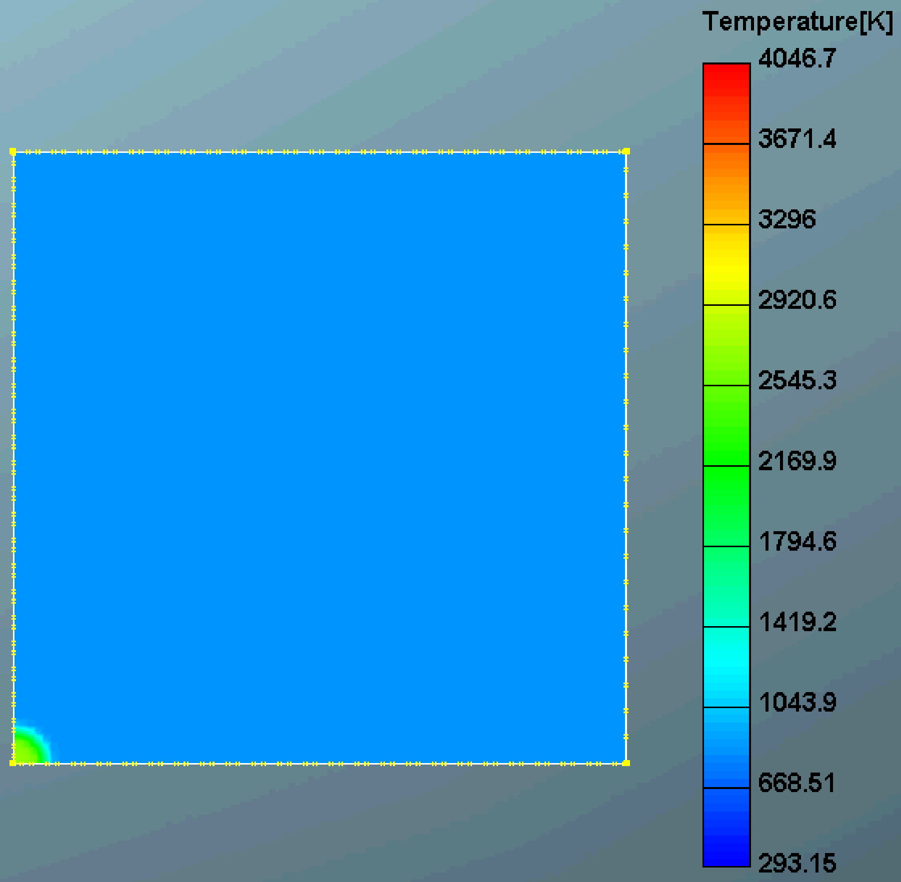




Flame propagation



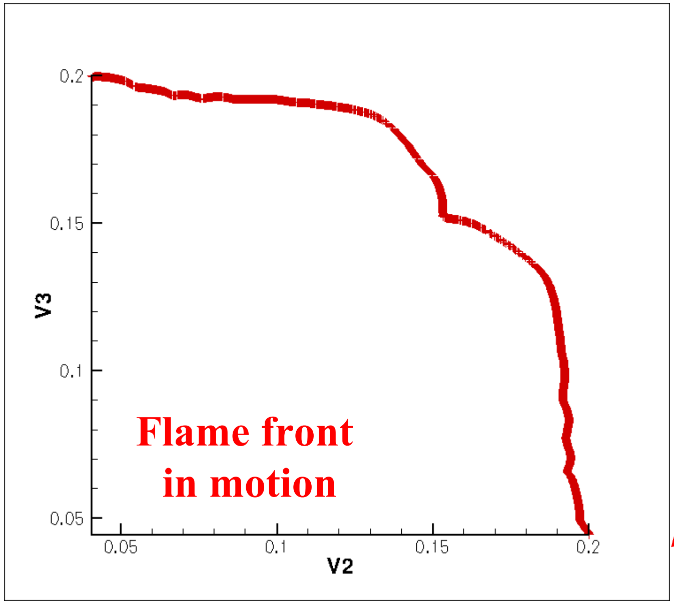




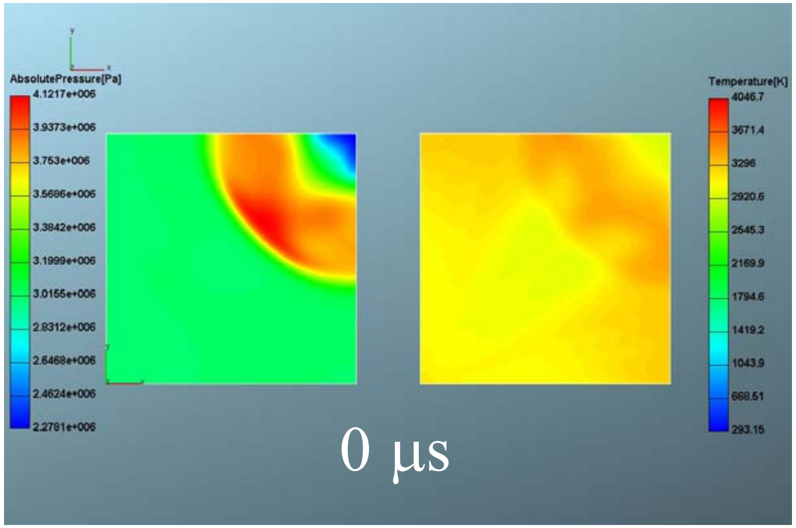
Pressure

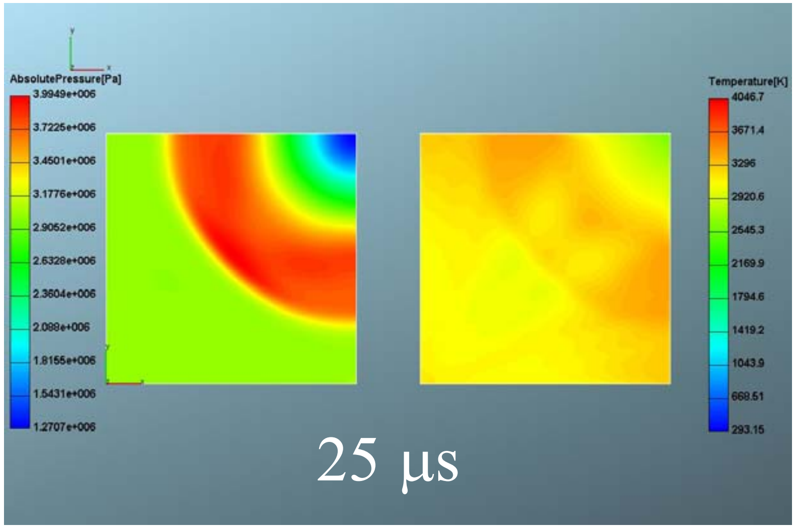
Temperature

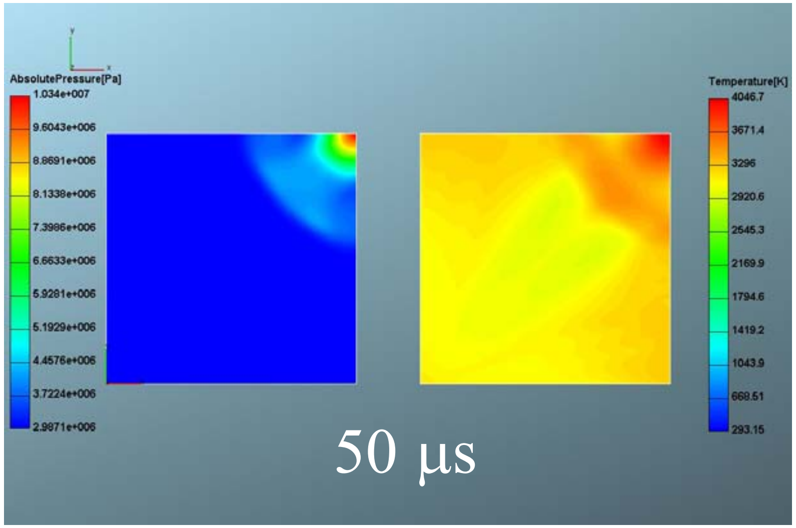
Snapshots of preflame autoignition



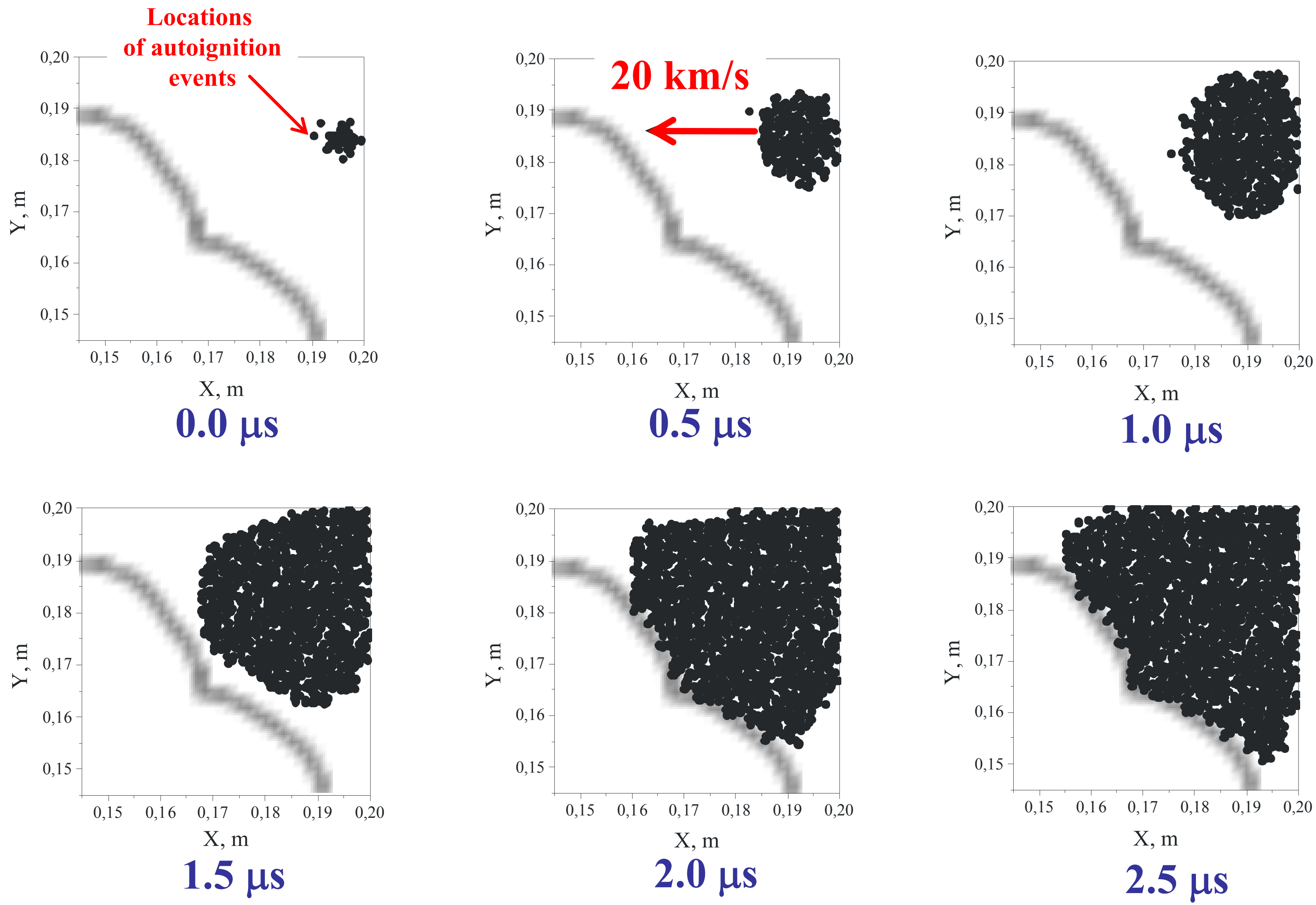
Flame
flashback



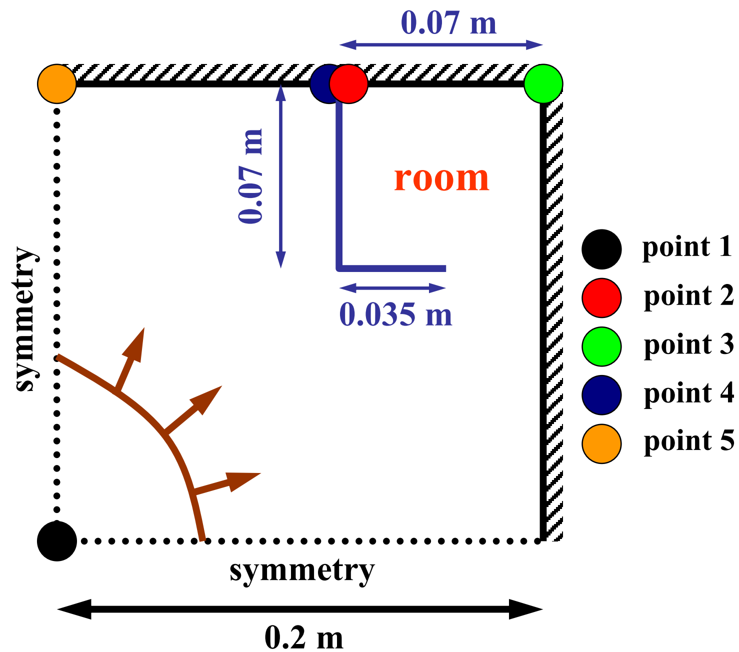


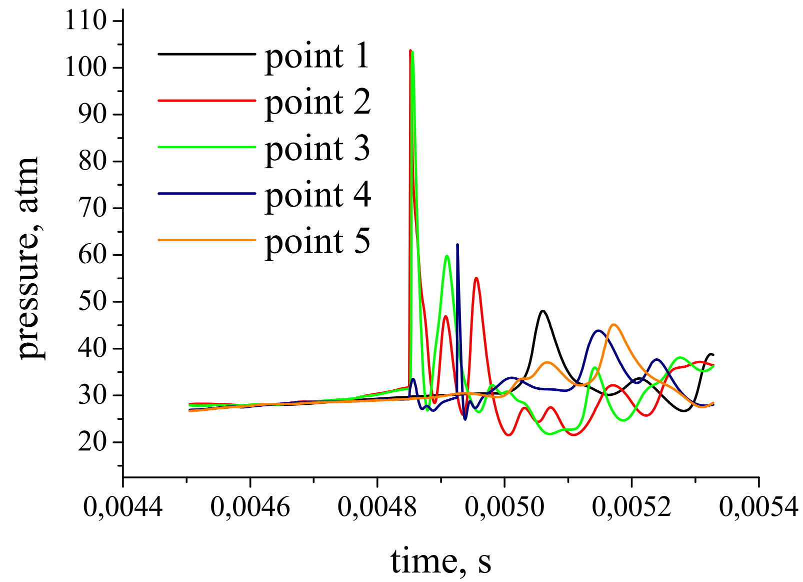


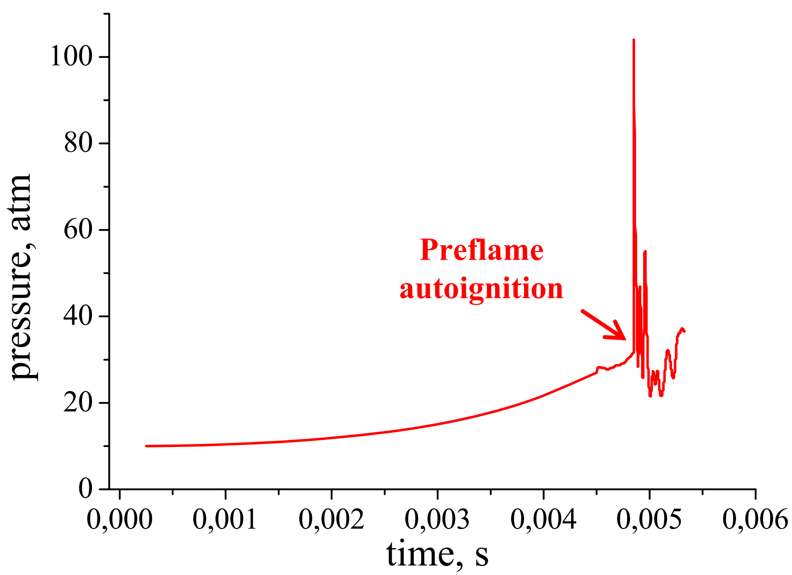
Localized autoignition dynamics

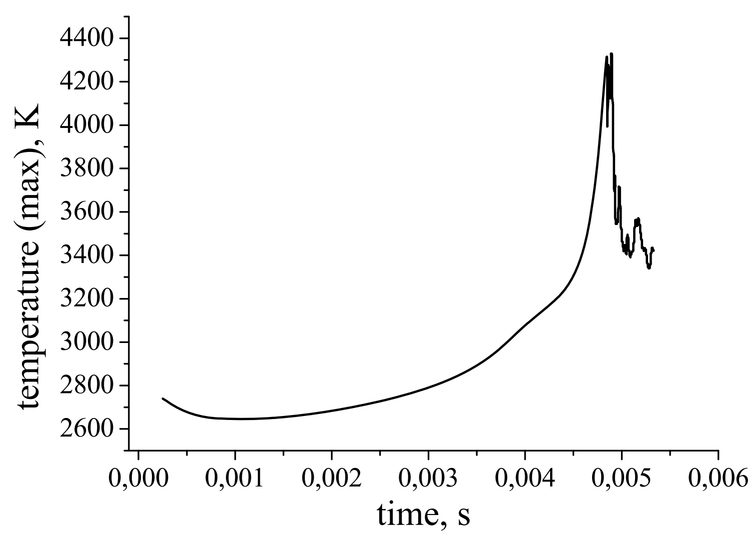


Results: Square domain with "room"

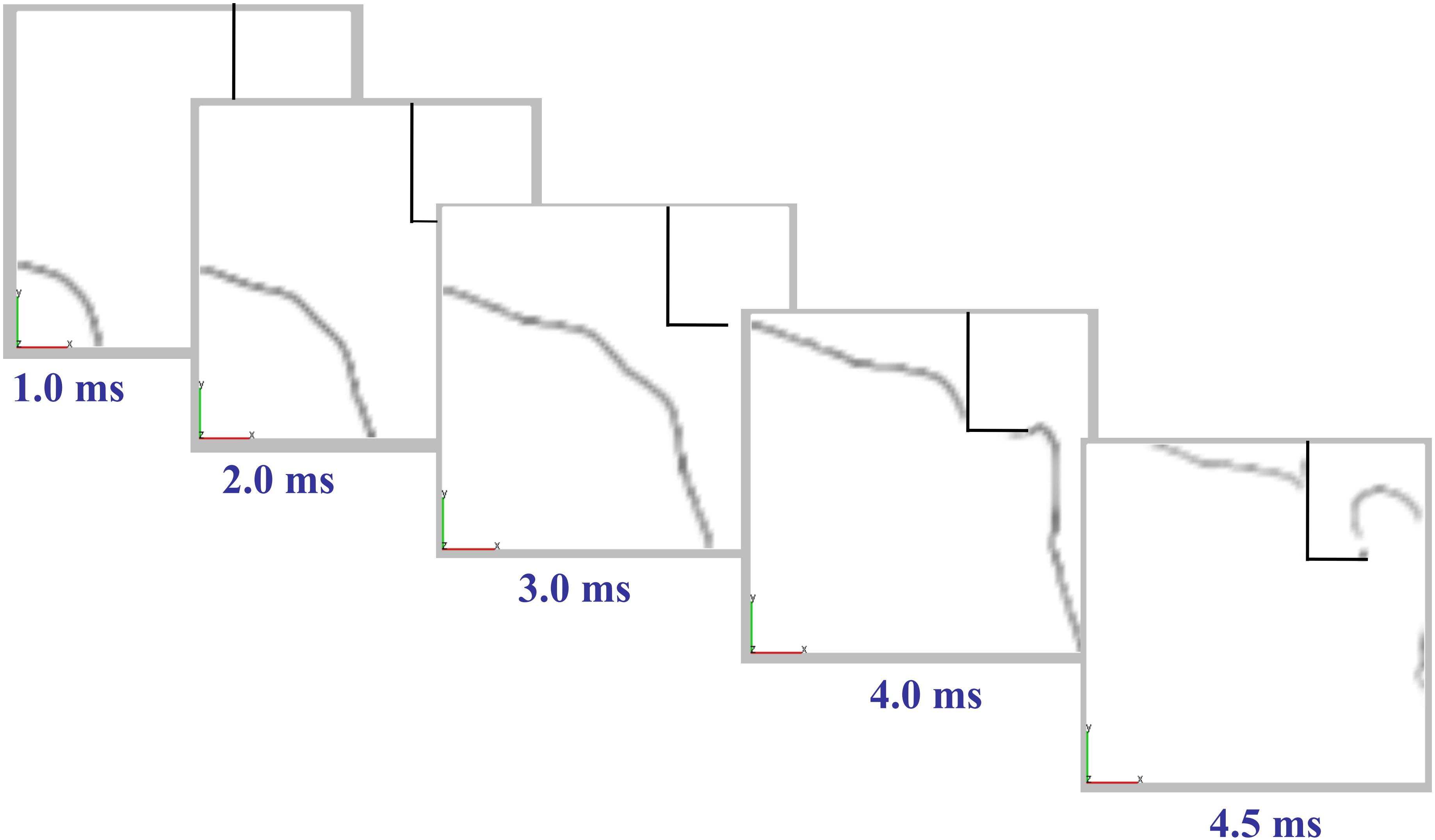


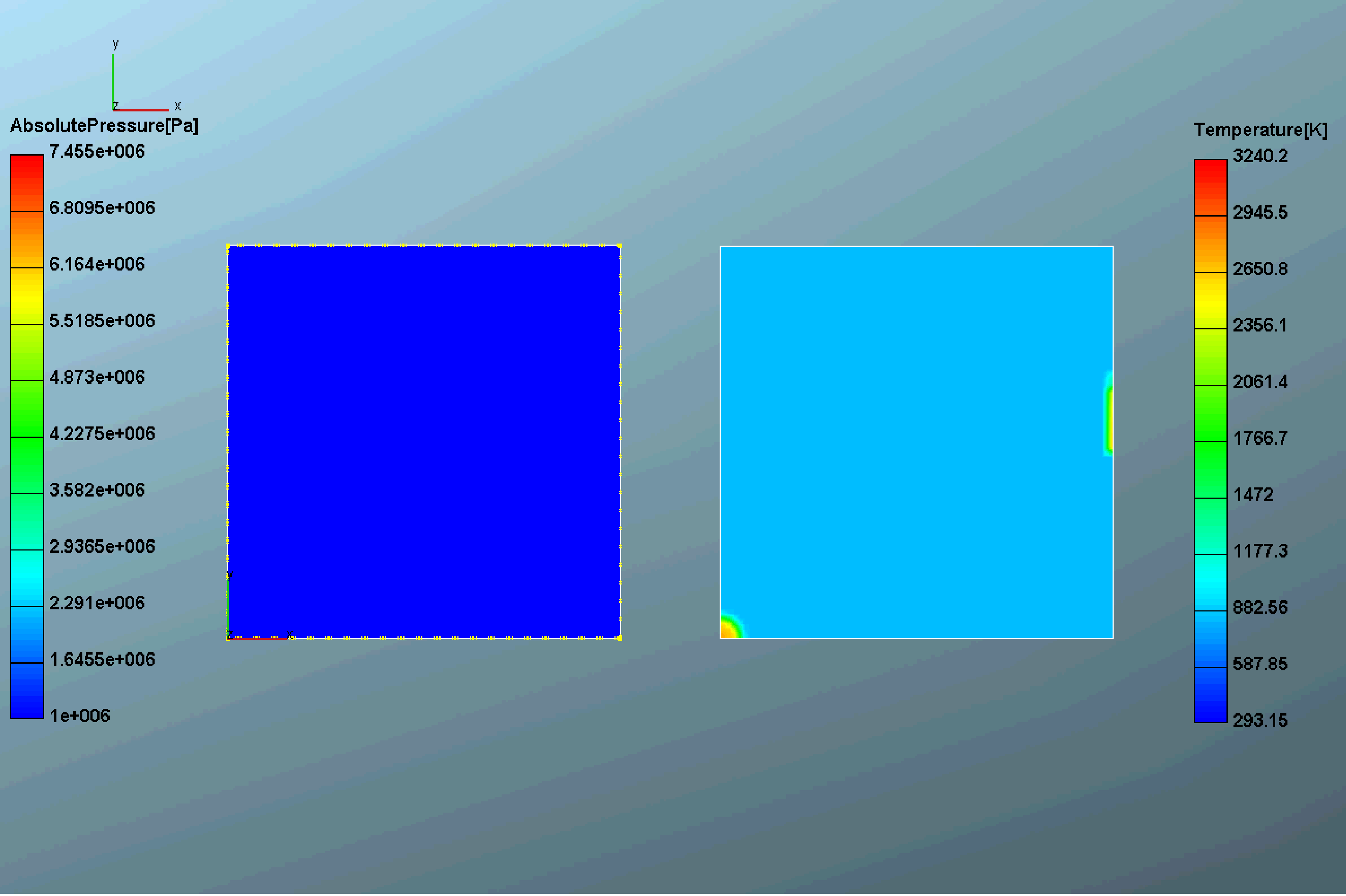






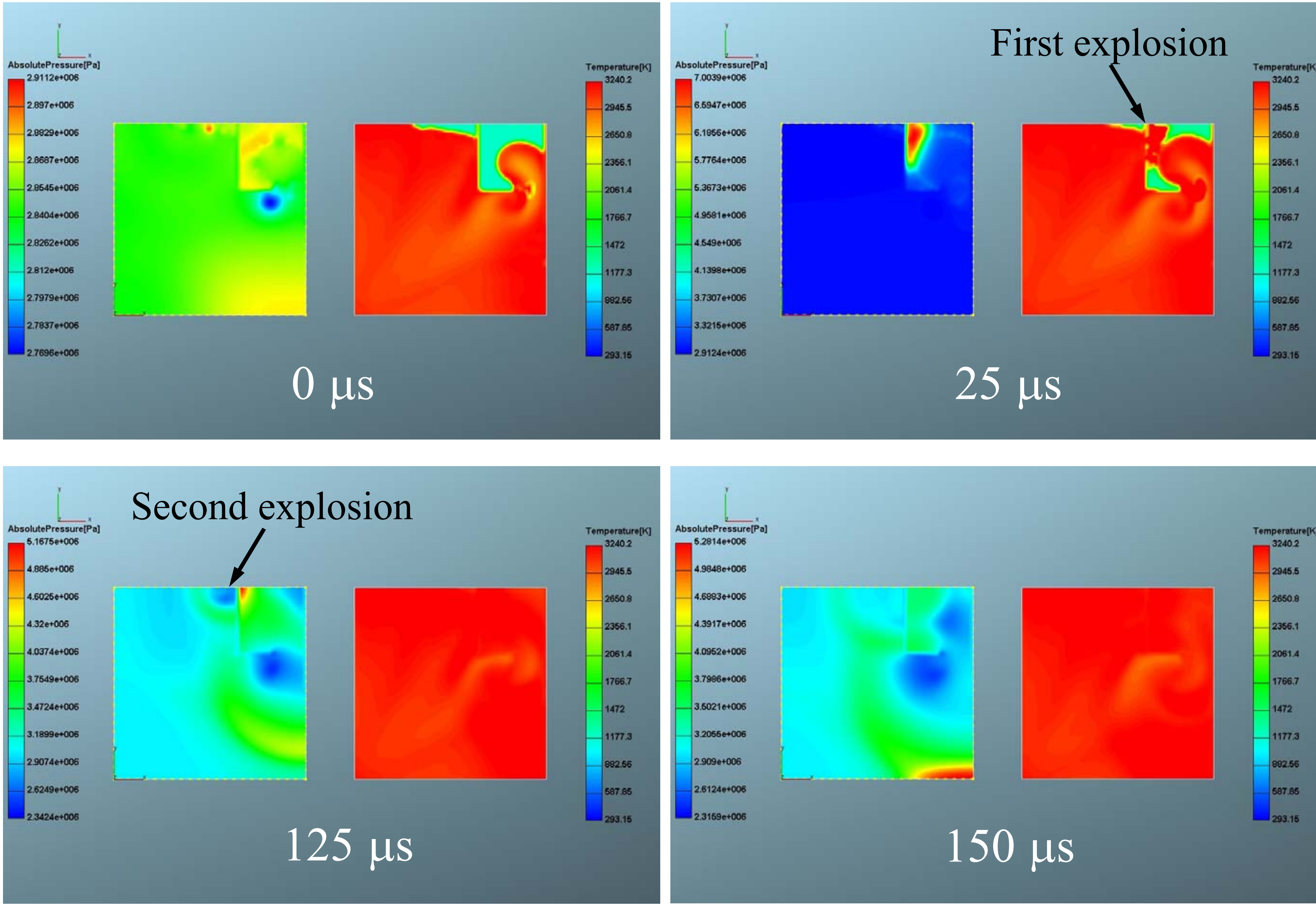
Flame propagation



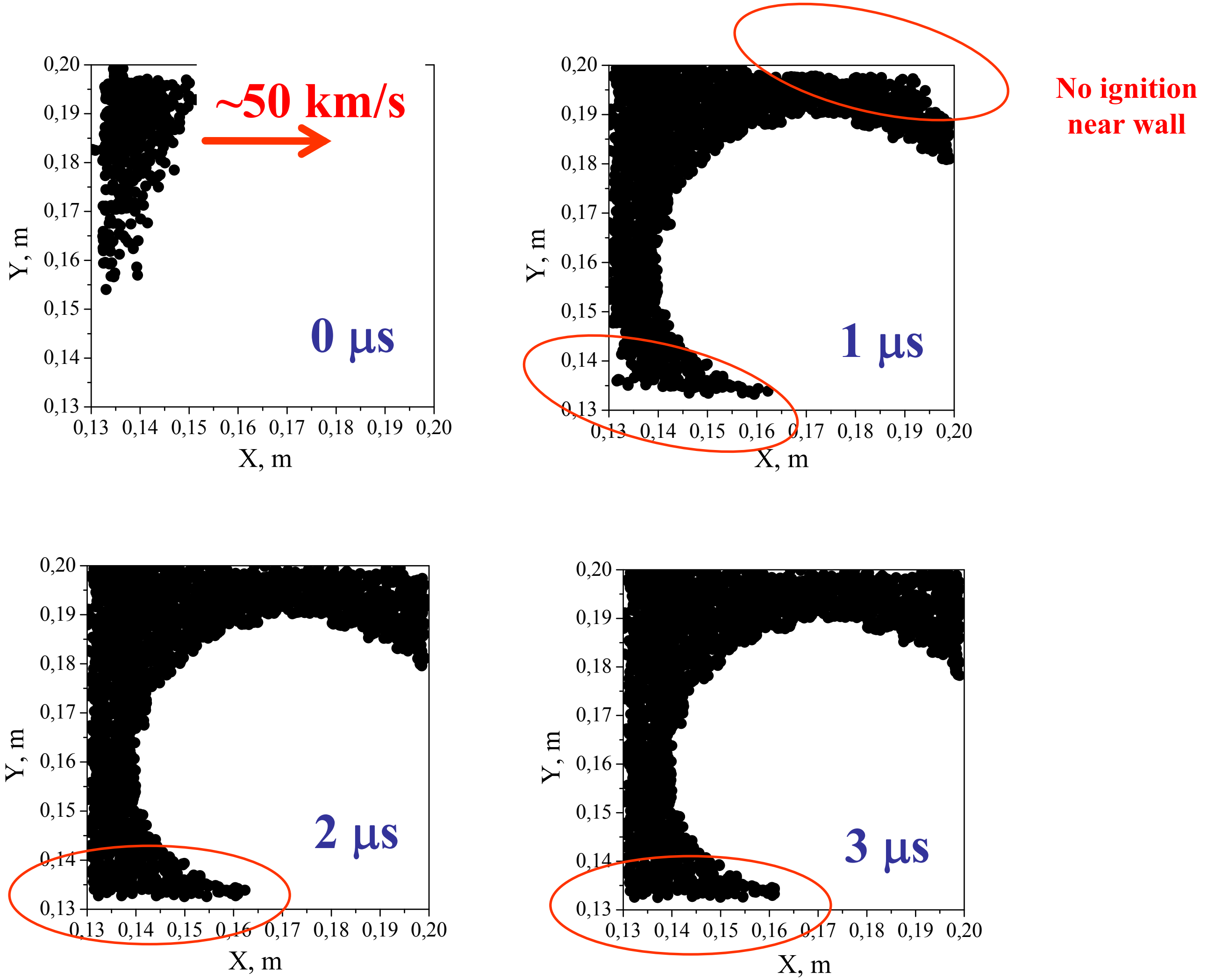


Pressure **Temperature**

Snapshots of preflame autoignition



Localized autoignition dynamics in "room"



Conclusions

- The algorithm of **Flame-Tracking – Particle method** in 2D geometries has been developed and implemented into a CFD code.
- The method is **(conditionally!) parameter free** and very efficient in terms of CPU requirements.
- The algorithm has been successfully **tested** for 2D configurations with flame acceleration in smooth-walled channels of different length.
- Results of calculations were **compared with experimental data for stoichiometric propane – air mixture**.
- The method has been applied for the problem of **hydrogen combustion in enclosures of complex shape**.
- The method is capable of predicting **spatial locations and development of preflame autoignition.**
- The method can be readily applied for studies of **hydrogen safety problems in enclosures of complex geometries.**

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