JAPAN-RUSSIA WORKSHOP ON SUPERCOMPUTER MODELING, INSTABILITY AND TURBULENCE IN FLUID DYNAMICS (JR SMIT 2015)

Numerical modelling of high speed reacting flows on multiprocessor computers

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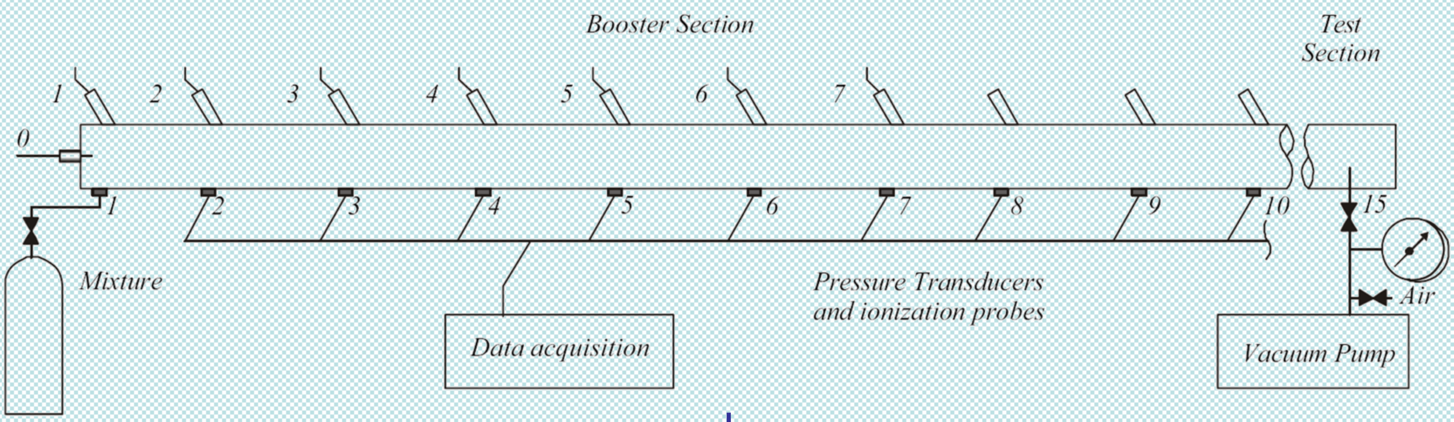
Detonation initiation in the reacting gaseous mixture

Motivation 1

The ways of detonation initiation

Direct initiation	Shock-to-detonation transition	Deflagration-to-detonation transition

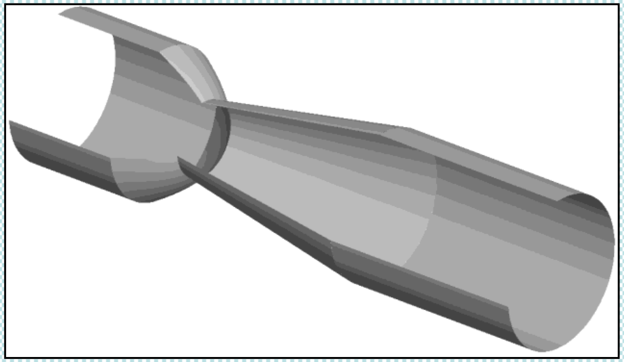
Initiation of detonation by «travelling ignition pulses»
(Frolov S.M. et al., 2004 – 2006)

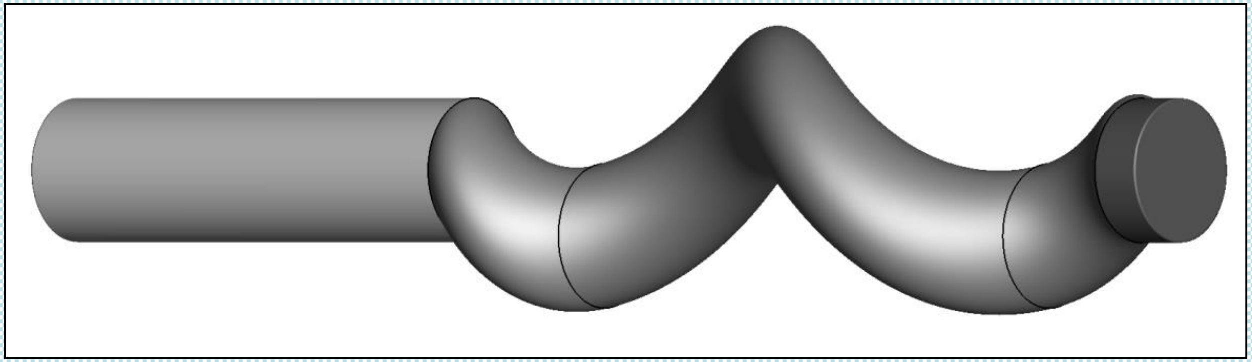


Special tube walls profiling

Motivation 1

New approaches to reducing the predetonation distance for pulse detonation engine (PDE) and burners applications. The underlying idea is to promote **fast DDT** by appropriate shaping of wall in the detonation device.
Numerical investigation of multidimensional instability of the detonation wave in tubes with complex geometry.





Developing of program complex for 3D numerical investigations of non-stationary transient regimes and effects of tube shape.
• CPU time and memory costs for 3D problems;
• unstructured or multi-block 3D grid generation for complex shapes;
• effective parallelization of the numerical algorithm which deals with unstructured grids.

Mathematical model for 3D flows with detonation waves

$$\frac{\partial \mathbf{q}}{\partial t}+\frac{\partial \mathbf{f}_1}{\partial x}+\frac{\partial \mathbf{f}_2}{\partial y}+\frac{\partial \mathbf{f}_3}{\partial z}=\mathbf{S},$$

$$\mathbf{q}=\begin{bmatrix}\rho_1\\ \dots\\ \rho_N\\ \rho U_x\\ \rho U_y\\ \rho U_z\\ \rho E\end{bmatrix},\ \mathbf{f}_1=\begin{bmatrix}\rho_1 U_x\\ \dots\\ \rho_N U_x\\ \rho U_x^2+p\\ \rho U_y U_x\\ \rho U_z U_x\\ (\rho E+p)U_x\end{bmatrix},\ \mathbf{f}_2=\begin{bmatrix}\rho_1 U_y\\ \dots\\ \rho_N U_y\\ \rho U_x U_y\\ \rho U_y^2+p\\ \rho U_z U_y\\ (\rho E+p)U_y\end{bmatrix},\ \mathbf{f}_3=\begin{bmatrix}\rho_1 U_z\\ \dots\\ \rho_N U_z\\ \rho U_x U_z\\ \rho U_y U_z\\ \rho U_z^2+p\\ (\rho E+p)U_z\end{bmatrix},\ \mathbf{S}=\begin{bmatrix}\dot{\omega}_1\\ \dots\\ \dot{\omega}_N\\ 0\\ 0\\ 0\\ 0\end{bmatrix},$$

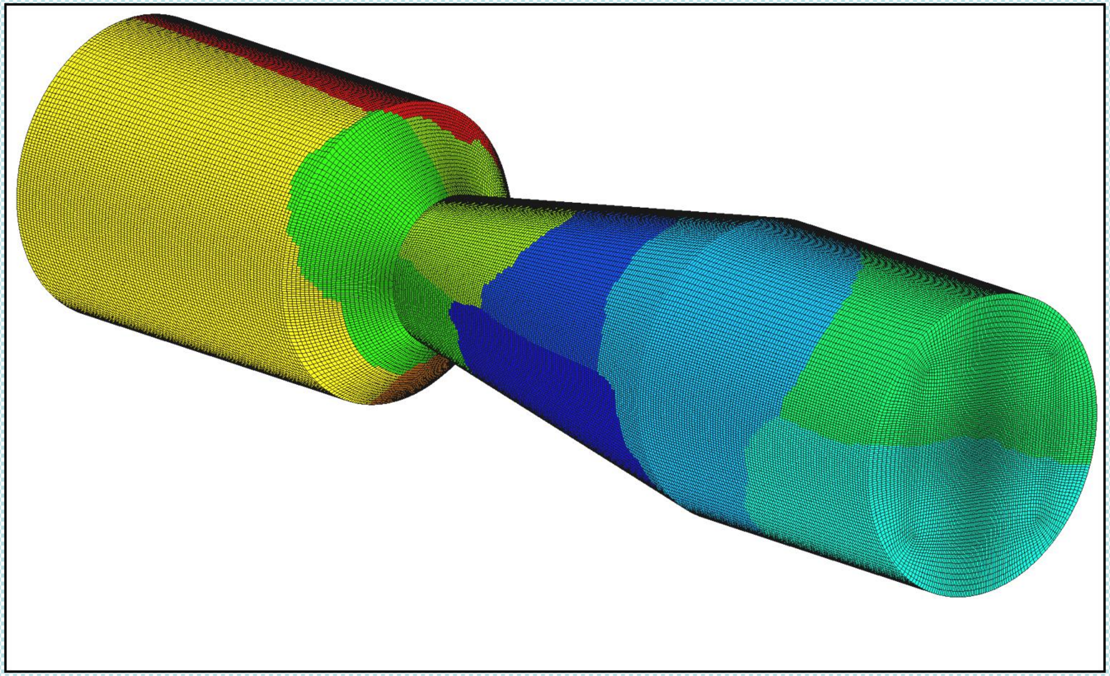
$$E=\frac{1}{2}\left(U_x^2+U_y^2+U_z^2\right)+\sum_{k=1}^{N}\rho_k h_k/\rho-p/\rho,\ h_k=h_{0k}+c_{Vk}T+p_k/\rho_k,\ k=1,\dots,N,$$

$$p=\sum_{k=1}^{N}p_k=\sum_{k=1}^{N}\rho_k R_k T,\ N-\text{mixture components number}$$

Numerical procedure

- Method of splitting with respect to physical processes
- Space discretization: finite-volume method, time integration: explicit predictor-corrector scheme with the second-order approximation
- Godunov’s method for fluxes calculation
- Enhancement of accuracy: MUSCL approach with upwind-biased third order scheme of interpolation and van Albada limiter
- Moving least squares method for gradients calculation
- Backward differentiation formulas for the solution of chemical kinetics system of ODE
- Unstructured hexahedral computational grids with up to 300 mln. cells, spatial resolution is 1.0 – 0.005 mm, time resolution is between 10 – 0.5 ns
- Parallel calculations with the use of up to 4000 cores on supercomputers Lomonosov MSU and MVS-100k at Joint Supercomputer Center RAS, domain decomposition method, MPI library

Parallelization



Example of computational O-grid (~ 3 mln cells) and its partition to 10 processors with the use of METIS library

- Domain decomposition with the use of METIS library (Karypis G., Kumar V. METIS 4.0: Unstructured graph partitioning and sparse matrix ordering system, 1998)
- CGNS (CFD General Notation System) as the format of computational grid representation

The models for **methane** oxidation kinetic mechanism

Single-stage overall kinetic mechanism model (V.Ya. Basevich, S.M. Frolov, 2009)

$$\begin{cases} CH_4 + 2(O_2 + 3.762N_2) \rightarrow CO_2 + 2H_2O + 7.524N_2, \\ \dot{\omega}_{CH_4} = \mu_{CH_4}\omega_{CH_4}^{mole} = \mu_{CH_4}\left(k\frac{\rho_{CH_4}}{\mu_{CH_4}}\cdot\left[\frac{\rho_{O_2}}{\mu_{O_2}}\right]^2\right), \\ k = -4\cdot 10^{14} p^{-1}\exp\left(-E^*/RT\right)\ \mathrm{l}^2/\left(\mathrm{mole}^2\cdot \mathrm{s}\right),\ E^* = 50\ \mathrm{kcal/mole} \end{cases}$$

Reduced kinetic mechanism model (V.Ya. Basevich, S.M. Frolov, 2006)

$$\begin{cases} CH_4 + 1.5O_2 \rightarrow CO + 2H_2O, \\ 2H_2 + O_2 \rightarrow 2H_2O, \\ 2CO + O_2 \rightarrow 2CO_2, \\ CO + H_2O \leftrightarrow CO_2 + H_2. \\ \omega_i = A_i \exp(E_i/RT)\prod_j n_{ij},\ i = 2, 3, 4, -4, \\ \omega_1 = A_1\frac{\rho_{CH_4}}{\mu_{CH_4}}\frac{\rho_{O_2}}{\mu_{O_2}}\exp(E_1/RT). \\ \mathrm{CH_4}(i=1), \mathrm{O_2}(i=2), \mathrm{N_2}(i=3), \\ \mathrm{CO_2}(i=4), \mathrm{H_2O}(i=5), \mathrm{CO}(i=6), \mathrm{H_2}(i=7). \end{cases}$$

$$A_1 = 4\cdot 10^{11}\cdot P^{-0.2264}\ \frac{l}{mole * s},\ \mathrm{E}_1 = 45\ \frac{kcal}{mole},$$

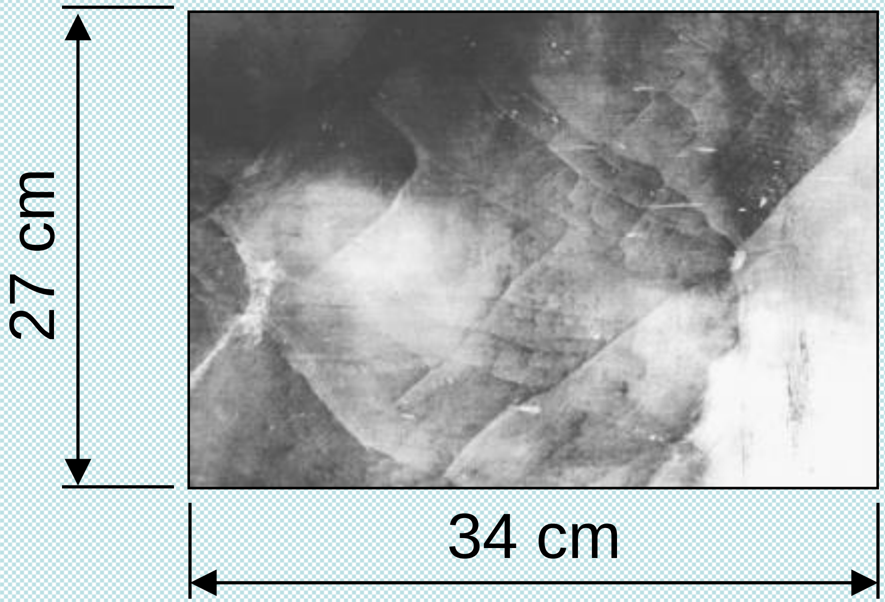
$$A_2 = 7\cdot 10^{13}\cdot P^{-0.5}\ \frac{l^2}{mole^2 * s},\ \mathrm{E}_2 = 21\ \frac{kcal}{mole},$$

$$A_3 = 8.5\cdot 10^{12}\cdot P^{-1.5}\ \frac{l^2}{mole^2 * s},\ \mathrm{E}_3 = 21\ \frac{kcal}{mole},$$

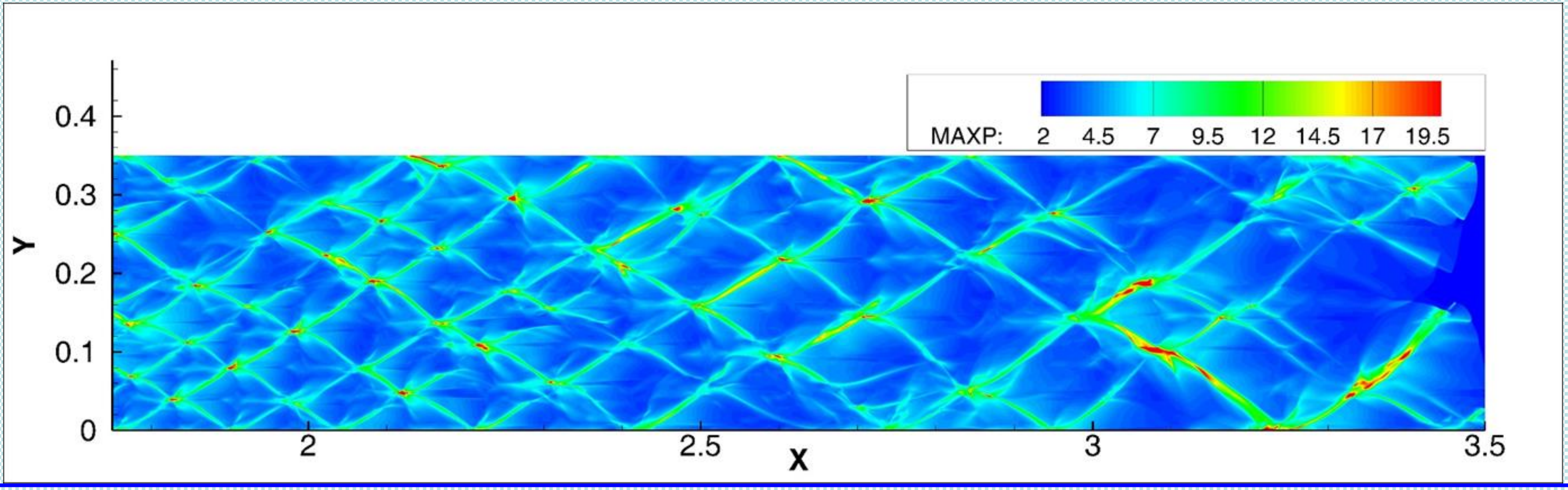
$$A_4 = 1\cdot 10^{12}\cdot P^{-1}\ \frac{l}{mole * s},\ \mathrm{E}_4 = 41.5\ \frac{kcal}{mole},$$

$$A_{-4} = 3.1\cdot 10^{13}\cdot P^{-1}\ \frac{l}{mole * s},\ \mathrm{E}_{-4} = 49.1\ \frac{kcal}{mole}.$$

Cellular structure of plane DW in methane-air mixture

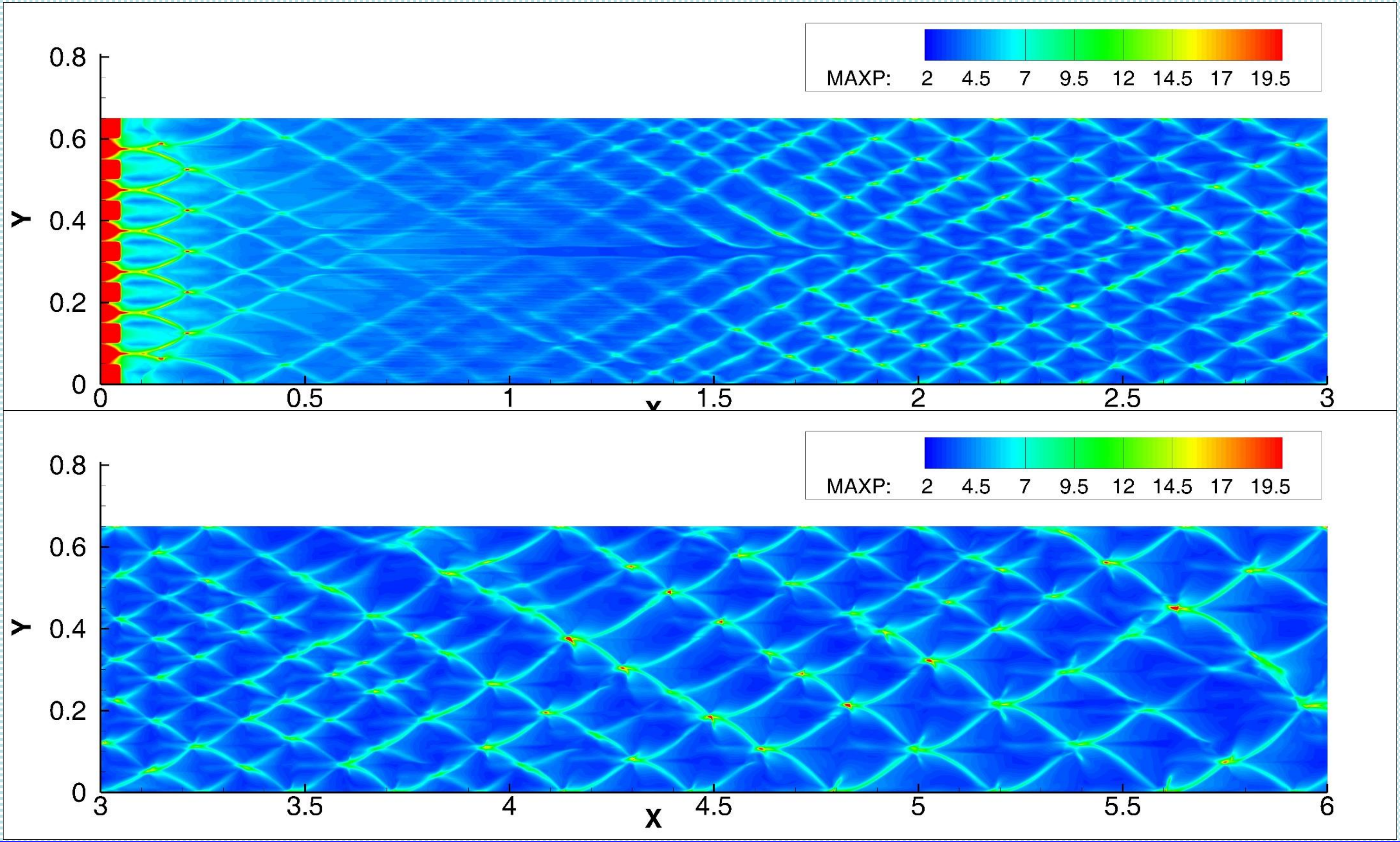


Experimental soot traces generated by detonations of mixture of natural gas and air in a 1.05 m diameter and 73 m long. Close-up view of a primary cell showing detailed secondary cellular structure for near-stoichiometric detonation. R.K. Zipf (NIOSH, 2010).



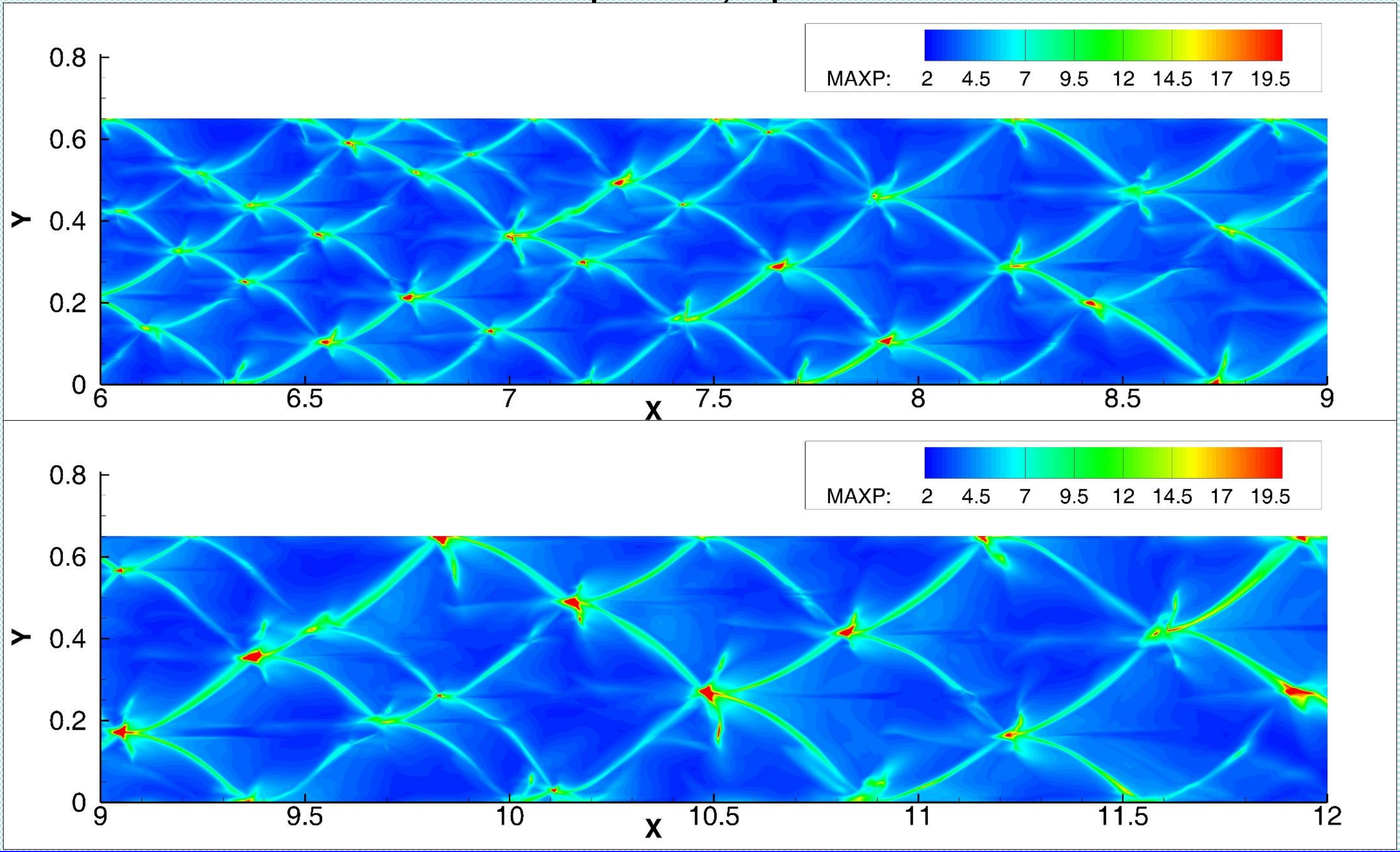
Cellular structure of plane DW in methane-air mixture

“Numerical soot footprints”, spatial resolution 1 mm



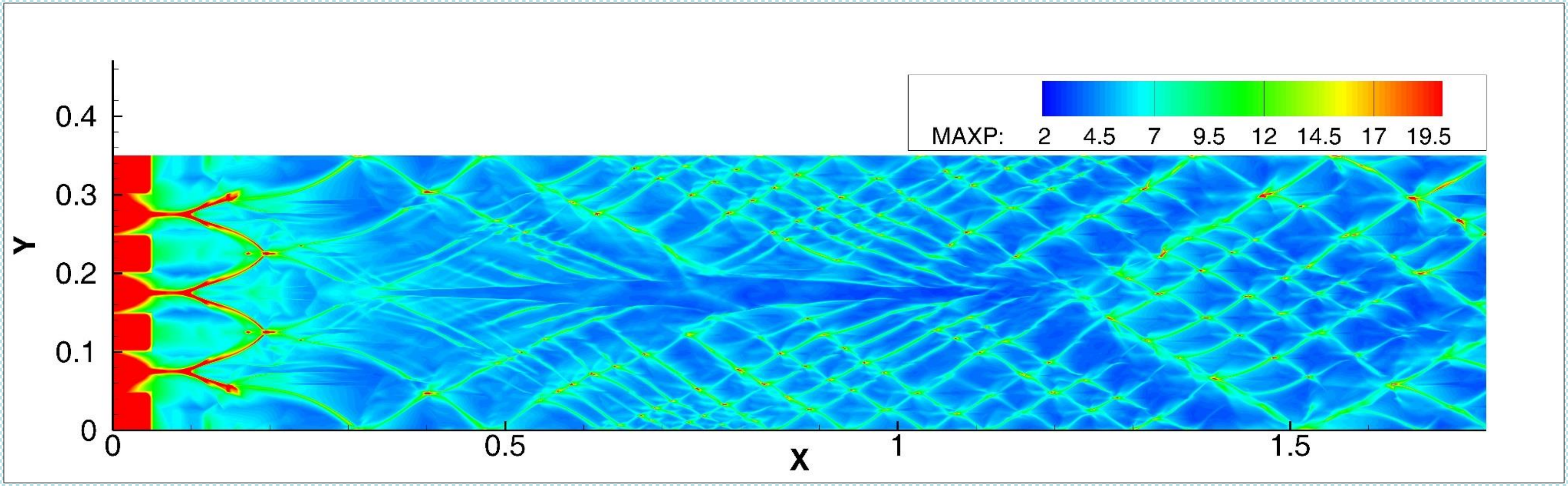
Cellular structure of plane DW in methane-air mixture

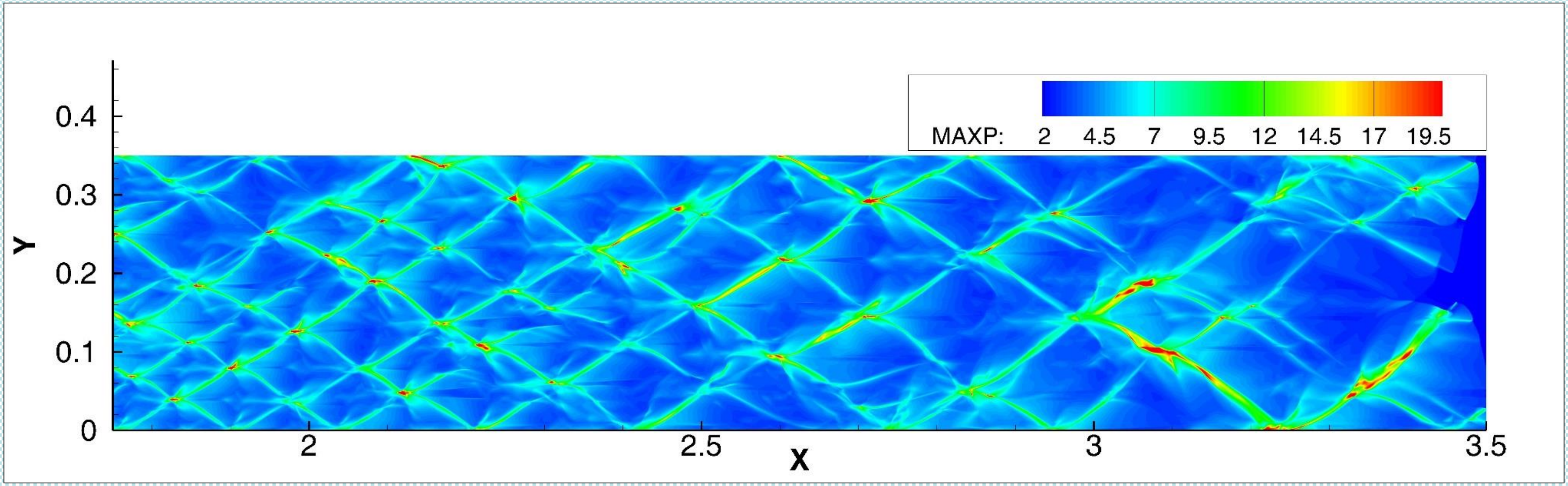
“Numerical soot footprints”, spatial resolution 1 mm



Cellular structure of plane DW in methane-air mixture

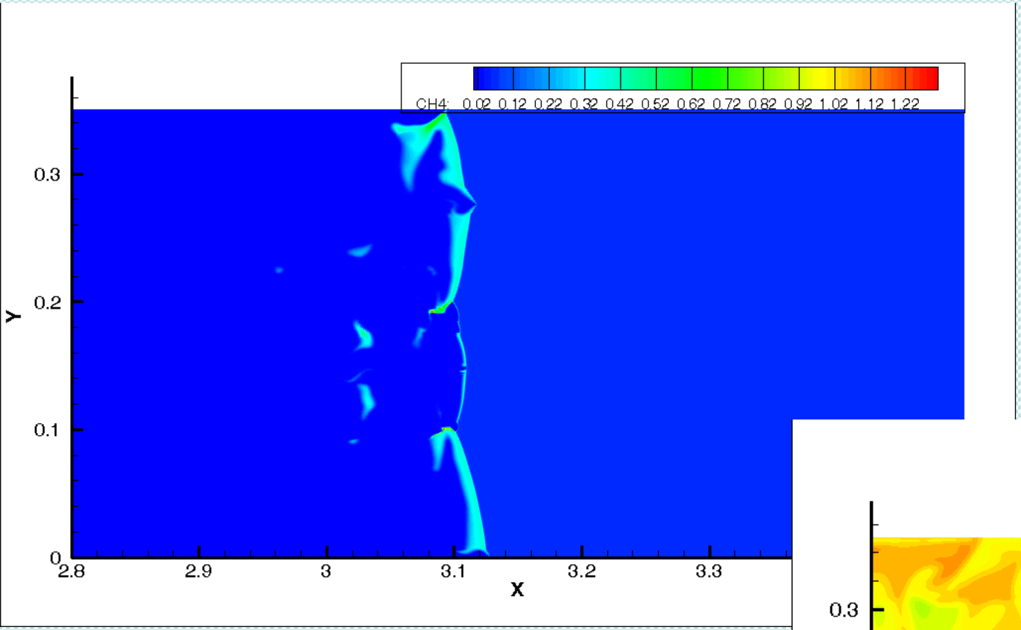
"Numerical soot footprints", spatial resolution 0.2 mm





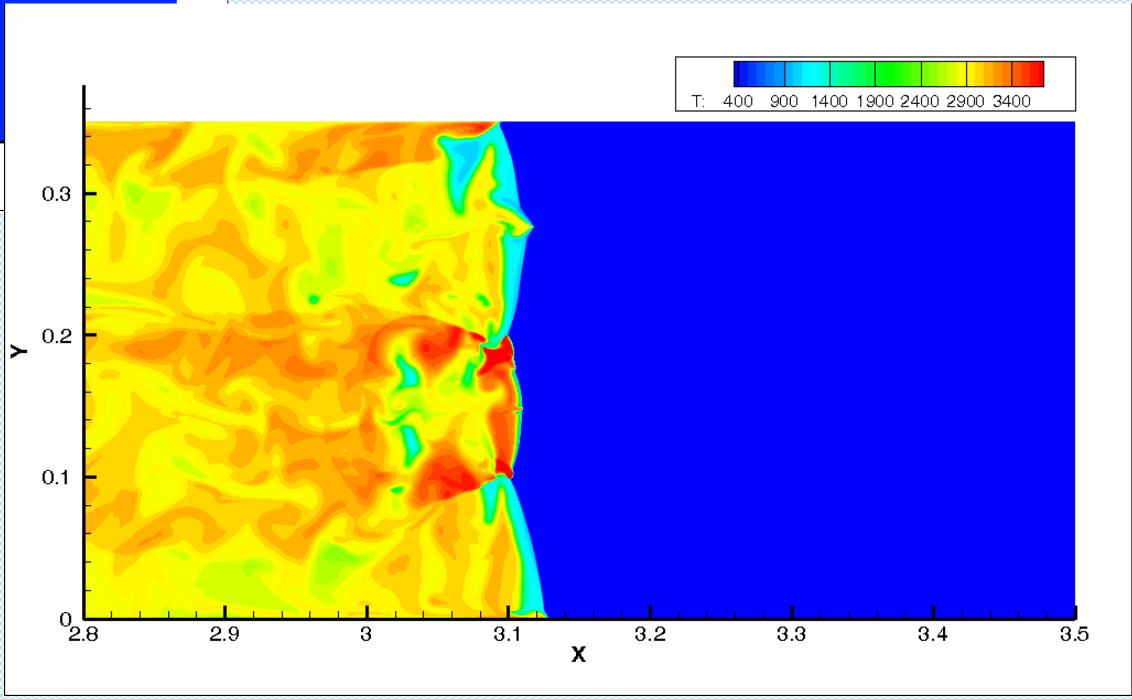
Cellular structure of plane DW in methane-air mixture

Spatial resolution 0.2 mm

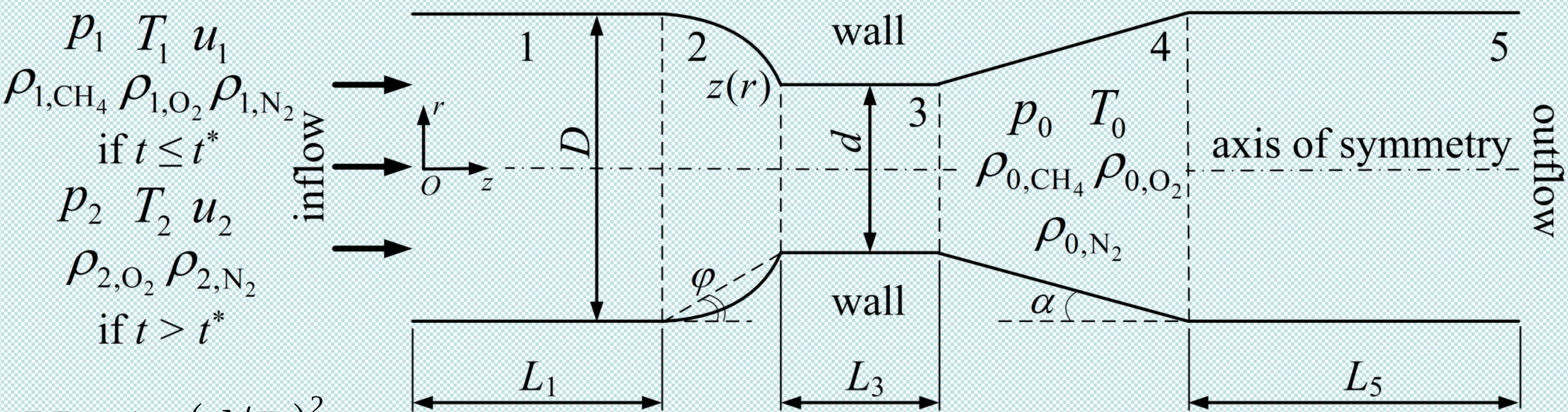


Methane density

Temperature (K)



Statement of the problem



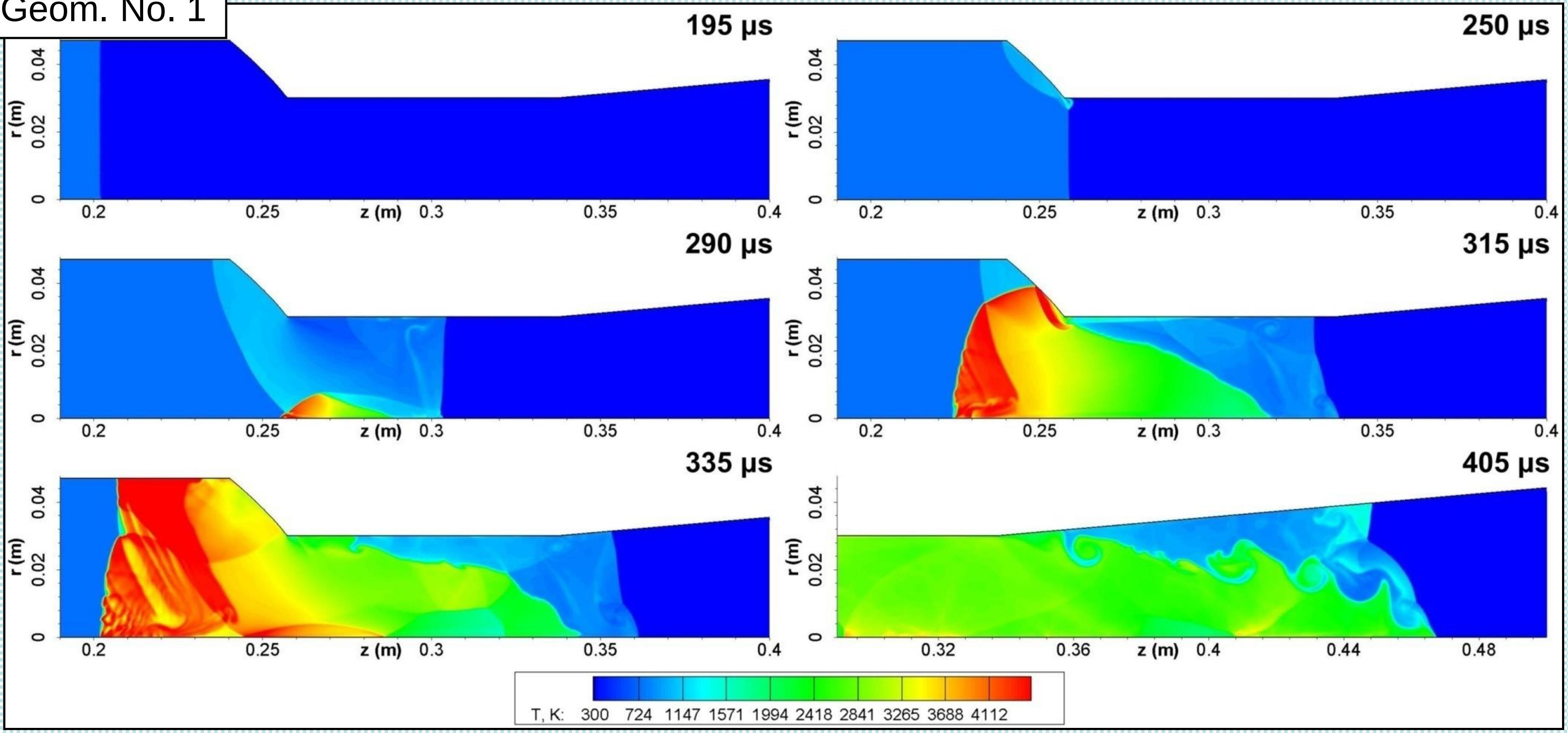
$$BR = 1 - \left(d/D\right)^2$$

$$D = 9.4 \cdot 10^{-2} \text{ m}, L_1 = 24 \cdot 10^{-2} \text{ m}, L_3 = 8 \cdot 10^{-2} \text{ m}, L_5 = 7 \cdot 10^{-2} \text{ m}$$

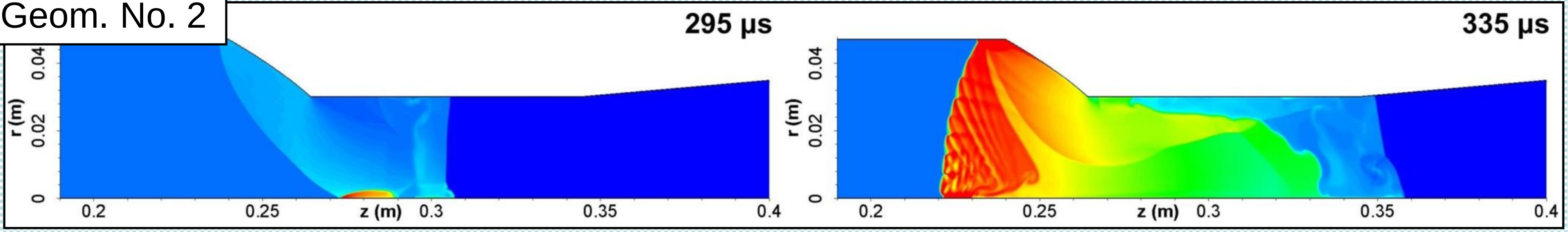
No.	φ, °	d, m	BR	α, °	Dimension	Initiating shock wave Mach number
1	45	$6 \cdot 10^{-2}$	0.6	5	2D	3.0
2	30	$6 \cdot 10^{-2}$	0.6	5	2D	3.0
3	45	$4.7 \cdot 10^{-2}$	0.75	5	2D	3.0
4	45	$4.7 \cdot 10^{-2}$	0.75	2.5	2D / 3D	3.0 / 3.3

2D case. Geometries No. 1 and 2.

Geom. No. 1



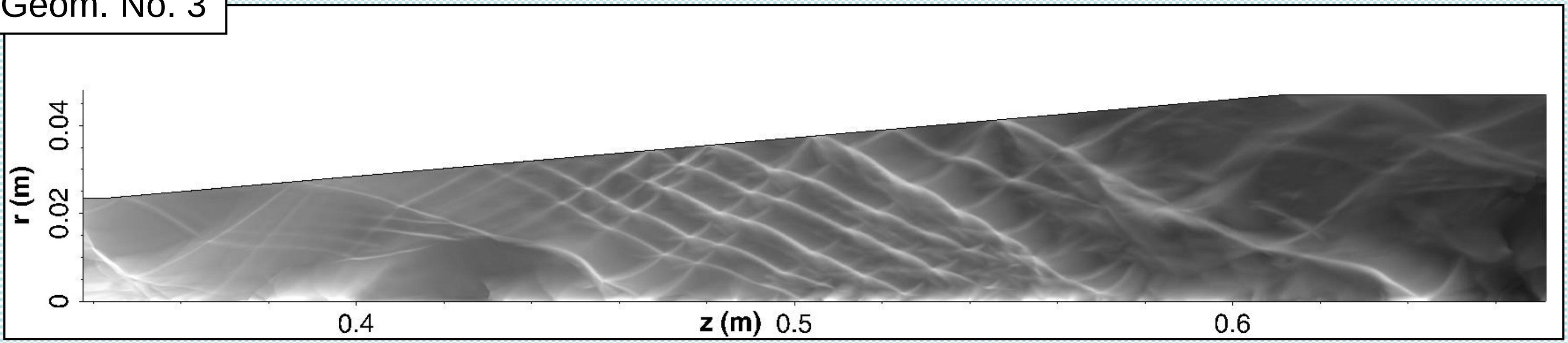
Geom. No. 2



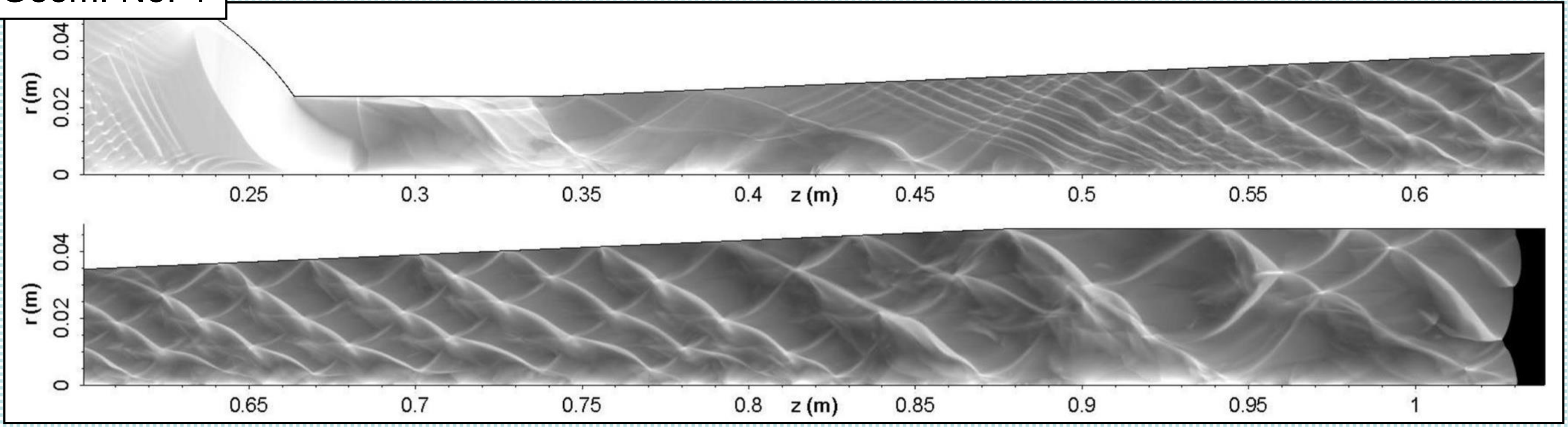
2D case. Geometries No. 3 and 4.

“Numerical soot footprints”

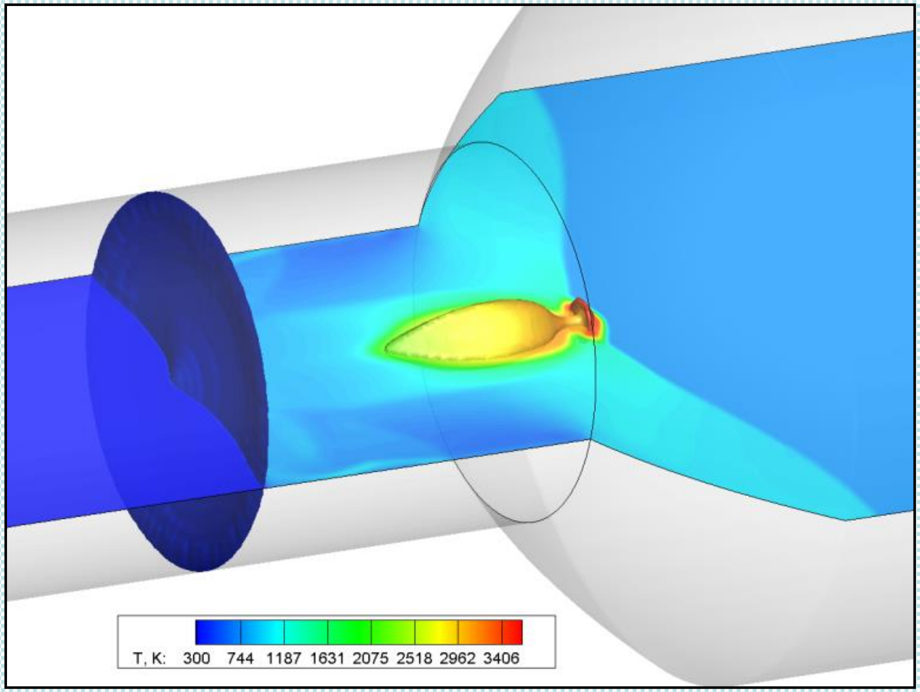
Geom. No. 3

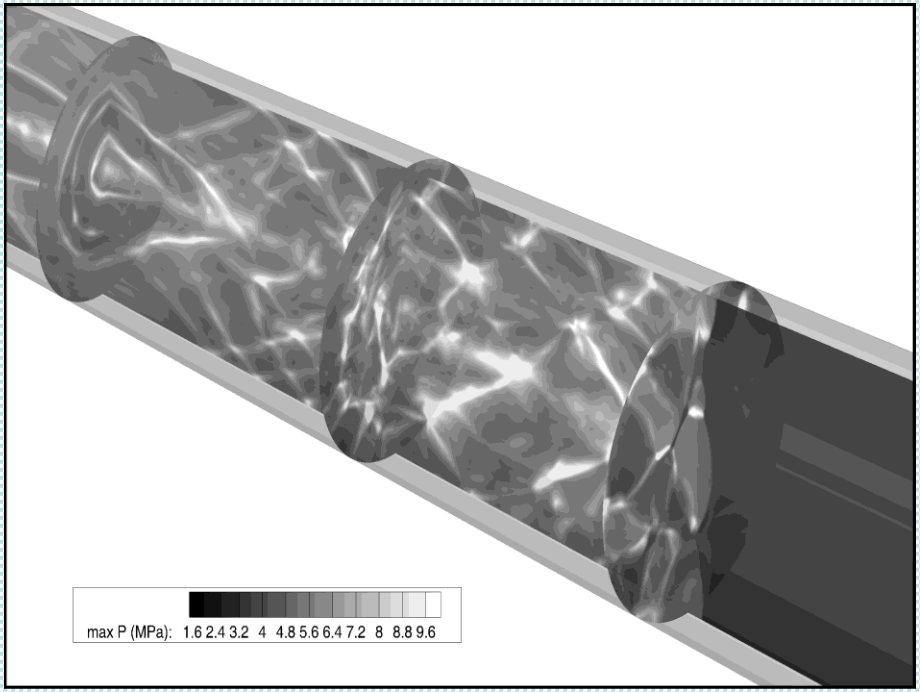


Geom. No. 4



3D case. Geometry No. 4.



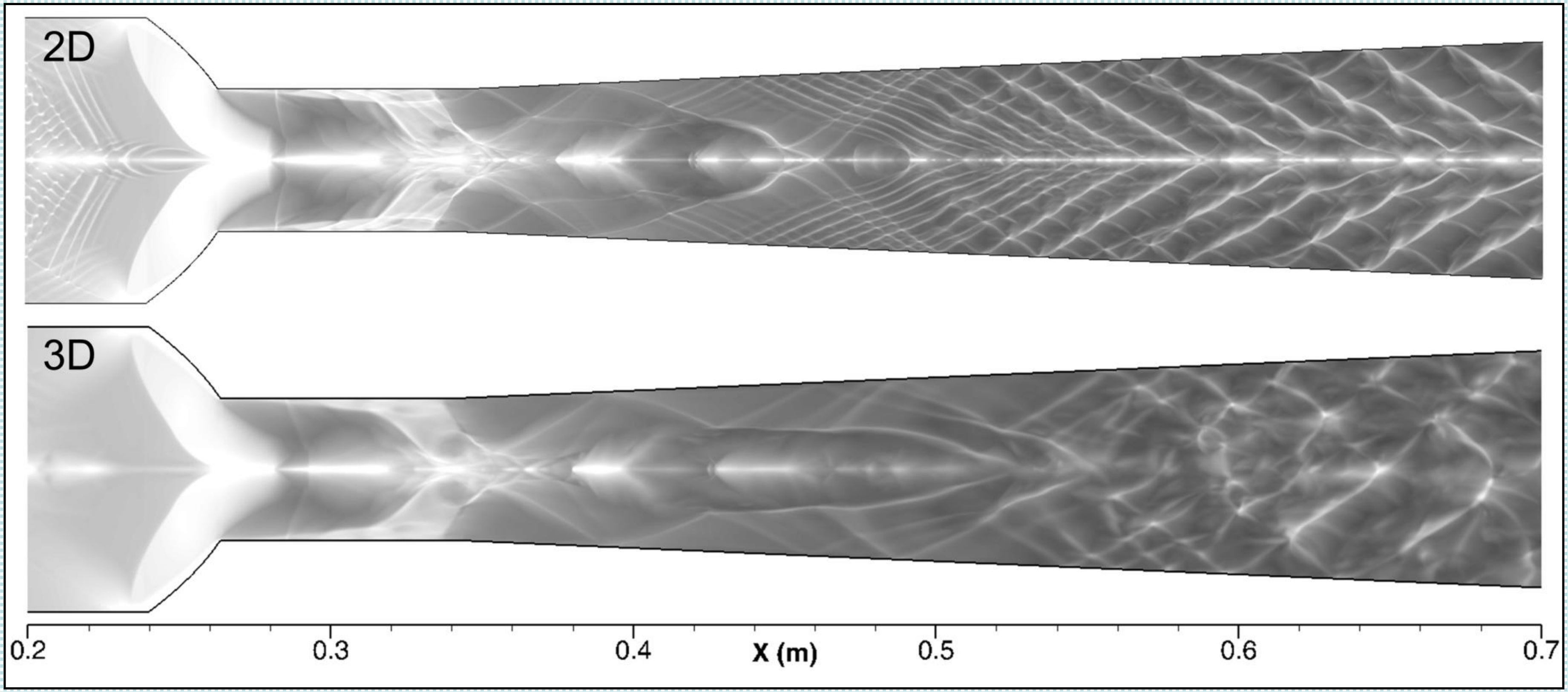


- Isosurfaces
  - Methane density, colored with temperature
    - ✓ Yellow part – blast wave
    - ✓ Red part – retonation wave
  - Temperature – leading shock wave
- Temperature field in section

“Numerical soot footprints” in several sections in cone expansion.

3D modeling results confirm qualitatively findings of the 2D modeling

Comparison of 2D and 3D calculations



Before the time moment when detonation wave moves to the conical expansion the mechanisms of detonation initiation in 2D and 3D approaches have no significant differences. At the same time after that time moment in 3D calculation the essential three-dimensional DW propagation character is observed.

Detonation initiation in coil with elbows (propane-air)

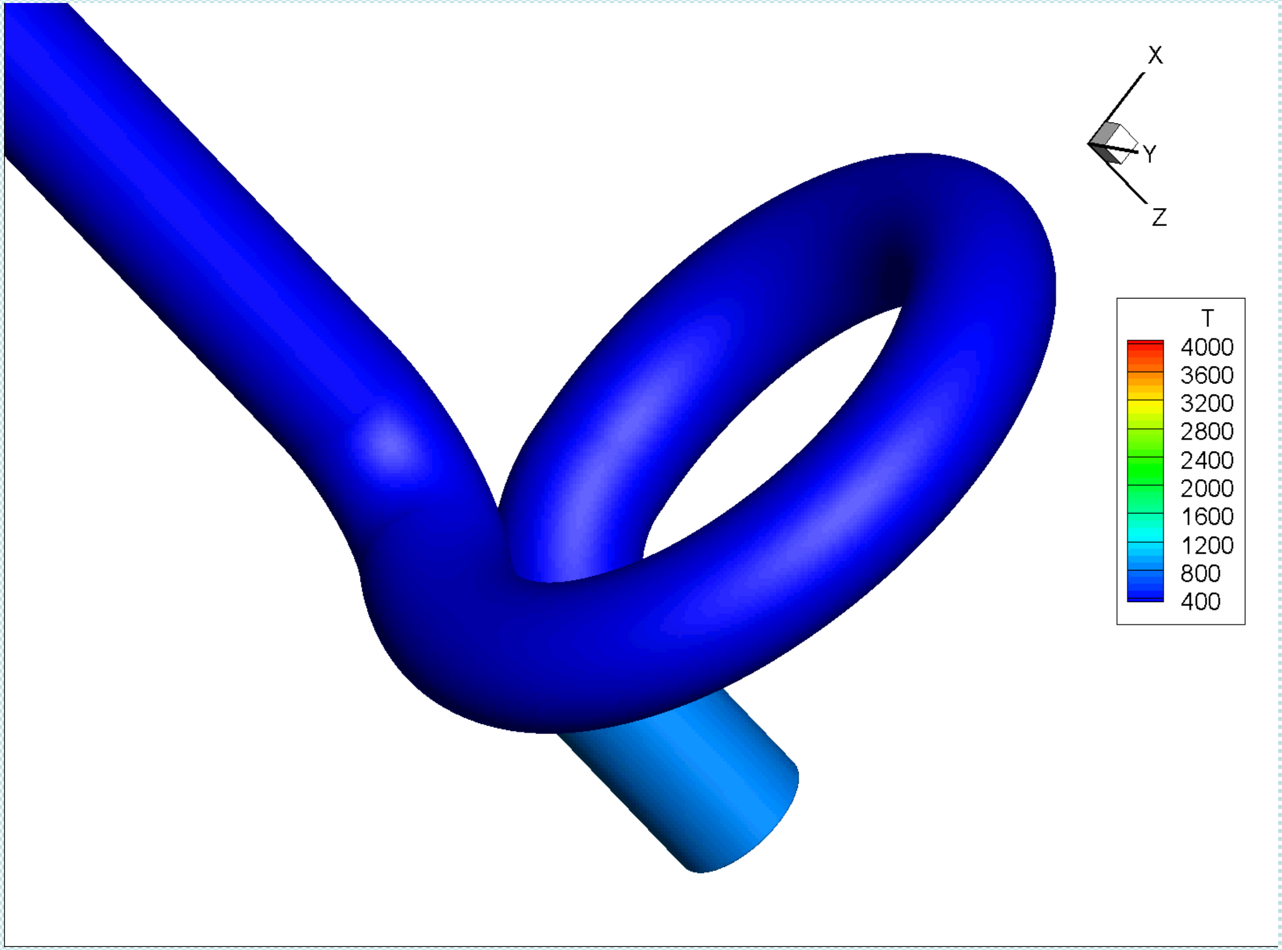
Time:
10-390 mcs

30 mln cells

Size ~ 0.15 mm

Hexahedral O-grid

D = 28 mm



Initial shock wave Mach number *M* = 3.4 (D =1139 m/s)
Dynamics of the temperature field, scales in Kelvin degrees

Conclusions 1

- The **mathematical model, numerical procedure and parallelization technique** for the problems of detonation initiation and propagation in 2D channels & 3D tubes of complex shapes are presented.
- 3D numerical investigations of detonation initiation in a tube with **parabolic contraction and conic expansion** confirm the mechanism of the process obtained earlier in 2D axisymmetric calculations.
- The shape of parabolic contraction and divergence angle of cone expansion are found which provide shock-to-detonation transition for the initiating shock wave Mach number about 3.3 in methane-air mixture. The **three-dimensional structure** of the formed detonation wave is obtained.
- The strong influence of the **computational cells size** on the detonation initiation and propagation (detonation cells structure) is revealed. The detonation wave front for **methane-air** stoichiometric mixtures is **highly irregular**. There are two different types of transverse waves: SW & DW.

Numerical Modelling of Dust-Layered Detonation

Motivation 2

WEST PHARMACEUTICAL SERVICES, INC.KINSTON
North Carolina, January 29, 2003

From U.S. Chemical Safety and Hazard Investigation Board (CSB). Investigation report. (6 Killed, 38 Injured)

(6th ISHPMIE, Halifax, 2006)

DUST EXPLOSION HAZARDS!

CSB concludes that accumulated ***polyethylene dust*** above the ceiling tiles fueled the explosion.

Overall dust accumulation ranged from 0.125 to 0.25 inch in depth.

Motivation 2

Numerous theoretical and experimental studies are devoted to the problem of dust-layered detonation (Klemens et al., 1990; Li et al., 1995; Korobeinikov et al., 2002;…)

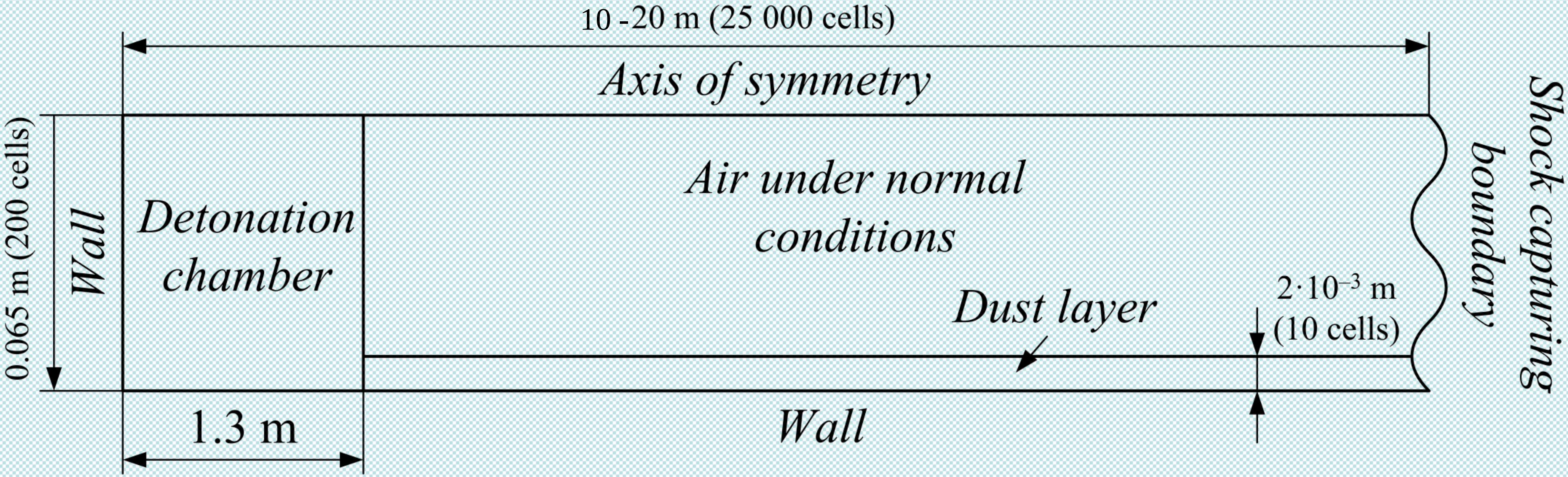
but

- the mechanism of initiation and self-sustained propagation of dust-layered detonation hasn't been studied yet;
- because of a lot of correlated subsequent processes such as dust-air mixture motion, dust lifting behind propagating SW, intensive mixing and heating of dust particles in the ambient air, devolatilization, ignition and combustion of carbon skeleton and volatiles;
- and also computational costs – the problem required large ratio of tube length to the diameter (up to 100),

so

The aim of the current work is the detailed large-scale modelling of layered detonation of coal dust to investigate and explain the mechanism of formation of self-sustained dust-layered detonation.

Problem formulation



- Initial blast wave in detonation chamber – self-similar Taylor solution about Chapman-Jouguet detonation of stoichiometric hydrogen-air mixture
- Coal particles properties
  - "Brown coal" (%wt.) – Methane 54.5, Carbon 39.1, Ash 3.7, Water 2.7
  - d_0 = 60 μm, ρ_{solid} = 1300 kg/m^3, ρ_{load} = 8 kg/m^3

(from Wolinski M., Wolanski P. Shock Wave-Induced Combustion of Dust Layer. Grain Dust Explosion and Control. Final Report. Warsaw, 1993)

Mathematical model (1). System of equations.

The mathematical statement of the problem was based on 2D equations of two-phase, viscous, reactive, compressible flow within a coupled two-velocity and two-temperature formulation (Nigmatulin, 1987):

$$
\begin{cases}
\rho_1 = \sum_{k=1}^{N_1} \rho_{1,k},\ \rho_2 = \sum_{k=1}^{N_2} \rho_{2,k}, \\
\partial_t \rho_{1,k} + \partial_m \rho_{1,k} u_{1,m} = -\partial_m J_{k,m} + \tilde{\omega}_{1,k},\ k = 1,\dots,N_1, \\
\partial_t \rho_{2,k} + \partial_m \rho_{2,k} u_{2,m} = \tilde{\omega}_{2,k},\ k = 1,\dots,N_2, \\
\partial_t n + \partial_m n u_{2,m} = 0, \\
\partial_t \left(\rho_1 \mathbf{u}_1\right) + \partial_m \left(\rho_1 \mathbf{u}_1 u_{1,m}\right) + \nabla p = -\mathbf{F} - \tilde{\omega}_2 \mathbf{u}_2 + \partial_m T_m, \\
\partial_t \left(\rho_2 \mathbf{u}_2\right) + \partial_m \left(\rho_2 \mathbf{u}_2 u_{2,m}\right) = \mathbf{F} + \tilde{\omega}_2 \mathbf{u}, \\
\partial_t E_1 + \partial_m \left(E_1 + p\right) u_{1,m} = -\mathbf{F}\mathbf{u}_2 - Q_T - Q_R - 0.5\tilde{\omega}_2 \mathbf{u}_2^2 - \sum_{l=1}^{N_2} \tilde{\omega}_{2,l} e_{2,l} - \dot{\omega}_{1,1} Q_v - \dot{\omega}_{2,2} Q_s - \partial_m \left(\sum_{k=1}^{N_1} h_{1,k} J_{k,m} + \mathbf{q} - \mathbf{T}\mathbf{u}_1 \right), \\
\partial_t E_2 + \partial_m E_2 u_{2,m} = \mathbf{F}\mathbf{u}_2 + Q_T + Q_R + 0.5\tilde{\omega}_2 \mathbf{u}_2^2 + \sum_{l=1}^{N_2} \tilde{\omega}_{2,l} e_{2,l}, \\
E_1 = 0.5\rho_1 \mathbf{u}_1^2 + \sum_{k=1}^{N_1} \rho_{1,k} e_{1,k},\ E_2 = 0.5\rho_2 \mathbf{u}_2^2 + \sum_{k=1}^{N_2} \rho_{2,k} e_{2,k},\ p = \sum_{k=1}^{N_1} \rho_{1,k} R_{1,k} T_1, \\
e_{2,k} = c_{2,k} T_2,\ k = 1,\dots,N_2,\ e_{1,k} = c_{1,k} T_1,\ k = 1,\dots,N_1,\ h_{1,\mathrm{k}} = e_{1,k} + R_{1,k} T_1,\ k = 1,\dots,N_1
\end{cases}
$$

Mathematical model (2). Kinetic equations.

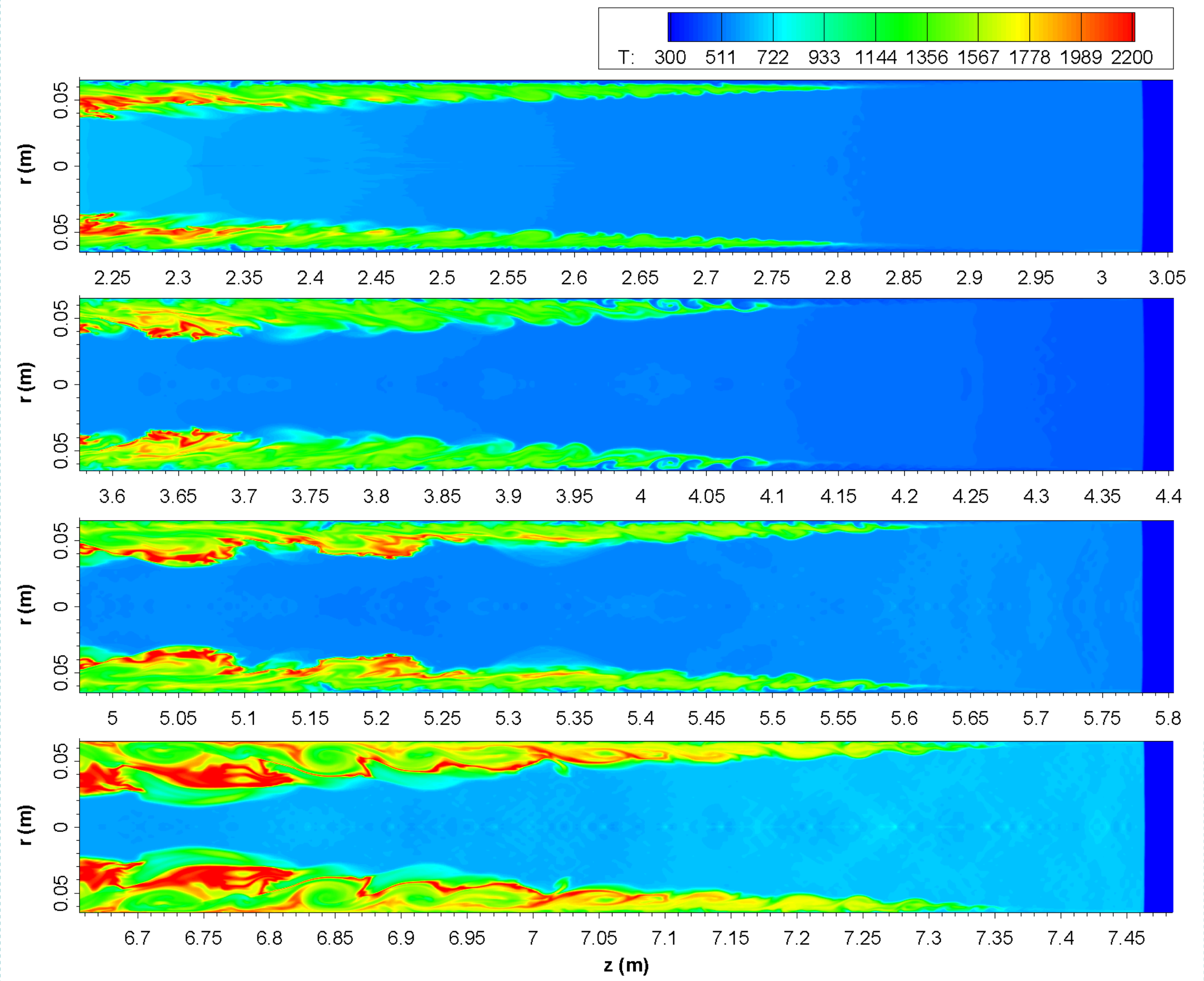
$CH_4 + 2O_2 = CO_2 + 2H_2O + Q_v$ (homogeneous) $Q_v = 47.9$ MJ/kg

$C + O_2 = CO_2 + Q_s$ (heterogeneous) $Q_s = 30$ MJ/kg

(Korobeinikov et al., 2002)

$$
\begin{cases}
\tilde{\omega}_{1,1} = \dot{\omega}_{1,1} - \dot{\omega}_{2,1}, \\
\dot{\omega}_{1,1} = -\rho_{1,2}\rho_{1,1}\sqrt{T_1}B_2 \exp\left(-\dfrac{E_g}{RT_1}\right),\ E_g = 60\ \text{kJ/mol},\ B_2 = 2.5\cdot 10^{10}\ \text{cm}^3\text{g}^{-1}\text{K}^{-1/2}\text{s}^{-1}, \\
\dot{\omega}_{2,1} = -\rho_{2,1}B_1 \exp\left(-\dfrac{E_v}{RT_2}\right),\quad E_v = 44\ \text{kJ/mol},\quad B_1 = 2.5\cdot 10^5\ \text{s}^{-1}, \\
\tilde{\omega}_{1,2} = 4\dot{\omega}_{1,1} + \dfrac{8}{3}\dot{\omega}_{2,2},\ \tilde{\omega}_{1,3} = 0,\ \tilde{\omega}_{1,4} = -\dfrac{11}{4}\dot{\omega}_{1,1} - \dfrac{11}{3}\dot{\omega}_{2,2},\ \tilde{\omega}_{1,5} = -\dfrac{9}{4}\dot{\omega}_{1,1}, \\
\tilde{\omega}_{2,1} = \dot{\omega}_{2,1}, \\
\tilde{\omega}_{2,2} = \dot{\omega}_{2,2} = -A_s F_s T_1 \rho_{1,2}\rho_{2,2} R_{O_2} \exp\left(-\dfrac{E_s}{RT_2}\right),\ R_{O_2} = \dfrac{R}{\mu_{O_2}}, \\
E_s = 144\ \text{kJ/mol},\ A_s = 8.71\cdot 10^3\ \text{cm}^{-2}\text{gs}^{-1}\text{bar}^{-1},\ F_s = 4.26\cdot 10^6\ \text{cm}^2\text{g}^{-1}
\end{cases}
$$

Dust-Layered detonation. Predicted fields of gas temperature (1).



Time

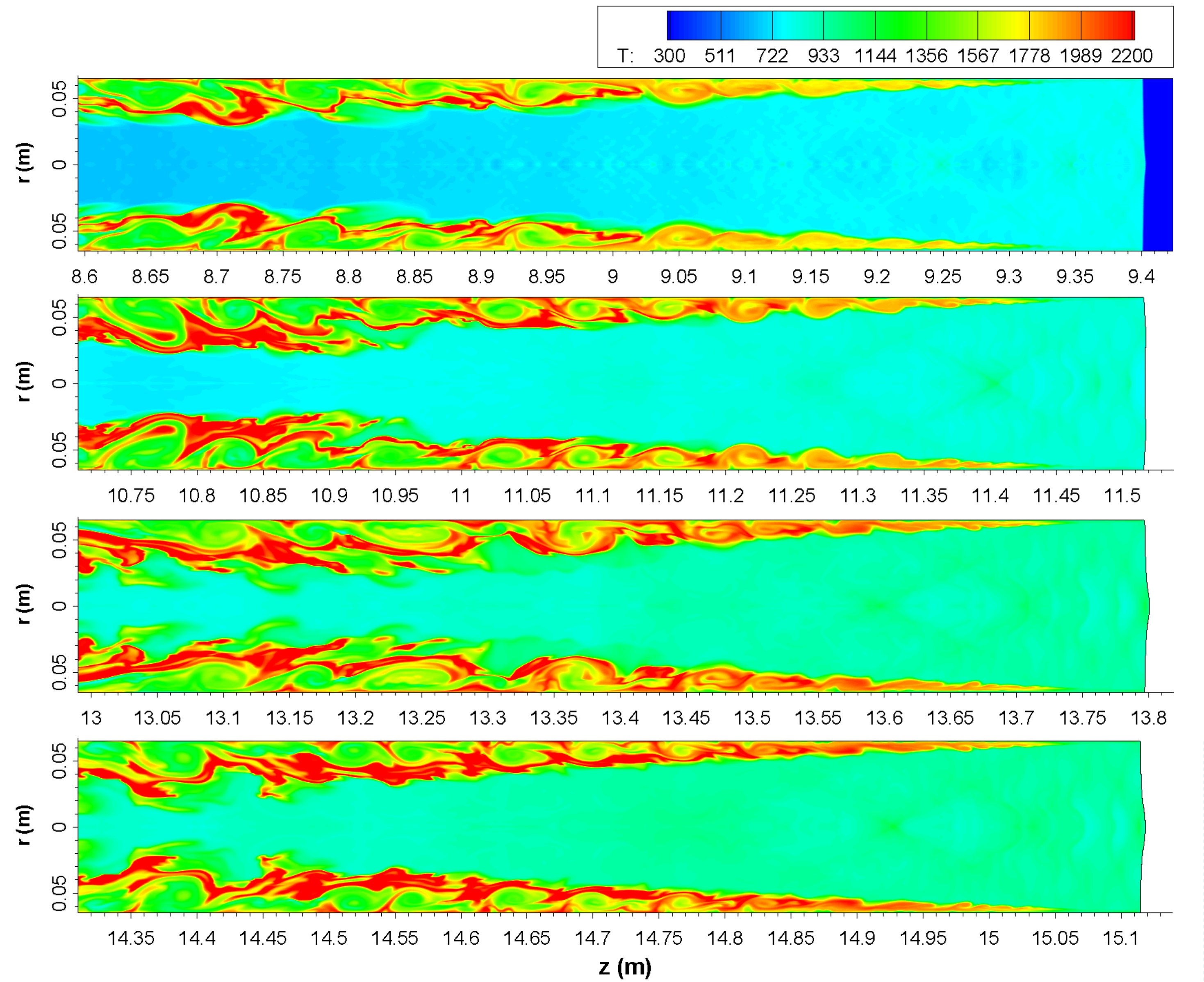
2 ms

4 ms

6 ms

8 ms

Dust-Layered detonation. Predicted fields of gas temperature (2).



Time

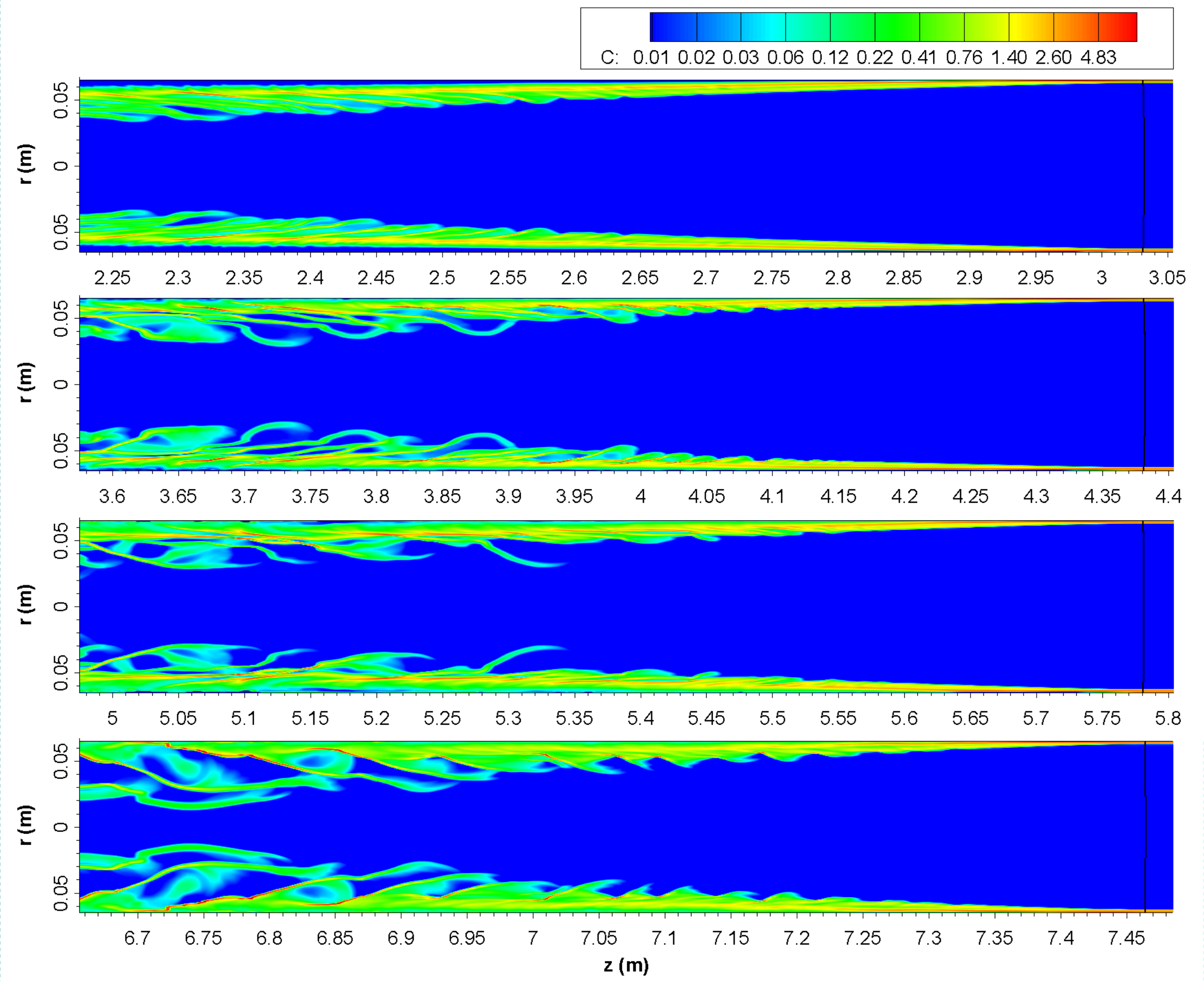
10 ms

12 ms

14 ms

16 ms

Dust-Layered detonation. Predicted fields of carbon density (1).



Time

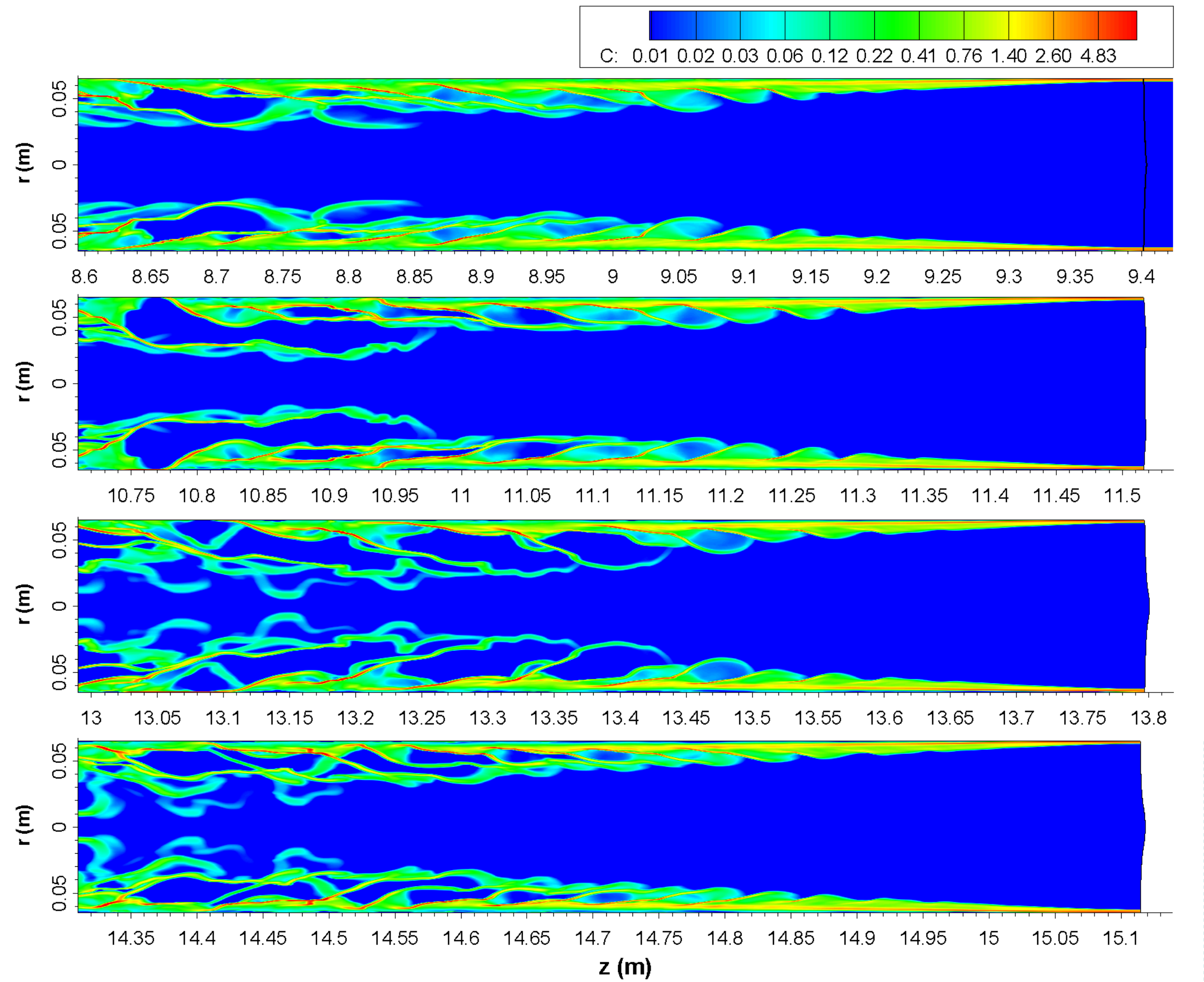
2 ms

4 ms

6 ms

8 ms

Dust-Layered detonation. Predicted fields of carbon density (2).



Time

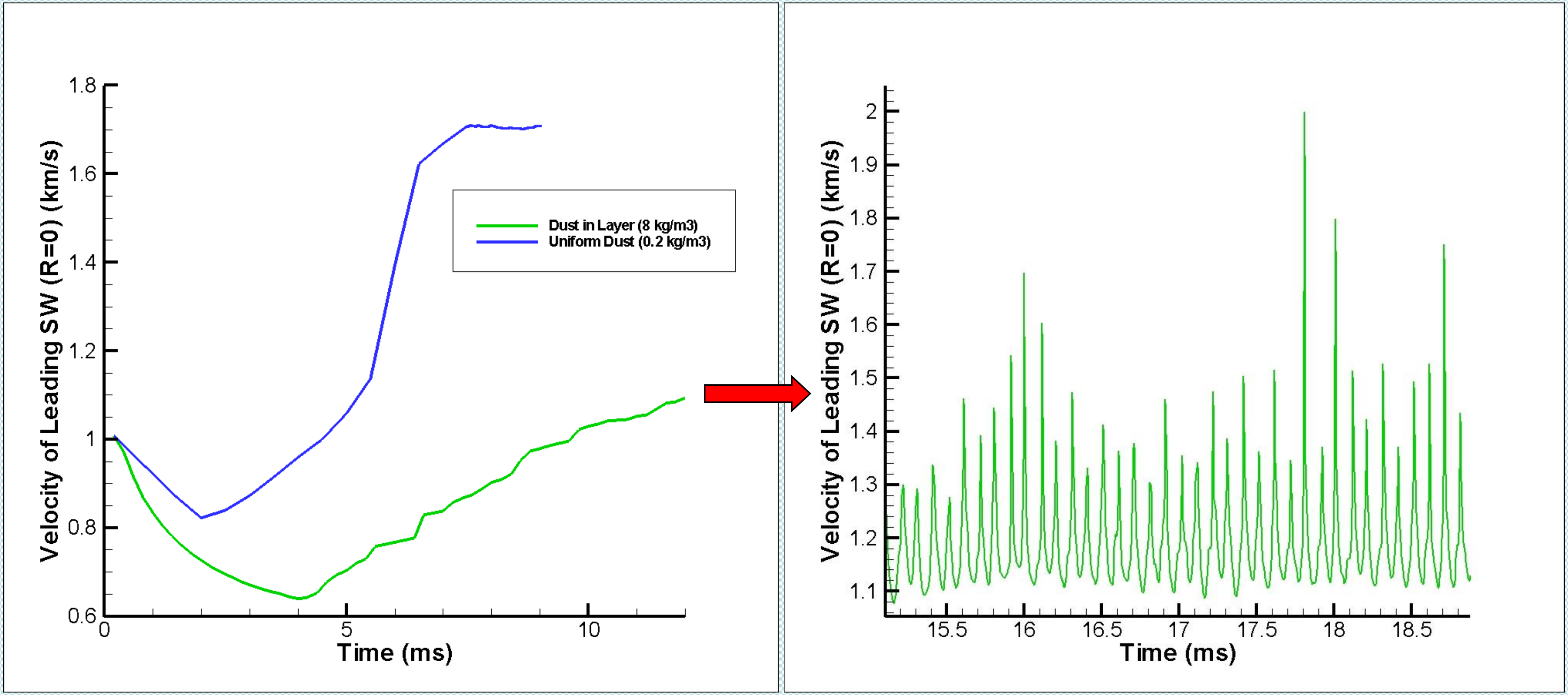
10 ms

12 ms

14 ms

16 ms

Time history of leading SW velocity

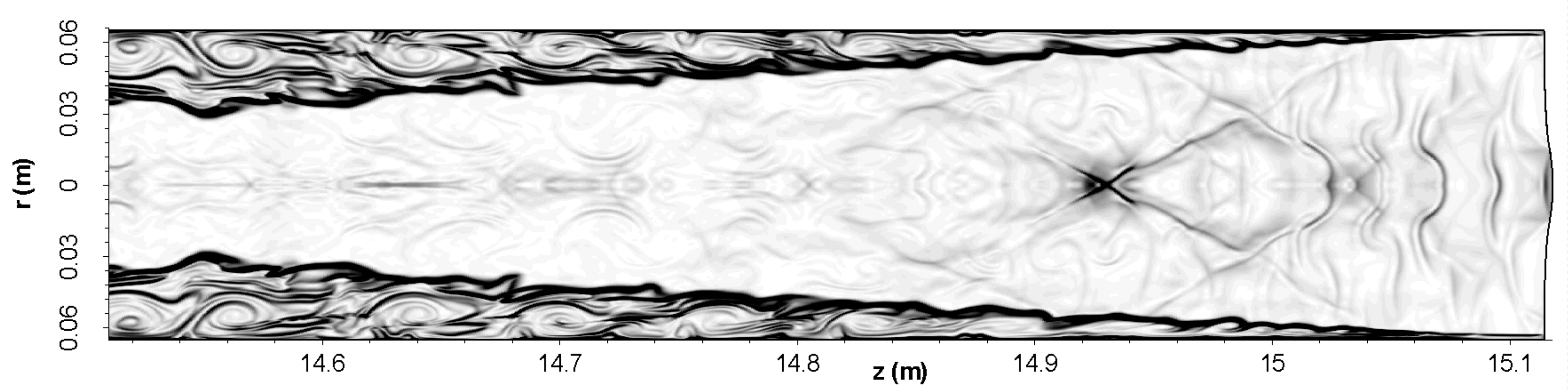


Transition to detonation

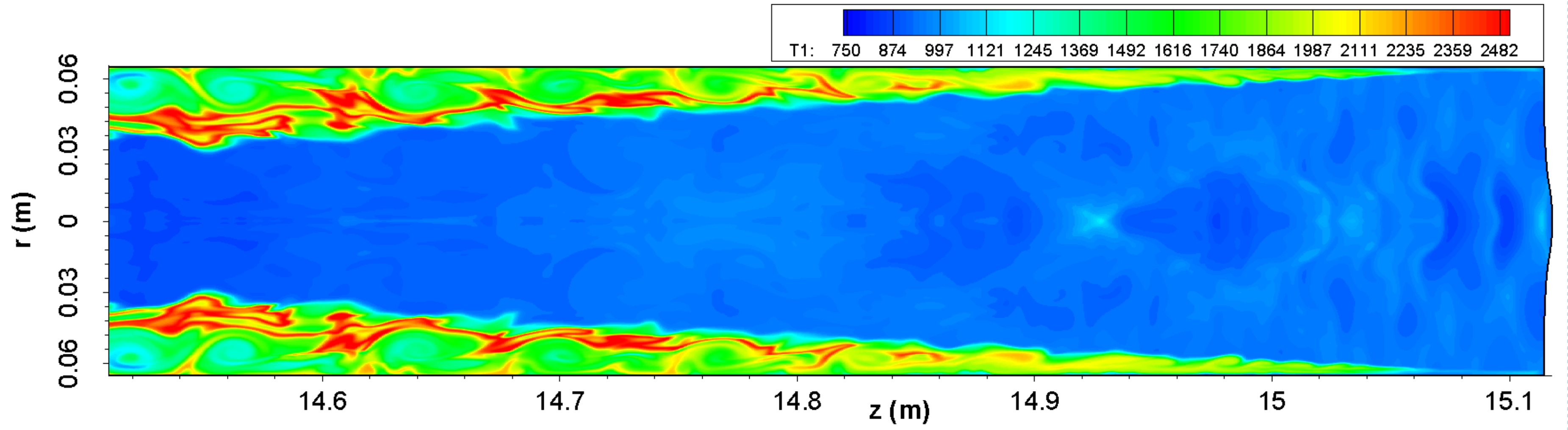
Self-sustained periodical regime

Dust-layered detonation

Self-sustained periodical regime



Normalized module of the density gradient

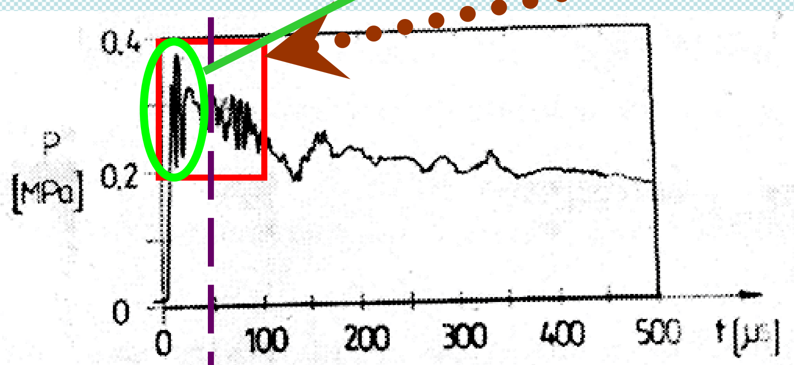


Predicted field of gas temperature

Pressure history

Reaction
zone starts

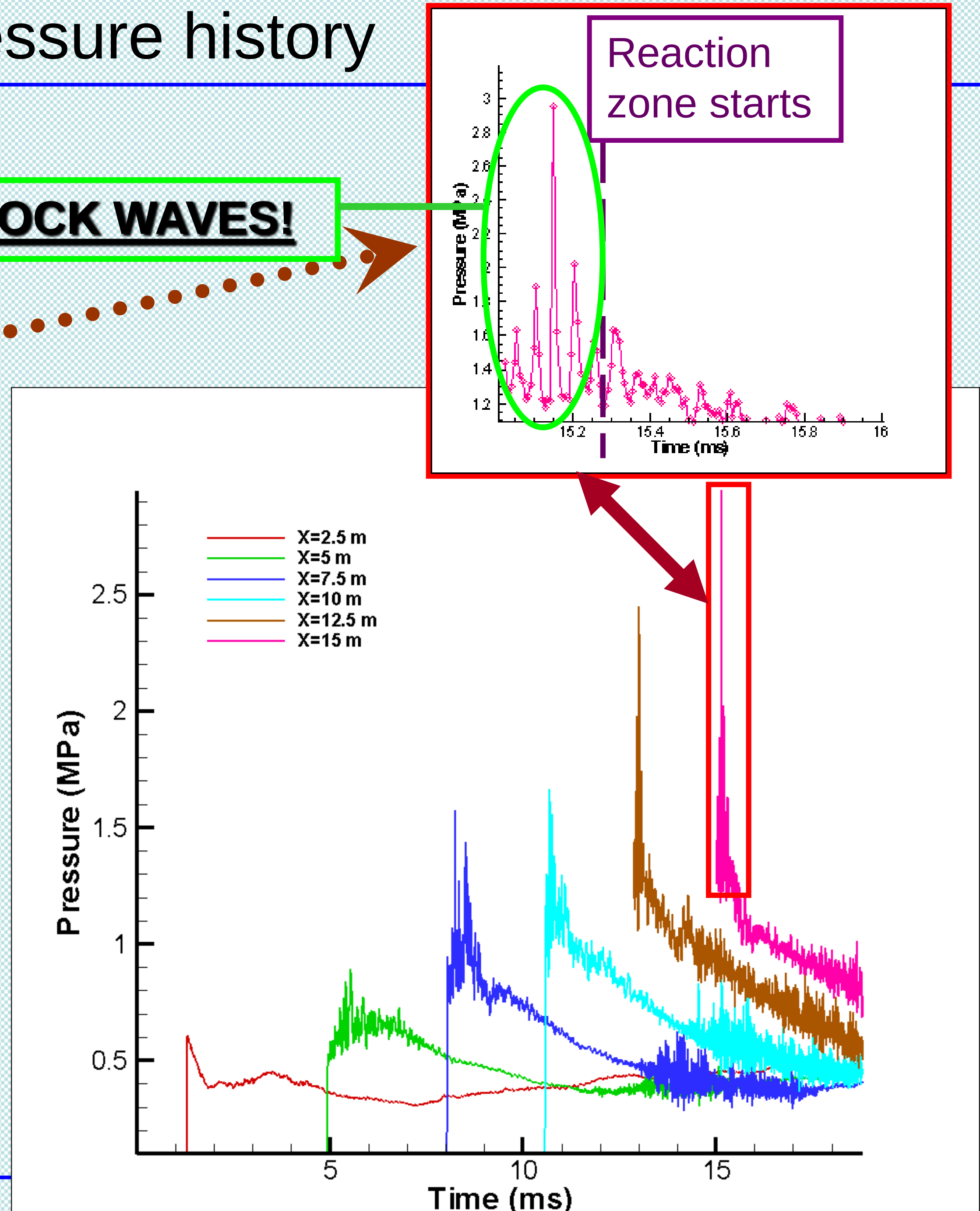
OBLIQUE SHOCK WAVES!



Experiment:

Pressure history for detonation brown coal dust layer with oxygen in square channel (35 mm x 35 mm)

Wolinski M. & Wolanski P., 1993



Conclusions 2

• Dust lifting model based on the Magnus force can provide reliable results at the initial stage of the dust entrainment. But we should take into account **volume fraction** of dust in the dense layer, **interaction between particles** and **turbulent dispersion**.

• It was observed that the period of leading SW's slowdown was followed by the period of leading SW's acceleration and layered DW formation. The layer detonation is formed at large distance from the place of the primary SW initiation (~100 diameters of the tube).

• The strong oblique shock waves caused by combustion zone were discovered.

• **The acceleration of leading SW's and dust layered detonation formation are connected with increasing and intensification of combustion zone, which strongly dependent on arising system of the oblique SWs due to development of the dust layer instabilities and vice versa**.

Thank you for your attention!