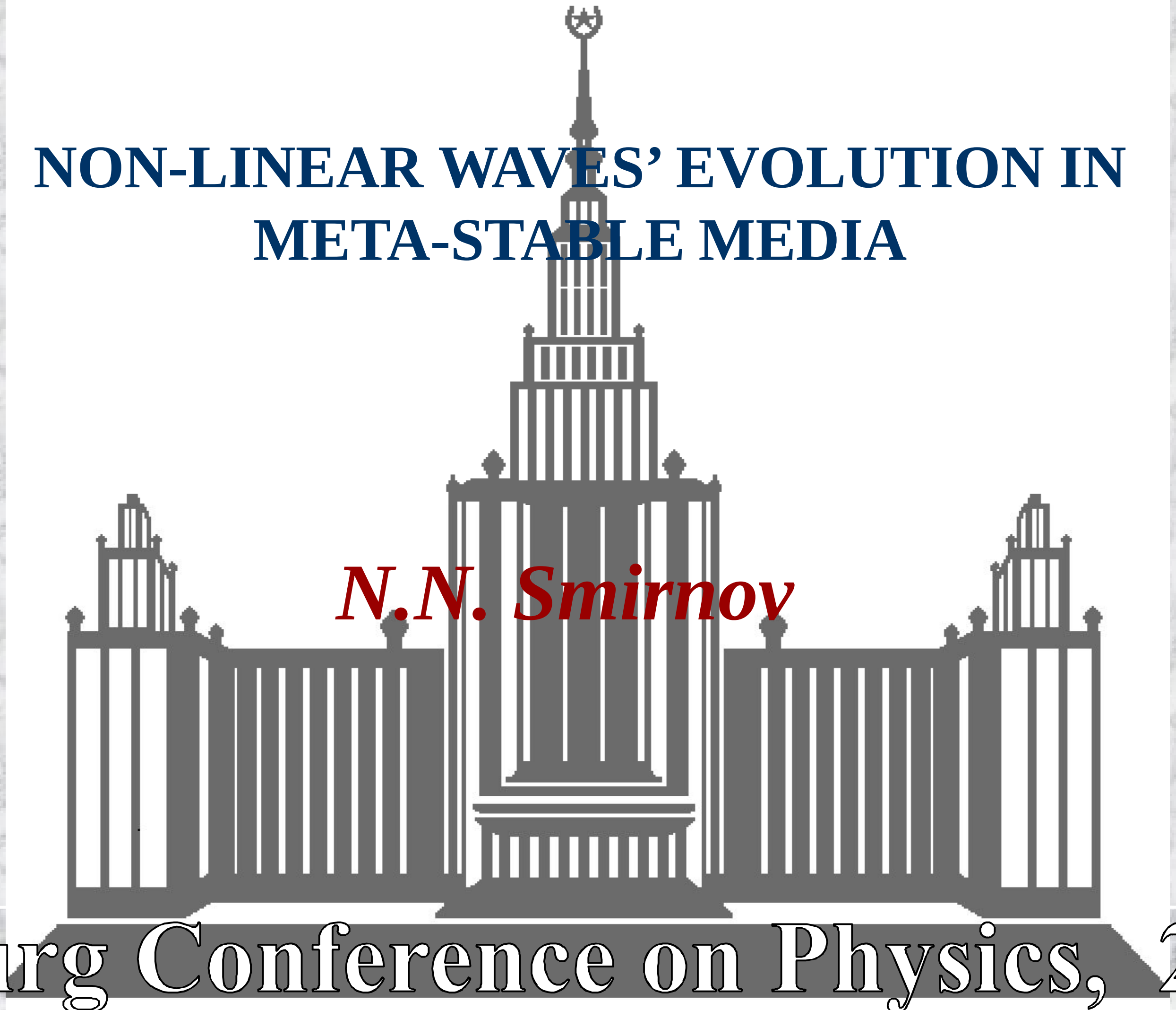
Wave Processes Laboratory
Faculty of Mechanics & Mathematics
Moscow M. V. Lomonosov State University

NON-LINEAR WAVES' EVOLUTION IN META-STABLE MEDIA

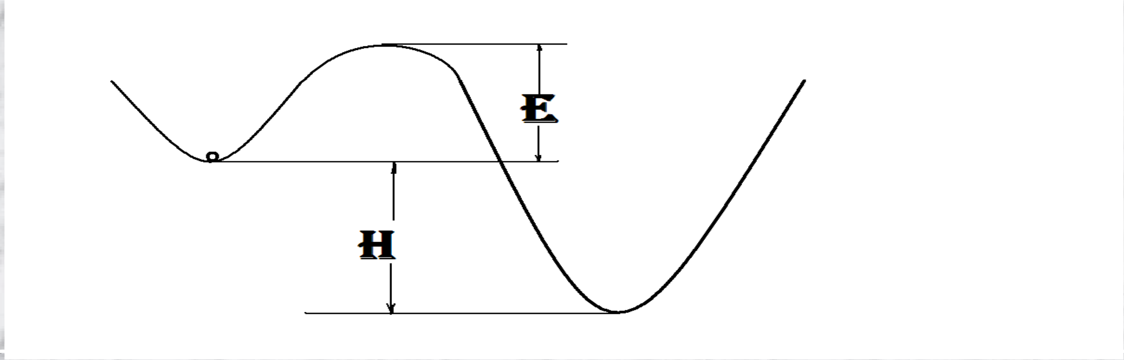


N.N. Smirnov

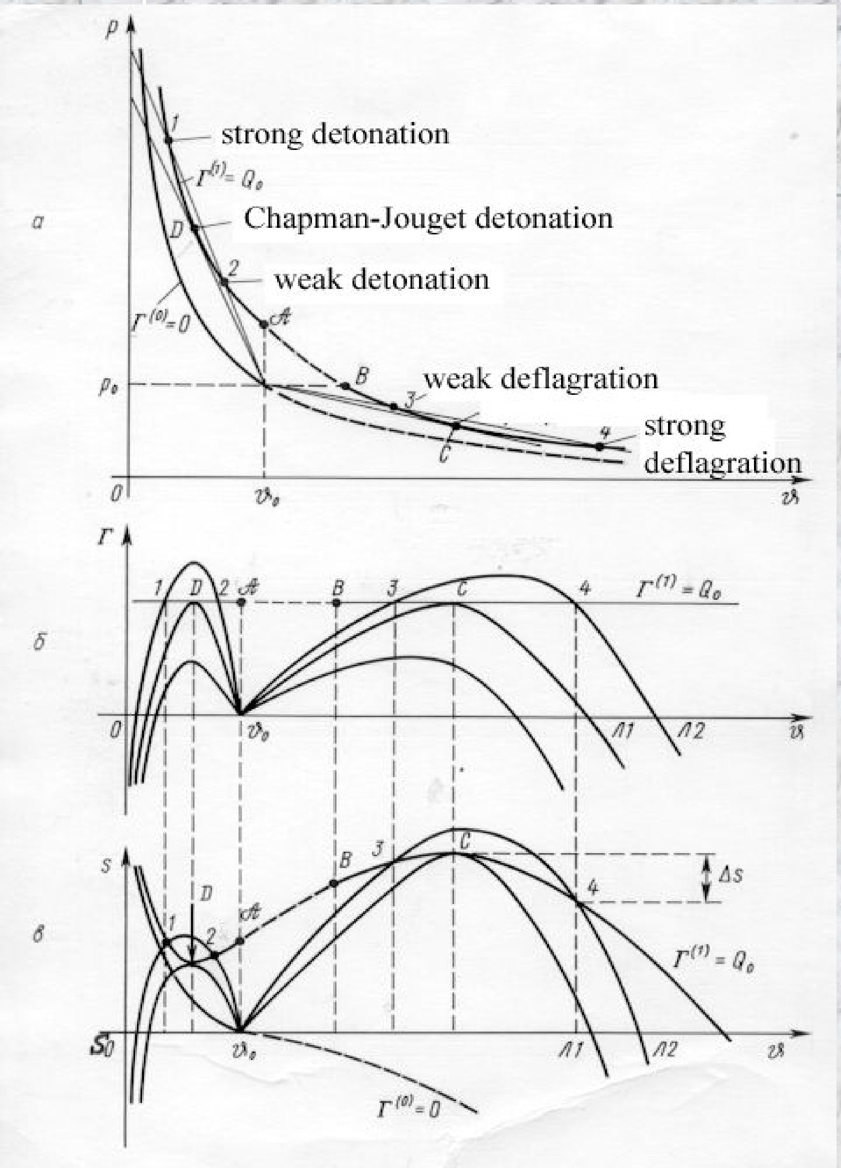
Ginzburg Conference on Physics, 2012

Self-sustaining waves in meta-stable media

- Energy needed to support such waves is released by the wave itself :
- waves of combustion,
- waves of boiling in overheated liquids,
- waves of thermonuclear fusion.



Two modes of combustion



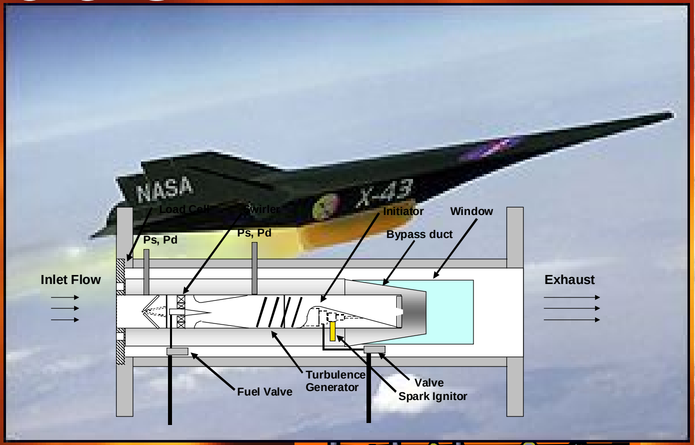
Advantages of detonation mode

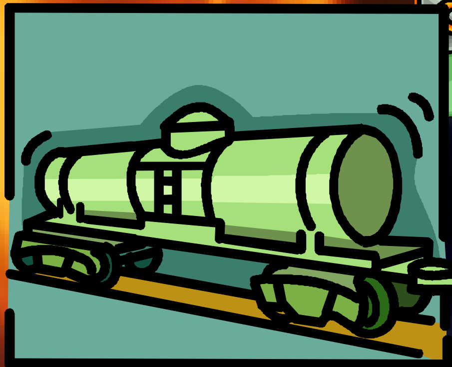
- High thermodynamic efficiency of Chapmen-Jouget detonation as compared to other combustion modes is due to the minimal entropy of the exhaust jet.
- CO emission reduction.
- High rate of energy conversion (10^3 times)
- Specific impulse increase

$$I_{PDE} / I_{RAM} \approx \sqrt{\gamma}$$

Practical importance of controlling detonation initiation

- working out effective preventive measures, such as suppressing deflagration to detonation transition (DDT) in case of combustible mixture ignition,
- the advantages of burning fuel in a detonation regime in comparison with slow burning at constant pressure attract increasing attention to pulse detonation engines.





Outline

- **Deflagration to detonation transition scenarios.**
- **Macro-kinetics mathematical model for DDT.**
- **Several new combustion modes in tubes incorporating cavities.**
- **The effect of volume ratio parameters on combustion modes.**
- **The effect of non-uniformity in cavities size distribution.**

Flame Acceleration Scenarios in Gases.

Macroscopical Kinetics for Modeling of DDT

- **Equations for multicomponent reacting compressible viscous flows.**
- **Three-equation turbulence model.**
- **Reduced chemistry modeling.**
- **Initial and boundary conditions.**
- **Confinement geometry: tubes with wider cavities.**

Governing equations for reacting turbulent flows

$$\partial_t(\rho) + \nabla\cdot(\rho\vec{u}) = 0$$

$$\partial_t(\rho Y_k) + \nabla\cdot(\rho\vec{u}Y_k) = -\nabla\cdot\vec{\mathrm{I}}_{\mathrm{k}} + \dot{\omega}_k$$

$$\partial_t(\rho\vec{u}) + \nabla\cdot(\rho\vec{u}\otimes\vec{u}) = \rho\vec{g} - \nabla p + \nabla\cdot\tau$$

$$\partial_t(\rho E) + \nabla\cdot(\rho\vec{u}E) = \rho\vec{u}\cdot\vec{g} - \nabla\cdot p\vec{u} - \nabla\cdot\vec{I}_q + \nabla\cdot(\tau\cdot\vec{u})$$

$$p = R_g\rho T\sum_k Y_k/W_k \qquad E = \sum_k Y_k(c_{vk}T + h_{0k}) + \frac{\vec{u}^2}{2} + k$$

$$\vec{I}_q = \vec{J}_q + \sum_k (c_{pk}T + h_{0k})\vec{I}_k \qquad \vec{I}_k = -\rho(D + (\nu^t/\sigma_d))\nabla\cdot Y_k \qquad \vec{J}_q = -(\lambda + \sum_k c_{pk}Y_k\rho(\nu^t/\sigma_t))\nabla\cdot T$$

$$\tau = (\mu + \rho\nu^t)(\nabla\vec{u} + \nabla\vec{u}^T - (2/3)(\nabla\cdot\vec{u})U) - (2/3)\rho kU$$

$$\nu^t = C_\mu\, {}^{k^2}\!/_{\varepsilon}.$$

Turbulence model.

$$\partial_t(\rho k)+\nabla\cdot(\rho\vec{u}k)=\nabla\cdot((\mu+\rho(\nu^t/\sigma_k))\nabla k)+\tau^t:\nabla\vec{u}-\rho\varepsilon$$

$$\partial_t(\rho\varepsilon)+\nabla\cdot(\rho\vec{u}\varepsilon)=\nabla\cdot((\mu+\rho(\nu^t/\sigma_\varepsilon))\nabla\varepsilon)+(\varepsilon/k)(C_{1\varepsilon}\tau^t:\nabla\vec{u}-C_{2\varepsilon}\rho\varepsilon)$$

$$\partial_t(\rho\tilde{c}_p\theta)+\nabla\cdot(\rho\vec{u}\tilde{c}_p\theta)=\nabla\cdot((\lambda+\sum_k c_{pk}Y_k\rho(\nu^t/\sigma_k))\nabla\theta)+P_\theta+W_\theta-D_\theta,$$

$$\theta=\overline{T'T'} \qquad T=\overline{T}+T'$$

$$P_\theta=2\rho\sum_k c_{pk}Y_k\left(\nu^t/\sigma_k\right)\left(\nabla T\right)^2 \qquad W_\theta=-\sum_k\overline{\dot{\omega}_k'T'}h_{0k}$$

$$D_\theta=C_g\rho\sum_k c_{pk}Y_k\frac{\varepsilon}{k}\frac{\theta}{\theta_m-\theta}, \quad \tilde{c}_p=\sum_k c_{pk}Y_k$$

Model parameters:

$k,\ \varepsilon,\ \theta$

$$C_\mu=0.09,\quad C_{1\varepsilon}=1.45,\quad C_{2\varepsilon}=1.92, \qquad \theta_m=\overline{T}^2/4. \quad C_g=2.8.$$

$$\sigma_d=1,\quad \sigma_t=0.9,\quad \sigma_k=1,\quad \sigma_\varepsilon=1.3.$$

Chemistry modeling.

$$O_2;\ C_nH_m; CO; CO_2; H_2; H_2O; N_2$$

$$C_nH_m + \left(\frac{n}{2} + \sigma\frac{m}{4}\right)O_2 \rightarrow nCO + \sigma\frac{m}{2}H_2O + (1-\sigma)\frac{m}{2}H_2$$

$$CO + 0.5O_2 \rightarrow CO_2$$

$$CO_2 + M \rightarrow CO + 0.5O_2 + M$$

$$H_2 + 0.5O_2 \rightarrow H_2O$$

$$H_2O + M \rightarrow H_2 + 0.5O_2 + M$$

$$\dot{\omega}_k = \sum_{j=1}^{B} \omega_{kj}$$

$$W_\theta = -T'\sum_{j=1}^{B}\sum_{k=1}^{K} h_k^0 \dot{\omega}_{kj}$$

$$A_j(T) = \begin{cases} K_j \exp\left(-\frac{T_{aj}}{T}\right), & T \geq T_{mj} \\ 0, & T < T_{mj} \end{cases}$$

$$\overline{T'A(T)} = \theta\,\frac{A(\overline{T} + \sqrt{3\theta}) - A(\overline{T} - \sqrt{3\theta})}{2\sqrt{3\theta}}.$$

$$\overline{A(T)} = \frac{1}{6}A(\overline{T} + \sqrt{3\theta}) + \frac{2}{3}A(\overline{T}) + \frac{1}{6}A(\overline{T} - \sqrt{3\theta}).$$

Boundary conditions.

Mean flow parameters

$x = 0,$

$x = x_i,\ r_i \le r \le R_i: \quad u_x = u_r = 0, \frac{\partial T}{\partial x} = 0, \frac{\partial Y_k}{\partial x} = 0$

$x = X,$

$r = R_i,\ x_i \le x \le x_{i+1}$

$r = r_i,\ x_{i-1} \le x \le x_i$

$i = 1, \ldots N-1,: \quad u_x = u_r = 0, \frac{\partial T}{\partial r} = 0, \frac{\partial Y_k}{\partial r} = 0$

$$r = 0, 0 \le x \le X: \quad u_r = 0, \frac{\partial u_x}{\partial r} = 0, \frac{\partial T}{\partial r} = 0, \frac{\partial Y_k}{\partial r} = 0$$

Turbulent parameters $k, \quad \varepsilon, \quad \theta$

$$k = 0, \quad \frac{\partial \varepsilon}{\partial \vec{n}} = 0, \quad \frac{\partial \theta}{\partial \vec{n}} = 0,$$

Lam-Bremhorst damping

$$f_\mu = [1 - \exp(-0.0165 R_y)]^2 \left(1 + \frac{20.5}{R_t}\right),$$

$$C_\mu = C_\mu^0 f_\mu,$$

$$C_{1\varepsilon} = C_{1\varepsilon}^0 f_1,$$

$$C_{2\varepsilon} = C_{2\varepsilon}^0 f_2,$$

$$f_1 = 1 + \left(\frac{0.05}{f_\mu}\right)^3,$$

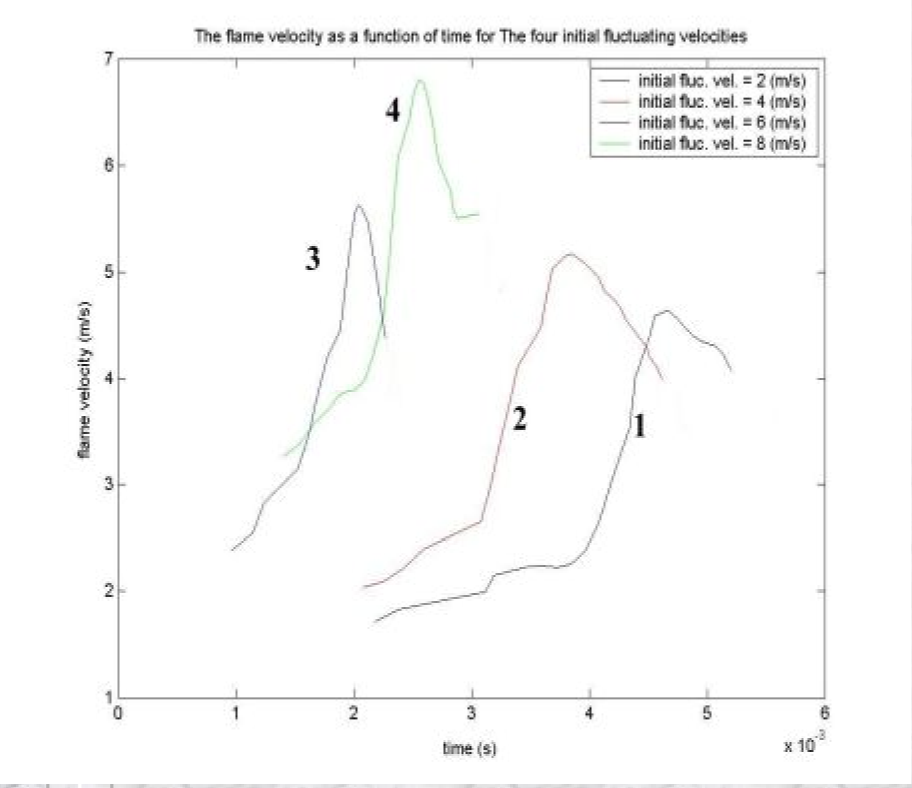
$$R_t = \frac{k^2}{\nu\varepsilon}, \quad R_y = \sqrt{k}\frac{y}{\nu},$$

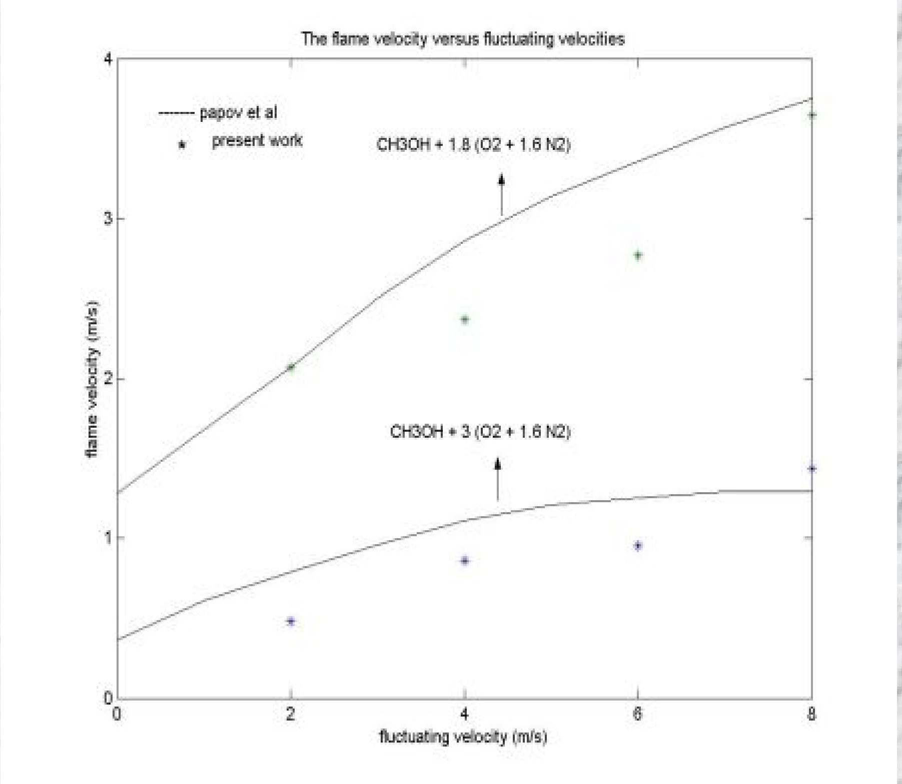
$$f_2 = 1 - \exp(-R_t^2).$$

Turbulent combustion model validation

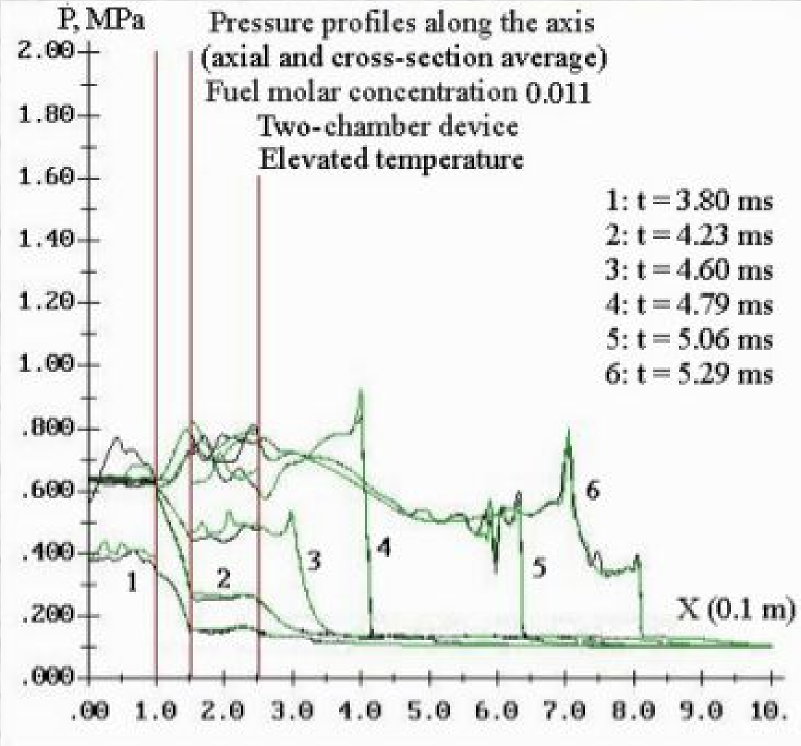
- **A problem was regarded of flame propagation in a tube of constant cross-section filled in with** $CH_3OH + 1.5\alpha(O_2 + 1.6N_2)$
- **The kinetic mechanism was based on the one suggested by Marinov N.M. (1999) and incorporated 129 elementary stages.**
- **Results were compared with experiments by Karpov V.P. et al.(1986)**

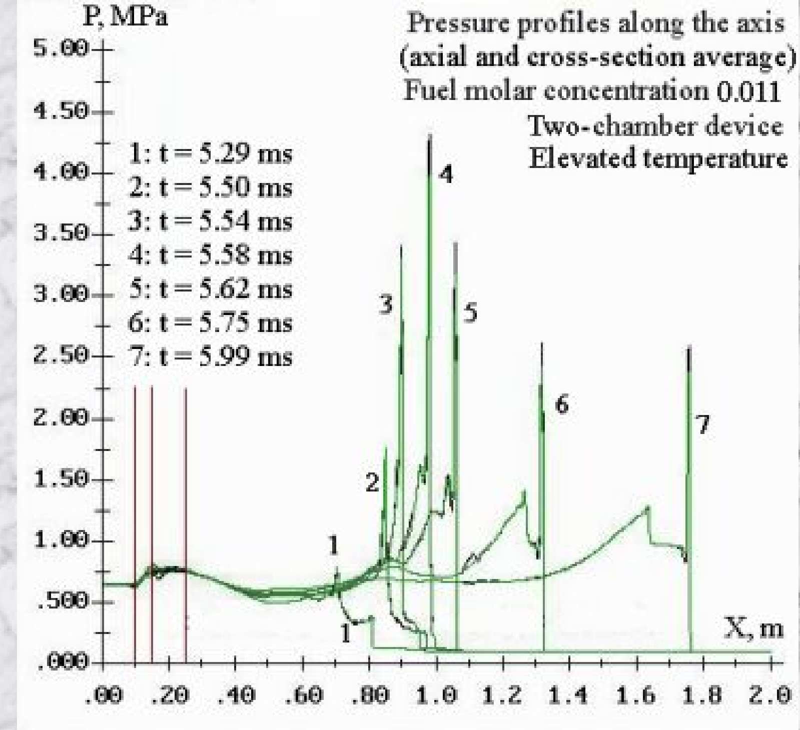
Turbulent combustion model validation II





Pressure profiles along the axis

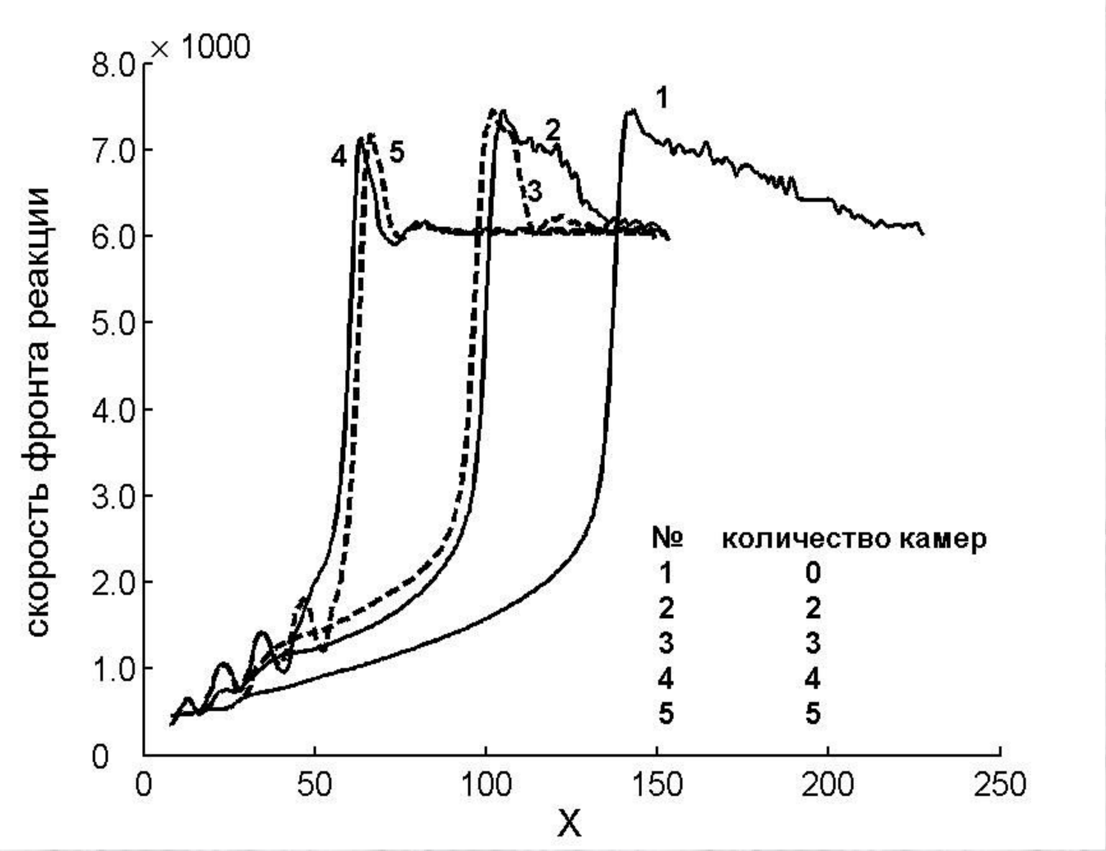




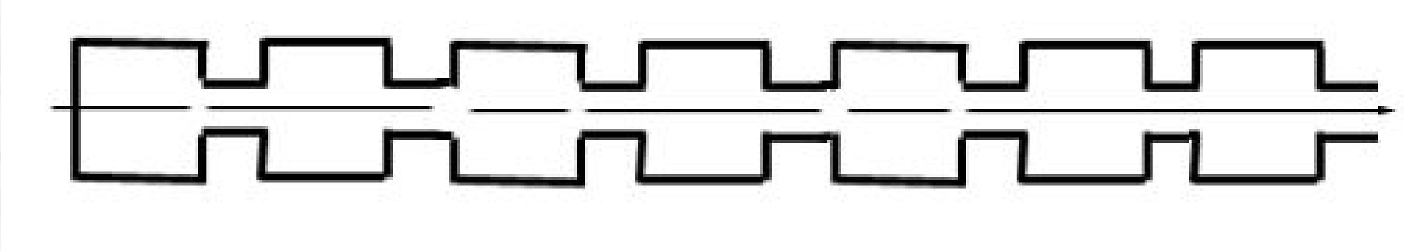
Onset of detonation via an overdriven regime

Deflagration to detonation transition simulation.

Reaction front velocity

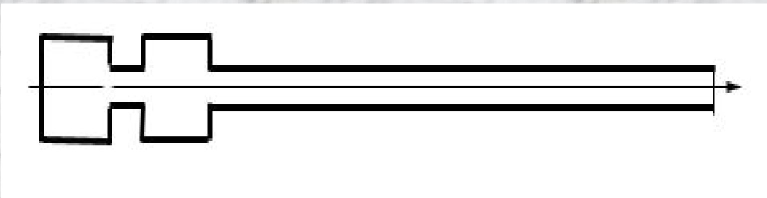


Studying the geometrical effect on the onset of detonation

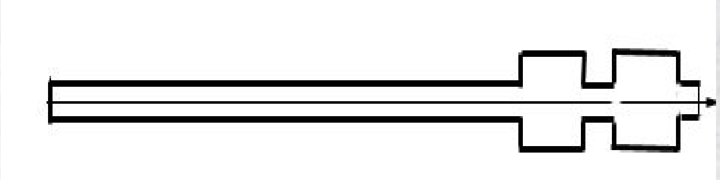


$$\beta_{ER} = \frac{S_{chamb} - S_{tube}}{S_{chamb}} \;\; ; \;\; \alpha_{ER} = \frac{S_{chamb} L_{chamb} + S_{tube} L_{tube}}{S_{chamb}(L_{chamb} + L_{tube})} \; ; \;\; \alpha_{ER} = 1 - \frac{\beta_{ER}}{1 + A}; \;\; A = \frac{L_{chamb}}{L_{tube}}$$

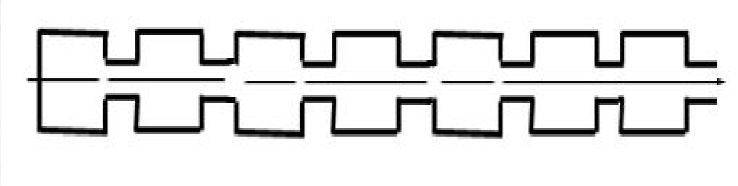
Different geometries



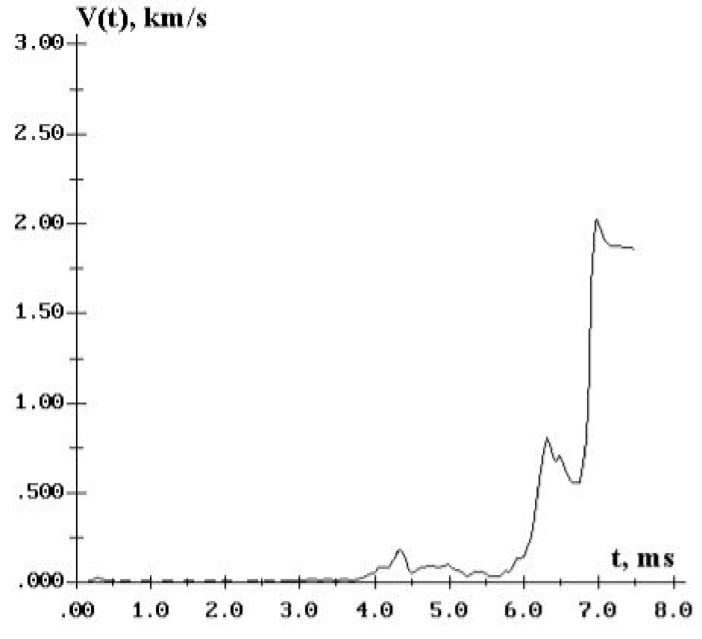
a) two chambers in the ignition section;

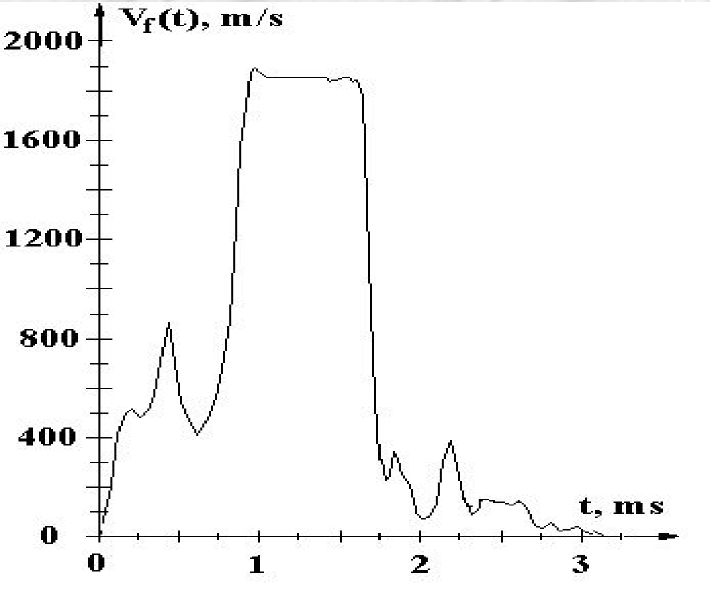


в) two chambers in the far end section of the tube;

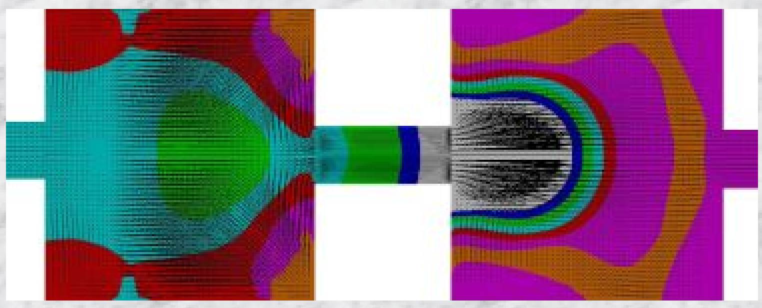


c) chambers incorporated into the tube along the whole length.

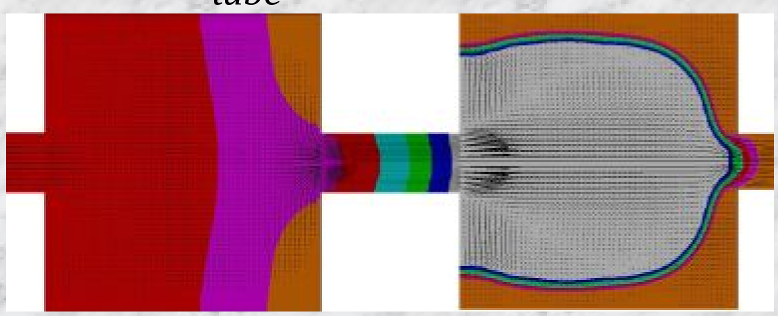


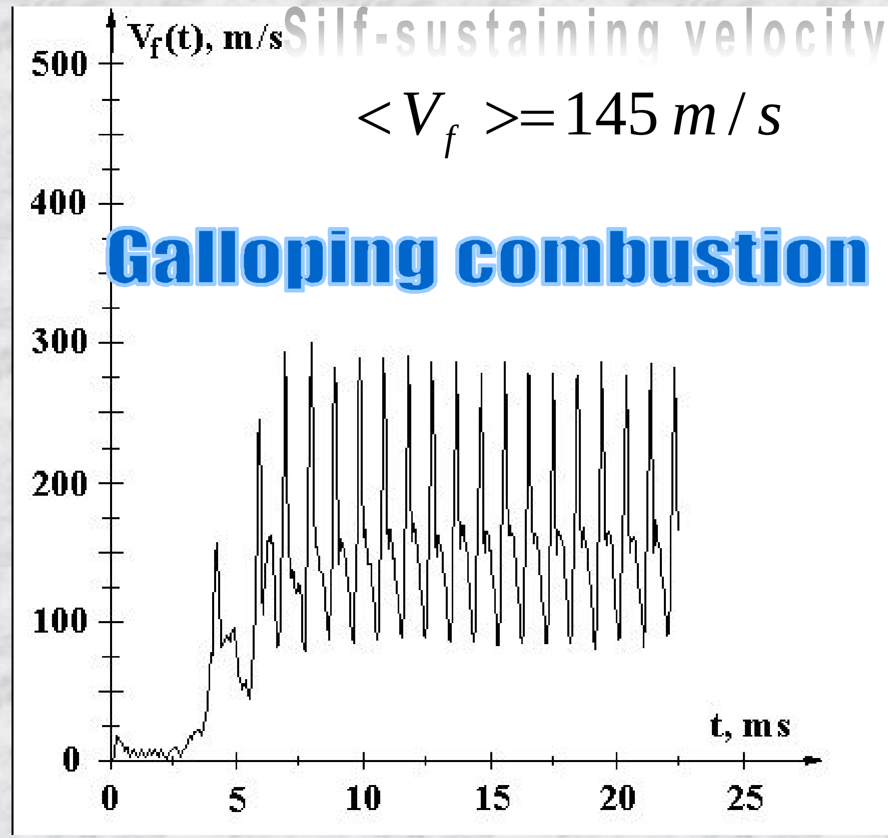


The influence of cavities incorporated into the tube along the whole length



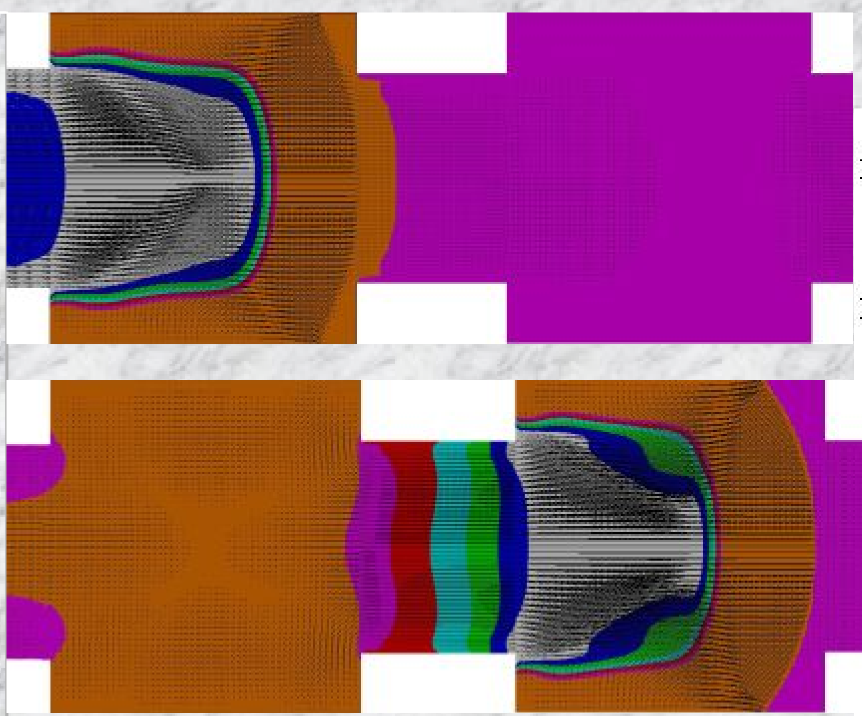
$$A = \frac{L_{chamb}}{L_{tube}}$$

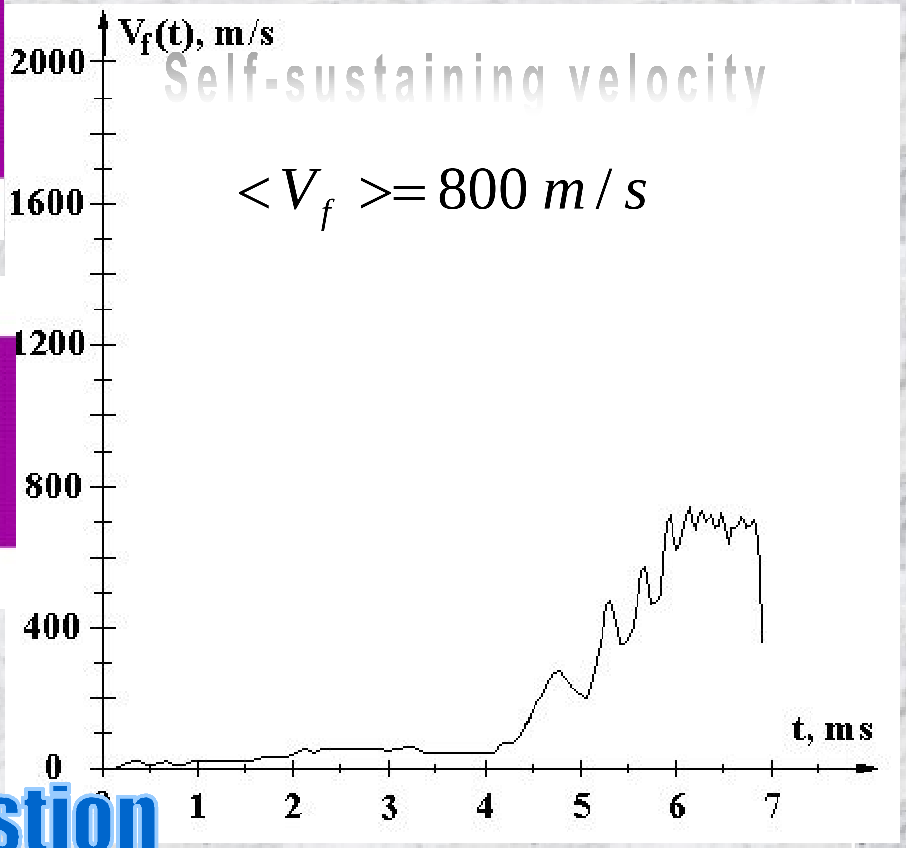




$$\beta_{ER} = \frac{S_{chamb} - S_{tube}}{S_{chamb}} \quad ; \quad \alpha_{ER} = \frac{S_{chamb} L_{chamb} + S_{tube} L_{tube}}{S_{chamb}(L_{chamb} + L_{tube})} \quad \beta_{ER} = 0.96, \ \alpha_{ER} = 1 - \frac{\beta_{ER}}{1 + A}$$

The effect of expansion ratio





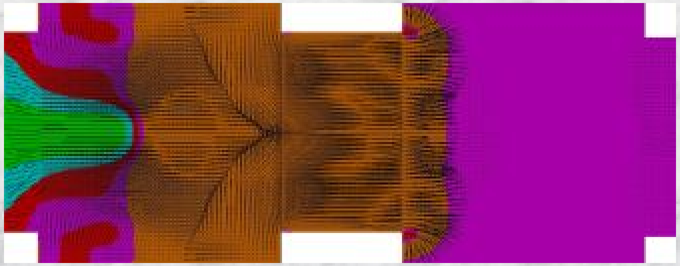
$< V_f >= 800\ m/s$

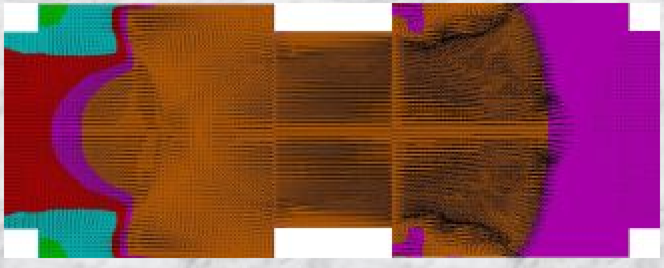
$\beta_{ER} = 0.60$

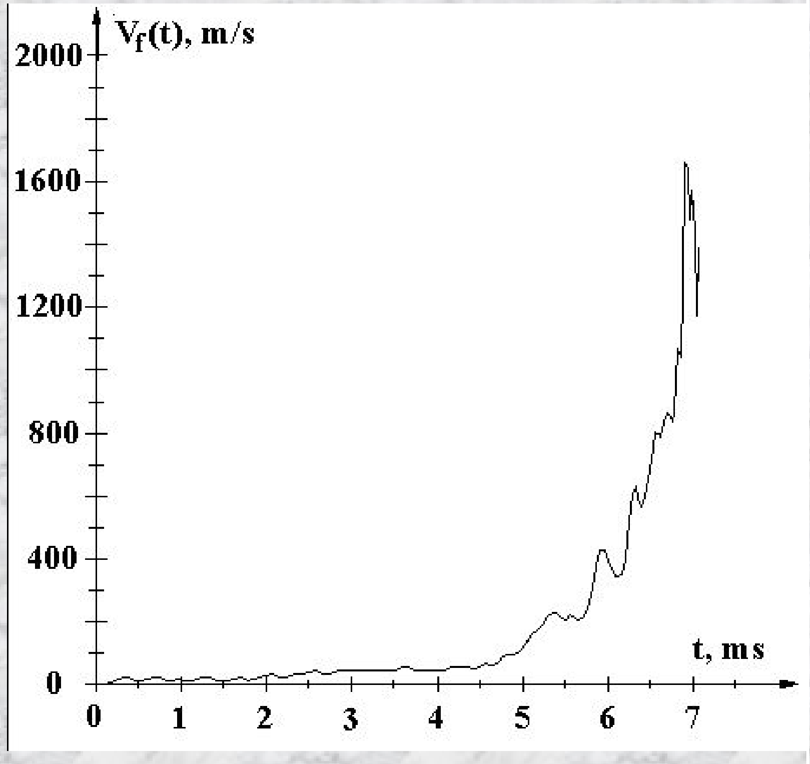
High speed galloping combustion

The effect of expansion ratio

$$\beta_{ER} = 0.40$$





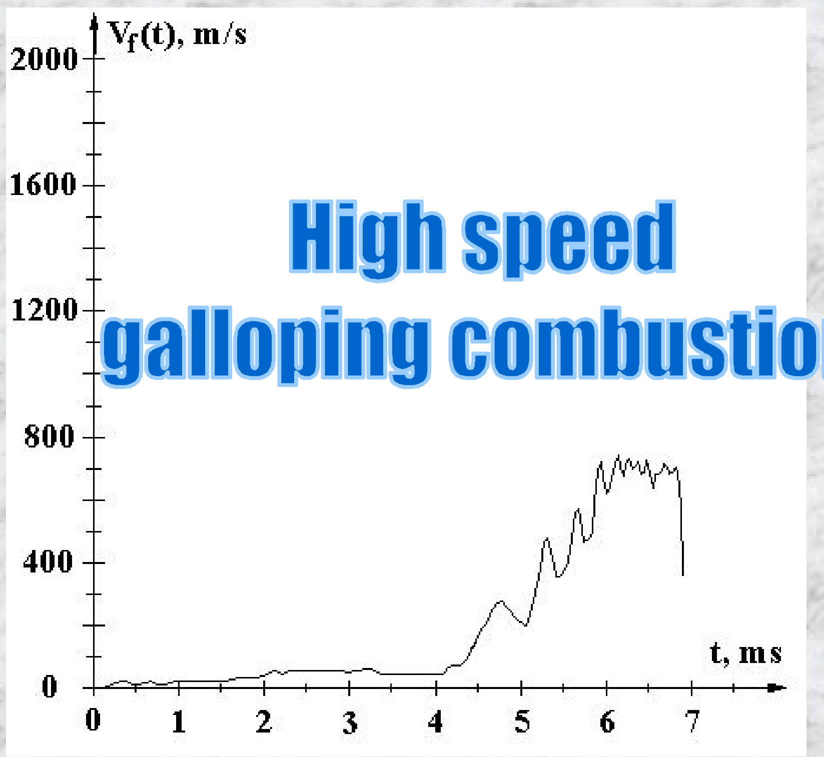


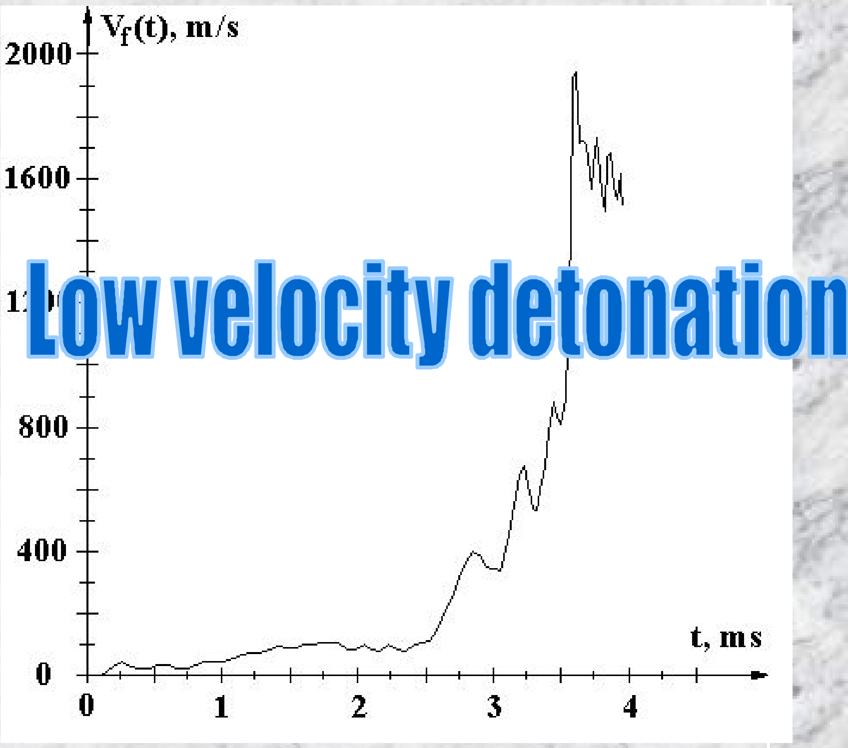
Silf-sustaining velocity

$$< V_f >= 1450\ m/s, \quad V_{\max} = 1700\ m/s$$

Low velocity detonation

The joint effect of expansion ratio and fuel concentration.

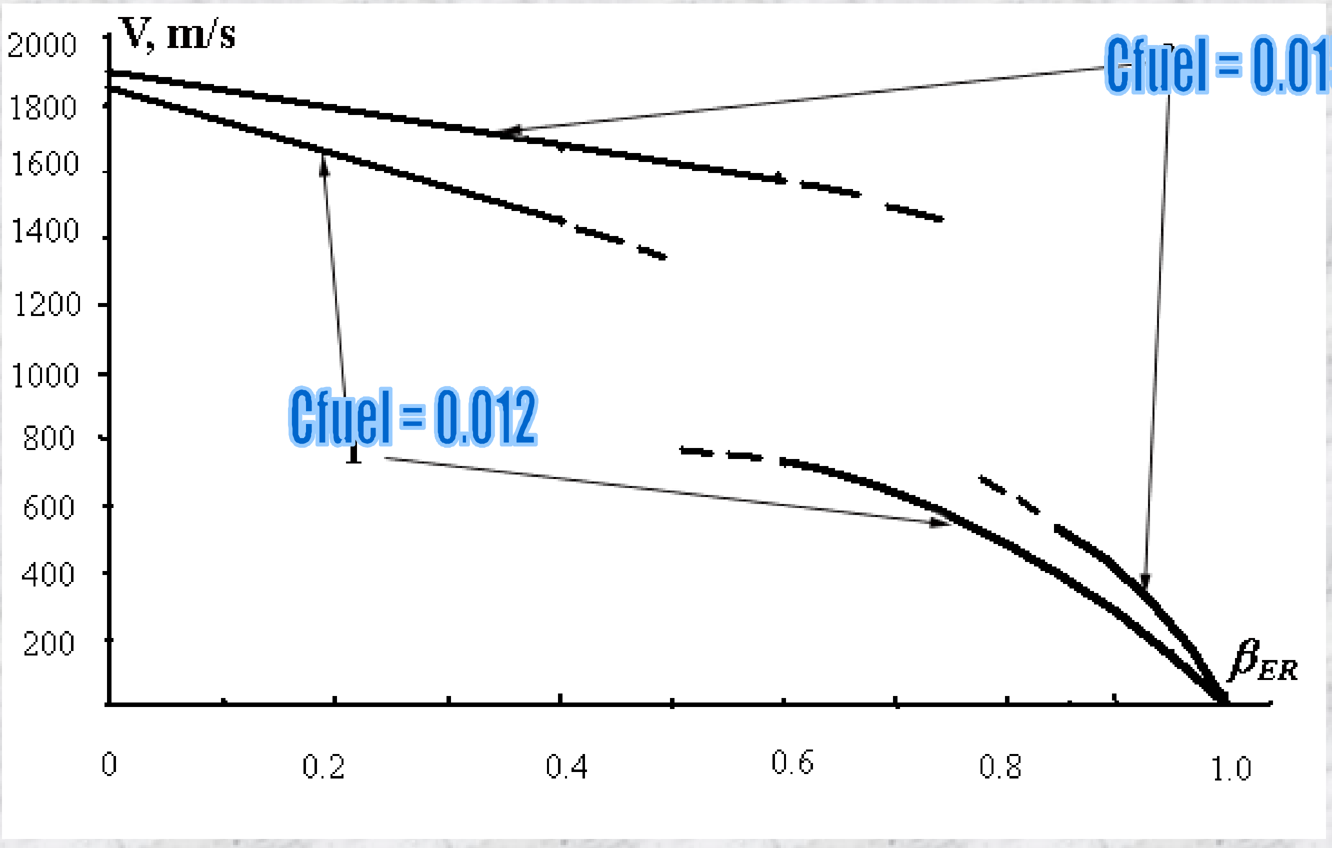




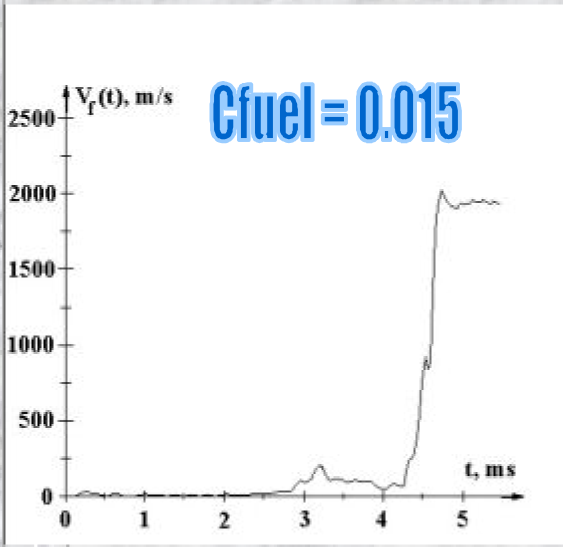
$\beta_{ER} = 0.60, \quad C_{\text{fuel}} = 0.012$

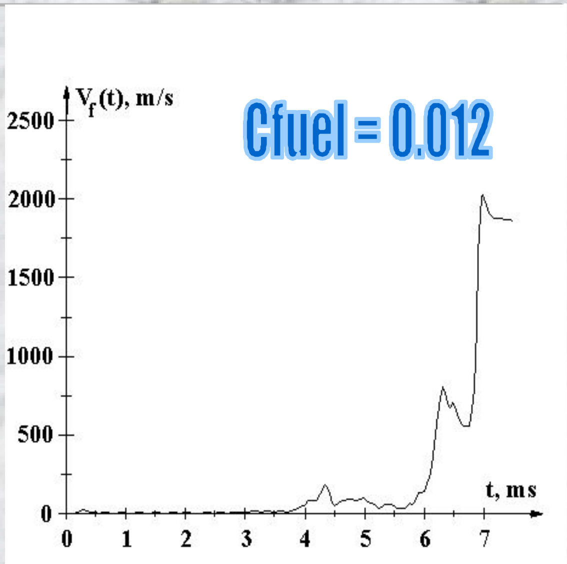
$\beta_{ER} = 0.60, \quad C_{\text{fuel}} = 0.015$

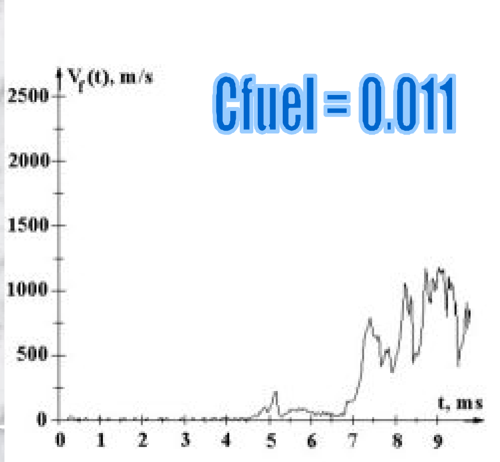
Self-sustaining velocity versus expansion ratio

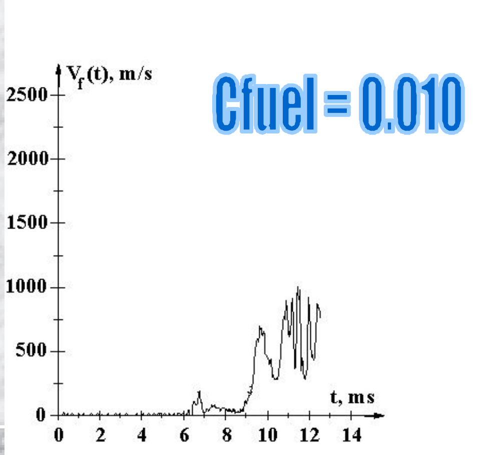


The effect of fuel concentration (two-chambers in ignition section)

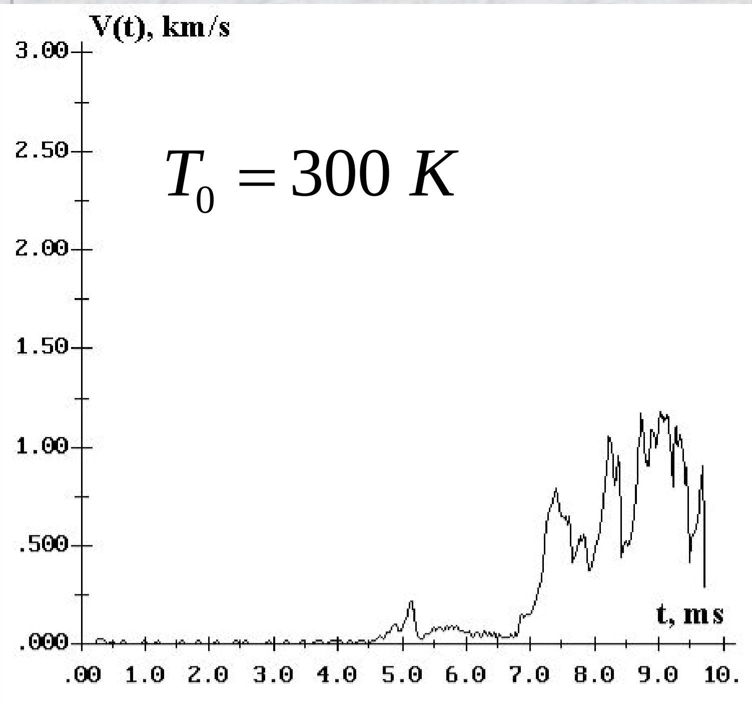




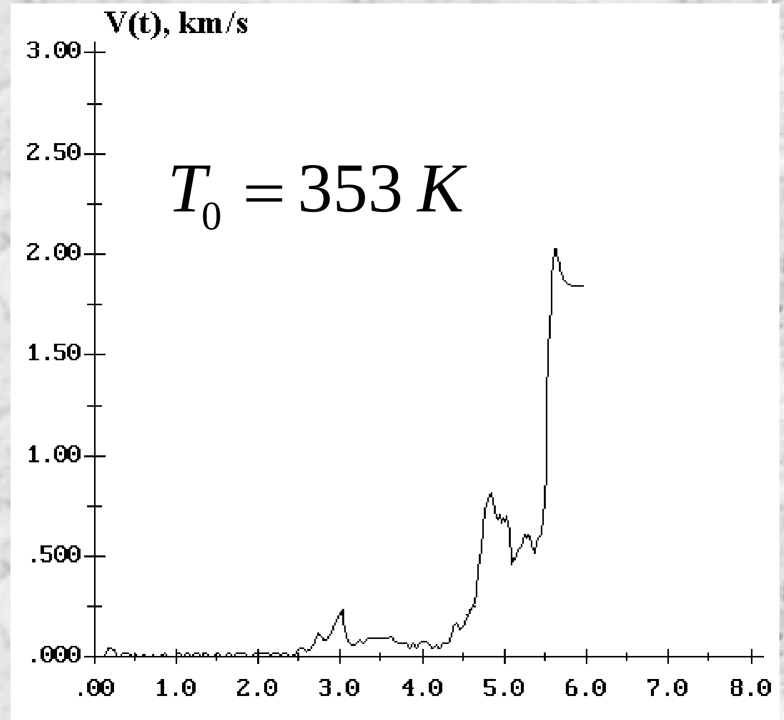




The influence of initial gas temperature on the DDT in tubes with 2 fore-chambers



$T_0 = 300\ K$



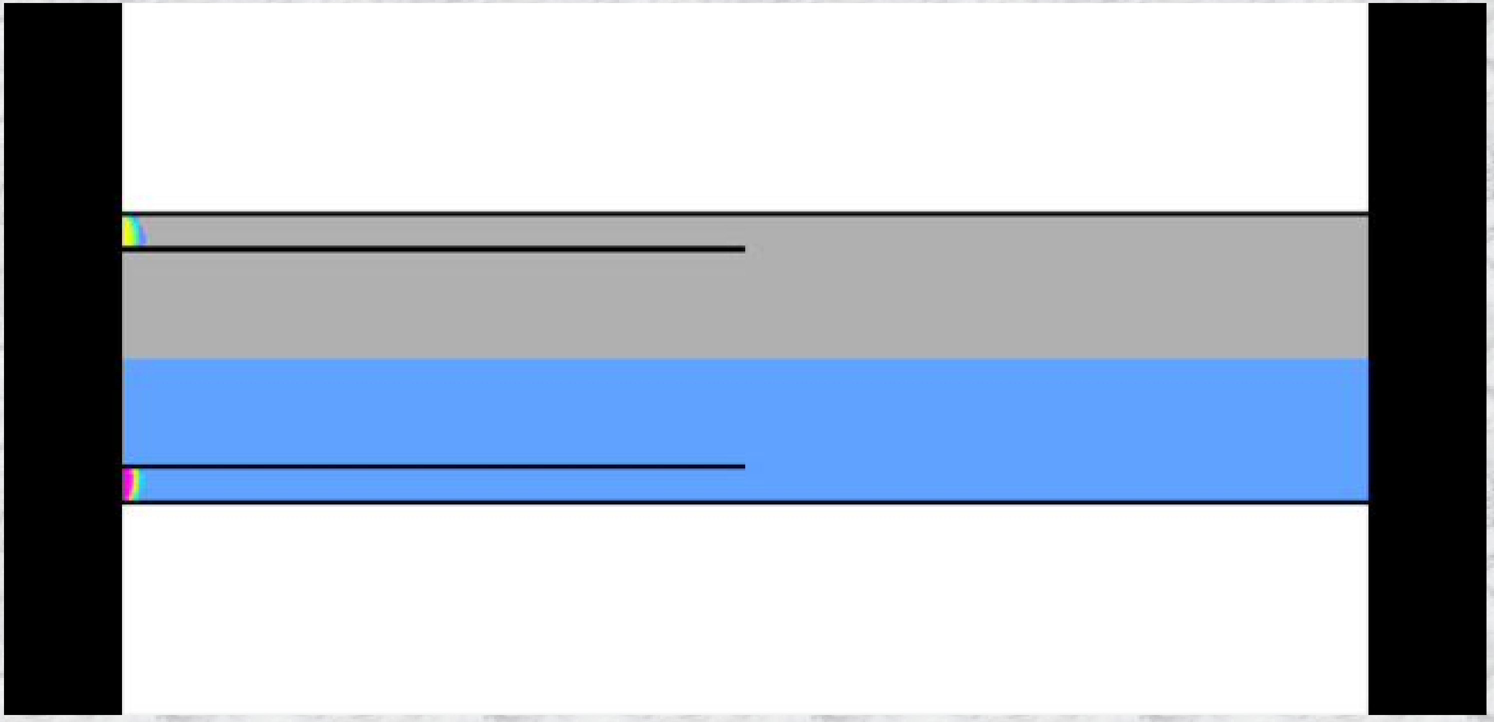
$T_0 = 353\ K$

Galloping combustion

Detonation onset

$$C_{fuel} = 0.011; \quad \beta_{ER} = 0.96$$

Combustion in detonation engine



Detonation wave transmission from thin gap into a cylinder. Upper part – pressure maps, lower part – temperature maps

Conclusions

- **Transition processes between two modes of self-sustainig waves propagation in meta-stable media are essentially controlled by:**
- **geometry of the channel,**
- **fuel concentration,**
- **mixture temperature.**