

**Распространение фронта  
пламени в канале с учетом  
обрыва реакционных цепей  
на стенке**

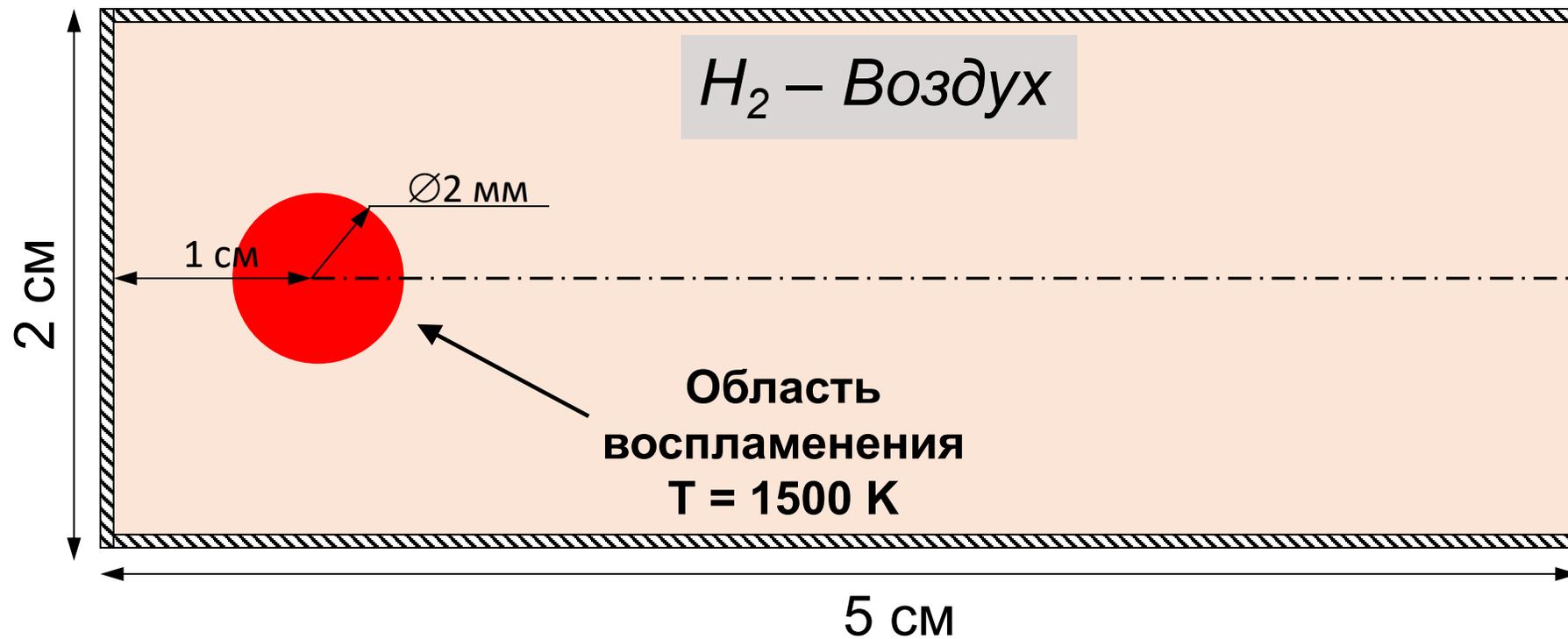
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Научный руководитель: н.с. Михальченко Е. В., доц. Никитин В.Ф.

# Постановка задачи

$$T_0 = 300K$$

$$H_2 : O_2 : N_2 = 1,19 : 1 : 3,7$$



# Математическая модель

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho v_i Y_k)}{\partial x_i} = \frac{\partial(\rho Y_k V_{k,i})}{\partial x_i} + \rho \dot{\omega}_k \quad H = \frac{|v|^2}{2} + \frac{\tilde{p}}{\rho} \quad \vec{\omega} = \frac{1}{2} \text{rot } \vec{v}$$

$$\frac{\partial v}{\partial t} - v \times \omega + \nabla H - \tilde{p} \nabla \left( \frac{1}{\rho} \right) = \frac{1}{\rho} \nabla \cdot \sigma$$

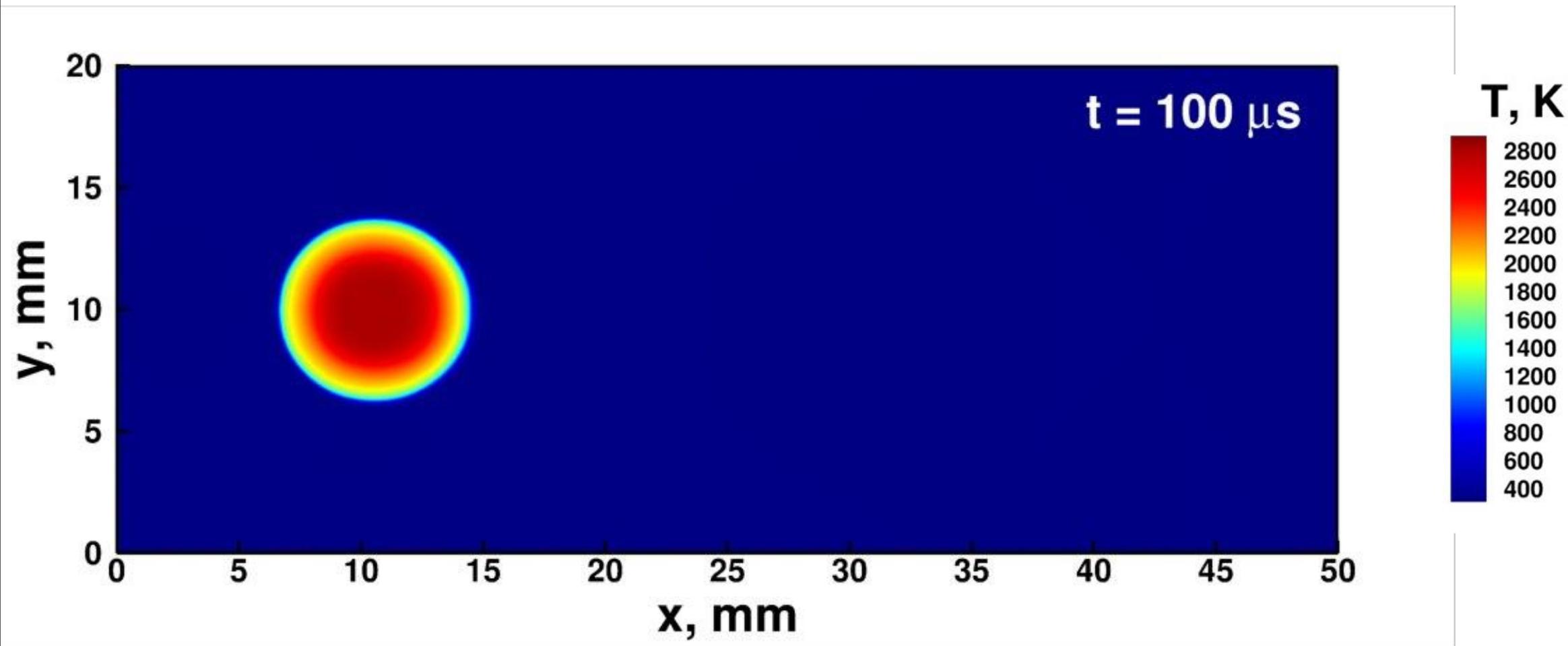
$$\frac{\partial \rho h_s}{\partial t} + \frac{\partial \rho v_i h_s}{\partial x_i} = \frac{\partial \bar{p}}{\partial t} - \sum_{k=1}^{N_c} \dot{\omega}_k h_{f,k}^0 - \frac{\partial}{\partial x_i} \left( \rho \sum_{k=1}^{N_c} h_{s,k} Y_k V_{k,i} \right) - \left( \kappa(T) \frac{\partial T}{\partial x_i} \right) + \sigma_{ij} \cdot \frac{\partial v_i}{\partial x_j}$$

$$\bar{p} = \rho R T \sum_{k=1}^{N_c} \frac{Y_k}{M_k} \quad dh_s = c_p(Y_k, T) dT \quad \sigma_{ij} = \mu(T) \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right)$$

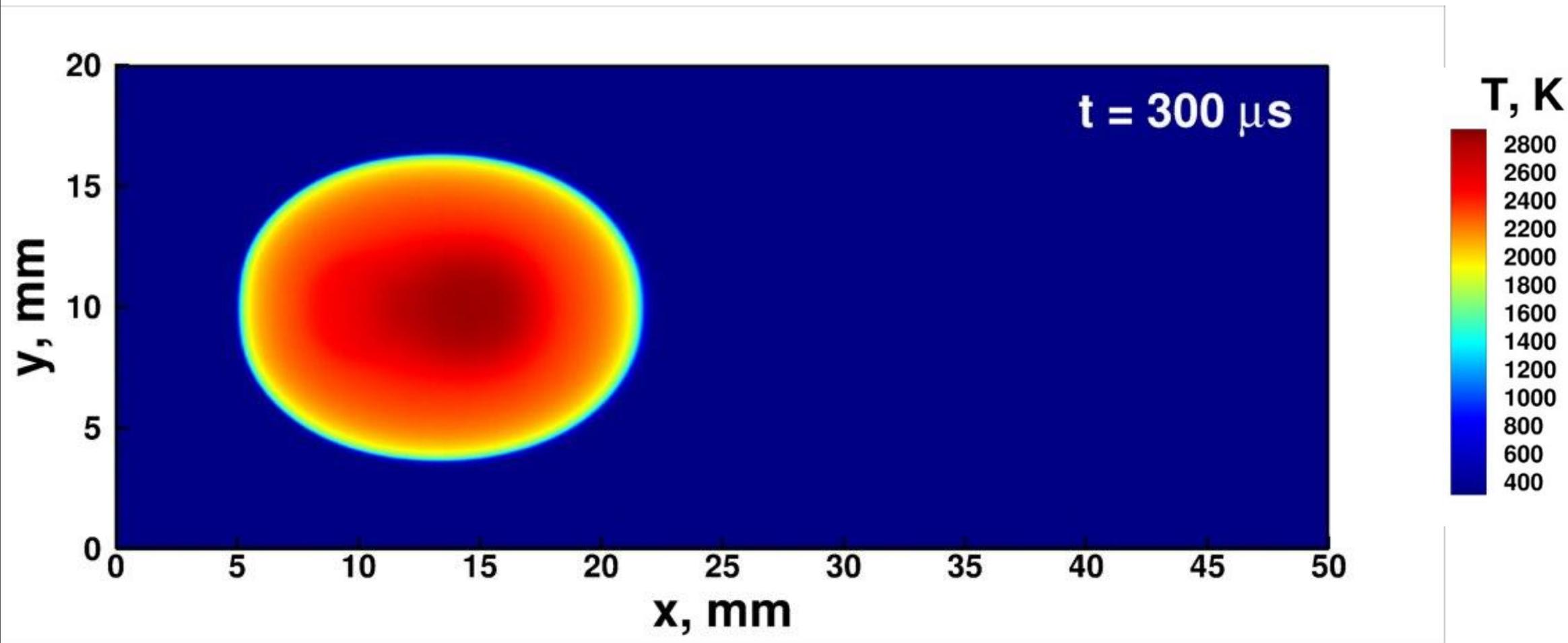
# Кинетический механизм (Alan Kéromnès)

#	Reaction	A	n	E <sub>A</sub>
1	H + O <sub>2</sub> = O + OH	1.040E+14	0.00	1.529E+04
2	O + H <sub>2</sub> = H + OH	5.080E+04	2.67	6.292E+03
3	OH + H <sub>2</sub> = H + H <sub>2</sub> O	4.380E+13	0.00	6.990E+03
4	O + H <sub>2</sub> O = OH + OH	2.970E+06	2.02	1.340E+04
5	H <sub>2</sub> + M = H + H + M	4.577E+19	-1.40	1.044E+05
	$\epsilon_{H_2} = 2.5, \epsilon_{H_2O} = 12, \epsilon_{CO} = 1.9, \epsilon_{CO_2} = 3.8, \epsilon_{He} = 0.83$			
6	O + O + M = O <sub>2</sub> + M	6.165E+15	-0.50	0.00
	$\epsilon_{H_2} = 2.5, \epsilon_{H_2O} = 12, \epsilon_{CO} = 1.9, \epsilon_{CO_2} = 3.8, \epsilon_{Ar} = 0.83, \epsilon_{He} = 0.83$			
7	O + H + M = OH + M	4.714E+18	-1.00	0.00
	$\epsilon_{H_2} = 2.5, \epsilon_{H_2O} = 12, \epsilon_{CO} = 1.5, \epsilon_{CO_2} = 2.0, \epsilon_{Ar} = 0.75, \epsilon_{He} = 0.75$			
8	H + OH + M = H <sub>2</sub> O + M	3.500E+22	-2.00	0.00
	$\epsilon_{H_2} = 0.73, \epsilon_{H_2O} = 3.65, \epsilon_{Ar} = 0.38, \epsilon_{He} = 0.38, \epsilon_{CO} = 1.9, \epsilon_{CO_2} = 3.8$			
9	H + O <sub>2</sub> (+M) = HO <sub>2</sub> (+M) <sup>a</sup>	4.65E+12	0.44	0.00
	Low-pressure limit	1.737E+19	-1.23	0.00
	$\epsilon_{H_2} = 1.3, \epsilon_{H_2O} = 10, \epsilon_{CO} = 1.9, \epsilon_{CO_2} = 3.8, \epsilon_{Ar} = 0.0, \epsilon_{He} = 0.0$			
	H + O <sub>2</sub> (+Ar) = HO <sub>2</sub> (+Ar) <sup>b</sup>	4.65E+12	0.44	0.00
	Low-pressure limit	6.81E+18	-1.20	0.0
	H + O <sub>2</sub> (+He) = HO <sub>2</sub> (+He) <sup>c</sup>	4.65E+12	0.44	0.00
	Low-pressure limit	9.19E+18	-1.20	0.0
10	H <sub>2</sub> + O <sub>2</sub> = H + HO <sub>2</sub>	5.176E+05	2.43	5.350E+04
11	HO <sub>2</sub> + H = OH + OH	7.079E+13	0.00	2.950E+02
12	HO <sub>2</sub> + O = OH + O <sub>2</sub>	3.250E+13	0.00	0.0
13	HO <sub>2</sub> + OH = H <sub>2</sub> O + O <sub>2</sub>	2.456E+13	0.00	-4.970E+02
14	HO <sub>2</sub> + HO <sub>2</sub> = H <sub>2</sub> O <sub>2</sub> + O <sub>2</sub>	1.300E+11	0.00	-1.630E+03
	HO <sub>2</sub> + HO <sub>2</sub> = H <sub>2</sub> O <sub>2</sub> + O <sub>2</sub>	3.658E+14	0.00	1.200E+04
15	H <sub>2</sub> O <sub>2</sub> (+M) = OH + OH (+M) <sup>d</sup>	2.000E+12	0.90	4.875E+04
	Low-pressure limit	2.490E+24	-2.30	4.875E+04
	$\epsilon_{H_2} = 3.7, \epsilon_{CO} = 2.8, \epsilon_{CO_2} = 1.6, \epsilon_{N_2} = 1.5, \epsilon_{O_2} = 1.2$			
	$\epsilon_{He} = 0.65, \epsilon_{H_2O_2} = 7.7, \epsilon_{H_2O} = 0.0$			
	H <sub>2</sub> O <sub>2</sub> (+H <sub>2</sub> O) = OH + OH (+H <sub>2</sub> O) <sup>e</sup>	2.000E+12	0.90	4.875E+04
	Low-pressure limit	1.865E+25	-2.30	4.875E+04
16	H <sub>2</sub> O <sub>2</sub> + H = H <sub>2</sub> O + OH	2.410E+13	0.00	3.970E+03
17	H <sub>2</sub> O <sub>2</sub> + H = H <sub>2</sub> + HO <sub>2</sub>	2.150E+10	1.00	6.000E+03
18	H <sub>2</sub> O <sub>2</sub> + O = OH + HO <sub>2</sub>	9.550E+06	2.00	3.970E+03
19	H <sub>2</sub> O <sub>2</sub> + OH = H <sub>2</sub> O + HO <sub>2</sub>	1.740E+12	0.00	3.180E+02
	H <sub>2</sub> O <sub>2</sub> + OH = H <sub>2</sub> O + HO <sub>2</sub>	7.590E+13	0.00	7.269E+03

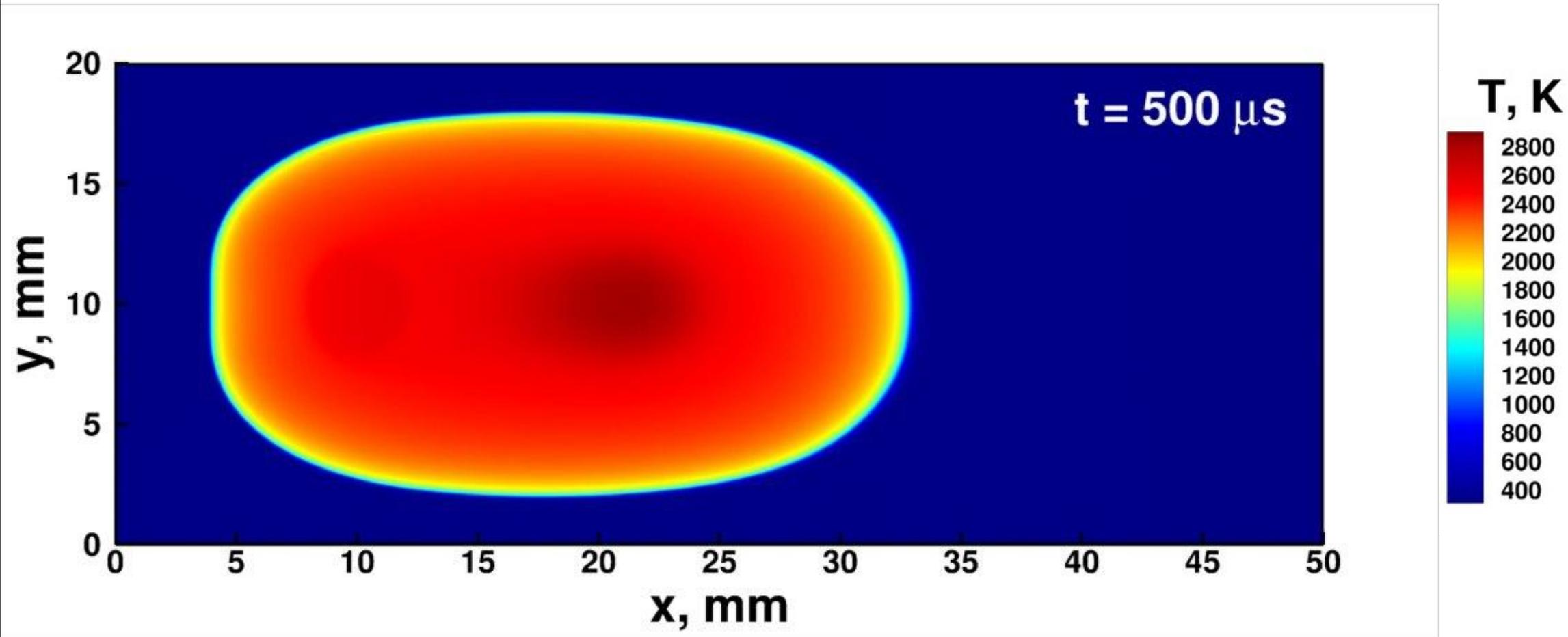
# Визуализация



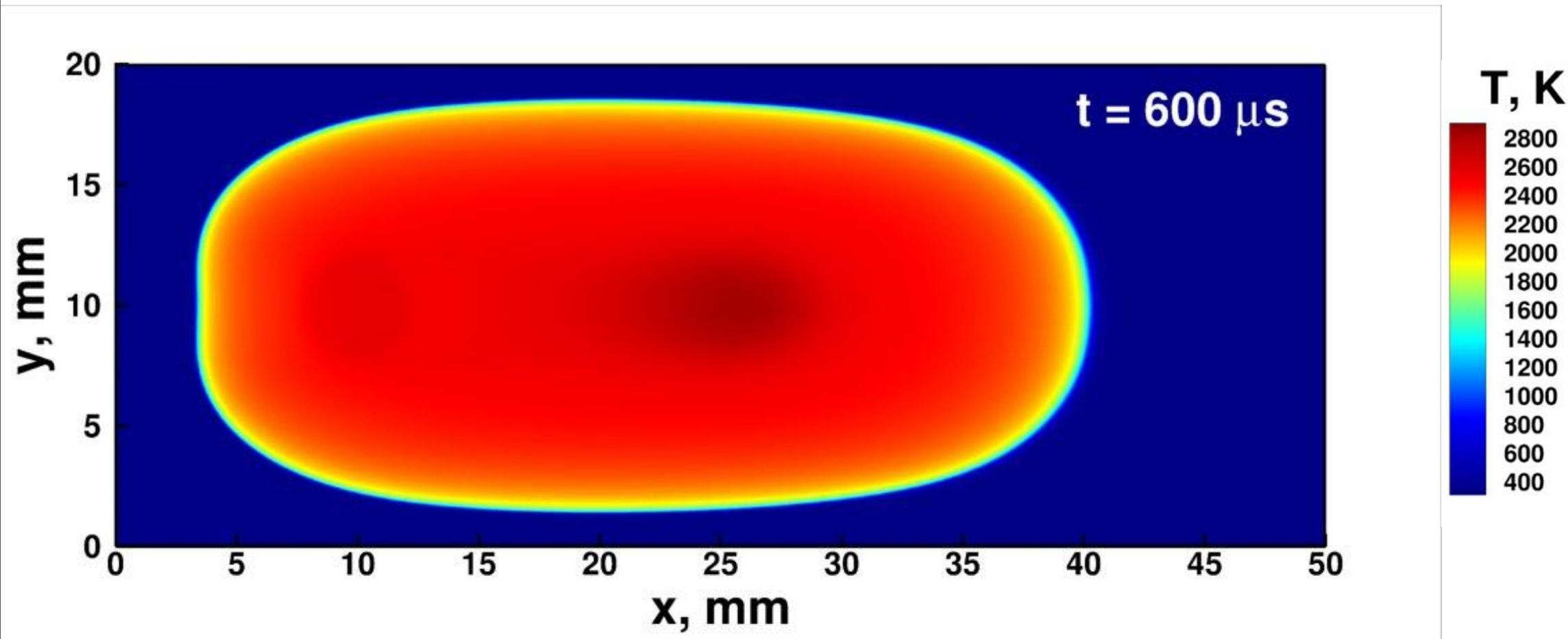
# Визуализация



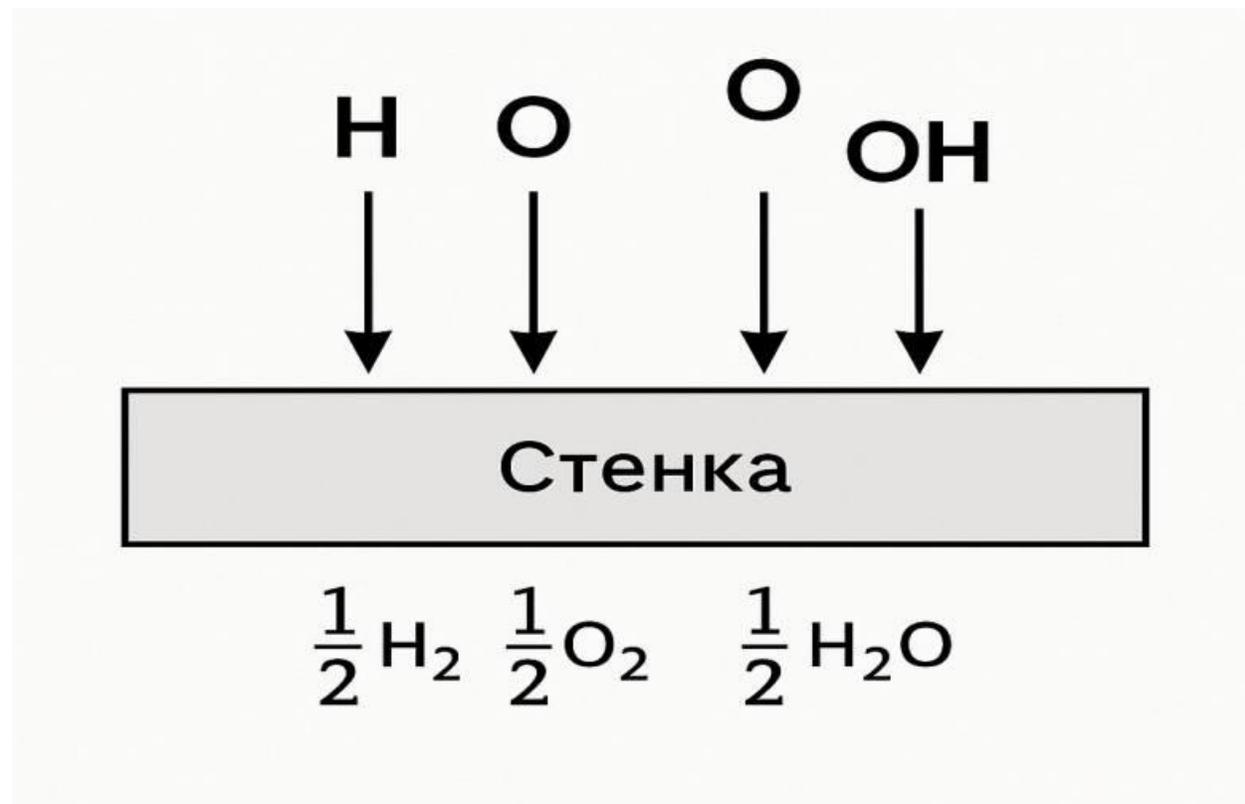
# Визуализация

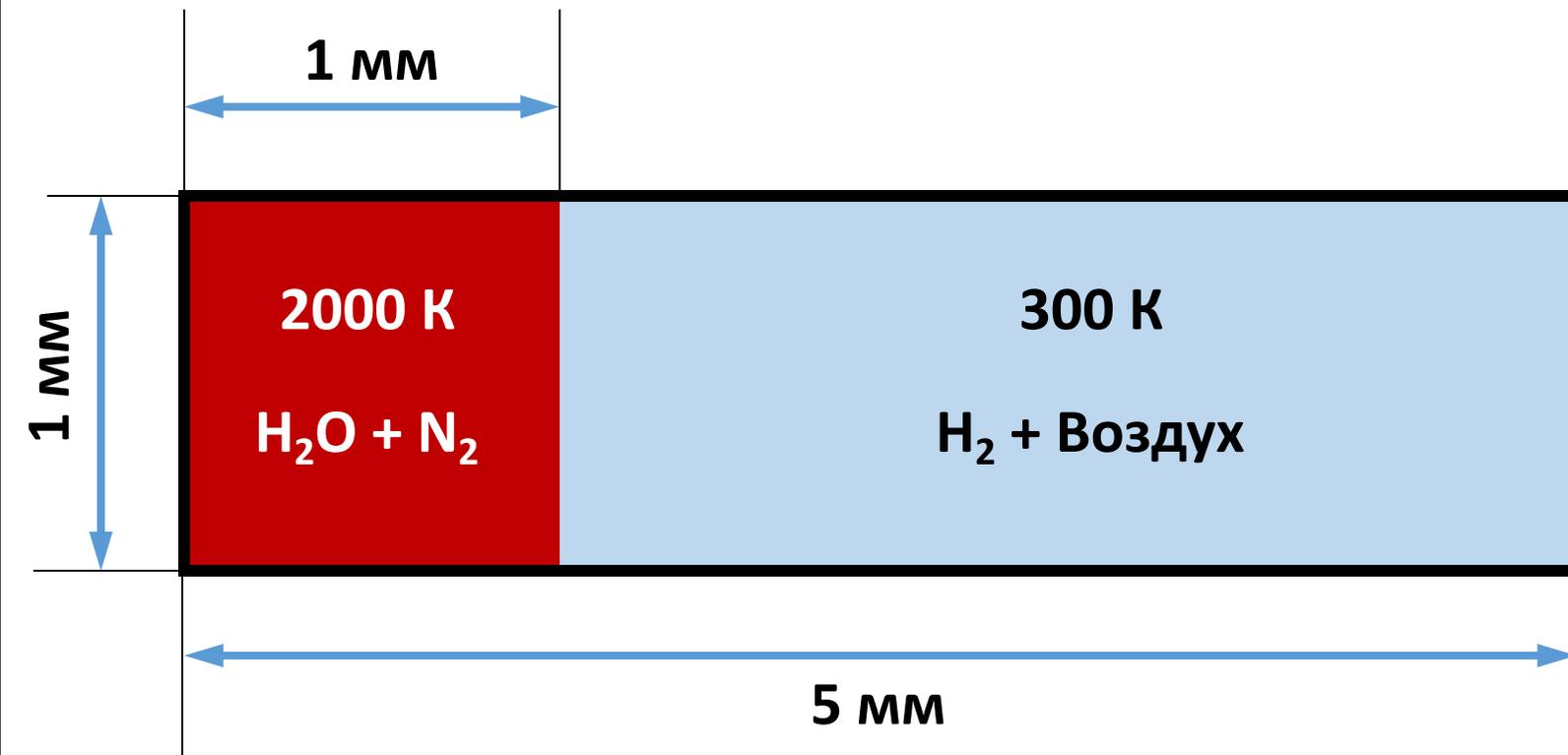


# Визуализация



## Схема каталитических реакций на стенке





Диффузионный поток  
атомарного водорода:

$$\vec{J}_H = D_H \left( \vec{\nabla} Y_H \right)$$

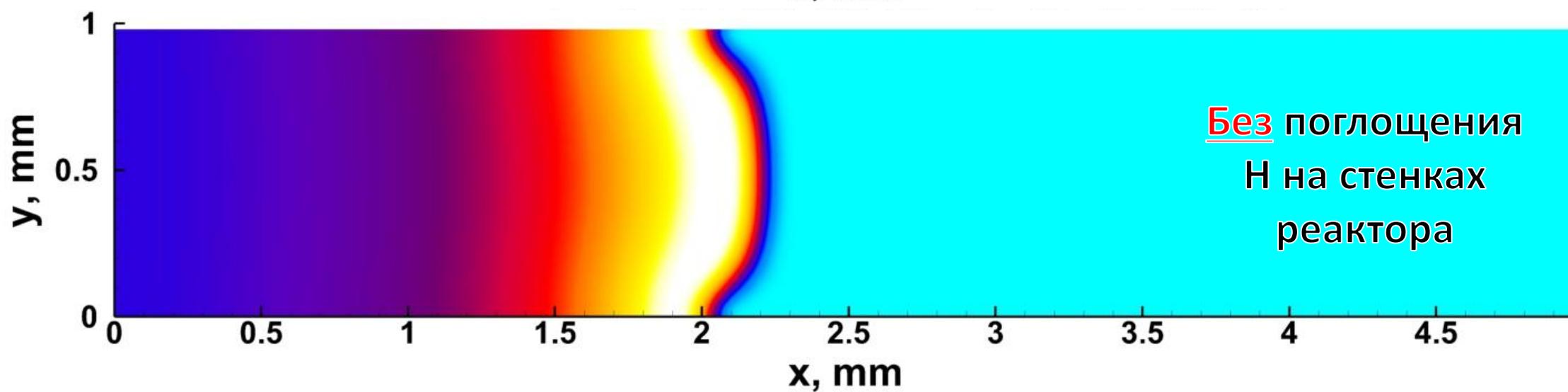
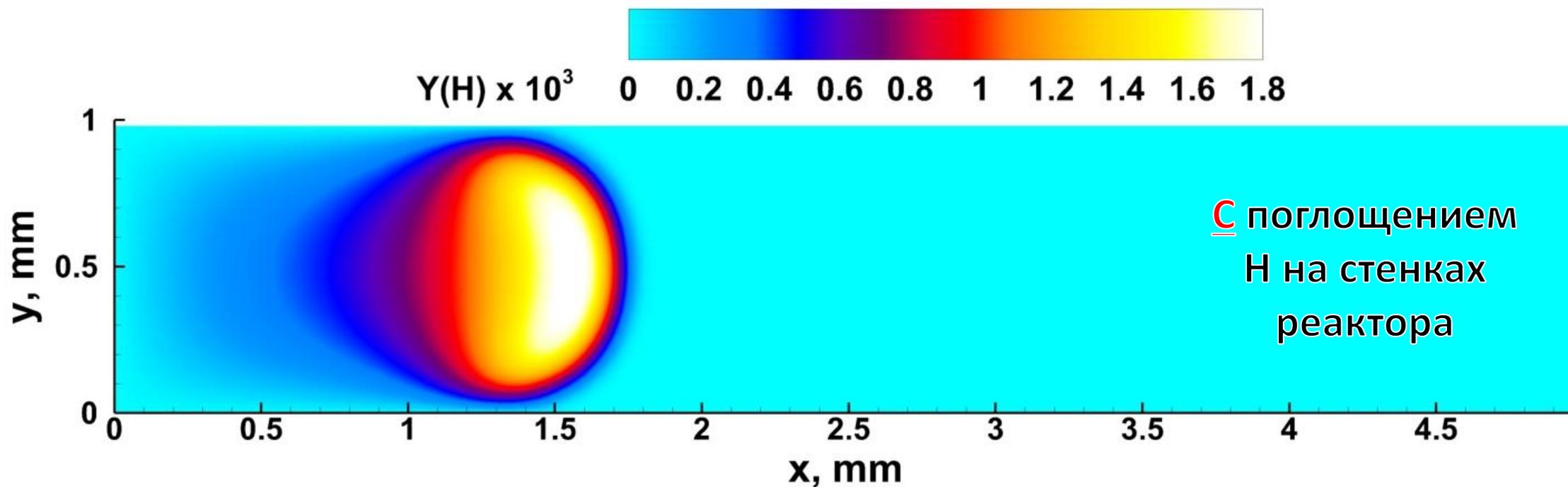
Имитация обрыва цепи  
на стенках:

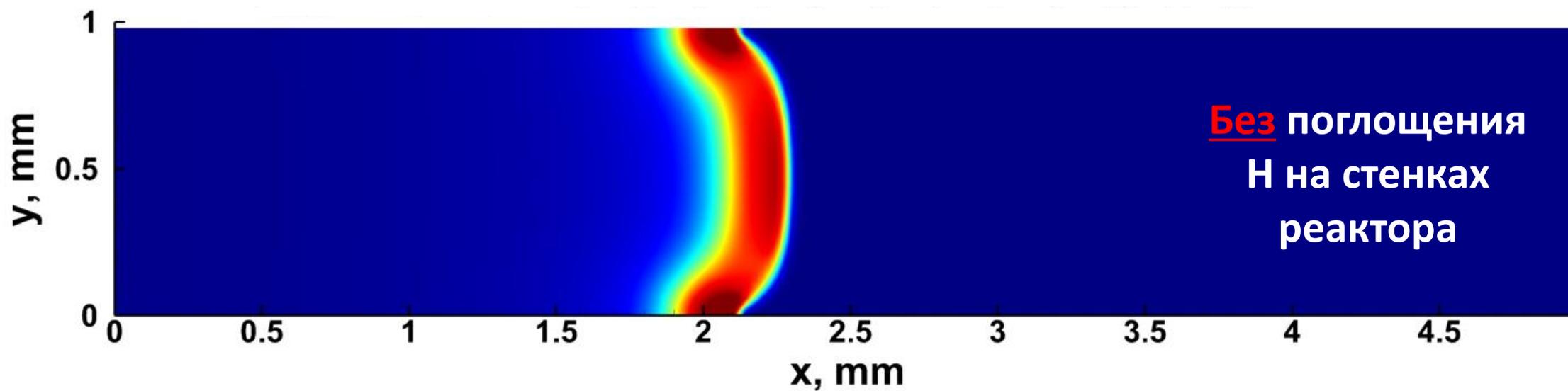
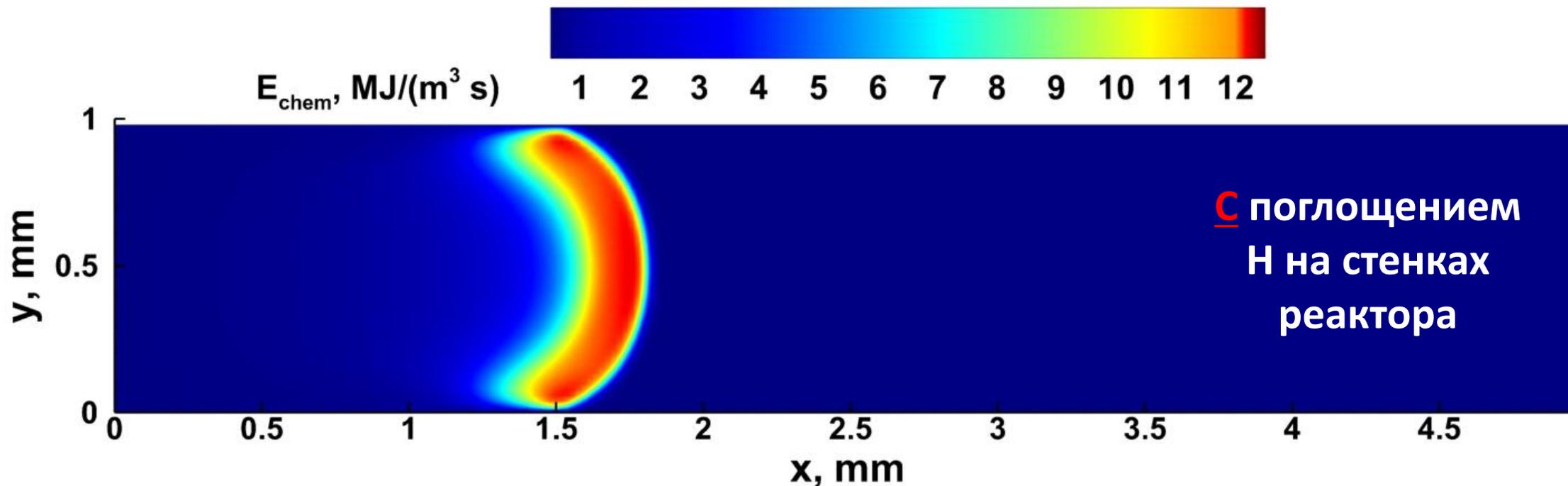
$$Y_{H,wall} = 0$$

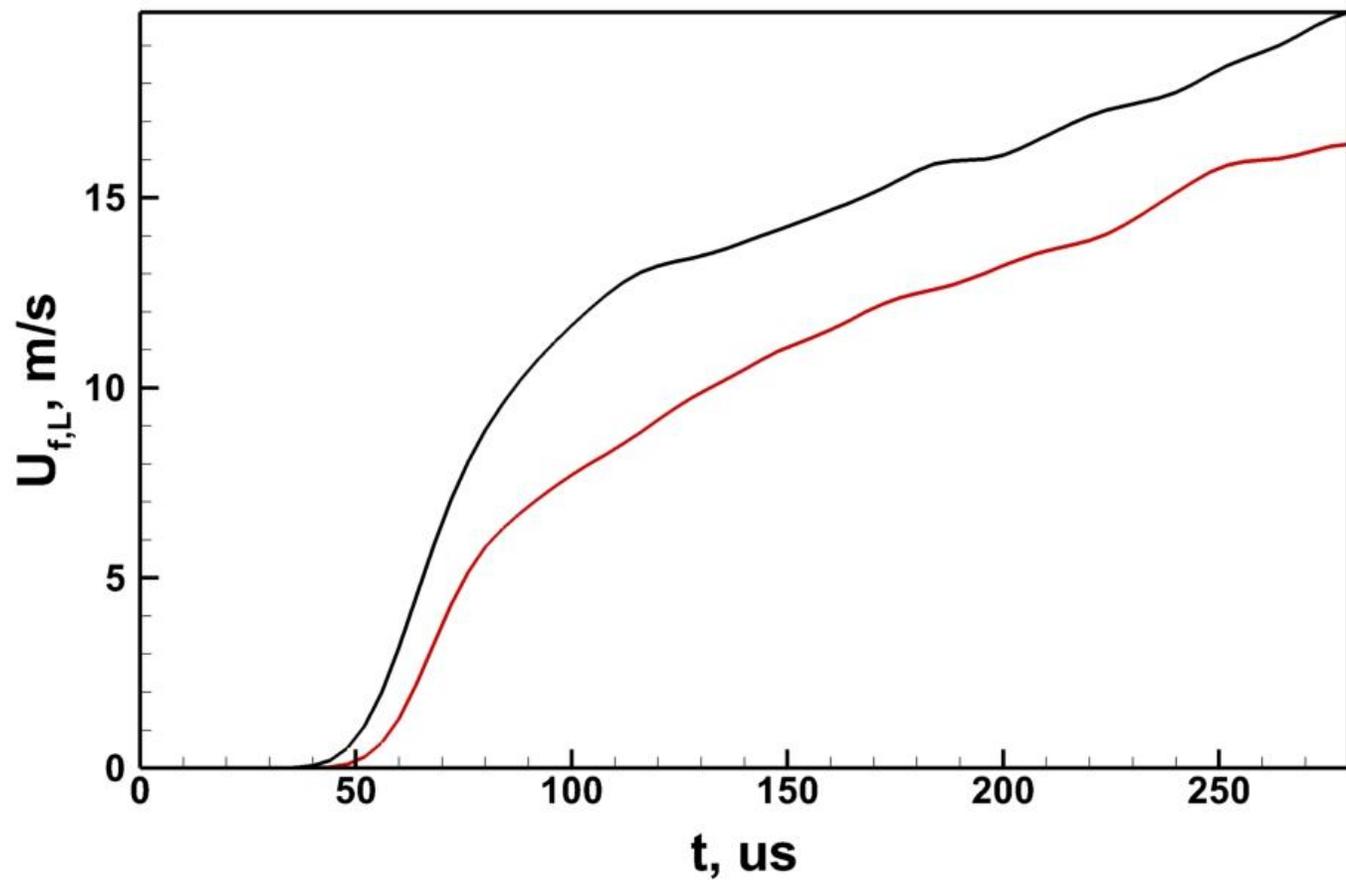
Модель газодинамики реагирующей смеси на основе полной системы уравнений Навье-Стокса, с учетом вязкости, теплопроводности, многокомпонентной диффузии и химической кинетики окисления водород-воздушной смеси [1]. Решение системы модельных уравнений выполняется с использованием метода КАБАРЕ [2].

[1] A. Keromnes et. al. // Combust. Flame, 2013, V. 160, pp. 995-1011

[2] S.A. Karabasov, V.M. Goloviznin // J. Comp. Phys., 2009, V. 228, pp. 7426-7451







**Черная – без поглощения  $N$  на стенках**  
**Красная – с поглощением  $N$  на стенках**