РОСАТОМ

ГОСУДАРСТВЕННАЯ КОРПОРАЦИЯ ПО АТОМНОЙ ЭНЕРГИИ «РОСАТОМ»

Calibration of k-ε model of turbulence for description of experiment on interaction of a hock wave with turbulent layer

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Work goals

When shock wave passing in gas phase through boundary of two components with different density, Richtmyer--Meshkov instability occurs, which leads to intensive mixing of this components.

The process can be modeled with help of special models of turbulence, which takes into account buoyancy production term:

$$G_b = \overline{u''} \cdot \vec{\nabla} \overline{p}$$

This work pursued following goals :

1. Adding k-ε model to existing multiphase gas dynamics model.
2. Simulation of experiments, that had investigated Richtmyer-Meshkov instability and calculation width of mixing zone.

Gas dynamic model

Modified system of gas dynamics equations for multiphase system, which was embodied in Focus programm*:

$$\frac{\partial\left(\overline{\rho_m}\cdot\alpha_i\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot\alpha_i\cdot\overrightarrow{\tilde{u}_m}\right)=\nabla\cdot\vec{\bar{J}}+\nabla\cdot\vec{J_t}$$

$$\frac{\partial\left(\alpha_i\right)}{\partial t}+\nabla\cdot\left(\alpha_i\cdot\overrightarrow{\tilde{u}_m}\right)=\alpha_i\cdot\nabla\cdot\overrightarrow{\tilde{u}_m}$$

$$\frac{\partial\left(\overline{\rho_m}\cdot\overrightarrow{\tilde{u}_m}\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot\overrightarrow{\tilde{u}_m}\otimes\overrightarrow{\tilde{u}_m}\right)+\vec{\nabla}\overline{P_m}=-\vec{\nabla}\left(\frac{2}{3}\cdot\overline{\rho_m}\cdot k\right)+\nabla\cdot\tau_d+\nabla\cdot\overline{\Omega}$$

$$\frac{\partial\left(\overline{\rho_m}\cdot\{E_m\}\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot\{E_m\}\cdot\overrightarrow{\tilde{u}_m}\right)+\nabla\cdot\left(P_m\cdot\overrightarrow{\tilde{u}_m}\right)=-\nabla\cdot\left(\overline{p}\cdot\overline{u''_m}-\overline{\Omega}\cdot\overline{u''_m}\right)+\nabla\cdot\left(\tau\cdot\overrightarrow{\tilde{u}_m}\right)$$
$$+\nabla\cdot\left(\overline{\Omega}\cdot\overrightarrow{\tilde{u}_m}\right)+\nabla\cdot\left(\left(\overline{\lambda}+\lambda_t\right)\cdot\vec{\nabla}\overline{T}+\frac{\mu_t}{\sigma}\cdot\vec{\nabla}\tilde{e}\right)+\nabla\cdot\left(\left(\overline{\mu}+\mu_t\right)\cdot\vec{\nabla}k\right)+\nabla\cdot\overline{H}$$

*Н. А. Михайлов, И. В. Глазырин, Метод укручения контактных границ для моделирования трёхмерных многофазных сжимаемых течений в эйлеровых переменных. Забабахинские научные чтения: Сборник тезисов XIII Международной конференции 20-24 марта 2017, Снежинск: Изд-во РФЯЦ-ВНИИТФ, с. 326, 2017

Turbulence model

k-ε model, proposed by J. T. Moran-Lopez and O. Schilling* for two component systems:

$$\frac{\partial\left(\bar{\rho}\cdot k\right)}{\partial t}+\nabla\cdot\left(\bar{\rho}\cdot k\cdot\tilde{\vec{u}}_m\right)-\nabla\cdot\left(\left(\bar{\mu}+\frac{\mu_t}{\sigma}\right)\cdot\vec{\nabla}k\right)=\tau_d:\vec{\nabla}\tilde{\vec{u}}_m-\overrightarrow{u''_m}\cdot\vec{\nabla}\bar{p}+$$

$$+\overrightarrow{u''_m}\cdot\nabla\cdot\bar{\Omega}-\frac{2}{3}\cdot\bar{\rho}\cdot k\cdot\nabla\cdot\tilde{\vec{u}}_m-\left(1+M_t^2\right)\cdot\bar{\rho}\cdot\varepsilon+\Pi_k$$

$$\frac{\partial\left(\bar{\rho}\cdot\varepsilon\right)}{\partial t}+\nabla\cdot\left(\bar{\rho}\cdot\varepsilon\cdot\tilde{\vec{u}}_m\right)-\nabla\cdot\left(\left(\bar{\mu}+\frac{\mu_t}{\sigma}\right)\cdot\vec{\nabla}\varepsilon\right)=C_{1\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\tau_d:\vec{\nabla}\tilde{\vec{u}}_m-$$

$$-C_{0\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\overrightarrow{u''_m}\cdot\vec{\nabla}\bar{p}+C_{0\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\overrightarrow{u''_m}\cdot\nabla\cdot\bar{\Omega}-C_{3\varepsilon}\cdot\frac{2}{3}\cdot\bar{\rho}\cdot\varepsilon\cdot\nabla\cdot\tilde{\vec{u}}_m-C_{2\varepsilon}\cdot\bar{\rho}\cdot\frac{\varepsilon^2}{k}+C_{4\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\Pi_k$$

*J. T. Moran-Lopez, O. Schilling, Multi-component Reynolds-averaged Navier-Stokes simulations of Richtmyer-Meshkov instability and mixing induced by reshock at different times, Shock Waves, 2014, Vol. 24(3), pp. 325-343

Division on processes

Solving Euler equations

↓

Solving PDE fo sources of k and ε

↓

Solving equations for other flows: diffusion of momentum, mass fraction, heat

Euler's equations

First system of equations is solved:

$$\frac{\partial\left(\overline{\rho_m}\cdot\alpha_i\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot\alpha_i\cdot\vec{\tilde{u}}_m\right)=0$$

$$\frac{\partial\left(\alpha_i\right)}{\partial t}+\nabla\cdot\left(\alpha_i\cdot\vec{\tilde{u}}_m\right)=0$$

$$\frac{\partial\left(\overline{\rho_m}\cdot\vec{\tilde{u}}_m\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot\vec{\tilde{u}}_m\otimes\vec{\tilde{u}}_m\right)+\vec{\nabla}\overline{P}_m=-\vec{\nabla}\left(\frac{2}{3}\cdot\overline{\rho_m}\cdot k\right)$$

$$\frac{\partial\left(\overline{\rho_m}\cdot E_m\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot E_m\cdot\vec{\tilde{u}}_m\right)+\nabla\cdot\left(\overline{P}_m\cdot\vec{\tilde{u}}_m\right)=-\nabla\cdot\left(\frac{2}{3}\cdot\overline{\rho_m}\cdot k\cdot\vec{\tilde{u}}_m\right)$$

$$\frac{\partial\left(\overline{\rho_m}\cdot k\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot k\cdot\vec{\tilde{u}}_m\right)=0$$

$$\frac{\partial\left(\overline{\rho_m}\cdot\varepsilon\right)}{\partial t}+\nabla\cdot\left(\overline{\rho_m}\cdot\varepsilon\cdot\vec{\tilde{u}}_m\right)=0$$

Making assumption about equal compressibility of phases, volum fraction is corrected:

$$\alpha_i=\frac{\alpha_i^*}{\sum_j\alpha_j^*}$$

α_i^* - volume fraction from Euler's equations

ODE for sources of k and ε

After that equation for *k* and *ε* are sold. Only sources are taking into account:

$$\frac{\partial\left(\overline{\rho}\cdot k\right)}{\partial t}=\tau_d:\vec{\vec{\nabla}}\tilde{\vec{u}}_m-\overrightarrow{u''}_m\cdot\vec{\nabla}\overline{p}+\overrightarrow{u''}_m\cdot\nabla\cdot\overline{\Omega}-$$

$$-\frac{2}{3}\cdot\rho\cdot k\cdot\nabla\cdot\tilde{\vec{u}}_m-\left(1+M_t^{\,2}\right)\cdot\rho\cdot\varepsilon+\Pi_k$$

$$\frac{\partial\left(\overline{\rho}\cdot\varepsilon\right)}{\partial t}=C_{1\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\tau_d:\vec{\vec{\nabla}}\tilde{\vec{u}}_m-C_{0\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\overrightarrow{u''}_m\cdot\vec{\nabla}\overline{p}+C_{0\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\overrightarrow{u''}_m\cdot\nabla\cdot\overline{\Omega}-$$

$$-C_{3\varepsilon}\cdot\frac{2}{3}\cdot\rho\cdot\varepsilon\cdot\nabla\cdot\tilde{\vec{u}}_m-C_{2\varepsilon}\cdot\rho\cdot\frac{\varepsilon^2}{k}+C_{4\varepsilon}\cdot\frac{\varepsilon}{k}\cdot\Pi_k$$

Other flows

Other are diffusion equations:

$$\frac{\partial\left(\overline{\rho_m}\cdot k\right)}{\partial t}=\nabla\cdot\left(\left(\overline{\mu}+\frac{\mu_t}{\sigma}\right)\cdot\vec{\nabla}k\right)$$

$$\frac{\partial\left(\overline{\rho_m}\cdot \varepsilon\right)}{\partial t}=\nabla\cdot\left(\left(\overline{\mu}+\frac{\mu_t}{\sigma}\right)\cdot\vec{\nabla}\varepsilon\right)$$

$$\frac{\partial\left(\overline{\rho_m}\cdot \overrightarrow{u_m}\right)}{\partial t}=\nabla\cdot\left(\tau_d+\overline{\Omega}\right)$$

$$\frac{\partial\left(\overline{\rho_m}\cdot \{E_m\}\right)}{\partial t}=-\nabla\cdot\left(\overline{p\cdot u''_m}-\overline{\Omega\cdot u''_m}\right)+\nabla\cdot\left(\tau_d\cdot\tilde{\tilde{u}}_m\right)+\nabla\cdot\left(\overline{\Omega}\cdot\tilde{\tilde{u}}_m\right)+\nabla\cdot\overline{H}$$

$$\frac{\partial\left(\overline{\rho_m}\cdot \tilde{e}_m\right)}{\partial t}=\nabla\cdot\left(\frac{\mu_t}{\sigma}\cdot\vec{\nabla}\tilde{e}\right)$$

$$\frac{\partial\tilde{e}_m}{\partial T}\cdot\frac{\partial\overline{T}}{\partial t}=\nabla\cdot\left(\left(\overline{\lambda}+\lambda_t\right)\cdot\vec{\nabla}\overline{T}\right)$$

$$\frac{\partial\left(\overline{\rho_m}\cdot \omega_i\right)}{\partial t}=\nabla\cdot\left(\overline{\vec{J}}+\vec{J}_t\right)$$

Closure model

$$\mu_t = C_\mu \cdot \overline{\rho_m} \cdot \frac{k^2}{\varepsilon}; \ \lambda_t = C_p \cdot \frac{\mu_t}{\sigma}$$

$$\tau = -\frac{2}{3} \cdot \overline{\rho_m} \cdot k + \tau_d$$

$$\tau_d = \mu_t \cdot \left(\vec{\nabla} \tilde{\vec{u}} + \vec{\nabla} \tilde{\vec{u}}^T - \frac{2}{3} \cdot \nabla \cdot \tilde{\vec{u}} \cdot I \right)$$

$$M_t^2 = \frac{2 \cdot k}{\overline{a}^2}$$

$$\overline{J_i} + J_t^i = \left(\overline{\rho_m} \cdot \frac{6}{5} \cdot \overline{\nu}_i + \frac{\mu_t}{\sigma} \right) \cdot \vec{\nabla} \omega_i$$

$$\overline{H} = \sum_i \overline{h_i} \cdot \left(\overline{J_i} + J_t^i \right)$$

$$\overline{h_i} \approx \overline{e}_i^{\alpha} + \frac{\{\alpha_i\} \cdot \overline{p}}{\{\omega\}_i \cdot \{\rho\}}$$

Closure model

Velocity fluctuation approximation:

$$\overline{u''} = \frac{\mu_t}{\overline{\rho} \cdot \sigma_\rho} \cdot \left(\frac{\nabla \overline{\rho}}{\overline{\rho}} - \frac{\nabla \overline{p}}{\overline{p}} \right)$$

Pressure-dilation correlation:

$$\Pi_k = \overline{p' \cdot \nabla \cdot \vec{u}'} = M_t^{\,2} \cdot \left(-\alpha_2 \cdot \left(\tau : \vec{\nabla} \tilde{\vec{u}} - \frac{2}{3} \cdot \overline{\rho} \cdot k \cdot \nabla \tilde{\vec{u}} \right) + \alpha_3 \cdot \overline{\rho} \cdot \varepsilon \right)$$

Constants:

$$C_\mu = 0.09;\ \sigma = 0.5;\ \sigma_\rho = 0.76;\ C_{0\varepsilon} = 0.84;$$

$$C_{1\varepsilon} = 1.44;\ C_{2\varepsilon} = 1.92;\ C_{3\varepsilon} = 2.;\ C_{4\varepsilon} = 1.1$$

$$\alpha_2 = 0.4;\ \alpha_3 = 0.2.$$

Connection between mass and volume fraction

Advection equations are solved in volume fractions:

$$\frac{\partial\left(\rho_m \cdot \alpha_i\right)}{\partial t} + \nabla \cdot \left(\rho_m \cdot \alpha_i \cdot \overrightarrow{u_m}\right) = 0; \quad \frac{\partial\left(\alpha_i\right)}{\partial t} + \nabla \cdot \left(\alpha_i \cdot \overrightarrow{u_m}\right) = \alpha_i \cdot \nabla \cdot \overrightarrow{u_m}$$

Diffusion equations — in mass fractions:

$$\frac{\partial\left(\overline{\rho_m} \cdot \omega_i\right)}{\partial t} = \nabla \cdot \left(\overline{\rho_m} \cdot \frac{6}{5} \cdot \overline{\nu}_i + \frac{\mu_t}{\sigma}\right) \cdot \vec{\nabla}\omega_i$$

After third stage only average pressure and temperature per cell:

$$\rho_i^{\alpha} = f\left(p_m^*, T_m^*\right)$$

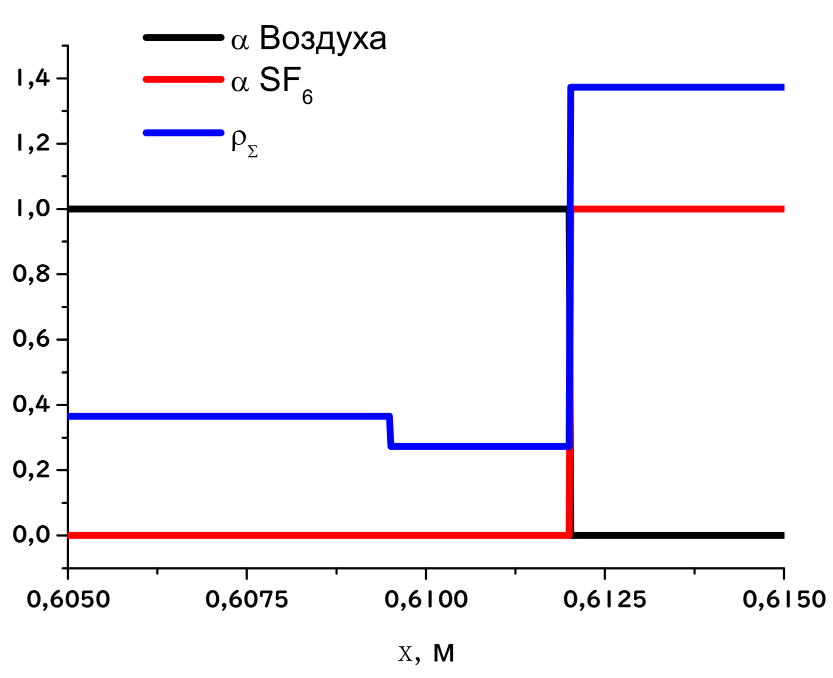
Then volume fraction on new time layer :

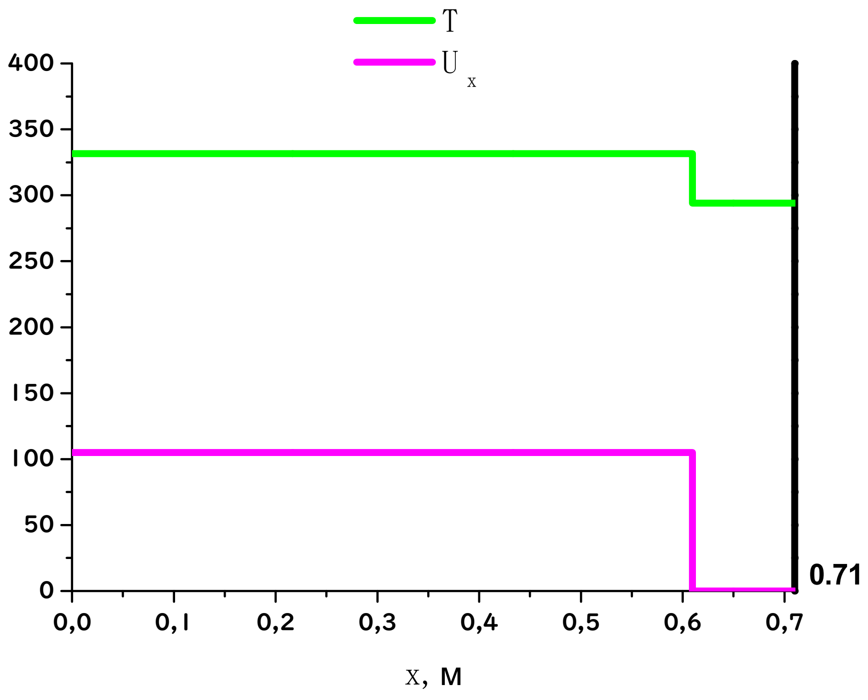
$$\alpha_i = \frac{\rho_i^{\alpha}}{\overline{\overline{\rho_m}} \cdot \omega_i}$$

After that pressure of the mixture and temperatures of phases are recalculated.

Comparision with experiment

Comparisions were made with experiment of E. Leinov and oth.*





*E. Leinov, G. Malamud, Y. Elbaz, L. A. Levin, G. Ben-Dor, D. Shvarts, O. Sadot, Experimental and numerical investigation of the Richtmeyer-Meshkov instability under re-shock conditions, J. Fluid Mech., 2009, Vol. 626, pp. 449-475

Comparision with experiment

One dimensional simulations were carried out for four variants of experiment.
Initial conditions:

- Pressure – 23 kPa.
- Temperature – 294 K.
- Density of air and sulfur hexafluoride – 0.2729 kg/m^3 and 1.3738 kg/m^3 correspondingly.
- Distance to wall 9.8, 13.2, 17.7 и 19.9 cm.
- Gases were taken as ideal with isochoric heat capacity:

$$C_V^{air} = 717.1 \text{ Дж/кг}$$

$$C_V^{SF_6} = 605.6 \text{ Дж/кг}$$

- Properties after the shock wave corresponded 1.2 Mach:

$$\overline{\rho}_0 = 0.366 \text{ кг/м}^3$$

$$\overline{p}_0 = 34806 \text{ Па}$$

$$\vec{\tilde{u}}_0 = (104.96; 0; 0) \text{ м/с}$$

Comparision with experiment

Initial *k* and *ε* were taken constan according to the equations:

$$k_0 = K^0 \cdot \left(\tilde{u}_0 \cdot At\right)^2 = 495 \text{ м}^2/\text{с}^2$$

$$\varepsilon_0 = k_0 \cdot \frac{2 \cdot \pi}{\lambda_{rms}} \cdot |At| \cdot \Delta\tilde{u} = 5.83 \cdot 10^7 \text{ м}^2/\text{с}^3$$

$$At = \frac{\rho_{SF_6} - \rho_a}{\rho_{SF_6} + \rho_a} = 0.67; \ \Delta\tilde{u} = (69.5; 0; 0)$$

$$\lambda_{rms} = 0.0025 \text{ м}; K^0 = 0.1$$

λ_{rms} – parameter about mean length of initial preturbation, Δu – change of velocity due to passing of shock wave.

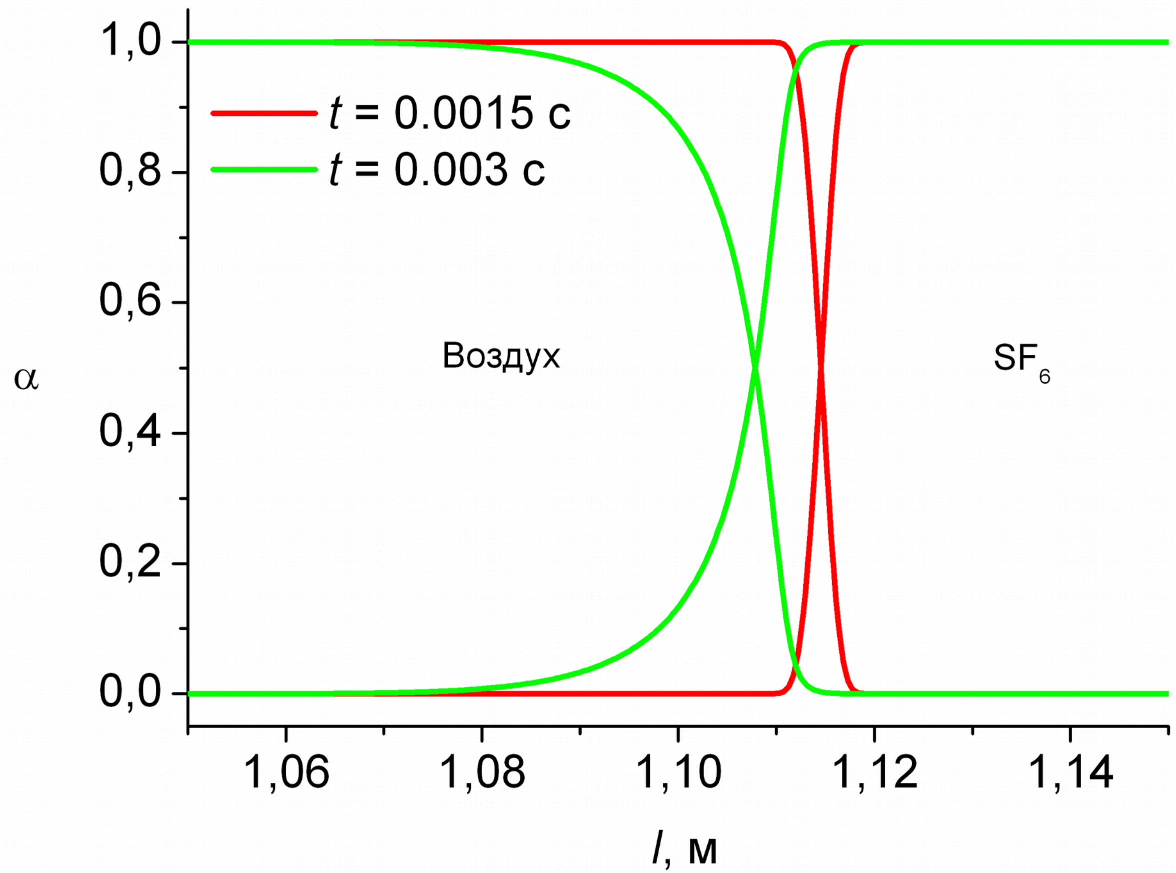
$$\tau_d = 0$$

$$\delta = l^a_{x=0.01} - l^a_{x=0.99}$$

Mixing zone width has been defined as distance between points, where molar fraction of air was 1% and 99%.

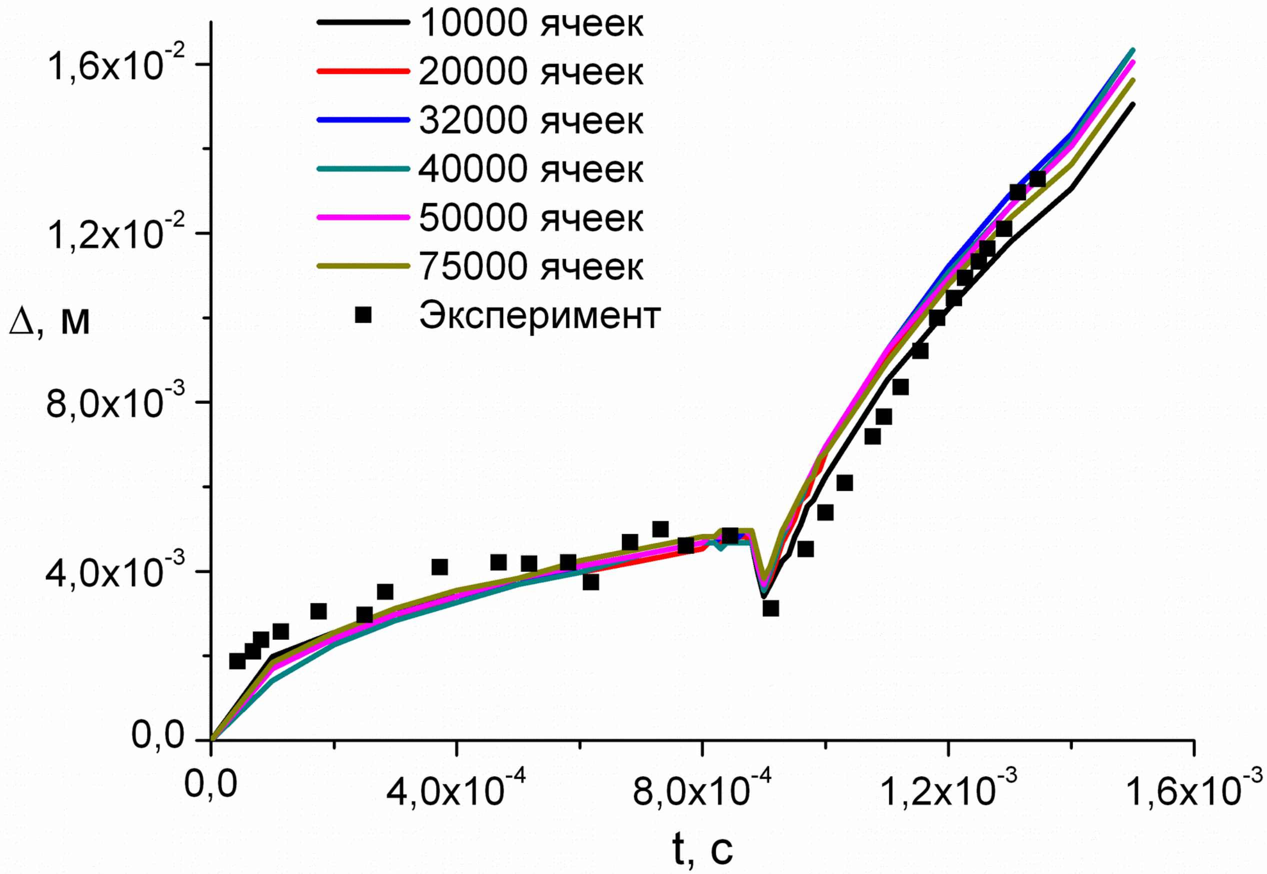
Comparision with experiment

Example of volume fraction profile:



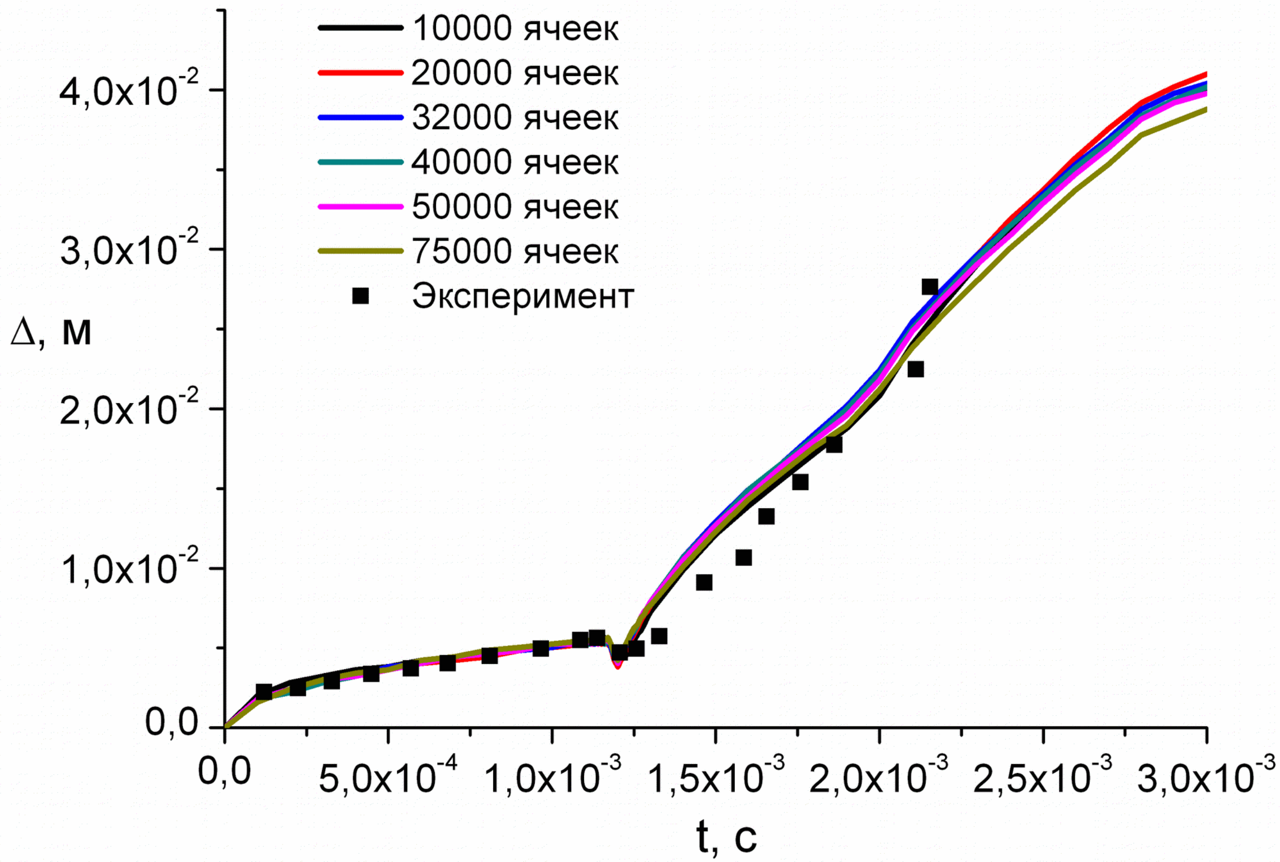
Comparision with experiment

Experiment with distance to wall 9.8 cm:



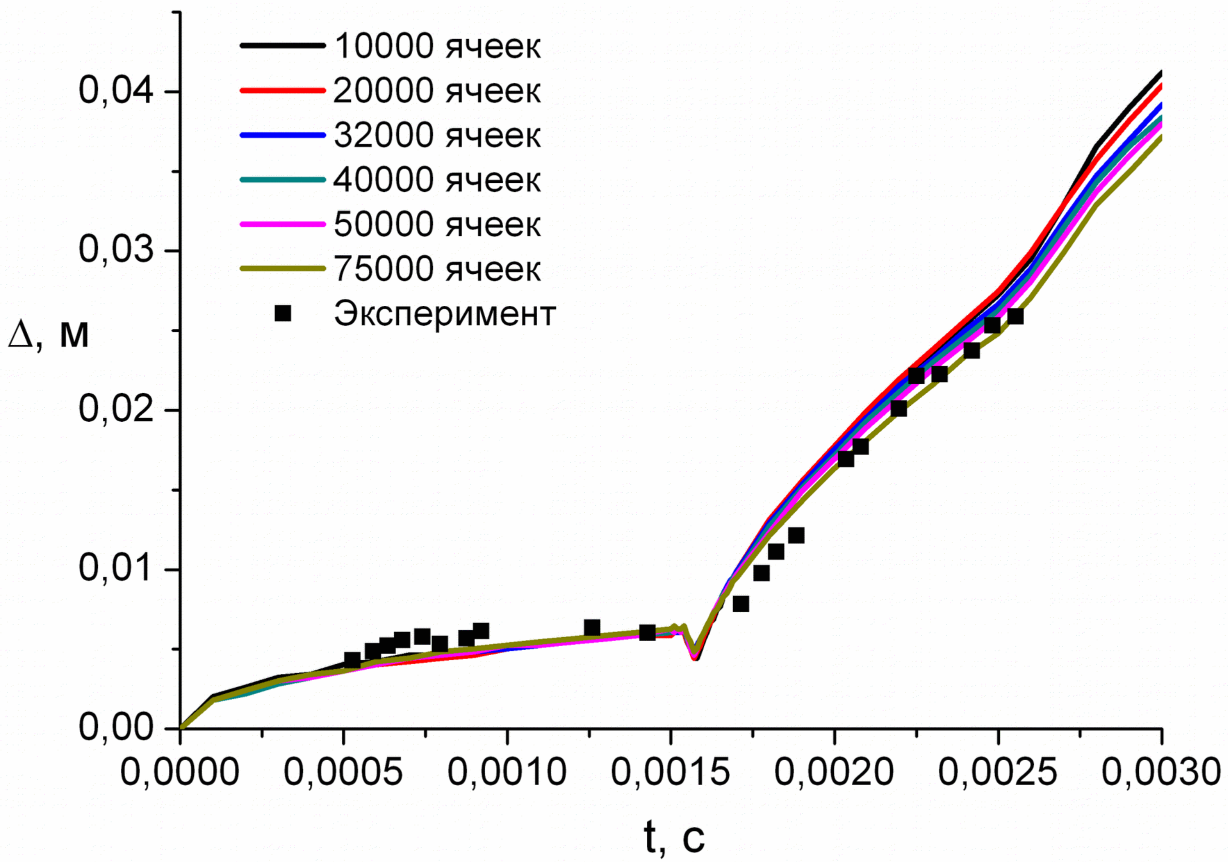
Comparision with experiment

Experiment with distance to wall 13.2 cm:



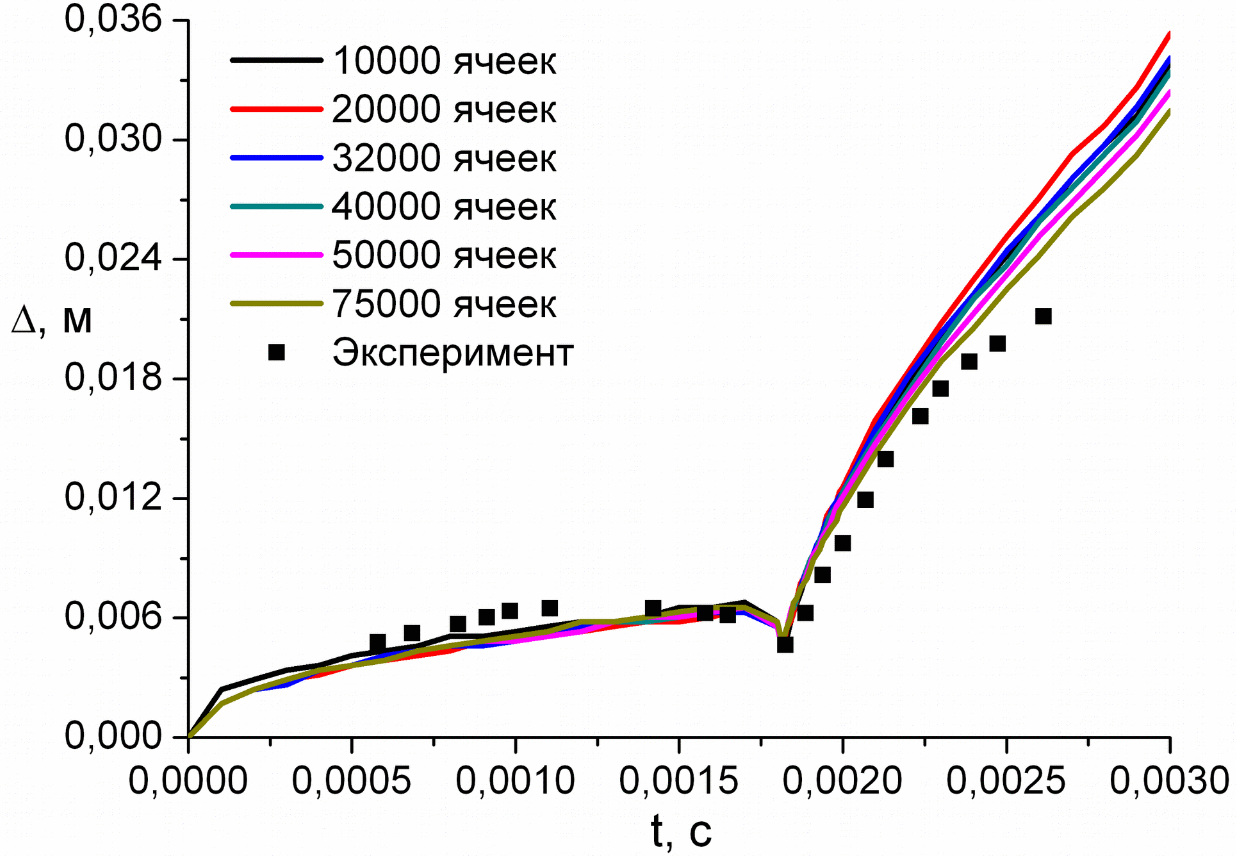
Comparision with experiment

Experiment with distance to wall 17.7 cm:



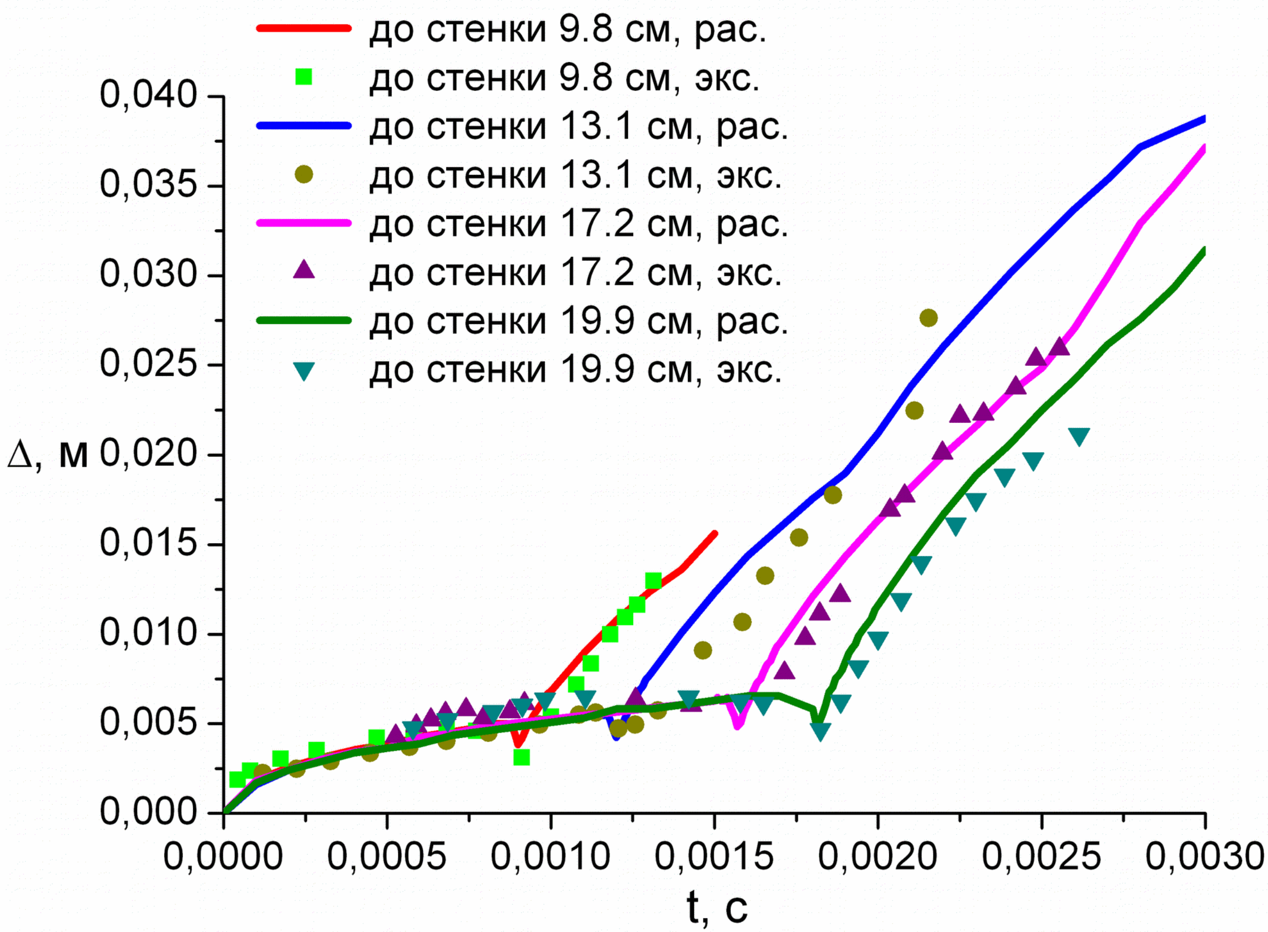
Comparision with experiment

Experiment with distance to wall 19.9 cm:



Comparision with experiment

Experiment with different distance to wall, 75000 cells:



Conclusion

- *K-ε model of turbulence was realised and parametrisation proposed.*

- **With help of this model one dimensional simulations of Richtmyer-Meshkov instability with 1. Mach were conducted.**

- **Model demonstrates good agreement with experiment achieved on width of mixing zone before reshocked wave. After reshocked wave agreement is satisfactory.**

Thank you for attention!

Numerical scheme

Time derivative approximation – Euler`s scheme:

$$\frac{\overline{\rho}^{j} \cdot y^{j+1} - \overline{\rho}^{j} \cdot y^{j}}{\Delta t}$$

Divegence and gradient approximation – Gauss theorem:

$$\nabla \varphi_i = \frac{1}{V_i} \cdot \int_s \varphi \cdot \vec{n} \cdot dS = \frac{1}{V} \cdot \sum_j \int_s \varphi \cdot \overrightarrow{n_j} \cdot dS_j = \frac{1}{V} \cdot \sum_j \varphi_j^c \cdot S_j \cdot \overrightarrow{n_j}$$

Approximation of quantities on surface centrea - linear:

$$\varphi_j^c = \sigma_j \cdot \varphi_P + \left(1 - \sigma_j\right) \cdot \varphi_N$$

$$\sigma_j = \frac{\overrightarrow{n_j} \cdot \overrightarrow{d_P}}{\overrightarrow{n_j} \cdot \left(\overrightarrow{d_P} + \overrightarrow{d_N}\right)}$$