

Квазигомогенная форма системы четырех уравнений динамики гетерогенных смесей газов и жидкостей, ее регуляризация и реализация

А.А. Злотник, Т.А. Ломоносов

НИУ Высшая школа экономики, департамент математики
ИПМ им. М.В. Келдыша

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- 1 A reduced system of PDEs for the dynamics of heterogeneous mixtures of stiffened gases and its further reduction
- 2 Regularized systems of PDEs for the dynamics of quasi-homogeneous mixtures of stiffened gases
- 3 Finite-difference schemes for the 1D regularized systems of PDEs
- 4 Numerical experiments
 - Water-to-air shock tube problem

The four-equation model: no volume fraction Eq.

Common velocity, common temperature and equal pressures:

S. Le Martelot, R. Saurel, B. Nkonga, Towards the direct numerical simulation of nucleate boiling flows, *Int. J. Multiphase Flow* **66**, 62–78 (2014).

R. Saurel, P. Boivin, O. Le Métayer, A general formulation for cavitating, boiling and evaporating flows, *Comput. Fluids* **128**, 53–64 (2016).

Our paper containing the results of the report:

A. Zlotnik, T. Lomonosov. On a doubly reduced model for dynamics of heterogeneous mixtures of stiffened gases, its regularizations and their implementations // *Chaos*. 2023. Vol. 33. No. 11. Article 113128.

The four-equation system of PDEs for the heterogeneous one-velocity and one-temperature compressible binary mixture consists of the balance PDEs for the mass of components, total momentum and total energy

$$\partial_t(\alpha_k r_k) + \operatorname{div}(\alpha_k r_k \mathbf{u}) = 0, \quad k = 1, 2, \quad (1)$$

$$\partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \operatorname{div} \Pi^{NS} + \rho \mathbf{f}, \quad (2)$$

$$\partial_t\left(\frac{1}{2}\rho |\mathbf{u}|^2 + \rho \varepsilon\right) + \operatorname{div}\left(\left(\frac{1}{2}\rho |\mathbf{u}|^2 + \rho \varepsilon + p\right)\mathbf{u}\right) = \operatorname{div}(-\mathbf{q}^F + \Pi^{NS} \mathbf{u}) + \rho \mathbf{u} \cdot \mathbf{f}. \quad (3)$$

Here the main sought functions are the density $r_k > 0$ and the volume fraction $0 < \alpha_k < 1$ of the heterogeneous component, $k = 1, 2$, the common velocity \mathbf{u} and absolute temperature $\theta > 0$ of the mixture. They depend on $x = (x_1, \dots, x_n) \in \Omega$ and $t \geq 0$, where Ω is a domain in \mathbb{R}^n , $n = 1, 2, 3$.

Hereafter vector-functions are written in bold,

$\operatorname{div} = \nabla \cdot$, $\nabla = (\partial_1, \dots, \partial_n)$, $\partial_t = \partial / \partial t$ and $\partial_i = \partial / \partial x_i$.

The symbols \otimes and \cdot correspond to the tensor and scalar products of vectors, the tensor divergence is taken with respect to its first index.

The following additional relations are used

$$\langle \alpha_k \rangle := \alpha_1 + \alpha_2 = 1, \quad \rho = \langle \alpha_k r_k \rangle, \quad \rho \varepsilon = \langle \alpha_k r_k \varepsilon_k(r_k, \theta) \rangle, \quad (4)$$

$$p = p_1(r_1, \theta) = p_2(r_2, \theta) > 0, \quad (5)$$

where $\langle \cdot \rangle$ means **the summation over index** $k = 1, 2$,

$p_k(r_k, \theta)$ and $\varepsilon_k = \varepsilon_k(r_k, \theta)$ are the pressure and specific internal energy of the k th component ($k = 1, 2$), ρ and ε are the density and specific internal energy of the mixture, and p is the common pressure of the components.

In particular, Eq. (5) means that the pressures p_k of the components are equal to each other, and this is the additional algebraic equation to PDEs (1)-(3) and formula $\langle \alpha_k \rangle = 1$ that is required to define all the sought functions listed above.

We apply **the stiffened gas equations of state** in the well-known form

$$p_k(r_k, \theta) = R_k r_k \theta - p_{*k}, \quad \varepsilon_k(r_k, \theta) = c_{V_k} \theta + \frac{p_{*k}}{r_k} + \varepsilon_{0k}, \quad (6)$$

$R_k > 0$, $c_{V_k} > 0$, $p_{*k} \geq 0$ and ε_{0k} are given physical constants, $k = 1, 2$. Also $R_k = (\gamma_k - 1)c_{V_k}$, where $\gamma_k > 1$; let $c_{p_k} = \gamma_k c_{V_k}$.

The perfect polytropic gas case corresponds to $p_{*k} = \varepsilon_{0k} = 0$.

The classical Navier-Stokes viscosity tensor and the Fourier heat flux

$$\Pi^{NS} = \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) + (\lambda - \frac{2}{3}\mu)(\operatorname{div} \mathbf{u})\mathbb{I}, \quad -\mathbf{q}^F = \varkappa \nabla \theta, \quad (7)$$

where $\mu \geq 0$, $\lambda \geq 0$ and $\varkappa \geq 0$ are the total viscosity and heat conductivity coefficients, $\nabla \mathbf{u} = \{\partial_i u_j\}_{i,j=1}^n$ and \mathbb{I} is the n -th order unit tensor. For $\mu = \lambda = 0$ and $\varkappa = 0$, these terms vanish.

Also \mathbf{f} is the given density of body forces.

We omit the phase transfer terms here but add the Navier-Stokes ones.

We define the alternative density $\rho_k = \alpha_k r_k$ of the k -th component.

Consider the following relations

$$\rho = \langle \rho_k \rangle, \quad \sigma^{(k)} = \sigma^{(k)}(\rho_1, \rho_2) = \frac{R_k \rho_k}{c_V \rho} > 0, \quad \langle \sigma^{(k)} \rangle = \frac{R}{c_V} = \gamma - 1, \quad (8)$$

$$\rho R = \langle \rho_k R_k \rangle, \quad \rho c_V = \langle \rho_k c_{V_k} \rangle.$$

For p , the quadratic equation holds

$$p^2 - bp - c = 0, \quad (9)$$

with the coefficients

$$b = \langle \sigma^{(k)}(\rho(\varepsilon - \varepsilon_0) - p_{*k}) - p_{*k} \rangle, \quad (10)$$

$$\begin{aligned} c &= \sigma^{(1)}(\rho(\varepsilon - \varepsilon_0) - p_{*1})p_{*2} + \sigma^{(2)}(\rho(\varepsilon - \varepsilon_0) - p_{*2})p_{*1} - p_{*1}p_{*2} \\ &= (\sigma^{(1)}p_{*2} + \sigma^{(2)}p_{*1})\rho(\varepsilon - \varepsilon_0) - \gamma p_{*1}p_{*2}. \end{aligned} \quad (11)$$

Let $d := b^2 + 4c$ be its discriminant. For $d > 0$, the quadratic Eq. (9) has the roots

$$p_{\pm} = p_{\pm}(\rho_1, \rho_2, \rho\varepsilon) = \frac{1}{2}(b \pm \sqrt{d}), \quad p_- < p_+. \quad (12)$$

But for $p_{*1}p_{*2} \neq 0$ (this case arises in some applications), the property $d > 0$ and the correct choice of the physical root are not obvious a priori and are analyzed below.

Proposition 1

Let $\Delta_* := p_{*2} - p_{*1}$. The following formulas hold

$$b = p_+ + p_-, \quad c = -p_+ p_- \geq 0, \quad (13)$$

where

$$p_+ = \langle \alpha_k p_k \rangle = R\rho\theta - \langle \alpha_k p_{*k} \rangle > 0, \quad p_- = -\left(\alpha_1 p_{*2} + \alpha_2 p_{*1} + \frac{\alpha_1 \alpha_2}{c_V \rho \theta} \Delta_*^2 \right) \leq 0. \quad (14)$$

Consequently, $d > 0$, thus, these p_{\pm} and those given by formula (12) are the same.

This Proposition guarantees that p_+ is the physical root and p_- is the parasitic one.

The found formula for p_- is also of interest since it allows to prove additional results.

The balance PDEs for the mass, kinetic and internal energies of the mixture

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = 0, \quad (15)$$

$$\frac{1}{2} \partial_t (\rho |\mathbf{u}|^2) + \frac{1}{2} \operatorname{div}(\rho |\mathbf{u}|^2 \mathbf{u}) + \mathbf{u} \cdot \nabla p = (\operatorname{div} \Pi^{NS}) \cdot \mathbf{u} + \rho \mathbf{f} \cdot \mathbf{u},$$

$$\partial_t (\rho \varepsilon) + \operatorname{div}(\rho \varepsilon \mathbf{u}) + p \operatorname{div} \mathbf{u} = \operatorname{div}(-\mathbf{q}^F) + \Pi^{NS} : \nabla \mathbf{u} + Q \quad (16)$$

are sequentially derived in a standard manner. Here $:$ denotes the scalar product of tensors. In particular, Eq. (15) arises by applying $\langle \cdot \rangle$ to Eqs. (1).

Proposition 2

The squared speed of sound and the balance PDE for p_+ hold

$$c_s^2 := \partial_\rho p_+ + \frac{p_+}{\rho^2} \partial_\varepsilon p_+ = \frac{\gamma(p_+ + p_{*1})(p_+ + p_{*2})}{\rho \sqrt{d}} > 0, \quad (17)$$

$$\partial_t p_+ + \mathbf{u} \cdot \nabla p_+ + \rho c_s^2 \operatorname{div} \mathbf{u} = \frac{c_s^2}{\gamma_{CV} \theta} (\operatorname{div}(-\mathbf{q}^F) + \Pi^{NS} : \nabla \mathbf{u} + Q), \quad (18)$$

where the derivatives ∂_ρ and ∂_ε are taken in assumption that ε_0 and $\sigma^{(k)}$, $k = 1, 2$, are constant in (10)-(11) following the literature.

The quasi-homogeneous four-equation statement. The balance PDEs for the mass of components, total momentum and total energy

$$\partial_t \rho_k + \operatorname{div}(\rho_k \mathbf{u}) = 0, \quad k = 1, 2, \quad (19)$$

$$\partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p = \operatorname{div} \Pi^{NS} + \rho \mathbf{f}, \quad (20)$$

$$\begin{aligned} \partial_t \left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho \varepsilon \right) + \operatorname{div} \left(\left(\frac{1}{2} \rho |\mathbf{u}|^2 + \rho \varepsilon + p \right) \mathbf{u} \right) \\ = \operatorname{div}(-\mathbf{q}^F + \Pi^{NS} \mathbf{u}) + \rho \mathbf{u} \cdot \mathbf{f}. \end{aligned} \quad (21)$$

Here the main sought functions are the alternative densities $\rho_k > 0$, $k = 1, 2$, the velocity \mathbf{u} and the specific internal energy ε of the mixture. Also $\rho = \langle \rho_k \rangle$, but formulas (4) for ρ_k and $\rho \varepsilon$ and (6) for p_k are not in use. The pressure p and temperature θ are given by the formulas

$$p(\rho_1, \rho_2, \varepsilon) = p_+ = \frac{1}{2}(b + \sqrt{d}), \quad \theta(\rho_1, \rho_2, \varepsilon) = \frac{\rho(\varepsilon - \varepsilon_0) + p}{\gamma c_V \rho}. \quad (22)$$

Recall that here $d = b^2 + 4c$, with $b = b(\rho_1, \rho_2, \varepsilon)$ and $c = c(\rho_1, \rho_2, \varepsilon)$ given in definitions (10), (11) and (8).

We emphasize that this system does not contain α_k and $r_k = \rho_k / \alpha_k$, $k = 1, 2$, although they can be computed a posteriori, we have

$$\alpha_k = \frac{R_k \rho_k \theta}{p_+ + p_{*k}}, \quad k = 1, 2. \quad (23)$$

This formula and the property $\langle \alpha_k \rangle = 1$ imply an alternative formula for θ :

$$\theta = \left\langle \frac{R_k \rho_k}{p_+ + p_{*k}} \right\rangle^{-1}, \quad (24)$$

that we apply in our computations below. For computing r_k , the formula $r_k = (p_+ + p_{*k}) / (R_k \theta)$ seems to be more reliable.

Importantly, the quasi-homogeneous form **is equivalent** to the original heterogeneous one. In particular, formulas (23) and (24) imply that

$$\langle \alpha_k \rangle = 1, \quad p_k = R_k r_k \theta - p_{*k} = R_k \frac{\rho_k}{\alpha_k} \theta - p_{*k} = p_+, \quad k = 1, 2,$$

see the first equation of state (6), and lead to Eqs. (5).

Regularized systems of PDEs for the dynamics of quasi-homogeneous mixtures of stiffened gases

Now we accomplish the formal regularization procedure first suggested in ¹ for the single-component gas. In the balance PDEs for the mass of components (19), the total momentum (20) and the total energy of the mixture (21), we accomplish respectively the following changes

$$\begin{aligned}\rho_k \mathbf{u} &\rightarrow \rho_k \mathbf{u} + \tau \partial_t (\rho_k \mathbf{u}), \\ \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \rho \mathbf{f} &\rightarrow \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + \tau \partial_t (\rho \mathbf{u} \otimes \mathbf{u})) \\ &\quad + \nabla(p + \tau \partial_t p) - (\rho + \tau \partial_t \rho) \mathbf{f}, \\ (E + p) \mathbf{u} &\rightarrow (E + p) \mathbf{u} + \tau \partial_t ((E + p) \mathbf{u}), \\ \rho \mathbf{u} \cdot \mathbf{f} &\rightarrow (\rho \mathbf{u} + \tau \partial_t (\rho \mathbf{u})) \cdot \mathbf{f},\end{aligned}$$

where $E = (1/2)\rho|\mathbf{u}|^2 + \rho\varepsilon$ is the total mixture energy and $\tau > 0$ is a regularization parameter which can depend on all the sought functions.

¹Злотник А. А. О построении квазигазодинамических систем уравнений и баротропной системе с потенциальной массовой силой // Матем. моделир. 2012. Т. 24. № 4. С. 65-79.

These changes lead from the original Navier-Stokes-Fourier-type system (19)-(21) to its following regularized QGD version

$$\partial_t \rho_k + \operatorname{div}(\rho_k(\mathbf{u} - \mathbf{w}_k)) = 0, \quad k = 1, 2,$$

$$\partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho(\mathbf{u} - \mathbf{w}) \otimes \mathbf{u}) + \nabla p = \operatorname{div}(\Pi^{NS} + \Pi^\tau) + (\rho - \tau \operatorname{div}(\rho \mathbf{u})) \mathbf{f},$$

$$\partial_t E + \operatorname{div}((E + p)(\mathbf{u} - \mathbf{w})) = \operatorname{div}(-\mathbf{q}^F - \mathbf{q}^\tau + (\Pi^{NS} + \Pi^\tau)\mathbf{u}) + \rho(\mathbf{u} - \mathbf{w}) \cdot \mathbf{f},$$

the unknown functions are the same. The regularizing velocities

$$\mathbf{w}_k := \frac{\tau}{\rho_k} \operatorname{div}(\rho_k \mathbf{u}) \mathbf{u} + \hat{\mathbf{w}}, \quad \hat{\mathbf{w}} = \tau \left((\mathbf{u} \cdot \nabla) \mathbf{u} + \frac{1}{\rho} \nabla p - \mathbf{f} \right), \quad (25)$$

$$\mathbf{w} := \left\langle \frac{\rho_k}{\rho} \mathbf{w}_k \right\rangle = \frac{\tau}{\rho} \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u} + \nabla p - \rho \mathbf{f}) = \frac{\tau}{\rho} \operatorname{div}(\rho \mathbf{u}) \mathbf{u} + \hat{\mathbf{w}}, \quad (26)$$

with $k = 1, 2$, the regularizing viscous stress and heat flux

$$\Pi^\tau := \rho \mathbf{u} \otimes \hat{\mathbf{w}} + \tau (\mathbf{u} \cdot \nabla p + \rho c_s^2 \operatorname{div} \mathbf{u}) \mathbb{I}, \quad (27)$$

$$-\mathbf{q}^\tau := \tau \left(\mathbf{u} \cdot \left(\rho \nabla \varepsilon - \frac{p}{\rho} \nabla \rho \right) \right) \mathbf{u}. \quad (28)$$

Finite-difference scheme

Further, we consider the 1D case with $\Omega = (-X, X)$ and define the main and auxiliary uniform meshes

$$\bar{\omega}_h = \{x_i = -X + ih; 0 \leq i \leq N\},$$

$$\omega_h^* = \{x_{i+1/2} = -X + (i + 0.5)h; 0 \leq i \leq N - 1\},$$

on $[-X, X]$, with the step $h = 2X/N$. Let $\omega_h = \bar{\omega}_h \setminus \{-X, X\}$.

We also define the nonuniform mesh $\bar{\omega}^{\Delta t} = \{t_0 = 0 < t_1 < \dots < t_m = t_{fin}\}$ in time, with the steps $\Delta t_m = t_{m+1} - t_m$. Let $\check{\omega}^{\Delta t} = \bar{\omega}^{\Delta t} \setminus \{t_{fin}\}$.

Denote by $H(\omega)$ the space of functions given on a mesh ω .

For $v \in H(\bar{\omega}_h)$, $w \in H(\omega_h^*)$ and $y \in H(\bar{\omega}^\tau)$, we introduce the averages and difference quotients

$$[v]_{i+1/2} = 0.5(v_i + v_{i+1}), \quad v_{i+1/2} = \frac{v_{i+1} - v_i}{h},$$

$$[w]_i^* = 0.5(w_{i-1/2} + w_{i+1/2}), \quad \delta^* w_i = \frac{w_{i+1/2} - w_{i-1/2}}{h}, \quad \delta_t y^m = \frac{y^{m+1} - y^m}{\Delta t_m},$$

where $v_i = v(x_i)$, $w_{i+1/2} = w(x_{i+1/2})$ and $y^m = y(t_m)$.

For the regularized QGD balance PDEs in the 1D case, we construct the explicit two-level in time and **symmetric three-point in space** discrete balance Eqs. **without limiters** for the mass of the components and the momentum and total energy of the gas mixture

$$\delta_t \rho_k + \delta^*([\rho_k]([u] - w_k)) = 0, \quad k = 1, 2, \quad (29)$$

$$\delta_t(\rho u) + \delta^*([\rho]([u] - w)[u] + [p]) = \delta^* \Pi, \quad (30)$$

$$\begin{aligned} \delta_t \left(\frac{1}{2} \rho u^2 + \rho \varepsilon \right) + \delta^* \left\{ \left(\frac{1}{2} [\rho] u_- u_+ + [\rho \varepsilon] + [p] \right) ([u] - w) - \frac{1}{4} h^2 (\delta p) \delta u \right\} \\ = \delta^* (-q + \Pi[u]) + [Q]^* \end{aligned} \quad (31)$$

on $\omega_h \times \check{\omega}^{\Delta t}$. The main sought functions $\rho_1 > 0, \rho_2 > 0, u, \varepsilon$ (in fact, $\rho \varepsilon$), and the functions p and θ , are defined on the main mesh $\bar{\omega}_h \times \bar{\omega}^{\Delta t}$.

Also p and θ (in the q -term) are given by the first formula (22) and formula (24), with $d = b^2 + 4c$ and their coefficients defined by (8), (10) and (11).

In Eq. (31), the nonstandard term $u_- u_+$ (like the geometric mean for u^2) instead of $[u^2]$ or $[u]^2$ and the additional term $-(1/4)h^2(\delta p)\delta u$ allows us to ensure a more natural form of the important discrete balance equation for the mixture internal energy without the spatial mesh imbalances.

We discretize the regularizing velocities (25)-(26) in the form

$$w_k = \frac{[\tau]}{[\rho_k]} [u] \delta(\rho_k u) + \widehat{w}, \quad \widehat{w} = \frac{[\tau]}{[\rho]} ([\rho][u] \delta u + \delta p), \quad (32)$$

$$w = \left\langle \frac{[\rho_k]}{[\rho]} w_k \right\rangle = \frac{[\tau]}{[\rho]} [u] \delta(\rho u) + \widehat{w} \quad (33)$$

with $k = 1, 2$ and the viscous stress and heat flux as follows

$$\begin{aligned} \Pi &= \nu \delta u + [u][\rho] \widehat{w} + [\tau] ([u] \delta p + [\rho c_s^2] \delta u), \\ -q &= \varkappa \delta \theta + [\tau] \left\{ \left(\delta(\rho \varepsilon) - \frac{[\rho \varepsilon] + [p]}{[\rho]} \delta \rho \right) [u]^2 \right\}. \end{aligned}$$

Here the squared speed of sound c_s^2 is given by the second formula in (17), and c_V and γ are introduced above.

The functions w_k , \widehat{w} , w , Π , $\nu = (4/3)\mu + \lambda$, q and \varkappa are defined on the auxiliary mesh $\bar{\omega}_h^* \times \bar{\omega}^{\Delta t}$, but τ is defined on $\bar{\omega}_h \times \bar{\omega}^{\Delta t}$.

We take τ , ν and \varkappa in the form

$$\tau = \frac{ah}{c_s}, \quad \nu = a_S[\tau][p], \quad \varkappa = a_{Pr}[\tau][c_p][p]$$

that is formally analogous to the single-component gas case.

So τ is h -dependent, ν and \varkappa are artificial viscosity coefficients, with the parameter $a > 0$, the Schmidt and inverse Prandtl numbers for the mixture $a_S \geq 0$ and $a_{Pr} > 0$ used as adjusting numerical parameters.

For the QGD regularization, in many tests, $a_S = 0$ is possible.

The initial data $(\rho_1, \rho_2, u, \rho\varepsilon) = (\rho_1^0, \rho_2^0, u^0, (\rho\varepsilon)^0)$ (or equivalent ones) are given on $\bar{\omega}_h$.

Below the time steps are chosen automatically according to the formulas

$$\Delta t_m = \frac{\beta h}{\max_i (c_{si}^m + |u_i^m|)}, \quad 0 \leq m < \bar{m} - 1,$$

$$\Delta t_{\bar{m}-1} = t_{fin} - t_{\bar{m}-1} \leq \frac{\beta h}{\max_i (c_{si}^{\bar{m}-1} + |u_i^{\bar{m}-1}|)},$$

where $\beta > 0$ is the Courant-type parameter.

Test B. Water-to-air shock tube problem

Таблица 1: Stiffened gas parameters

Substance	γ	c_V , J/(kg K)	p_* , Pa	ϵ_0 , J/kg
Air	1.4	720	0	0
Water	2.8	1495	$8.5 \cdot 10^8$	0

In this test ², we have a 10 m long tube separated into two halves, both of which contain a mixture of air and water but in different proportions, with

$$(p_0, u_0, \theta_0) = \begin{cases} (2 \cdot 10^7 \text{ Pa}, 0 \text{ m/s}, 308.15 \text{ K}), & -5 \leq x < 0 \\ (10^7 \text{ Pa}, 0 \text{ m/s}, 308.15 \text{ K}), & 0 < x \leq 5 \end{cases},$$

and we have $\alpha_1 = 0.25$ in the left half and $\alpha_1 = 0.75$ in the right half. Notice that $a = 2$ is taken, thus, $a > 1$.

²Q. Li, S. Fu, A gas-kinetic BGK scheme for gas-water flow, *Comput. Math. Appl.* **61**, 3639–3652 (2011).

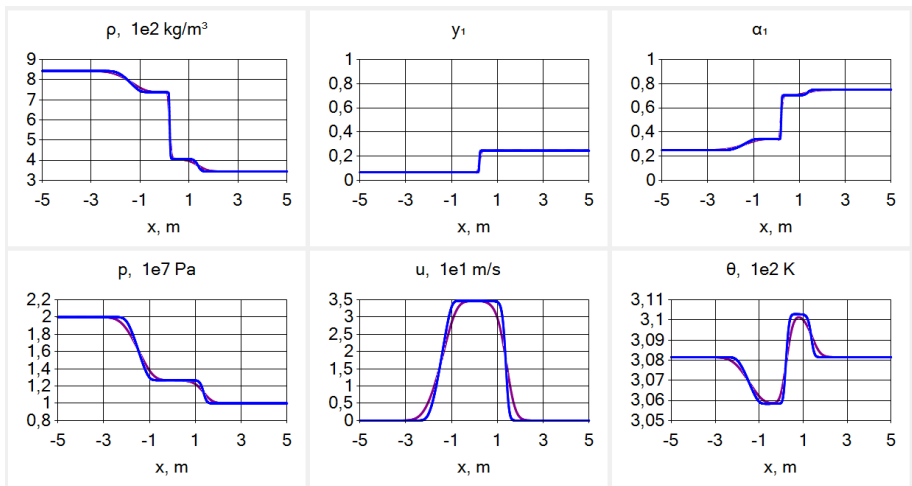


Рис. 1: Numerical results for water-to-air shock tube (test B) for $N = 500$ (dark magenta), 2500 (blue), $a = 2$ and $\beta = 0.1$, $t_{fin} = 6$ ms (the QGD regularization)