ISSN 0965-5425, Computational Mathematics and Mathematical Physics, 2019, Vol. 59, No. 11, pp. 1832–1847. © Pleiades Publishing, Ltd., 2019.
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Regularized Equations for Numerical Simulation of Flows of Homogeneous Binary Mixtures of Viscous Compressible Gases

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Received June 26, 2019; revised June 26, 2019; accepted July 8, 2019

Abstract—Regularized equations for binary mixtures of viscous compressible gases (in the absence of chemical reactions) are considered. Two new simpler systems of equations are constructed for the case of a homogeneous mixture, when the velocities and temperatures of the components coincide. In the case of moderately rarefied gases, such a system is obtained by aggregating previously derived general equations for binary mixtures of polyatomic gases. In the case of relatively dense gases, the regularizing terms in these equations are subjected to a further substantial modification. For both cases, balance equations for the total mass, kinetic, and internal energy and new balance equations for total entropy are derived from the constructed equations; additionally, the entropy production is proved to be non-negative. As an example of successful use of the new equations, the two-dimensional Rayleigh–Taylor instability of relatively dense gas mixtures is numerically simulated in a wide range of Atwood numbers.

Keywords: homogeneous binary mixture of compressible gases, regularized equations, entropy balance equation, Rayleigh–Taylor instability, computer simulation

DOI: 10.1134/S0965542519110058

INTRODUCTION

Most gaseous substances found in nature are mixtures of different gases, so the description of flows of gas mixtures is clearly of interest to researchers. There is a wide variety of mathematical models for describing flows of mixtures of compressible gases [1–5]. Even wider is the variety of numerical algorithms intended for computer simulation of such flows. New approaches to the numerical simulation of mixture flows are of both theoretical and practical interest. In this paper, we describe and test a new approach of this kind.

A mathematical model frequently used to describe flows of gas mixture is an Eulerian-type model of a homogeneous mixture consisting of mass balance equations for each of components of the mixture, together with balance equations for momentum and total energy of the mixture as a whole (rather than of individual components). Various numerical methods can be used to implement this model. The mutual diffusion of the gases involved is not taken into account in these mathematical models and numerical methods (see, e.g., [5]). Accordingly, special algorithms for describing the boundary between the species of the mixture are applied, if necessary. Models taking into account diffusive mass fluxes for the species of the mixture can be found, for example, in [2–4].

A model kinetic equation was used in [6, 7] to construct a regularized or quasi-gasdynamic (QGD), system of equations for describing flows of binary gas mixture (for more detail on QGD models of one-component gases, see [7, 8]). It was assumed that each component of the gas mixture has its own density, velocity, and temperature. In the absence of chemical reactions (cold gas approximation), there were no exchange terms in the mass balance equations for the components, while the momentum and total energy balance equations for each components contained such terms, which described the interaction between the components of the mixture. The form of the exchange terms was based on that in kinetic equations, and the gases were assumed to be monatomic. Therefore, these QGD equations for mixtures were

intended for describing simple monatomic gases. This system of equations was tested by computing one-dimensional rarefied gas flows, namely, the problem of a stationary shock wave and the gas flow between two tanks. The results were compared with those based on direct simulation Monte Carlo computations [9] and were found sufficiently accurate. Additional applications were given in [10].

These equations were used in [7] to construct a homogeneous (one-fluid) approximation, assuming that all components of the mixture have identical velocities and temperatures. Moreover, the adiabatic exponents γ and the Prandtl numbers α_{Pr} of the components were also assumed to be identical and the internal energy of the mixture was not introduced in explicit form. The performance of this model was also tested as applied to the same two problems.

In [11] the exchange terms in the QGD system were generalized to the case of polyatomic gas flows with arbitrary γ and α_{Pr}. Additionally, the QGD equations for a gas mixture were written in a different form that is more conventional for gas dynamics, which is especially convenient for their subsequent discretization. It was also shown in [11] that the QGD system for a gas mixture satisfies the total energy conservation law and has a nondecreasing total entropy. A physical interpretation of the proposed generalization of the exchange terms was given in [12].

The application of the complete QGD system to flow simulation for mixtures of rather dense gases showed that, with an increasing number of intermolecular collisions, the exchange terms in the equations grow rapidly, which means that the temperatures and velocities of the components quickly equalize and there is a possibility of passing to a homogeneous mixture in the model. Moreover, the use of the complete QGD system led to computational instability, so the homogeneous model seems preferable from both physical and computational points of view.

In this paper, firstly a system of equations for a homogeneous binary mixture of polyatomic gases is constructed by aggregating the equations from [11]. The resulting model has the following properties: natural formulas (involving the component concentrations) hold for the specific heat capacities, the adiabatic index, and the total pressure of the mixture; the mass balance equations for each component involve regularizing diffusive fluxes for the components of the mixture; natural balance equations for the total mass and total kinetic and internal energy of the mixture are satisfied; they are used to derive a new balance equation for the total entropy of a binary gas mixture with a nonnegative entropy production (Theorem 1); this model is quite easy to implement numerically by using the corresponding implementation of the one-component gas model; and the model can be naturally generalized to a larger number of gas components in the mixture.

However, attempts to use this model in numerical simulation of homogeneous binary mixtures of relatively dense gases, for example, in the Rayleigh–Taylor instability problem have revealed a rather high numerical diffusion in the component mass balance equations caused by the large jumps in the component pressure. Accordingly, the regularizing terms in all equations of motion for such gas mixtures were substantially modified. As a result, another regularized system of equations for a homogeneous binary mixture was constructed for the case of relatively dense gases. Note that this modification has some elements similar to a substantially simpler (than in this paper) quasi-hydrodynamic regularization in flow problems for a binary (i.e., two-component) mixture under small variations in total density, but with additional allowance for interphase effects (described by the Navier–Stokes–Cahn–Hilliard equations for a compressible fluid) [13, 14]. The second system of equations constructed in this paper mainly preserves the above-noted properties of the first one, but involves only total regularizing diffusive fluxes. It should be emphasized that the total entropy balance equation for the mixture again holds together with a nonnegative entropy production (Theorem 2). Note that the equation itself differs substantially from its counterpart in the first system of equations. The indicated property is of key importance, since it ensures the physical consistency of the model. It was not simple to achieve this property in such a regularization for mixtures.

The simulation of Rayleigh–Taylor instability arising in the gravity field at the interface between a heavy and a light gas (the latter being beneath the former) is often used as a test in order to analyze the properties of mathematical and numerical mixture models. Another type of test problem is Richtmyer–Meshkov instability arising when a shock wave propagates through the interface of two gases. Both types of instability were extensively overviewed in the recent paper [15]. A numerical study and a detailed analysis of results concerning Rayleigh–Taylor instability for compressible gases can be found in [16]. In this work, we focus on gravitational instability, including examples like those presented in [16]. An important point is that various binary mixtures are numerically simulated in the entire range (0,1) of the Atwood number, which characterizes the difference in the molecular weights of the components in the mixture.

1. REGULARIZED EQUATIONS OF MOTION FOR GENERAL AND HOMOGENEOUS BINARY MIXTURES OF MODERATELY RAREFIED GASES

1.1. Following [11], the regularized QGD system of equations for a binary mixture of moderately rarefied gases consists of the following mass, momentum, and total energy balance equations for gases $\alpha = a, b$:

$$\partial_t \rho_\alpha + \operatorname{div}[\rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha)] = 0, \tag{1.1}$$

$$\partial_t(\rho_\alpha \mathbf{u}_\alpha) + \operatorname{div}[\rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha) \otimes \mathbf{u}_\alpha] + \nabla p_\alpha = \operatorname{div}\Pi_\alpha + [\rho_\alpha - \tau \operatorname{div}(\rho_\alpha \mathbf{u}_\alpha)]\mathbf{F}_\alpha + \mathbf{S}_{u,\alpha}, \tag{1.2}$$

$$\partial_t E_\alpha + \operatorname{div}[(E_\alpha + p_\alpha)(\mathbf{u}_\alpha - \mathbf{w}_\alpha)] = \operatorname{div}(-\mathbf{q}_\alpha + \Pi_\alpha \mathbf{u}_\alpha) + \rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha) \cdot \mathbf{F}_\alpha + Q_\alpha + S_{E,\alpha}. \tag{1.3}$$

Here and below, ∂_t and ∂_i denote partial derivatives with respect to t and x_i; the operators div and ∇ are taken with respect to the spatial coordinates $x = (x_1, \ldots, x_n)$, where $n = 1, 2, 3$ (the divergence of a tensor is taken with respect to its first index); and $\otimes$ and $\cdot$ denote the tensor and scalar product of vectors, respectively.

The basic sought functions are $\rho_\alpha > 0$, $\mathbf{u}_\alpha = (u_{1\alpha}, \ldots, u_{n\alpha})$, and $\theta_\alpha > 0$, i.e., the density, velocity, and absolute temperature of gas α, which depend on (x, t). Additionally, we deal with the total energy, pressure, and specific internal energy of gas α, which is assumed to be perfect and polytropic:

$$E_\alpha = \frac{1}{2}\rho_\alpha |\mathbf{u}_\alpha|^2 + \rho_\alpha \varepsilon_\alpha, \quad p_\alpha = R_\alpha \rho_\alpha \theta_\alpha, \quad \varepsilon_\alpha = c_{V\alpha}\theta_\alpha. \tag{1.4}$$

Here, $R_\alpha = R_0/M_\alpha > 0$ is a constant, where R_0 is the universal gas constant and M_α is the molecular weight, and $c_{V\alpha}$ is the specific heat at constant volume. The pressure can also be written as

$$p_\alpha = (\gamma_\alpha - 1)\rho_\alpha \varepsilon_\alpha, \quad \gamma_\alpha = \frac{c_{p\alpha}}{c_{V\alpha}} = \frac{R_\alpha}{c_{V\alpha}} + 1,$$

where γ_α is the adiabatic index and $c_{p\alpha}$ is the specific heat at constant pressure.

In these equations, $\Pi_\alpha = \Pi_\alpha^{NS} + \Pi_\alpha^{\tau}$ is the viscous stress tensor, where Π_α^{NS} is the classical Navier–Stokes viscous stress tensor:

$$\Pi_\alpha^{NS} \equiv \Pi_\alpha^{NS}(\mathbf{u}_\alpha) = \mu_\alpha[2\mathbb{D}(\mathbf{u}_\alpha) - \frac{2}{3}(\operatorname{div}\mathbf{u}_\alpha)\mathbb{I}] + \lambda_\alpha(\operatorname{div}\mathbf{u}_\alpha)\mathbb{I}, \quad \mathbb{D}_{ij}(\mathbf{u}_\alpha) = \frac{1}{2}(\partial_i u_{j\alpha} + \partial_j u_{i\alpha}) \tag{1.5}$$

with dynamic viscosity $\mu_\alpha = \mu_\alpha(\rho_\alpha, \theta_\alpha) > 0$, bulk viscosity $\lambda_\alpha = \lambda_\alpha(\rho_\alpha, \theta_\alpha) \geq 0$, and unit tensor $\mathbb{I}$ (of order n). Additionally,

$$\Pi_\alpha^{\tau} = \rho_\alpha \mathbf{u}_\alpha \otimes \hat{\mathbf{w}}_\alpha + \tau[\mathbf{u}_\alpha \cdot \nabla p_\alpha + \gamma_\alpha p_\alpha \operatorname{div}\mathbf{u}_\alpha - (\gamma_\alpha - 1)Q_\alpha]\mathbb{I} \tag{1.6}$$

is a regularizing tensor. Note that, in the last formula, $\gamma_\alpha p_\alpha = c_{s\alpha}^2 \rho_\alpha$, where $c_{s\alpha}^2 = \gamma_\alpha(\gamma_\alpha - 1)\varepsilon_\alpha$ is the squared speed of sound of the component α. The quantities $\mathbf{F}_\alpha$ and $Q_\alpha \geq 0$ are the body force density and the heat source strength, which are assumed to be given, and $\tau > 0$ is a relaxation parameter that may depend on all the sought functions ρ_a, $\mathbf{u}_a$, θ_a and ρ_b, $\mathbf{u}_b$, θ_b.

The quantities $\mathbf{S}_{u,\alpha}$ and $S_{E,\alpha}$ are exchange terms; they depend on all sought functions and relate the equations for the gases a and b. They are such that

$$\mathbf{S}_{u,a} + \mathbf{S}_{u,b} = 0, \quad S_{E,a} + S_{E,b} = 0. \tag{1.7}$$

Expressions for $\mathbf{S}_{u,\alpha}$ and $S_{E,\alpha}$ can be found in [11] (see also the physical motivation in [12]). In what follows, they are not used and, for this reason, are omitted.

The regularizing velocities $\mathbf{w}_\alpha$ and $\hat{\mathbf{w}}_\alpha$ are given by

$$\mathbf{w}_\alpha = \frac{\tau}{\rho_\alpha}[\operatorname{div}(\rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha) + \nabla p_\alpha - \rho_\alpha \mathbf{F}_\alpha], \quad \hat{\mathbf{w}}_\alpha = \frac{\tau}{\rho_\alpha}[\rho_\alpha(\mathbf{u}_\alpha \cdot \nabla)\mathbf{u}_\alpha + \nabla p_\alpha - \rho_\alpha \mathbf{F}_\alpha], \tag{1.8}$$

where $\rho_\alpha(\mathbf{u}_\alpha - \mathbf{w}_\alpha)$ is the mass flux density of gas α.

The heat flux $\mathbf{q}_\alpha$ can be expressed by the formulas

$$-\mathbf{q}_\alpha = \varkappa_\alpha \nabla\theta_\alpha - \mathbf{q}_\alpha^{\tau}, \tag{1.9}$$

$$-\mathbf{q}_\alpha^\tau = \tau\left[\rho_\alpha \mathbf{u}_\alpha \cdot \left(\nabla\varepsilon_\alpha - \frac{p_\alpha}{\rho_\alpha^2}\nabla\rho_\alpha\right) - Q_\alpha\right]\mathbf{u}_\alpha = \tau[\mathbf{u}_\alpha \cdot (c_{V\alpha}\rho_\alpha\nabla\theta_\alpha - R_\alpha\theta_\alpha\nabla\rho_\alpha) - Q_\alpha]\mathbf{u}_\alpha, \tag{1.10}$$

where $\varkappa_\alpha = \varkappa_\alpha(\rho_\alpha, \theta_\alpha) > 0$ is the thermal conductivity and $\mathbf{q}_\alpha^\tau$ is a regularizing heat flux.

The regularized equations can involve physical or artificial viscosity and thermal conductivity coefficients. The artificial coefficients are usually given by the formulas (see [7])

$$\mu_\alpha = \alpha_{S\alpha}\tau p_\alpha, \quad \lambda_\alpha = 0, \quad \varkappa_\alpha = \frac{\gamma_\alpha c_{V\alpha}}{\alpha_{\mathrm{Pr}\,\alpha}}\tau p_\alpha, \tag{1.11}$$

where $\alpha_{S\alpha} > 0$ and $\alpha_{\mathrm{Pr}\alpha} > 0$ are the Schmidt and Prandtl numbers of the component α, respectively.

The above-presented system of regularized equations for a binary mixture is rather complicated and contains $2(n+2)$ sought scalar functions ρ_α, $\mathbf{u}_\alpha = (u_{1\alpha}, \ldots, u_{n\alpha})$, and θ_α for $\alpha = a, b$. Therefore, simplified models of a binary mixture flow are of practical interest.

1.2. For a *homogeneous* binary mixture, we set $\mathbf{u}_a = \mathbf{u}_b = \mathbf{u}$ and $\theta_a = \theta_b = \theta$ (see [1]). Additionally, let $\mathbf{F}_a = \mathbf{F}_b = \mathbf{F}$. The equations of motion for a such mixture are derived by aggregating the equations written above for $\alpha = a, b$. The mass balance equation (1.1) is rewritten as

$$\partial_t\rho_\alpha + \operatorname{div}[\rho_\alpha(\mathbf{u} - \mathbf{w}^{(\alpha)})] = 0, \quad \alpha = a, b, \tag{1.12}$$

by setting

$$\mathbf{w}^{(\alpha)} = \frac{\tau}{\rho_\alpha}[\operatorname{div}(\rho_\alpha\mathbf{u}\otimes\mathbf{u}) + \nabla p_\alpha - \rho_\alpha\mathbf{F}], \quad p_\alpha = R_\alpha\rho_\alpha\theta, \quad \hat{\mathbf{w}}^{(\alpha)} = \frac{\tau}{\rho_\alpha}[\rho_\alpha(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p_\alpha - \rho_\alpha\mathbf{F}];$$

the quantity $\hat{\mathbf{w}}^{(\alpha)}$ will be used later.

Introducing the total density $\rho = \rho_a + \rho_b$ and the total pressure $p = p_a + p_b$ and summing the momentum balance equations of form (1.2) with $\mathbf{u}_a = \mathbf{u}_b = \mathbf{u}$ and $\theta_a = \theta_b = \theta$ over $\alpha = a, b$, we obtain the following aggregated momentum balance equation of the homogeneous mixture:

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}[\rho(\mathbf{u} - \mathbf{w})\otimes\mathbf{u}] + \nabla p = \operatorname{div}\Pi + [\rho - \tau\operatorname{div}(\rho\mathbf{u})]\mathbf{F}. \tag{1.13}$$

Here, the total regularizing velocities and the terms in the viscous stress tensor $\Pi = \Pi^{NS} + \Pi^\tau$ are given by

$$\mathbf{w} := \frac{\rho_a}{\rho}\mathbf{w}^{(a)} + \frac{\rho_b}{\rho}\mathbf{w}^{(b)} = \frac{\tau}{\rho}[\operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p - \rho\mathbf{F}], \tag{1.14}$$

$$\hat{\mathbf{w}} := \frac{\rho_a}{\rho}\hat{\mathbf{w}}^{(a)} + \frac{\rho_b}{\rho}\hat{\mathbf{w}}^{(b)} = \frac{\tau}{\rho}[\rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \rho\mathbf{F}], \tag{1.15}$$

$$\begin{gathered}\Pi^{NS} := \Pi_a^{NS}(\mathbf{u}) + \Pi_b^{NS}(\mathbf{u}) = (\mu_a + \mu_b)\left[2\mathbb{D}(\mathbf{u}) - \frac{2}{3}(\operatorname{div}\mathbf{u})\mathbb{I}\right] + (\lambda_a + \lambda_b)(\operatorname{div}\mathbf{u})\mathbb{I},\\ \Pi^\tau := \Pi_a^\tau + \Pi_b^\tau = \rho\mathbf{u}\otimes\hat{\mathbf{w}} + \tau[\mathbf{u}\cdot\nabla p + (\gamma_a p_a + \gamma_b p_b)\operatorname{div}\mathbf{u} - (\gamma_a Q_a + \gamma_b Q_b) + Q]\mathbb{I}\end{gathered} \tag{1.16}$$

with $Q := Q_a + Q_b$; here, we took into account the important (though obvious) property that the regularizing momenta are additive:

$$\rho\mathbf{w} = \rho_a\mathbf{w}^{(a)} + \rho_b\mathbf{w}^{(b)}, \quad \rho\hat{\mathbf{w}} = \rho_a\hat{\mathbf{w}}^{(a)} + \rho_b\hat{\mathbf{w}}^{(b)}. \tag{1.17}$$

The total specific internal energy and the total heat capacity at constant volume are defined as

$$\varepsilon := \frac{\rho_a}{\rho}\varepsilon_a + \frac{\rho_b}{\rho}\varepsilon_b = c_V\theta, \quad c_V := \frac{\rho_a}{\rho}c_{Va} + \frac{\rho_b}{\rho}c_{Vb}. \tag{1.18}$$

Summing the total energy balance equations of form (1.3) with $\mathbf{u}_a = \mathbf{u}_b = \mathbf{u}$ and $\theta_a = \theta_b = \theta$ over $\alpha = a, b$, we obtain the following aggregated total energy balance equation of a homogeneous mixture:

$$\begin{gathered}\partial_t E + \operatorname{div}\left[\frac{1}{2}\rho|\mathbf{u}|^2(\mathbf{u} - \mathbf{w}) + (\rho_a\varepsilon_a + p_a)(\mathbf{u} - \mathbf{w}^{(a)}) + (\rho_b\varepsilon_b + p_b)(\mathbf{u} - \mathbf{w}^{(b)})\right]\\ = \operatorname{div}(-\mathbf{q} + \Pi\mathbf{u}) + \rho(\mathbf{u} - \mathbf{w})\cdot\mathbf{F} + Q.\end{gathered} \tag{1.19}$$

Here, the total energy, heat flux, and its regularizing component are given by the formulas

$$E = \frac{1}{2}\rho|\mathbf{u}|^2 + \rho\varepsilon, \quad -\mathbf{q} := -\mathbf{q}_a - \mathbf{q}_b = (\varkappa_a + \varkappa_b)\nabla\theta - \mathbf{q}^\tau, \tag{1.20}$$

$$-\mathbf{q}^\tau := -\mathbf{q}_a^\tau - \mathbf{q}_b^\tau = \tau\{\mathbf{u}\cdot[c_V\rho\nabla\theta - \theta(R_a\nabla\rho_a + R_b\nabla\rho_b)] - Q\}\mathbf{u}, \tag{1.21}$$

where we took into account the additivity of ρ, $\rho\varepsilon$, $c_V\rho$, and $\rho\mathbf{w}$. The exchange terms in Eqs. (1.13) and (1.19) canceled out by virtue of properties (1.7).

The derived system of regularized equations for a homogeneous binary mixture is much simpler than the original system and contains only $n + 3$ sought scalar functions ρ_a, ρ_b, $\mathbf{u} = (u_1, \ldots, u_n)$, and θ.

Additionally, the total heat capacities at constant pressure, gas constant, and adiabatic index can be introduced using the formulas

$$c_p := \frac{\rho_a}{\rho}c_{pa} + \frac{\rho_b}{\rho}c_{pb}, \quad R := \frac{\rho_a}{\rho}R_a + \frac{\rho_b}{\rho}R_b = c_p - c_V, \quad \gamma := \frac{c_p}{c_V}. \tag{1.22}$$

Then $\gamma - 1 = R/c_V$ and, hence, other natural formulas hold for the pressure of the mixture

$$p = R\rho\theta = (\gamma - 1)\rho\varepsilon. \tag{1.23}$$

To avoid misunderstanding, the following remark has to be made: although the formulas for a homogeneous binary mixture are similar in form to the equations of state of a homogeneous perfect polytropic gas, the quantities R, c_p, c_V, and γ in the former are not constants, but rather functions of the component concentrations ρ_a/ρ and $\rho_b/\rho = 1 - \rho_a/\rho$.

In (1.16) and (1.19), we can use the formulas

$$\gamma_a p_a + \gamma_b p_b = \rho c_s^2, \quad c_s^2 = \frac{\rho_a}{\rho}c_{sa}^2 + \frac{\rho_b}{\rho}c_{sb}^2, \tag{1.24}$$

$$(\rho_a\varepsilon_a + p_a)(\mathbf{u} - \mathbf{w}^{(a)}) + (\rho_b\varepsilon_b + p_b)(\mathbf{u} - \mathbf{w}^{(b)}) = c_{pa}\rho_a\theta(\mathbf{u} - \mathbf{w}^{(a)}) + c_{pb}\rho_b\theta(\mathbf{u} - \mathbf{w}^{(b)}). \tag{1.25}$$

Here, c_s^2 plays the role of the squared speed of sound of the mixture.

Note that, in the aggregation procedure, some quantities are taken additively, i.e., they are summed up (e.g., ρ_α, p_α, etc.), while others are taken as linear combinations with concentrations ρ_α/ρ used as weights (e.g., $\mathbf{w}^{(\alpha)}$, ε_α, etc.).

For control of the result, we note that, in the simplest case of gases with identical $c_{V\alpha}$ and $c_{p\alpha}$, we have

$$c_V = c_{V\alpha}, \quad c_p = c_{p\alpha}, \quad R = R_\alpha, \quad \gamma = \gamma_\alpha, \quad \alpha = a, b.$$

As a consequence, $\varepsilon = \varepsilon_\alpha = c_V\theta$ and, in view of formulas (1.17), the total energy balance equation and the expression for $\mathbf{q}^\tau$ take the standard form for a one-component gas:

$$\partial_t E + \operatorname{div}[(E + p)(\mathbf{u} - \mathbf{w})] = \operatorname{div}(-\mathbf{q} + \Pi\mathbf{u}) + \rho(\mathbf{u} - \mathbf{w})\cdot\mathbf{F} + Q,$$
$$-\mathbf{q}^\tau = \tau[\mathbf{u}\cdot(c_V\rho\nabla\theta - R\theta\nabla\rho) - Q]\mathbf{u},$$

cf. (1.3) and (1.10) (here, Π and $\mathbf{q}$ involve the total viscosity and thermal conductivity coefficients).

For $\tau = 0$ (without using formulas (1.11)), the resulting system (1.12), (1.13), (1.19) turns into the Navier–Stokes-type equations for the binary mixture:

$$\partial_t\rho_\alpha + \operatorname{div}(\rho_\alpha\mathbf{u}) = 0, \quad \alpha = a, b, \tag{1.26}$$

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p = \operatorname{div}\Pi^{NS} + \rho\mathbf{F}, \tag{1.27}$$

$$\partial_t E + \operatorname{div}[(E + p)\mathbf{u}] = \operatorname{div}(-\mathbf{q} + \Pi^{NS}\mathbf{u}) + \rho\mathbf{u}\cdot\mathbf{F} + Q, \tag{1.28}$$

where p, Π^{NS}, Q, and $-\mathbf{q} = (\varkappa_a + \varkappa_b)\nabla\theta$ were introduced above. If $\mu_\alpha = \lambda_\alpha = \varkappa_\alpha = 0$, then we obtain a system of Euler-type equations for the binary mixture, namely,

$$\partial_t\rho_\alpha + \operatorname{div}(\rho_\alpha\mathbf{u}) = 0, \quad \partial_t(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla p = \rho\mathbf{F}, \quad \partial_t E + \operatorname{div}[(E + p)\mathbf{u}] = \rho\mathbf{u}\cdot\mathbf{F} + Q.$$

From the obtained regularized equations, we derive a set of consequences of standard type. Adding Eqs. (1.12) over α and taking into account the additivity of ρ and $\rho\mathbf{w}$ yields the natural total density balance equation

$$\partial_t\rho + \operatorname{div}[\rho(\mathbf{u}-\mathbf{w})] = 0. \tag{1.29}$$

It can be used as an equivalent substitute for one of the component mass balance equations in (1.12). This substitution is often used for numerically solving of such systems of equations.

Taking the inner product of the momentum balance equation (1.13) and $\mathbf{u}$ and applying the product rule and Eq. (1.29), we derive the kinetic energy balance equation

$$\partial_t\left(\frac{1}{2}\rho|\mathbf{u}|^2\right) + \operatorname{div}\left[\frac{1}{2}\rho|\mathbf{u}|^2(\mathbf{u}-\mathbf{w})\right] + \nabla p\cdot\mathbf{u} = \operatorname{div}\Pi\cdot\mathbf{u} + (\rho - \tau\operatorname{div}(\rho\mathbf{u}))\mathbf{F}\cdot\mathbf{u}. \tag{1.30}$$

Subtracting the last equation from the total energy balance equation (1.19) and taking into account the formula $\rho\mathbf{w} = \tau\operatorname{div}(\rho\mathbf{u})\mathbf{u} + \rho\hat{\mathbf{w}}$ lead to the internal energy balance equation

$$\begin{gathered}\partial_t(\rho\varepsilon) + \operatorname{div}(\rho\varepsilon\mathbf{u} - \rho_a\varepsilon_a\mathbf{w}^{(a)} - \rho_b\varepsilon_b\mathbf{w}^{(b)}) + p\operatorname{div}\mathbf{u} - \operatorname{div}(p_a\mathbf{w}^{(a)} + p_b\mathbf{w}^{(b)}) \\ = -\operatorname{div}\mathbf{q} + \Pi : \nabla\mathbf{u} - \rho\hat{\mathbf{w}}\cdot\mathbf{F} + Q,\end{gathered} \tag{1.31}$$

where $\nabla\mathbf{u} = \{\partial_i u_j\}_{i,j=1}^n$ and : denotes the scalar product of tensors.

The entropies of the species α and the mixture are defined as

$$s_\alpha = S_{0\alpha} - R_\alpha\ln\rho_\alpha + c_{V\alpha}\ln\varepsilon_\alpha, \quad \alpha = a, b, \quad s = \frac{\rho_a}{\rho}s_a + \frac{\rho_b}{\rho}s_b, \tag{1.32}$$

where $S_{0\alpha} = \text{const}$. Let $|\mathbb{D}(\mathbf{u})|^2 = \mathbb{D}(\mathbf{u}) : \mathbb{D}(\mathbf{u})$.

Theorem 1. *The following regularized entropy balance equation for a homogeneous binary mixture of moderately rarefied gases holds*:

$$\partial_t(\rho s) + \operatorname{div}[\rho s\mathbf{u} - (\rho_a s_a\mathbf{w}^{(a)} + \rho_b s_b\mathbf{w}^{(b)})] = \operatorname{div}\left(-\frac{\mathbf{q}}{\theta}\right) + \mathcal{P}^{NS} + \mathcal{P}_a^\tau + \mathcal{P}_b^\tau, \tag{1.33}$$

with entropy production $\mathcal{P}^{NS} + \mathcal{P}_a^\tau + \mathcal{P}_b^\tau$, *where*

$$\mathcal{P}^{NS} = 2\frac{\mu_a+\mu_b}{\theta}|\mathbb{D}(\mathbf{u})|^2 + \left(\lambda_a + \lambda_b - \frac{2}{3}(\mu_a+\mu_b)\right)\frac{1}{\theta}(\operatorname{div}\mathbf{u})^2 + \frac{\varkappa_a+\varkappa_b}{\theta^2}|\nabla\theta|^2 \geq 0, \tag{1.34}$$

$$\begin{gathered}\mathcal{P}_\alpha^\tau = \tau\frac{\rho_\alpha}{\theta}\left|\frac{\hat{\mathbf{w}}^{(\alpha)}}{\tau}\right|^2 + \tau\frac{R_\alpha}{\rho_\alpha}[\operatorname{div}(\rho_\alpha\mathbf{u})]^2 \\ + \tau c_{V\alpha}\rho_\alpha\left[\mathbf{u}\cdot\nabla\ln\theta + (\gamma_\alpha - 1)\operatorname{div}\mathbf{u} - \frac{(\gamma_\alpha-1)Q_\alpha}{2p_\alpha}\right]^2 + \frac{Q_\alpha}{\theta}\left(1 - \frac{\tau(\gamma_\alpha-1)Q_\alpha}{4p_\alpha}\right),\end{gathered} \tag{1.35}$$

moreover, $\mathcal{P}_\alpha^\tau \geq 0$ *if* $\tau(\gamma_\alpha - 1)Q_\alpha \leq 4p_\alpha$ *for* $\alpha = a, b$.

Proof. Clearly, taking into account the additivity of ρs and using the component mass balance equation (1.12), we have

$$\begin{gathered}\partial_t(\rho s) + \operatorname{div}[\rho s\mathbf{u} - (\rho_a s_a\mathbf{w}^{(a)} + \rho_b s_b\mathbf{w}^{(b)})] \\ = \sum_{\alpha=a,b}\partial_t(\rho_\alpha s_\alpha) + \operatorname{div}[\rho_\alpha s_\alpha(\mathbf{u}-\mathbf{w}^{(\alpha)})] = \sum_{\alpha=a,b}\rho_\alpha[\partial_t s_\alpha + (\mathbf{u}-\mathbf{w}^{(\alpha)})\cdot\nabla s_\alpha].\end{gathered} \tag{1.36}$$

Using the definition of s_α and applying Eq. (1.12) twice yield

$$\begin{gathered}\rho_\alpha[\partial_t s_\alpha + (\mathbf{u}-\mathbf{w}^{(\alpha)})\cdot\nabla s_\alpha] \\ = \rho_\alpha\left\{-\frac{R_\alpha}{\rho_\alpha}[\partial_t\rho_\alpha + (\mathbf{u}-\mathbf{w}^{(\alpha)})\cdot\nabla\rho_\alpha] + \frac{1}{\theta}[\partial_t\varepsilon_\alpha + (\mathbf{u}-\mathbf{w}^{(\alpha)})\cdot\nabla\varepsilon_\alpha]\right\} \\ = R_\alpha\rho_\alpha\operatorname{div}(\mathbf{u}-\mathbf{w}^{(\alpha)}) + \frac{1}{\theta}\{\partial_t(\rho_\alpha\varepsilon_\alpha) + \operatorname{div}[\rho_\alpha\varepsilon_\alpha(\mathbf{u}-\mathbf{w}^{(\alpha)})]\}.\end{gathered} \tag{1.37}$$

Using the internal energy balance equation (1.31) for the mixture, applying the formula

$$-\frac{1}{\theta}\operatorname{div}\mathbf{q} = -\operatorname{div}\frac{\mathbf{q}}{\theta} + \mathbf{q}\cdot\nabla\frac{1}{\theta},$$

and performing the deaggregation of some of the above-introduced total quantities, we derive

$$\partial_t(\rho s) + \operatorname{div}[\rho s\mathbf{u} - (\rho_a s_a \mathbf{w}^{(a)} + \rho_b s_b \mathbf{w}^{(b)})] = \operatorname{div}\left(-\frac{\mathbf{q}}{\theta}\right) + \frac{1}{\theta}\Pi^{NS} : \nabla\mathbf{u} + \mathcal{P}_a^\tau + \mathcal{P}_b^\tau,$$

where

$$\mathcal{P}^{NS} = \frac{1}{\theta}\Pi^{NS} : \nabla\mathbf{u} - (\varkappa_a + \varkappa_b)\nabla\theta\cdot\nabla\frac{1}{\theta},$$

$$\mathcal{P}_\alpha^\tau = \frac{1}{\theta}\left[p_\alpha \operatorname{div}(\mathbf{u} - \mathbf{w}^{(\alpha)}) - p_\alpha \operatorname{div}\mathbf{u} + \operatorname{div}(p_\alpha \mathbf{w}^{(\alpha)}) - \mathbf{q}_\alpha^\tau\cdot\frac{1}{\theta}\nabla\theta + \Pi_\alpha^\tau : \nabla\mathbf{u} - \rho_\alpha\hat{\mathbf{w}}^{(\alpha)}\cdot\mathbf{F} + Q_\alpha\right].$$

As it is easy to see, $\mathcal{P}^{NS}$ can be rewritten in the form of (1.34). Additionally, $\mathcal{P}_\alpha^\tau$ can be simplified to

$$\mathcal{P}_\alpha^\tau = \frac{1}{\theta}\left(\nabla p_\alpha\cdot\mathbf{w}^{(\alpha)} - \mathbf{q}_\alpha^\tau\cdot\frac{1}{\theta}\nabla\theta + \Pi_\alpha^\tau : \nabla\mathbf{u} - \rho_\alpha\hat{\mathbf{w}}^{(\alpha)}\cdot\mathbf{F} + Q_\alpha\right).$$

It is well known that this expression can be transformed into the form of (1.35); for $Q_\alpha = 0$, see, for example, [7] and the short derivation in [17, Proposition 2]. The case $Q_\alpha \neq 0$ is treated in the same manner as in [18] (see also the proof of Theorem 2 below).

The derived entropy balance equation makes the constructed model physically correct. Moreover, it looks as if this model was obtained by summing the entropy balance equations for the species with $\mathbf{S}_{u,\alpha} = 0$ at $\mathbf{u}_a = \mathbf{u}_b = \mathbf{u}$ and $\theta_a = \theta_b = \theta$ (cf. [11, Theorem 1]). Of course, this is not the case, since, for a homogeneous binary mixture, the momentum, total energy, and entropy balance equations for individual components are no longer satisfied.

Let us discuss the nature of the regularization in the constructed equations. The component mass balance equation (1.12) involves the nonaggregated regularizing momenta $\rho_\alpha\mathbf{w}^{(\alpha)}$, which depend only on the density and pressure of the same component. By contrast, the momentum balance equation (1.13) and the total mass balance equation (1.29) involve only the total regularizing momenta $\rho\mathbf{w}$ and $\rho\hat{\mathbf{w}}$. Moreover, in the formula for Π^τ (see (1.16) and (1.24)), the squared speeds of sound for the species can be regarded as aggregated in combination with the use of the total density. The convective terms of the total energy balance equation (1.19) (and the total entropy balance equation (1.33) as well) contain nonaggregated regularizing momenta $\rho_a\mathbf{w}^{(a)}$ and $\rho_b\mathbf{w}^{(b)}$ (see also (1.25)). In formula (1.21) for $\mathbf{q}^\tau$, the quantities $c_{V\alpha}$ are aggregated (to produce c_V) and the quantities $R_\alpha\nabla\rho_\alpha$ are summed.

Note that regularized equations for a homogeneous binary mixture can also be constructed by applying procedures different from the one described above. Instead of aggregating the regularized equations of the (whole) binary mixture, we can try to construct such equations by applying the binary-mixture Navier–Stokes type equations (1.26)–(1.28), including by analogy with the procedures from [19] or [20] used in the case of a one-component gas. They even yield a simpler (than (1.25)) regularizing expression on the left-hand side of the total energy balance equation (1.19) for the mixture, but fail to ensure a nonnegative entropy production in the entropy balance equation for the mixture.

An additional important feature of the above-described aggregation method for deriving equations of a homogeneous binary mixture is that the resulting equations are easy to implement numerically if there is a software code for the corresponding equations of a one-component gas. For illustrative purposes, suppose that the latter equations are solved numerically by applying an explicit Euler method of the form

$$\hat{\rho} = \rho - \Delta t A_1[\mathbf{d}](\rho,\mathbf{u},\theta), \quad \hat{\rho}\hat{\mathbf{u}} = \rho\mathbf{u} - \Delta t\mathbf{A}_2[\mathbf{d}](\rho,\mathbf{u},\theta), \quad \hat{E} = E - \Delta t A_3[\mathbf{d}](\rho,\mathbf{u},\theta),$$

where $(\rho,\mathbf{u},\theta)$ and $(\hat{\rho},\hat{\mathbf{u}},\hat{\theta})$ are the values of the sought functions at the current and next time levels; $\hat{E} = \frac{1}{2}\hat{\rho}|\hat{\mathbf{u}}|^2 + c_V\hat{\rho}\hat{\theta}$; Δt is the time step; and $\mathbf{d}$ is the vector consisting of the gas parameters R, c_V, α_{Sc}, α_{Pr} and function Q. Here, $A_1[\mathbf{d}](\rho,\mathbf{u},\theta)$, $A_2[\mathbf{d}](\rho,\mathbf{u},\theta)$, and $A_3[\mathbf{d}](\rho,\mathbf{u},\theta)$ are approximations, at the current time level, of all terms of the mass balance, momentum, and total energy equations, respectively, except for the terms involving time derivatives.

Then the explicit Euler method as applied to the constructed equations of a homogeneous binary mixture can be written as

$$\hat{\rho}_a = \rho_a - \Delta t A_1[\mathbf{d}_a](\rho_a, \mathbf{u}, \theta), \quad \hat{\rho}_b = \rho_b - \Delta t A_1[\mathbf{d}_b](\rho_b, \mathbf{u}, \theta),$$
$$(\hat{\rho}_a + \hat{\rho}_b)\hat{\mathbf{u}} = \rho\mathbf{u} - \Delta t(\mathbf{A}_2[\mathbf{d}_a](\rho_a, \mathbf{u}, \theta) + \mathbf{A}_2[\mathbf{d}_b](\rho_b, \mathbf{u}, \theta)),$$
$$\hat{E} = E - \Delta t(A_3[\mathbf{d}_a](\rho_a, \mathbf{u}, \theta) + A_3[\mathbf{d}_b](\rho_b, \mathbf{u}, \theta)),$$

where $\rho = \rho_a + \rho_b$ and $\mathbf{d}_\alpha$ is the value of the parameter vector for the gas α. The unknowns $(\hat{\rho}_a, \hat{\rho}_b, \hat{\mathbf{u}}, \hat{\theta})$ at the new time level are easy to find sequentially from the formulas presented above. Here, $E = \frac{1}{2}\rho|\mathbf{u}|^2 + (c_{Va}\rho_a + c_{Vb}\rho_b)\theta$ and $\hat{E} = \frac{1}{2}(\hat{\rho}_a + \hat{\rho}_b)|\hat{\mathbf{u}}|^2 + (c_{Va}\hat{\rho}_a + c_{Vb}\hat{\rho}_b)\hat{\theta}$.

Note that the addition of the first two formulas gives

$$\hat{\rho}_a + \hat{\rho}_b = \rho_a + \rho_b - \Delta t(A_1[\mathbf{d}_a](\rho_a, \mathbf{u}, \theta) + A_1[\mathbf{d}_b](\rho_b, \mathbf{u}, \theta)),$$

which corresponds to an approximation of the total density equation (1.29).

2. REGULARIZED EQUATIONS FOR A HOMOGENEOUS BINARY MIXTURE OF RELATIVELY DENSE GASES

Presented at the beginning of Section 1, system (1.1)–(1.10) for describing flows of a inhomogeneous binary mixture can be used to compute flows of moderately rarefied gases (see [6, 7, 10]). However, numerical simulations show that, as the gas density grows, which is accompanied by an increase in the number of molecular collisions for individual components, the exchange terms in this system increase very rapidly, which leads to the instability of the numerical algorithm. For such flows, we can use the equations constructed in Section 1 for a homogeneous binary mixture, namely, Eqs. (1.12)–(1.16), (1.18)–(1.21). However, these equations become invalid as the Knudsen number is reduced, since the pressure gradients of the individual components increase near the interfaces between the species.

For this reason, for simulation of flows of relatively dense homogeneous binary gas mixtures, in this section we construct an alternative regularized model in which, in contrast to the other two systems described in Section 1, the regularizers involve the pressure and density of the entire mixture, rather than the pressures and densities of its components. Note that the use of a single regularizing mixture velocity $\hat{\mathbf{w}}$ was proposed in [13] and was successfully implemented in [14] in 3D isothermal computations for a substantially simpler (than in this paper) quasi-hydrodynamic regularization intended for flows of binary mixtures under small total density variations, but with additional allowance for interphase effects (described by the Navier–Stokes–Cahn–Hilliard equations for a compressible fluid).

The regularized (QGD) equations for a homogeneous binary mixture of relatively dense gases are constructed as follows. The mass balance equation (1.12) for components is modified by substituting $\mathbf{w}$ for $\mathbf{w}^{(\alpha)}$. The same substitution is made in the total energy balance equation (1.19) for the mixture. Additionally, the regularizing terms in the momentum balance and total energy equations for the mixture are modified so that the entropy balance equation for the mixture holds true with a nonnegative entropy production (this is a nontrivial task in the present model). Specifically, the regularized equations for a homogeneous binary mixture of relatively dense gases are given by

$$\partial_t\rho_\alpha + \operatorname{div}[\rho_\alpha(\mathbf{u} - \mathbf{w})] = 0, \quad \alpha = a, b, \tag{2.1}$$

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}[\rho(\mathbf{u} - \mathbf{w}) \otimes \mathbf{u}] + \nabla p = \operatorname{div}\Pi + [\rho - \tau\operatorname{div}(\rho\mathbf{u})]\mathbf{F}, \tag{2.2}$$

$$\begin{gathered}\partial_t E + \operatorname{div}[(E + p)(\mathbf{u} - \mathbf{w})] \\ = \operatorname{div}(-\mathbf{q} + \Pi\mathbf{u}) - \tau\delta R\operatorname{div}(\rho\mathbf{u})(\mathbf{u}\cdot\nabla C)\theta + \rho(\mathbf{u} - \mathbf{w})\cdot\mathbf{F} + Q.\end{gathered} \tag{2.3}$$

Here, as before, $\rho = \rho_a + \rho_b$, $p = p_a + p_b$, $E = \frac{1}{2}\rho|\mathbf{u}|^2 + \rho\varepsilon$, and we use formulas (1.18) for ε. Note that Eq. (2.3) contains a new regularizing term with the difference of the gas constants, $\delta R := R_a - R_b$, and with the concentration $C = \rho_a/\rho$ of the component a. Additionally, we use the previous regularizing mixture velocities

$$\mathbf{w} = \frac{\tau}{\rho}[\operatorname{div}(\rho\mathbf{u} \otimes \mathbf{u}) + \nabla p - \rho\mathbf{F}], \quad \hat{\mathbf{w}} = \frac{\tau}{\rho}[\rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p - \rho\mathbf{F}], \tag{2.4}$$

the viscous stress tensor $\Pi = \Pi^{NS} + \tilde{\Pi}^{\tau}$, and the heat flux $-\mathbf{q} = (\varkappa_a + \varkappa_b)\nabla\theta - \tilde{\mathbf{q}}^{\tau}$ with the following modified regularizing terms:

$$\tilde{\Pi}^{\tau} = \rho\mathbf{u} \otimes \hat{\mathbf{w}} + \tau\left(R\mathbf{u} \cdot \nabla \frac{p}{R} + \gamma p \operatorname{div} \mathbf{u} - (\gamma - 1)Q\right)\mathbb{I}, \tag{2.5}$$

$$-\tilde{\mathbf{q}}^{\tau} = \tau[\mathbf{u} \cdot (c_V \rho\nabla\theta - R\theta\nabla\rho) - Q]\mathbf{u}, \tag{2.6}$$

where, as before, c_V, R, and γ are given by formulas (1.18) and (1.22). All three terms in (2.5) with the tensor $\mathbb{I}$ used as a factor and the term $R\theta\nabla\rho$ in (2.6) are also modified. According to the modified term $\gamma p \operatorname{div} \mathbf{u} = \tilde{c}_s^2 \rho \operatorname{div} \mathbf{u}$, the speed of sound in the mixture is now computed using the conventional formula $\tilde{c}_s = \sqrt{\gamma(\gamma - 1)\varepsilon}$. In the special case of $R_a = R_b$, the term with δR in Eq. (2.3) vanishes and, as usual, we obtain $R\mathbf{u} \cdot \nabla(p/R) = \mathbf{u} \cdot \nabla p$ in (2.5).

Adding the new density balance equations (2.1) for the species over $\alpha = a, b$ leads, as before, to the total density balance equation (1.29). Therefore, the kinetic energy balance equation (1.30) for the mixture also preserves its form.

Subtracting the last equation from the total energy balance equation (2.3) for the mixture yields the following internal energy balance equation for the mixture:

$$\begin{aligned} &\partial_t(\rho\varepsilon) + \operatorname{div}[\rho\varepsilon(\mathbf{u} - \mathbf{w})] + p \operatorname{div} \mathbf{u} - \operatorname{div}(p\mathbf{w}) \\ &= -\operatorname{div} \mathbf{q} + \Pi : \nabla\mathbf{u} - \tau\delta R \operatorname{div}(\rho\mathbf{u})(\mathbf{u} \cdot \nabla C) - \rho\hat{\mathbf{w}} \cdot \mathbf{F} + Q. \end{aligned} \tag{2.7}$$

The entropy of the mixture is given, as before, by formulas (1.32).

Theorem 2. *The regularized entropy balance equation for a homogeneous binary mixture of relatively dense gases is given by*

$$\partial_t(\rho s) + \operatorname{div}[\rho s(\mathbf{u} - \mathbf{w})] = \operatorname{div}\left(-\frac{\mathbf{q}}{\theta}\right) + \mathcal{P}^{NS} + \mathcal{P}^{\tau},$$

with entropy production $\mathcal{P}^{NS} + \mathcal{P}^{\tau}$, where $\mathcal{P}^{NS}$ is defined by formula (1.34), *and $\mathcal{P}^{\tau}$, by the formula*

$$\begin{aligned} \mathcal{P}^{\tau} &= \tau\frac{\rho}{\theta}\left|\frac{\hat{\mathbf{w}}}{\tau}\right|^2 + \tau\frac{R}{\rho}[\operatorname{div}(\rho\mathbf{u})]^2 \\ &+ \tau c_V \rho\left[\mathbf{u} \cdot \nabla \ln\theta + (\gamma - 1)\operatorname{div} \mathbf{u} - \frac{(\gamma - 1)Q}{2p}\right]^2 + \frac{Q}{\theta}\left(1 - \frac{\tau(\gamma - 1)Q}{4p}\right), \end{aligned} \tag{2.8}$$

moreover, $\mathcal{P}^{\tau} \geq 0$ if $\tau(\gamma - 1)Q \leq 4p$.

Proof. Owing to the additivity of ρs and the new mass balance equation (2.1) for species, in perfect analogy with (1.36) and (1.37) (omitting the superscripts of $\mathbf{w}^{(a)}$, $\mathbf{w}^{(b)}$, and $\mathbf{w}^{(\alpha)}$), we obtain

$$\begin{aligned} \partial_t(\rho s) + \operatorname{div}[\rho s(\mathbf{u} - \mathbf{w})] &= \sum_{\alpha=a,b} \partial_t(\rho_\alpha s_\alpha) + \operatorname{div}[\rho_\alpha s_\alpha(\mathbf{u} - \mathbf{w})] \\ &= \sum_{\alpha=a,b} R_\alpha \rho_\alpha \operatorname{div}(\mathbf{u} - \mathbf{w}) + \frac{1}{\theta}\{\partial_t(\rho_\alpha\varepsilon_\alpha) + \operatorname{div}[\rho_\alpha\varepsilon_\alpha(\mathbf{u} - \mathbf{w})]\}. \end{aligned}$$

From this, taking into account the additivity of p and $\rho\varepsilon$ and using the internal energy balance equations (2.7) for the mixture, we derive

$$\partial_t(\rho s) + \operatorname{div}[\rho s(\mathbf{u} - \mathbf{w})] = \frac{p}{\theta}\operatorname{div}(\mathbf{u} - \mathbf{w}) + \frac{1}{\theta}\{\partial_t(\rho\varepsilon) + \operatorname{div}[\rho\varepsilon(\mathbf{u} - \mathbf{w})]\} = \operatorname{div}\left(-\frac{\mathbf{q}}{\theta}\right) + \mathcal{P}^{NS} + \mathcal{P}^{\tau},$$

where, by virtue of the formula $p \operatorname{div}(\mathbf{u} - \mathbf{w}) - p \operatorname{div} \mathbf{u} + \operatorname{div}(p\mathbf{w}) = \nabla p \cdot \mathbf{w}$,

$$\mathcal{P}^{\tau} = \frac{1}{\theta}\left(\nabla p \cdot \mathbf{w} - \tilde{\mathbf{q}}^{\tau} \cdot \frac{1}{\theta}\nabla\theta + \tilde{\Pi}^{\tau} : \nabla\mathbf{u} - \tau\delta R \operatorname{div}(\rho\mathbf{u})(\mathbf{u} \cdot \nabla C)\theta - \rho\hat{\mathbf{w}} \cdot \mathbf{F} + Q\right).$$

With the help of the formulas

$$\mathbf{w} = \tau\frac{1}{\rho}\operatorname{div}(\rho\mathbf{u})\mathbf{u} + \hat{\mathbf{w}}, \quad \nabla p = \frac{p}{\rho}\nabla\rho + \rho\nabla\frac{p}{\rho}, \quad R\mathbf{u}\cdot\nabla\frac{p}{R} = R\rho\mathbf{u}\cdot\nabla\theta + \frac{p}{\rho}\mathbf{u}\cdot\nabla\rho,$$
$$\mathbf{u}\cdot\nabla\rho + \rho\operatorname{div}\mathbf{u} = \operatorname{div}(\rho\mathbf{u}),$$

where we took into account that $p = R\rho\theta$ (see (1.23)), we perform the following transformations in order to generate partial quadratic terms:

$$\begin{aligned}
\mathfrak{R}_0^\tau &:= \nabla p\cdot\mathbf{w} + [\tilde{\Pi}^\tau + \tau(\gamma-1)Q\mathbb{I}] : \nabla\mathbf{u} - \rho\hat{\mathbf{w}}\cdot\mathbf{F} \\
&= \frac{\tau}{\rho}\operatorname{div}(\rho\mathbf{u})\nabla p\cdot\mathbf{u} + \nabla p\cdot\hat{\mathbf{w}} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u}\cdot\hat{\mathbf{w}} + \tau\left(R\mathbf{u}\cdot\nabla\frac{p}{R} + \gamma p\operatorname{div}\mathbf{u}\right)\operatorname{div}\mathbf{u} - \rho\hat{\mathbf{w}}\cdot\mathbf{F} \\
&= \tau\rho\left|\frac{\hat{\mathbf{w}}}{\tau}\right|^2 + \frac{\tau p}{\rho^2}\operatorname{div}(\rho\mathbf{u})\mathbf{u}\cdot\nabla\rho + \tau\operatorname{div}(\rho\mathbf{u})\mathbf{u}\cdot\nabla\frac{p}{\rho} + \tau\left[R\rho\mathbf{u}\cdot\nabla\theta + \frac{p}{\rho}\operatorname{div}(\rho\mathbf{u}) + (\gamma-1)p\operatorname{div}\mathbf{u}\right]\operatorname{div}\mathbf{u} \\
&= \tau\left\{\rho\left|\frac{\hat{\mathbf{w}}}{\tau}\right|^2 + \frac{p}{\rho^2}[\operatorname{div}(\rho\mathbf{u})]^2 + \operatorname{div}(\rho\mathbf{u})\mathbf{u}\cdot\nabla\frac{p}{\rho} + R\rho(\mathbf{u}\cdot\nabla\theta)\operatorname{div}\mathbf{u} + (\gamma-1)p(\operatorname{div}\mathbf{u})^2\right\}.
\end{aligned}$$

Next, by sequentially applying the formulas

$$\nabla\frac{p}{\rho} = R\nabla\theta + (\nabla R)\theta = R\nabla\theta + \delta R(\nabla C)\theta,$$
$$\operatorname{div}(\rho\mathbf{u})\mathbf{u}\cdot\nabla\frac{p}{\rho} = R(\mathbf{u}\cdot\nabla\rho)\mathbf{u}\cdot\nabla\theta + R\rho(\mathbf{u}\cdot\nabla\theta)\operatorname{div}\mathbf{u} + \delta R\operatorname{div}(\rho\mathbf{u})(\mathbf{u}\cdot\nabla C)\theta,$$
$$R\rho(\mathbf{u}\cdot\nabla\theta)\operatorname{div}\mathbf{u} = c_V\rho\theta(\mathbf{u}\cdot\nabla\ln\theta)(\gamma-1)\operatorname{div}\mathbf{u},$$

where we took into account that $R = c_V(\gamma-1)$ (see (1.22)), and using the formulas

$$\begin{aligned}
-\tilde{\mathbf{q}}^\tau\cdot\frac{1}{\theta}\nabla\theta &= \tau\frac{c_V\rho}{\theta}(\mathbf{u}\cdot\nabla\theta)^2 - \tau R(\mathbf{u}\cdot\nabla\rho)\mathbf{u}\cdot\nabla\theta - \tau\frac{Q}{\theta}\mathbf{u}\cdot\nabla\theta \\
&= \tau c_V\rho\theta(\mathbf{u}\cdot\nabla\ln\theta)^2 - \tau R(\mathbf{u}\cdot\nabla\rho)\mathbf{u}\cdot\nabla\theta - \tau Q\mathbf{u}\cdot\nabla\ln\theta
\end{aligned}$$

and $p = c_V(\gamma-1)\rho\theta$ (see (1.23)), the generation of quadratic terms is completed as follows:

$$\begin{aligned}
\theta\mathcal{P}^\tau &= \mathfrak{R}_0^\tau - \tau(\gamma-1)Q\operatorname{div}\mathbf{u} - \tilde{\mathbf{q}}^\tau\cdot\frac{1}{\theta}\nabla\theta - \tau\delta R\operatorname{div}(\rho\mathbf{u})(\mathbf{u}\cdot\nabla C)\theta + Q \\
&= \tau\left\{\rho\left|\frac{\hat{\mathbf{w}}}{\tau}\right|^2 + \frac{R\theta}{\rho}[\operatorname{div}(\rho\mathbf{u})]^2 + c_V\rho\theta[\mathbf{u}\cdot\nabla\ln\theta + (\gamma-1)\operatorname{div}\mathbf{u}]^2\right\} \\
&\quad - \tau Q[\mathbf{u}\cdot\nabla\ln\theta + (\gamma-1)\operatorname{div}\mathbf{u}] + Q \\
&= \tau\left[\rho\left|\frac{\hat{\mathbf{w}}}{\tau}\right|^2 + \frac{R\theta}{\rho}[\operatorname{div}(\rho\mathbf{u})]^2 + c_V\rho\theta\left[\mathbf{u}\cdot\nabla\ln\theta + (\gamma-1)\operatorname{div}\mathbf{u} - \frac{(\gamma-1)Q}{2p}\right]^2\right] + Q\left(1 - \tau\frac{(\gamma-1)Q}{4p}\right).
\end{aligned}$$

Formula (2.8) has been derived, and the theorem has been proved.

Let us discuss a substantially simpler quasi-hydrodynamic regularization (which is also easier to compare with [13]) that also can be used in applications, but for a much narrow class of flows at moderate Mach numbers. The corresponding system of equations involves only one regularizing velocity $\hat{\mathbf{w}}$ (see (2.4)) and has the form

$$\partial_t\rho_\alpha + \operatorname{div}[\rho_\alpha(\mathbf{u} - \hat{\mathbf{w}})] = 0, \quad \alpha = a, b,$$
$$\partial_t(\rho\mathbf{u}) + \operatorname{div}[\rho(\mathbf{u} - \hat{\mathbf{w}})\otimes\mathbf{u}] + \nabla p = \operatorname{div}\Pi + \rho\mathbf{F},$$
$$\partial_t E + \operatorname{div}[(E + p)(\mathbf{u} - \hat{\mathbf{w}})] = \operatorname{div}(-\mathbf{q} + \Pi\mathbf{u}) + \rho(\mathbf{u} - \hat{\mathbf{w}})\cdot\mathbf{F} + Q.$$

Here, $\Pi = \Pi^{NS} + \tilde{\Pi}^\tau$, but the regularizing viscous stress tensor is much simpler: $\tilde{\Pi}^\tau = \rho\mathbf{u}\otimes\hat{\mathbf{w}}$, while the heat flux does not contain a regularizing term at all: $-\mathbf{q} = (\varkappa_a + \varkappa_b)\nabla\theta$.

Table 1. Gas parameters

Gas	γ	μ (Pa s)	α_{Pr}	M
Helium He	5/3	1.86×10^{-5}	0.67	4.003
Air	7/5	1.71×10^{-5}	0.715	28.96
Argon Ar	5/3	2.26×10^{-5}	0.669	39.91657
Ozone O_3	4/3	1.55×10^{-5}	0.9	47.998
Sulfur hexafluoride SF_6	1.0937	1.57×10^{-5}	0.736	146.0554

For this system, the entropy balance equation for the mixture is much easier to derive and is much simpler in form:

$$\partial_t(\rho s) + \operatorname{div}[\rho s(\mathbf{u} - \hat{\mathbf{w}})] = \operatorname{div}\left(-\frac{\mathbf{q}}{\theta}\right) + \mathcal{P}^{NS} + \mathcal{P}^{\tau}, \quad \mathcal{P}^{\tau} = \tau\frac{\rho}{\theta}\left|\frac{\hat{\mathbf{w}}}{\tau}\right|^2 + \frac{Q}{\theta},$$

once again, the entropy production is $\mathcal{P}^{NS} + \mathcal{P}^{\tau} \geq 0$.

3. NUMERICAL SIMULATION OF HOMOGENEOUS BINARY MIXTURES OF RELATIVELY DENSE GASES IN THE RAYLEIGH–TAYLOR-TYPE PROBLEM

By applying the equations derived in Section 2, the instability of a homogeneous binary mixture of relatively dense gases was simulated in two dimensions (in coordinates (x, z)) under the gravity field $\mathbf{F} = (0, -g)$ (where $g = 9.82$ m/s^2 is the acceleration of gravity) in a domain of width $L = 0.125$ m and height $H = 0.5$ m. The interface between two gases was initially along the line $z = 0$ with the heavier gas occupying the upper part $0 < z < H_2 = 0.2$ of the domain and with the lighter gas being in the lower part $H_1 = -0.3 < z < 0$.

The gas parameters used for the simulation are given in Table 1. The viscosity and thermal conductivity coefficients were specified as $\mu = \text{const}$, $\lambda = 0$, and $\varkappa = (\gamma/(\gamma-1))R_0\mu/(M\alpha_{Pr})$. Recall that R_0 is the universal gas constant and M is the molecular weight of a gas.

A difference approximation of the equations was constructed according to [7]. The regularization parameter and the time step were computed using the formulas

$$\tau = \frac{\mu}{p} + \alpha\frac{\sqrt{h_x^2 + h_z^2}}{\tilde{c}_s}, \quad \Delta t = \beta\min\left\{\frac{h_x}{\tilde{c}_s + |u_x|}, \frac{h_z}{\tilde{c}_s + |u_z|}\right\},$$

where $\tilde{c}_s = \sqrt{\gamma(\gamma-1)\varepsilon}$ is the speed of sound of the mixture, h_x and h_z are the mesh sizes in x and z, and the minimum is taken over all nodes of the spatial grid. Here, α and β (Courant number) are parameters from the interval $(0,1)$.

Initial conditions. The initial state of the gas at the time $t = 0$ was determined by the hydrostatic equilibrium under the adiabatic assumption: $\partial_z p = -g\rho$ and $\mathbf{u} = 0$. For it, the dependences of the density and pressure of the gas species on the height z were specified by the formulas

$$\frac{p_a}{p_0} = \left(\frac{\rho_a}{\rho_{a0}}\right)^{\gamma_a} = \left(1 - \frac{\rho_{a0}gz}{\gamma'_a p_0}\right)^{\gamma'_a}, \quad 0 \leq z \leq H_2; \quad \frac{p_b}{p_0} = \left(\frac{\rho_b}{\rho_{b0}}\right)^{\gamma_b} = \left(1 - \frac{\rho_{b0}gz}{\gamma'_b p_0}\right)^{\gamma'_b}, \quad z < 0, \tag{3.1}$$

where $\gamma'_\alpha := \gamma_\alpha/(\gamma_\alpha - 1)$. Relying on them, the temperature θ was computed using the state equations of the gases. For $z = 0$, we specified normal atmospheric parameters, namely, $p_a = p_b = p_0 = 101325$ Pa and $\theta = 273$ K, which were used to compute the densities ρ_{a0} and ρ_{b0} according to the state equations of the gases. Note that the values of $p_a(z)$, $p_b(z)$, and $\theta(z)$ differed weakly from the their indicated values at $z = 0$.

In the part of the domain where one of the gases was nearly absent at the initial time, its density was set to a small value of 10^{-8}.

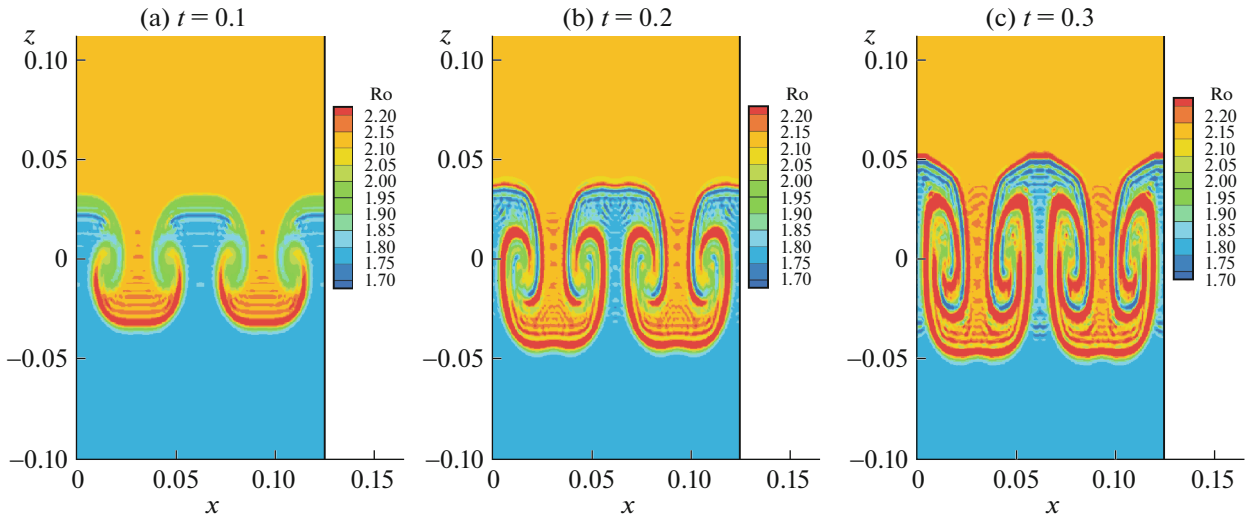

Fig. 1. Density of an Ar–O_3 mixture with $At = 0.091$ at the times $t = 0.1, 0.2, 0.3$ for a grid of 125×400 nodes.

To initialize the process, an x-symmetric oscillating perturbation of vertical velocity with a large amplitude was specified near the interface of the gases, namely, $u_z|_{0 \le z \le z_0} = 10\cos(4\pi x/L)$, where $z_0 = 0.0025$.

Note that the values of the molecular weights M have to taken with a sufficiently high accuracy, so that the hydrostatic equilibrium conditions for both gases at $t = 0$ are satisfied with appropriate accuracy. Otherwise, the gas layers begin to move immediately.

Boundary conditions. On the vertical (lateral) and lower boundaries of the computational domain, we set the impermeability and slip conditions

$$(\partial_x \rho_\alpha, \partial_x p, u_x, \partial_x u_z)|_{x=0,L} = 0, \quad (\partial_z \rho_\alpha, \partial_z p, \mathbf{u})|_{z=-H_1} = 0, \quad \alpha = a, b,$$

where $\mathbf{u} = (u_x, u_z)$. Additionally, we set $\mathbf{F}|_{z=-H_1} = 0$ to ensure the mass impermeability of the lower wall.

On the upper boundary of the domain, we specified the free atmosphere condition for pressure, drift for density and velocity, and no heat flux for temperature:

$$p|_{z=H_2} = p_{H_2}, \quad \partial_z \rho_\alpha|_{z=H_2} = 0 \quad (\alpha = a, b), \quad \partial_z \mathbf{u}|_{z=H_2} = 0, \quad \partial_z \theta|_{z=H_2} = 0,$$

where p_{H_2} is found at $z = H_2$ according to (3.1). These conditions allow solution perturbations to leave the computational domain through the upper boundary.

Numerical results. The computations were performed for three mixtures (pairs) of gases frequently considered in the literature (see, e.g., [15, 16]) with the Atwood number $At = (M_a - M_b)/(M_a + M_b)$ equal to 0.091, 0.57, and 0.947, i.e., all characteristic values of At, including the most complicated regime $At \approx 1$, were covered.

Figure 1 shows the distributions of the total density ρ for the Ar–O_3 mixture with $At = 0.091$ at three characteristic times $t = 0.1, 0.2, 0.3$ s. The mixture temperature and the component densities are mainly similar to the mixture density distributions, so they are not shown for brevity.

It can well be seen that the ascending light-gas bubbles and descending heavy-gas bubbles have mushroom shapes; moreover, their edges are curved inside and become thinner over time. The fine structure of the developing structures suggests that the numerical algorithm has a very low artificial viscosity. An advantage of this algorithm is that the symmetry of the numerical solution with respect to x is maintained to high accuracy.

It is also well seen that acoustic disturbances are formed in the gasdynamic fields of the light and heavy gases in the course of their evolution.

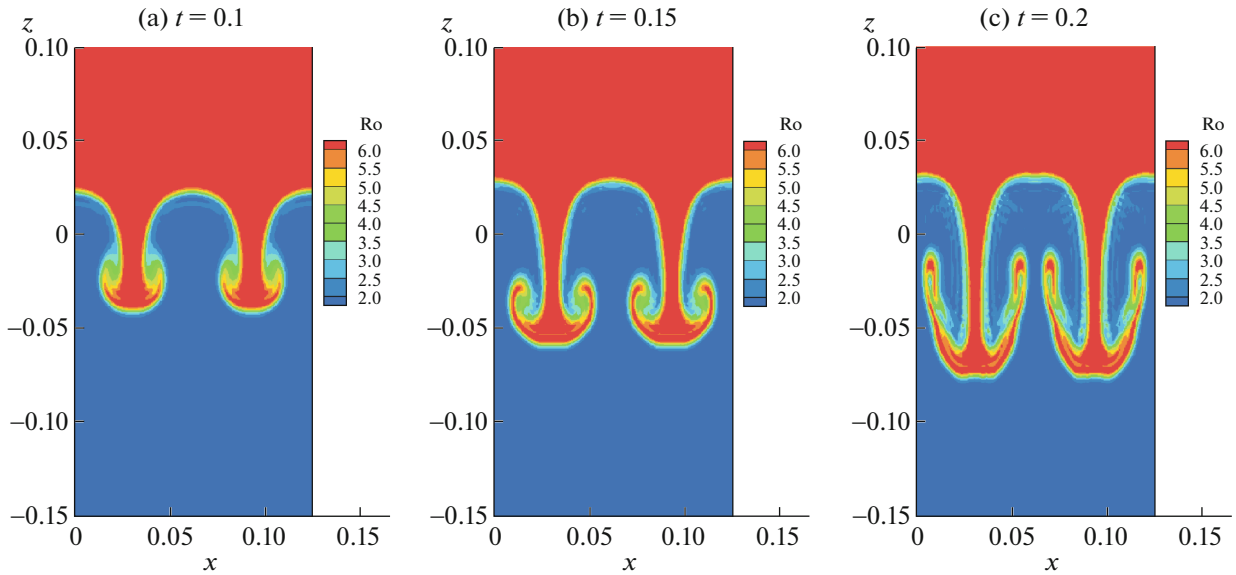

Fig. 2. Density of the Ar–SF_6 mixture with $At = 0.57$ at the times $t = 0.1, 0.15, 0.2$ for a grid of 125×400 nodes.

Additionally, the temperature distributions (not shown) exhibit higher temperature zones near the boundaries of the bubbles, which are associated with the heating of the light gas caused by its compression in the emerging structures.

Over time, the gravity-based gas mixing process exhibits a progressively more complicated pattern with finer details and vortex structures appearing in it. Eventually, these new details become comparable in size with the spatial mesh size, which leads to the termination of the computation.

Since the Rayleigh–Taylor problem is unstable, the results of its simulation depend strongly on numerous parameters, including the Atwood number, the adiabatic indices γ_a and γ_b, the shape and type of the initial perturbation of the data, a particular moment of time, etc. Therefore, the results can be only qualitatively compared with data of other authors. Nevertheless, we can note that the computed density fields are typical for problems of this type; specifically, they are similar to the fields at $At = 0.1$ presented in [16].

The basic computations were performed on a mesh of 125×400 nodes with the parameters $\alpha = 0.2$ and $\beta = 0.3$. Note that their values were not optimized in these computations, so, possibly, the artificial dissipation coefficient α can be reduced, while the Courant number can be increased.

Figure 2 presents the numerical results obtained for an Ar–SF_6 mixture with $At = 0.57$ at the times $t = 0.1, 0.15, 0.2$ s. A comparison with the preceding computation shows that the overall picture of instability development is generally preserved. However, with increasing At, mushroom bubbles are generated more intensively, the acoustic disturbances increase in value, the descending bubbles of the heavy SF_6 gas become narrower, and thin jets develop over time whose upper parts tend to shed from the basic flow to form separate drops. Moreover, the ascending light-gas bubbles become wider. These bubble shapes agree with the data available in [5, 15, 16].

The additional results obtained for the air–SF_6 mixture with $At = 0.66$ were found to be overall similar to the last data, so they are omitted.

The numerical results obtained for the He–SF_6 mixture with $At = 0.947$ are presented in Fig. 3. We can see intensive development of instability. Ascending mushroom bubbles and zones of a descending heavy gas are formed at a significantly higher rate than in the case of smaller At. For this reason, the mixture density distributions are shown at earlier times, namely, at $t = 0.06, 0.10, 0.12$ s. Note that the computation of such problems faces serious difficulties because of the huge difference in the gas densities and the high rates of the processes involved.

It can be seen that the heavy gas SF_6 rapidly sinks into the zone of light helium with the formation of downward jets of SF_6. Additionally, mushroom-shaped structures emerge at the ends of the heavy-gas jets, and the latter tend to split to form drops.

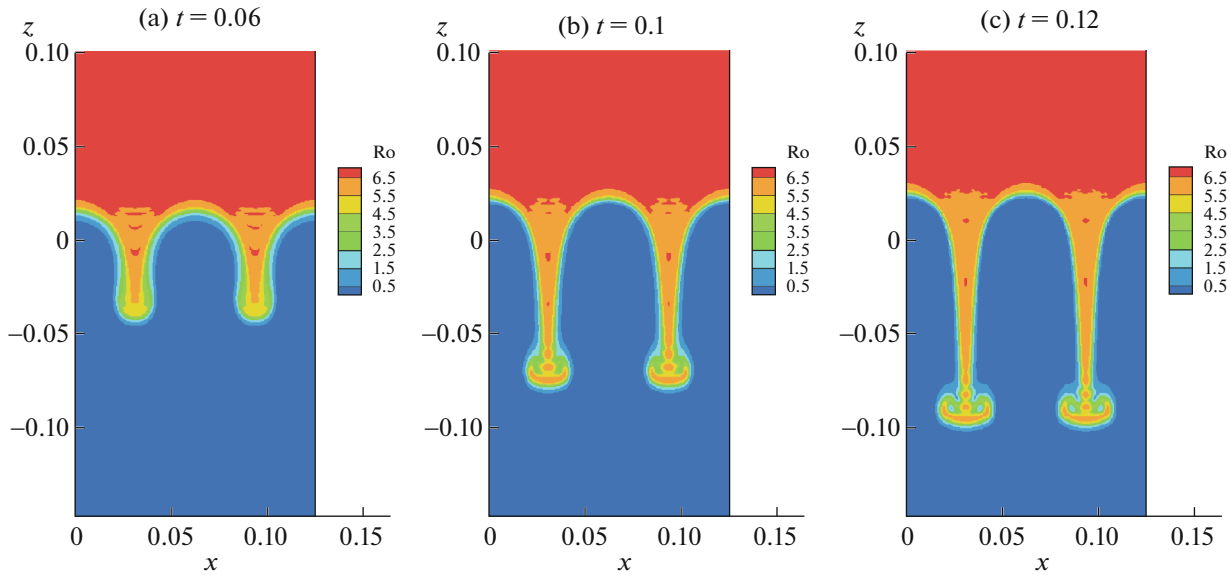

Fig. 3. Density of the He–SF_6 mixture with $At = 0.947$ at the times $t = 0.06, 0.10, 0.12$ for a grid of 125×400 nodes.

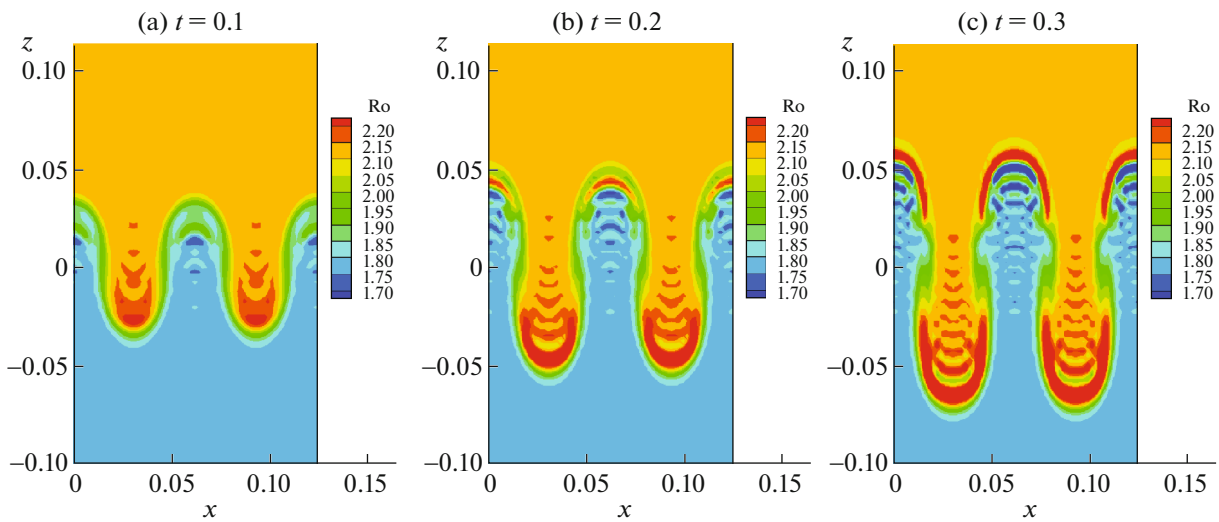

Fig. 4. Density of the Ar–O_3 mixture of with $At = 0.091$ at the times $t = 0.1, 0.2, 0.3$ for a grid of 60×200 nodes.

The temperature isolines exhibit rapid heating of helium due to its compression caused by the influence of the heavy gas playing the role of a piston. At larger t, the formed heavy-gas bubbles interact with the lower boundary of the domain and the flow pattern ceases to be typical for the gravitational instability problem. These computations were performed again on the mesh of 125×400 nodes at $\alpha = 0.4$ and smaller $\beta = 0.03$.

To analyze the dependence of the numerical solution on the spatial mesh size, Figs. 4 and 5 show the results obtained for the first version of mixture (i.e., for Ar–O_3) with $At = 0.091$ at the same times $t = 0.1, 0.2, 0.3$ s for grids of 60×200 and 250×800 nodes, respectively. The results demonstrate that the characteristic features of the flow are resolved even on the coarse grid, except for the specific curved boundaries of the mushrooms, since this boundary contains only one or several grid cells. Under mesh refinement, additional finer details can be observed in the formation of mushroom structures. Additionally, the structures of the twisted flows obtained on the fine mesh are more roundish and have more spiral turns than in the flow pattern obtained on the coarser mesh.

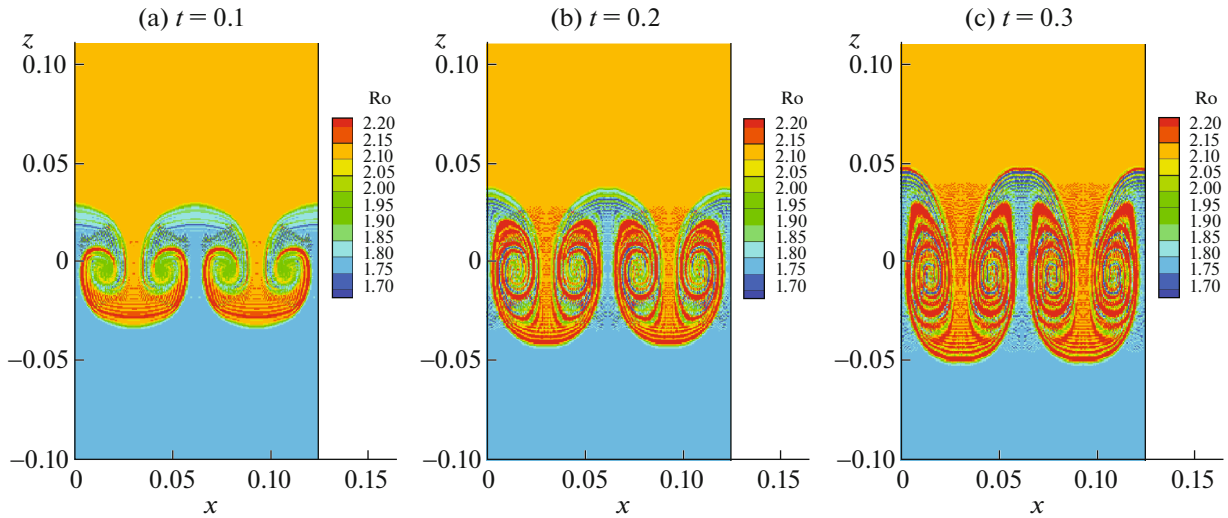

Fig. 5. Density of the Ar–O_3 mixture with $At = 0.091$ at the times $t = 0.1, 0.2, 0.3$ for a grid of 250×800 nodes.

4. CONCLUSIONS

To describe flows of inhomogeneous binary mixtures of nonreacting gases, regularized equations were presented taking into account momentum and energy exchange between the gas components. New simpler regularized equations for homogeneous binary mixtures of polyatomic gases were derived by applying an aggregation procedure. Both systems of equations are applicable to describe flows of moderately rarefied gases.

A new regularized system of equations for homogeneous binary mixtures of polyatomic relatively dense gases was also constructed. For both systems of equations for homogeneous mixture flows, natural formulas were derived for the specific heat capacities, the adiabatic index, and the total pressure of mixture. Natural balance equations for the total mass and kinetic and internal energy of mixtures hold for these systems. They were used to derive new balance equations for the total entropy of binary gas mixtures with a nonnegative entropy production.

The last system of equations was used to develop a numerical method for computing the Rayleigh–Taylor-type instability problem in the entire range of actual Atwood numbers from small values to ones close to the maximum value of 1. The obtained results qualitatively agree with data presented in the literature. The numerical solution has an appropriate symmetry. Its quality is improved under spatial mesh refinement.

The numerical algorithm has also been implemented for the computation of 3D flows. Moreover, the 2D computations described above were performed using the 3D code with a minimum number of nodes in the third spatial direction.

The first version of the algorithm based on the regularized equations for a one-component gas has recently been incorporated into the open software platform OpenFOAM [21]. The algorithm developed in this paper for simulation of flows of gas mixtures can also be included in this platform.

The developed technique can be extended to multicomponent homogeneous mixtures and can be applied to other flows of gas mixtures, including subsonic and supersonic jets, and to geophysical flows at atmospheric scales.

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Translated by I. Ruzanova