

# Regularized Isothermal Phase-Field Type Model of a Two-Phase Compressible Fluid and Its One-Dimensional Spatial Discretization

V. A. Balashov<sup>1\*</sup> and E. B. Savenkov<sup>1\*\*</sup>

<sup>1</sup>*Keldysh Institute of Applied Mathematics, Moscow, 125047 Russia*

*e-mail: \*vladislav.balashov@gmail.com, \*\*e.savenkov@gmail.com*

Received February 9, 2020; revised February 18, 2020; accepted April 17, 2020

**Abstract**—We consider a quasi-hydrodynamic regularized model of the phase field type that describes the dynamics of an isothermal compressible two-phase viscous mixture with allowance for interphase effects. The dissipativity of the model, i.e., the lack of growth in the complete energy of the closed system as it tends to an equilibrium state, is discussed. A spatially discrete approximation to the one-dimensional model that possesses the dissipativity property with respect to total energy is constructed for the plane-parallel case. The working capacity of the discretization constructed is demonstrated using the spinodal decomposition of the two-phase mixture.

**DOI:** 10.1134/S0012266120070058

## INTRODUCTION

Multiphase multicomponent microflows, in which capillary effects play a significant role, often occur in nature and technology. They are encountered in motors, reactors, pipelines, pores of container rocks, living organisms, and many other natural and technical systems. Therefore, creating new and perfecting the existing mathematical models to describe such systems and developing counterpart numerical methods is a topical problem.

Depending on the typical spatial scale of the problem, various approaches are used to construct the mathematical model for describing the multiphase system. In the present paper, we consider models in which the interface and its dynamics are resolved. All such models can be divided into two groups. The first group includes models that represent the interface as a mathematical surface (of “zero” thickness) with prescribed contact conditions. These conditions determine the nature of interaction between the phases and are an indispensable part of the model. The interface position can be tracked both explicitly (on Lagrangian meshes) and implicitly (on Eulerian meshes). In the latter case, one can use, for example, the Volume of Fluid (VoF) method [1] or the level set method [2]. The second group incorporates models with a diffuse boundary [3–7], in which the interface is described by a thin layer of finite thickness within which the properties of the medium undergo “rapid” but smooth changes.

These models are based on using a specially defined (in space) function, referred to as the order parameter, that plays the role of a phase indicator. The order parameter can be one of the medium characteristics (for example, density or concentration) or, alternatively, some artificially introduced variable. Note that there can be several order parameters and they can be scalars or quantities of a higher tensor dimension. One can consider phase-field models [8, 9] as a particular case of models with diffuse boundary. The nature of interaction between the phases is determined in these models by a special form of the Helmholtz free energy (or another thermodynamic potential of the system): it depends on both the order parameter and its spatial derivatives (this is why such models are sometimes called “weakly nonlocal” or “gradient”); in this case, the dependence on the order parameter is nonconvex. The indicated special form of free energy determines the thickness of the interface and the interphase energy (the surface tension coefficient in problems of hydrodynamics). Phase field models quite naturally, from the viewpoint of the original mathematical model, describe such phenomena as coagulation and fragmentation of droplets (which are topological changes in the spatial distribution of phases).

Note that no explicit concept of a phase is introduced in the models under consideration. However, in view of the special form of free energy, subdomains with virtually uniform (in space) composition form the flow range. It is these subdomains that are interpreted as separate phases. Phase-field type models are exemplified by the Navier–Stokes–Cahn–Hilliard (NSCH) equations [3, 5], which describe the dynamics of a two-component two-phase mixture. The mass or volume concentration of one of the components serves as the order parameter in the NSCH equations. Another example of frequently used phase field models is Navier–Stokes–Korteweg (NSK) equations [3, 4, 10], which describe the dynamics of a one-component two-phase system (a liquid and its vapor). The mass density is considered in this model as the order parameter.

Liu et al. [11] (see also [12]) considered a system that describes the dynamics of a compressible two-phase two-component mixture. In this case, the medium is treated as one-velocity. The order parameters in this system are the mass densities of components (rather than concentrations as in the NSCH model). This choice of phase fields in some sense combines the NSCH and NSK systems. Similar systems in which molar densities are taken for the phase fields were considered in [12–16]. The model in [13–15] was constructed with the use of the density functional method.

In the present paper, for the isothermal case, we suggest a QHD-regularized version of the system proposed in [11] (see Eqs. (1) and (2) below). The dissipativity (in the sense of the lack of growth of total energy) of the system under study is discussed. The problem of constructing a spatial discretization is considered for the one-dimensional plane-parallel case. In this case, the discretization is constructed with allowance for the conservation of the system total energy for a discrete analog of the property of dissipativity. It is important that this property be satisfied at the discrete level. In particular, as was noted in [4, 17, 18], this allows one to get rid of the so-called “parasitic currents,” a numerical artifact that is an eddy-like velocity field in a neighborhood of the interface that does not fade as the system approaches the equilibrium state. To this end, it was proposed in [4, 17, 18] to use a representation of capillary stresses in a potential form. In its turn, such a representation leads to a momentum-nonconservative difference scheme, but this is not critical in view of no shock waves or other strong discontinuities being present. Such discretizations were constructed for QHD-regularized NSCH equations in the papers [19, 20].

QHD-regularization of various models in the continuum mechanics presumes that, in the general case, the mass density of the flow of a mixture differs from the average momentum of unit volume, with the case of the two being equal *not excluded*. Thus, QHD-regularized models include original models as a special case. In view of the above assumption, additional terms of dissipative nature arise in the equations of the original model. On the one hand, these terms allow one to solve relatively simple-to-implement explicit stable central difference schemes. On the other hand, in some cases they ensure more precise coincidence with the results of experiments [21–23]. Note that similar regularization techniques were also considered in the papers [24, 25].

QHD-regularized (and also related quasi-gasdynamics) models of the dynamics of viscous fluid, magnetic hydrodynamics, shallow water etc. have been successfully applied before [21–23, 26]. For multiphase multicomponent models with surface effects, a QHD-regularization was constructed in [27]. Its particular case corresponding to the isothermal Navier–Stokes–Cahn–Hilliard model was considered in the papers [19, 20, 28, 29].

This paper is organized as follows. Section 1 introduces the notation used in the paper. In Sec. 2, we present the isothermal two-component phase-field model in [11] and its QHD-regularization. In Sec. 3, we discuss the potential form of capillary stresses. Section Sec. 4 proves the dissipativity of the regularized model. In Sec. 5, we propose a space-discrete difference scheme for the one-dimensional plane-parallel case and prove its dissipativity. In Sec. 6, following the paper [11], the equations of the model are rendered dimensionless. In the concluding section 7, we carry out numerical modeling of the spinodal decomposition and analyze the dynamics of the system total energy.

## 1. NOTATION

For convenience, let us list the notation used in the paper. Consider a bounded domain  $\Omega \subset \mathbb{R}^n$  ( $n = 1, 2, \text{ or } 3$ ) with piecewise smooth boundary  $\partial\Omega$ ,  $\bar{\Omega} = \Omega \cup \partial\Omega$ . In  $\mathbb{R}^n$ , define a Cartesian coordinate system  $Ox_1 \dots x_n$  with basis unit vectors  $e_1, \dots, e_n$ . For a vector (point)  $\mathbf{x} \in \mathbb{R}^n$ , we denote its  $i$ th component in this basis by  $x_i$ , i.e.,  $\mathbf{x} := (x_1, \dots, x_n)^T$ , and the time variable, by  $t$ . Hereinafter the symbol “:=” designates equality by definition.

We will index the spatial coordinates by Latin letters  $i$  and  $j$  and use Greek letters  $\alpha, \beta, \kappa$ , and  $v$  for the numbers of mixture components. In this case, if not stated otherwise, repeated indices  $i$  and  $j$  assume summation from 1 to  $n$  and repeated indices  $\alpha$  and  $\beta$  indicate summation from 1 to 2 (according to the number of mixture components); no summation is performed over repeated indices  $\kappa$  and  $v$ .

Let  $\mathbf{u} = u_i \mathbf{e}_i$  and  $\mathbf{v} = v_i \mathbf{e}_i$  be arbitrary smooth vector fields, let  $\mathbf{A} = A_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$  and  $\mathbf{B} = B_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$  be arbitrary smooth tensor fields of the second rank, and let  $\mathbf{e}_i \otimes \mathbf{e}_j$  be the basis dyad. In the sequel, we will use the following notation and operations:  $\partial_i := \partial/\partial x_i$ ,  $\partial_t := \partial/\partial t$ ,  $\mathbf{u} \cdot \mathbf{v} := u_i v_i$  is the inner product,  $|\mathbf{u}|^2 := \mathbf{u} \cdot \mathbf{u}$ ,  $\mathbf{A}\mathbf{u} \equiv \mathbf{A} \cdot \mathbf{u} := A_{ij} u_j \mathbf{e}_i$ ,  $\mathbf{u} \cdot \mathbf{A} := A_{ij} u_i \mathbf{e}_j$ ,  $\nabla := (\partial_i) \mathbf{e}_i$  stands for the gradient,  $\operatorname{div} \mathbf{A} \equiv \nabla \cdot \mathbf{A} := (\partial_i A_{ij}) \mathbf{e}_j$  is the divergence of a tensor,  $\mathbf{A} : \mathbf{B} := A_{ij} B_{ij}$  is the double inner product,  $|\mathbf{A}|^2 := \mathbf{A} : \mathbf{A}$ ,  $\mathbf{u} \otimes \mathbf{v} := u_i v_j \mathbf{e}_i \otimes \mathbf{e}_j$  stands for the tensor product of vectors,  $\delta_{ij}$  is Kronecker's delta, and  $\mathbf{I} = \delta_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$  is the identity tensor.

## 2. REGULARIZED MODEL OF A TWO-COMPONENT TWO-PHASE FLUID

The system of equations describing the dynamics of a two-component two-phase isothermal compressible viscous fluid in the domain  $\Omega$  allowing for interphase effects and neglecting gravity has the form [11]:

$$\partial_t \rho_\alpha + \operatorname{div}(\rho_\alpha \mathbf{u}) = (-1)^{\alpha+1} \operatorname{div}(M \nabla \hat{\mu}_{12}), \quad \alpha = 1, 2, \tag{1}$$

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

where  $\mathbf{u}(\mathbf{x}, t)$  is the mass-averaged fluid velocity,  $\rho_\alpha(\mathbf{x}, t) > 0$  is the density of component  $\alpha$ , and  $\rho := \rho_1 + \rho_2$  is the total density of the mixture. To determine the remaining variables in this system, we preliminarily introduce the *volume* density of the Helmholtz free energy  $\psi$  [11]

$$\psi(\rho_1, \rho_2, \nabla \rho_1, \nabla \rho_2) := \psi_0(\rho_1, \rho_2) + \frac{1}{2} \lambda_{\alpha\beta} \nabla \rho_\alpha \cdot \nabla \rho_\beta, \tag{3}$$

$$\psi_0(\rho_1, \rho_2) := k_B T \frac{\rho_\alpha}{m_\alpha} \ln \left[ \frac{\rho_\alpha \Lambda_\alpha^3}{m_\alpha (1 - \phi)} \right] - k_B T \frac{\rho_\alpha}{m_\alpha} - a_{\alpha\beta} \frac{\rho_\alpha}{m_\alpha} \frac{\rho_\beta}{m_\beta}, \tag{4}$$

where  $m_\alpha$  is the molecular mass of component  $\alpha$ ,  $\Lambda_\alpha = (2\pi m_\alpha k_B T)^{-1/2} \hbar$ ,  $\hbar$  is the Planck constant,  $\phi = b_\alpha \rho_\alpha / m_\alpha$  is the volume fraction occupied by the molecules,  $b_\alpha$  is the molecular volume of component  $\alpha$ , and  $k_B$  is the Boltzmann constant. The function  $\psi_0(\rho_1, \rho_2)$  is the *volume* density of the *homogeneous* part of Helmholtz' free energy of the mixture. The capillary coefficients  $\lambda_{\kappa v} > 0$  are constants calculated by the formula  $\lambda_{\kappa v} := k_B T D_{\kappa v} / (m_\kappa m_v)$ ,  $\kappa, v = 1, 2$ , where  $D_{\kappa v} = D_{v\kappa} > 0$  are constant coefficients. Recall that no summation is performed over the indices  $\kappa$  and  $v$ .

The pressure  $p$  is linked to the densities  $\rho_1$  and  $\rho_2$  by the relation

$$p(\rho_1, \rho_2) = \rho_1 \mu_1 + \rho_2 \mu_2 - \psi_0(\rho_1, \rho_2),$$

where  $\mu_\alpha(\rho_1, \rho_2) = \partial_{\rho_\alpha} \psi_0$  is the (classical) chemical potential of component  $\alpha$ .

The Navier–Stokes viscous stress tensor is prescribed in the form

$$\mathbf{\Pi}^{\text{NS}} := 2\eta \mathbf{D} + \left( \zeta - \frac{2}{3} \eta \right) (\operatorname{div} \mathbf{u}) \mathbf{I}, \quad \mathbf{D}(\mathbf{u}) := \frac{1}{2} (\nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^T),$$

where  $\eta(\rho_1, \rho_2) > 0$  and  $\zeta(\rho_1, \rho_2) \geq 0$  are the dynamic and volume viscosity coefficients, respectively. Further, we set  $\eta(\rho_1, \rho_2) = \rho_\alpha \nu_\alpha$ , where the  $\nu_\alpha > 0$  are the constant kinematic viscosity coefficients of component  $\alpha = 1, 2$ .

The capillary stress tensor has the form

$$\mathbf{\Pi}^c := \left( \lambda_{\alpha\beta} \rho_\alpha \Delta \rho_\beta + \frac{1}{2} \lambda_{\alpha\beta} \nabla \rho_\alpha \cdot \nabla \rho_\beta \right) \mathbf{I} - \lambda_{\alpha\beta} \nabla \rho_\alpha \otimes \nabla \rho_\beta.$$

Note that  $\mathbf{\Pi}^c \approx 0$  in domains where  $\rho_\alpha \approx \text{const}$ . Thus, the tensor  $\mathbf{\Pi}^c$  significantly differs from zero only within the interphase boundary. The tensor  $\mathbf{\Pi}^c$ , together with the nonconvex dependence of the function  $\psi_0$  on  $\rho_1$  and  $\rho_2$ , permits one to take the interphase tension into account.

On the right-hand side of Eqs. (1), the coefficient  $M(\rho_1, \rho_2) := M_0 \rho_1 \rho_2 / \rho^2$  is the mobility of components, where  $M_0 > 0$  is a constant;  $\hat{\mu}_{12} := T^{-1}(\hat{\mu}_1 - \hat{\mu}_2)$ , where  $T > 0$  is the temperature, which is a constant parameter by virtue of the assumption about the problem being isothermal;  $\hat{\mu}_\alpha$  is the generalized chemical potential of component  $\alpha$ , and

$$\hat{\mu}_\alpha(\rho_1, \rho_2, \Delta\rho_1, \Delta\rho_2) = \mu_\alpha(\rho_1, \rho_2) - \lambda_{\alpha\beta} \Delta\rho_\beta. \tag{5}$$

System (1), (2) is equipped with the boundary conditions

$$\mathbf{u} = \mathbf{0}, \quad \mathbf{n} \cdot \nabla \rho_\alpha = 0, \quad \mathbf{n} \cdot \nabla \hat{\mu}_\alpha = 0 \quad \text{on} \quad \partial\Omega \tag{6}$$

and the initial conditions

$$\rho_\alpha(\mathbf{x}, 0) = \rho_{\alpha,0}(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}) \quad \text{in} \quad \Omega.$$

Here  $\mathbf{n}$  is the unit outward normal to the domain boundary  $\partial\Omega$ . The first condition in (6) corresponds to the standard no-slip condition, the second condition prescribes a neutral wetting angle (the interface is perpendicular to the domain boundary at the points where they intersect), and the third condition ensures the lack of mass flux of the component  $\alpha$  through the domain boundary.

Consider the QHD-regularization of system (1), (2):

$$\partial_t \rho_\alpha + \operatorname{div}(\rho_\alpha \mathbf{u}_m) = (-1)^{\alpha+1} \operatorname{div}(M \nabla \hat{\mu}_{12}), \quad \alpha = 1, 2, \tag{7}$$

$$\partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u}_m \otimes \mathbf{u}) + \nabla p = \operatorname{div} \mathbf{\Pi}^c + \operatorname{div} \mathbf{\Pi}^{\text{NS}} + \operatorname{div} \mathbf{\Pi}^\tau. \tag{8}$$

In both equations (7) and (8), the expression  $\rho \mathbf{u}$  has been replaced by  $\rho \mathbf{u}_m$ , where  $\mathbf{u}_m = \mathbf{u} - \mathbf{w}$  is the regularized velocity. Also, on the right-hand side of the momentum balance equation (8) we added the term  $\operatorname{div} \mathbf{\Pi}^\tau$ , where  $\mathbf{\Pi}^\tau := \rho \mathbf{u} \otimes \mathbf{w}$  is the regularizing stress tensor. A thermodynamically consistent derivation of Eqs. (7) and (8) can be conducted by analogy with the paper [27].

The presence of the auxiliary term  $\mathbf{w}$  in  $\mathbf{u}_m$  provides a basis for the QHD-regularization of various models of continuum mechanics and corresponds to the mass flux density  $\rho \mathbf{u}_m$  being, in general, distinct from the average momentum of the volume unit  $\rho \mathbf{u}$ , with them being equal not ruled out. In other words, we do not presume the standard hypothesis about the average momentum of a unit volume being equal to the mass flux density to be satisfied [23]. Similar to other QHD-regularized models (see, e.g., [23, 27, 20]), the expression for  $\mathbf{w}$  (see the proof of Theorem 1 below) is constructed taking into account the necessity of the condition of dissipativity of total energy (entropy in the nonisothermal case) to be satisfied and has the form

$$\mathbf{w} = \rho^{-1} \tau [\rho(\mathbf{u} \cdot \nabla) \mathbf{u} + \rho_\alpha \nabla \hat{\mu}_\alpha]. \tag{9}$$

Here the relaxation parameter  $\tau(\rho_1, \rho_2) > 0$  has the dimension of time. Terms having the order  $\mathcal{O}(\tau)$  can be considered as physically motivated regularizers ensuring the stability of explicit central difference approximations to Eqs. (7), (8). Obviously,  $\mathbf{w} = \mathbf{0}$  for  $\tau = 0$ , and system (7), (8) becomes system (1), (2).

Performing summation of Eq. (7) over  $\alpha$ , we obtain the total mass balance equation

$$\partial_t \rho + \operatorname{div}(\rho \mathbf{u}_m) = 0. \tag{10}$$

Throughout the rest of the paper, the parameter  $\tau$  in (9) will be calculated using the formula  $\tau(\rho_1, \rho_1) = \alpha^* \eta(\rho_1, \rho_2) / p(\rho_1, \rho_2)$ , where  $\alpha^* > 0$  is a dimensionless parameter whose value is chosen from the considerations of stability of numerical calculations.

**Remark.** The boundary conditions (6) being satisfied implies the equality  $\mathbf{n} \cdot \mathbf{w} = 0$  on the domain boundary; this implies that  $\mathbf{n} \cdot \mathbf{u}_m = 0$ . Therefore, for system (7), (8), conditions (6) ensure the lack of flux through the boundary in the form of the total mass of the mixture as well as the mass of its separate components. Taking this into account, we have the relations

$$\int_{\Omega} \rho_\alpha(\mathbf{x}, t) d\mathbf{x} = \int_{\Omega} \rho_{\alpha,0}(\mathbf{x}) d\mathbf{x}, \quad \alpha = 1, 2; \quad \int_{\Omega} \rho(\mathbf{x}, t) d\mathbf{x} = \int_{\Omega} (\rho_{1,0}(\mathbf{x}) + \rho_{2,0}(\mathbf{x})) d\mathbf{x},$$

which express the law of conservation of the total mass of the mixture and the total mass of individual components.

3. POTENTIAL FORM OF CAPILLARY STRESSES

Below we will use a representation for capillary stresses in the so-called *potential* form. This form is based on the following assertion, which we provide here with its proof for the presentation to be complete.

**Assertion.** *Under the condition that the capillary coefficients be symmetrical,  $\lambda_{\alpha\beta} = \lambda_{\beta\alpha}$ , one has the relation*

$$\nabla p - \operatorname{div} \mathbf{\Pi}^c = \rho_\alpha \nabla \hat{\mu}_\alpha. \tag{11}$$

**Proof.** By virtue of  $\lambda_{\alpha\beta} = \lambda_{\beta\alpha}$  and  $\partial_i \partial_j = \partial_j \partial_i$ , we obtain

$$\begin{aligned} \lambda_{\alpha\beta} \nabla \rho_\alpha \cdot (\nabla \otimes \nabla \rho_\beta) &= \lambda_{\alpha\beta} (\partial_i \rho_\alpha) (\partial_i \partial_j \rho_\beta) \mathbf{e}_j \\ &= \lambda_{\alpha\beta} (\partial_i \rho_\alpha) (\partial_j \partial_i \rho_\beta) \mathbf{e}_j \\ &= \lambda_{\alpha\beta} \partial_j (\partial_i \rho_\alpha \partial_i \rho_\beta) \mathbf{e}_j - \lambda_{\alpha\beta} (\partial_i \rho_\beta) (\partial_j \partial_i \rho_\alpha) \mathbf{e}_j \\ &= \lambda_{\alpha\beta} \partial_j (\partial_i \rho_\alpha \partial_i \rho_\beta) \mathbf{e}_j - \lambda_{\alpha\beta} (\partial_i \rho_\alpha) (\partial_i \partial_j \rho_\beta) \mathbf{e}_j \\ &= \nabla (\lambda_{\alpha\beta} \nabla \rho_\alpha \cdot \nabla \rho_\beta) - \lambda_{\alpha\beta} \nabla \rho_\alpha \cdot (\nabla \otimes \nabla \rho_\beta). \end{aligned} \tag{12}$$

It readily follows from (12) that

$$\lambda_{\alpha\beta} \nabla \rho_\alpha \cdot (\nabla \otimes \nabla \rho_\beta) = \frac{1}{2} \nabla (\lambda_{\alpha\beta} \nabla \rho_\alpha \cdot \nabla \rho_\beta);$$

the last relation and the Leibniz rule imply that

$$\operatorname{div} (\lambda_{\alpha\beta} \nabla \rho_\alpha \otimes \nabla \rho_\beta) = \lambda_{\alpha\beta} (\nabla \rho_\beta) \Delta \rho_\alpha + \nabla \left( \frac{1}{2} \lambda_{\alpha\beta} \nabla \rho_\alpha \cdot \nabla \rho_\beta \right). \tag{13}$$

Using the representation  $\nabla \psi_0 = (\partial_{\rho_\alpha} \psi_0) \nabla \rho_\alpha \equiv \mu_\alpha \nabla \rho_\alpha$ , we write the pressure gradient in the form

$$\nabla p = \nabla (\rho_\alpha \mu_\alpha) - \nabla \psi_0 = \mu_\alpha \nabla \rho_\alpha + \rho_\alpha \nabla \mu_\alpha - \nabla \psi_0 = \rho_\alpha \nabla \mu_\alpha. \tag{14}$$

In what follows, considering relation (13), the Leibniz rule, and the fact that the coefficients  $\lambda_{\alpha\beta}$  are symmetric, we obtain the relation

$$\operatorname{div} \mathbf{\Pi}^c = \nabla \left( \lambda_{\alpha\beta} \rho_\alpha \Delta \rho_\beta + \frac{1}{2} \lambda_{\alpha\beta} \nabla \rho_\alpha \cdot \nabla \rho_\beta \right) - \operatorname{div} (\lambda_{\alpha\beta} \nabla \rho_\alpha \otimes \nabla \rho_\beta) = \rho_\alpha \nabla (\lambda_{\alpha\beta} \Delta \rho_\beta).$$

Subtracting this relation from relation (14) and using the expression for the *generalized* chemical potential in (5), we arrive at relation (11). The proof of the assertion is complete.

By applying formula (11), we write the momentum balance equation (8) in the form

$$\partial_t (\rho \mathbf{u}) + \operatorname{div} (\rho \mathbf{u}_m \otimes \mathbf{u}) + \rho_\alpha \nabla \hat{\mu}_\alpha = \operatorname{div} \mathbf{\Pi}^{\text{NS}} + \operatorname{div} \mathbf{\Pi}^\tau. \tag{15}$$

Thus, in the representation (15), the capillary forces have a nondivergence (potential) representation. It was noted in the papers [4, 17, 18] that writing the momentum balance equation in such a form permits one to construct energy-dissipative approximations even if they lead to a momentum-nonconservative difference scheme, with the latter not being critical in view of the absence of shock waves and other strong discontinuities. The representation (15) (for  $\tau = 0$ ) was used in the papers [17, 12].

4. DISSIPATIVITY OF QHD-REGULARIZED EQUATIONS

One fundamental property described by systems (1), (2) and (7), (8) is their dissipativity. For isothermal processes, this implies the lack of growth in the total energy  $\mathcal{E}_{\text{tot}}(t)$  of the closed system as the system moves to the equilibrium state. In this section, we prove the dissipativity of the system of QHD-regularized equations (7), (8) with the boundary conditions (6). The following assertion holds.

**Theorem 1.** *For the QHD-regularized system of equations (7), (8) (or (15)), one has the total-energy local balance equation*

$$\partial_t e_{\text{tot}} + \operatorname{div} \mathbf{a} + TM|\nabla \hat{\mu}_{12}|^2 + 2\eta|\mathbf{D}|^2 + \left(\zeta - \frac{2}{3}\eta\right)(\operatorname{div} \mathbf{u})^2 + \rho\tau^{-1}|\mathbf{w}|^2 = 0. \tag{16}$$

Here  $e_{\text{tot}} := \psi_0 + (\lambda_{\alpha\beta}/2)\nabla\rho_\beta \cdot \nabla\rho_\alpha + (\rho|\mathbf{u}|^2)/2$  is the volume density of total energy of the system and

$$\begin{aligned} \mathbf{a} = & (\partial_{\rho_\alpha}\psi_0)\rho_\alpha\mathbf{u}_m - TM\hat{\mu}_{12}\nabla\hat{\mu}_{12} - \partial_t(\lambda_{\alpha\beta}\rho_\alpha)\nabla\rho_\beta \\ & - (\lambda_{\alpha\beta}\Delta\rho_\beta)\rho_\alpha\mathbf{u}_m + \left(\frac{1}{2}|\mathbf{u}|^2\rho\mathbf{u}_m - \mathbf{\Pi}^\tau\mathbf{u} - \mathbf{\Pi}^{\text{NS}}\mathbf{u}\right) \end{aligned} \tag{17}$$

is the total-energy flux vector.

**Proof.** 1. Multiply Eq. (7) by  $\mu_\alpha \equiv \partial_{\rho_\alpha}\psi_0$  and perform summation over  $\alpha$ . Then, taking into account the relation  $\partial_t\psi_0 = (\partial_{\rho_\alpha}\psi_0)\partial_t\rho_\alpha$ , we have

$$\partial_t\psi_0 + \mu_\alpha \operatorname{div}(\rho_\alpha\mathbf{u}_m) = \mu_\alpha(-1)^{\alpha+1} \operatorname{div}(M\nabla\hat{\mu}_{12}). \tag{18}$$

Let us transform the second term on the left-hand side in relation (18) using the Leibniz rule:

$$\mu_\alpha \operatorname{div}(\rho_\alpha\mathbf{u}_m) = \operatorname{div}(\mu_\alpha\rho_\alpha\mathbf{u}_m) - \rho_\alpha\mathbf{u}_m \cdot \nabla\mu_\alpha, \tag{19}$$

and represent the right-hand side of relation (18) in the form

$$\begin{aligned} \mu_\alpha(-1)^{\alpha+1} \operatorname{div}(M\nabla\hat{\mu}_{12}) &= (\mu_1 - \mu_2) \operatorname{div}(M\nabla\hat{\mu}_{12}) \\ &= (T\hat{\mu}_{12} + \lambda_{1\beta}\Delta\rho_\beta - \lambda_{2\beta}\Delta\rho_\beta) \operatorname{div}(M\nabla\hat{\mu}_{12}) \\ &= \operatorname{div}(TM\hat{\mu}_{12}\nabla\hat{\mu}_{12}) - TM|\nabla\hat{\mu}_{12}|^2 + (\lambda_{1\beta} - \lambda_{2\beta})\Delta\rho_\beta \operatorname{div}(M\nabla\hat{\mu}_{12}), \end{aligned} \tag{20}$$

where we have also used the Leibniz rule when deriving the last expression.

Let us substitute the expressions (19) and (20) into (18) to arrive at the relation

$$\begin{aligned} \partial_t\psi_0 + \operatorname{div}(\mu_\alpha\rho_\alpha\mathbf{u}_m - TM\hat{\mu}_{12}\nabla\hat{\mu}_{12}) - \rho_\alpha\mathbf{u}_m \cdot \nabla\mu_\alpha \\ = -TM|\nabla\hat{\mu}_{12}|^2 + (\lambda_{1\beta} - \lambda_{2\beta})\Delta\rho_\beta \operatorname{div}(M\nabla\hat{\mu}_{12}). \end{aligned} \tag{21}$$

2. Multiply Eq. (7) by  $-\lambda_{\alpha\beta}\Delta\rho_\beta$  and perform summation over  $\alpha$  to obtain

$$-(\lambda_{\alpha\beta}\Delta\rho_\beta)\partial_t\rho_\alpha - (\lambda_{\alpha\beta}\Delta\rho_\beta) \operatorname{div}(\rho_\alpha\mathbf{u}_m) = (-1)^{\alpha+2}(\lambda_{\alpha\beta}\Delta\rho_\beta) \operatorname{div}(M\nabla\hat{\mu}_{12}). \tag{22}$$

Let us transform the first term on the left-hand side in relation (22) as

$$-(\lambda_{\alpha\beta}\Delta\rho_\beta)\partial_t\rho_\alpha = -\operatorname{div}(\nabla\rho_\beta)\lambda_{\alpha\beta}\partial_t\rho_\alpha = -\operatorname{div}(\lambda_{\alpha\beta}\partial_t\rho_\alpha\nabla\rho_\beta) + \partial_t\left(\frac{1}{2}\lambda_{\alpha\beta}\nabla\rho_\beta \cdot \nabla\rho_\alpha\right), \tag{23}$$

where we have used the Leibniz rule as well as the identity  $\partial_t\nabla = \nabla\partial_t$  and the relation

$$\lambda_{\alpha\beta}\nabla\rho_\beta \cdot \partial_t\nabla\rho_\alpha = \partial_t(\lambda_{\alpha\beta}\nabla\rho_\beta \cdot \nabla\rho_\alpha/2), \tag{24}$$

which holds by virtue of the condition  $\lambda_{\alpha\beta} = \lambda_{\beta\alpha}$ . Recall that that repeated indices  $\alpha$  and  $\beta$  assume summation from 1 to 2.

We bring the second term on the left-hand side in relation (22) to the form

$$-(\lambda_{\alpha\beta}\Delta\rho_\beta) \operatorname{div}(\rho_\alpha\mathbf{u}_m) = -\operatorname{div}[(\lambda_{\alpha\beta}\Delta\rho_\beta)\rho_\alpha\mathbf{u}_m] + \rho_\alpha\mathbf{u}_m \cdot \nabla(\lambda_{\alpha\beta}\Delta\rho_\beta). \tag{25}$$

Substituting the expressions (23) and (25) into (22), we arrive at the relation

$$\begin{aligned} \partial_t\left(\frac{1}{2}\lambda_{\alpha\beta}\nabla\rho_\beta \cdot \nabla\rho_\alpha\right) + \rho_\alpha\mathbf{u}_m \cdot \nabla(\lambda_{\alpha\beta}\Delta\rho_\beta) - \operatorname{div}[\partial_t(\lambda_{\alpha\beta}\rho_\alpha)\nabla\rho_\beta + (\lambda_{\alpha\beta}\Delta\rho_\beta)\rho_\alpha\mathbf{u}_m] \\ = -(\lambda_{1\beta} - \lambda_{2\beta})\Delta\rho_\beta \operatorname{div}(M\nabla\hat{\mu}_{12}), \end{aligned} \tag{26}$$

where we have also used the identity  $(-1)^{\alpha+2}(\lambda_{\alpha\beta}\Delta\rho_\beta) \equiv -(\lambda_{1\beta} - \lambda_{2\beta})\Delta\rho_\beta$ .

3. Let us obtain the kinetic-energy balance equation. First, note that by virtue of the Leibniz rule, one has the formulas

$$\mathbf{u} \cdot \partial_t(\rho \mathbf{u}) = \frac{1}{2} |\mathbf{u}|^2 \partial_t \rho + \partial_t \left( \frac{1}{2} |\mathbf{u}|^2 \rho \right) = -\frac{1}{2} |\mathbf{u}|^2 \operatorname{div}(\rho \mathbf{u}_m) + \partial_t \left( \frac{1}{2} |\mathbf{u}|^2 \rho \right), \tag{27}$$

$$\mathbf{u} \cdot \operatorname{div}(\rho \mathbf{u}_m \otimes \mathbf{u}) = \frac{1}{2} |\mathbf{u}|^2 \operatorname{div}(\rho \mathbf{u}_m) + \operatorname{div} \left( \frac{1}{2} |\mathbf{u}|^2 \rho \mathbf{u}_m \right), \tag{28}$$

$$\mathbf{u} \cdot \operatorname{div} \mathbf{\Pi}^{\text{NS}} + \mathbf{u} \cdot \operatorname{div} \mathbf{\Pi}^\tau = \operatorname{div}(\mathbf{\Pi}^\tau \mathbf{u} + \mathbf{\Pi}^{\text{NS}} \mathbf{u}) - \mathbf{\Pi}^{\text{NS}} : (\nabla \otimes \mathbf{u}) - \mathbf{\Pi}^\tau : (\nabla \otimes \mathbf{u}), \tag{29}$$

where, in relation (27), we have also used the total-mass balance equation (10). Let us transform the last two terms on the right-hand side in relation (29) as

$$\mathbf{\Pi}^{\text{NS}} : (\nabla \otimes \mathbf{u}) = 2\eta |\mathbf{D}|^2 + \left( \zeta - \frac{2}{3} \eta \right) (\operatorname{div} \mathbf{u})^2, \quad \mathbf{\Pi}^\tau : (\nabla \otimes \mathbf{u}) = \rho \boldsymbol{\omega} \cdot [(\mathbf{u} \cdot \nabla) \mathbf{u}], \tag{30}$$

where the first relation is derived taking into account the identity  $\mathbf{D} : (\nabla \otimes \mathbf{u}) \equiv |\mathbf{D}|^2$ , which holds in view of the tensor  $\mathbf{D}$  being symmetric.

Taking the inner product of the momentum balance equation (15) by  $\mathbf{u}$  and using the relations in (27)–(30), we obtain

$$\begin{aligned} \partial_t \left( \frac{1}{2} \rho |\mathbf{u}|^2 \right) + \operatorname{div} \left( \frac{1}{2} |\mathbf{u}|^2 \rho \mathbf{u}_m - \mathbf{\Pi}^{\text{NS}} \mathbf{u} - \mathbf{\Pi}^\tau \mathbf{u} \right) + \rho_\alpha \mathbf{u} \cdot \nabla \hat{\mu}_\alpha \\ = -2\eta |\mathbf{D}|^2 - \left( \zeta - \frac{2}{3} \eta \right) (\operatorname{div} \mathbf{u})^2 - \rho \boldsymbol{\omega} \cdot [(\mathbf{u} \cdot \nabla) \mathbf{u}]. \end{aligned} \tag{31}$$

Adding relations (21), (26), and (31), we arrive at Eq. (16), and this completes the proof of the theorem. Note that it is at this stage that it becomes clear that the vector  $\boldsymbol{\omega}$  has the form (9) and the vector  $\mathbf{a}$  has the form (17).

**Corollary 1.** *For system (7), (8) (or (15)) with the boundary conditions (6), one has the law of lack of growth in the system total energy ,*

$$\frac{d\mathcal{E}_{\text{tot}}}{dt} = - \int_{\Omega} \left( 2\eta |\mathbf{D}|^2 + \left( \zeta - \frac{2}{3} \eta \right) (\operatorname{div} \mathbf{u})^2 + TM |\nabla \hat{\mu}_{12}|^2 + \rho \tau^{-1} |\boldsymbol{\omega}|^2 \right) d\mathbf{x} \leq 0, \tag{32}$$

where  $\mathcal{E}_{\text{tot}}(t) := \int_{\Omega} e_{\text{tot}}(\mathbf{x}, t) d\mathbf{x}$  is the total energy of the system.

**Proof.** The proof is conducted by a straightforward integration of Eq. (16) over the domain  $\Omega$  and application of the Gauss divergence theorem with allowance for conditions (6) and the relation

$$|\mathbf{D}|^2 - \frac{1}{3} (\operatorname{div} \mathbf{u})^2 \equiv \left| \mathbf{D} - \frac{1}{3} (\operatorname{tr} \mathbf{D}) \mathbf{I} \right|^2 \geq 0.$$

**Corollary 2.** *System (1), (2) with the boundary conditions (6) is dissipative.*

**Proof.** The proof follows from the fact that for  $\tau = 0$  system (7), (8) transforms into system (1), (2), while inequality (32) remains true.

### 5. SPATIAL APPROXIMATION

The dissipativity is a fundamental property of system (7), (8) (or (15)) that determines its thermodynamic correctness. Therefore, among all feasible numerical algorithms for solving this system, one should prefer the ones that ensure this property (in one or another form) at the discrete

level. This section is devoted to constructing such a spatial discretization of Eqs. (7), (8) that is dissipative in the above-indicated sense for the one-dimensional plane-parallel case.

Consider the spatial domain  $\Omega = [0, L] \subset \mathbb{R}$ . We will use uniform difference meshes with step  $h = L/N$ . The mesh nodes with integer indices will be denoted by  $x_i = hi$  and those with half-integer ones, by  $x_{i-1/2} = h(i - 1/2)$ , with  $x_0 = 0$  and  $x_N = L$ . Here and below, the subscripts  $i, j$ , and  $k$  are reserved for node numbers. In  $\Omega$ , introduce the main mesh  $\bar{\omega}_h := \{x_i\}_{i=0}^N$  and internal meshes  $\omega_h := \{x_i\}_{i=1}^{N-1}$  and  $\omega_h^* := \{x_{i-1/2}\}_{i=1}^N$ . We will need the auxiliary *extended* meshes  $\bar{\omega}_h^* := \{x_{i-1/2}\}_{i=0}^{N+1}$ ,  $\bar{\omega}_h^{**} := \{x_{i-1/2}\}_{i=-1}^{N+2}$ , and  $\bar{\omega}_h := \{x_i\}_{i=-1}^{N+1}$ . Note that not all the nodes of the extended meshes lie in the domain  $\Omega$ .

Let  $H(\omega)$  be the set of functions defined on some mesh  $\omega$ . We introduce the mesh averaging operators  $s : H(\bar{\omega}_h) \rightarrow H(\bar{\omega}_h^*)$ ,  $s^* : H(\bar{\omega}_h^{**}) \rightarrow H(\bar{\omega}_h)$  and difference relations  $\delta : H(\bar{\omega}_h) \rightarrow H(\bar{\omega}_h^*)$ ,  $\delta^* : H(\bar{\omega}_h^*) \rightarrow H(\bar{\omega}_h)$  by the formulas

$$\begin{aligned} (su)_{i+1/2} &:= \frac{1}{2}(u_{i+1} + u_i), & (s^*v)_i &:= \frac{1}{2}(v_{i+1/2} + v_{i-1/2}), \\ (\delta u)_{i+1/2} &:= \frac{1}{h}(u_{i+1} - u_i), & (\delta^*v)_i &:= \frac{1}{h}(v_{i+1/2} - v_{i-1/2}). \end{aligned}$$

Let  $u$  and  $v$  be some mesh functions in  $H(\bar{\omega}_h)$  and let  $\tilde{u}$  and  $\tilde{v}$  be mesh functions in  $H(\bar{\omega}_h^*)$ . Define the inner products  $(u, v)$  on  $H(\omega_h)$ ,  $(u, v)_{\bar{x}}$  on  $H(\bar{\omega}_h)$ , and  $(\tilde{u}, \tilde{v})_*$  on  $H(\omega_h^*)$  by the formulas

$$(u, v) := h \sum_{i=1}^{N-1} u_i v_i, \quad (u, v)_{\bar{x}} := \frac{1}{2} h v_0 u_0 + (u, v) + \frac{1}{2} h v_N u_N, \quad (\tilde{u}, \tilde{v})_* := h \sum_{i=1}^N \tilde{u}_{i-1/2} \tilde{v}_{i-1/2}.$$

For the inner products thus introduced, one has the identities

$$\begin{aligned} (\delta v, \tilde{u})_* &= -(v, \delta^* \tilde{u})_{\bar{x}} + (s^* \tilde{u})_N v_N - (s^* \tilde{u})_0 v_0, \\ (sv, \tilde{u})_* &= (v, s^* \tilde{u})_{\bar{x}} + \frac{1}{4} h^2 v_0 (\delta^* \tilde{u})_0 - \frac{1}{4} h^2 v_N (\delta^* \tilde{u})_N. \end{aligned}$$

In particular, if  $v_0 = v_N = 0$ , then  $(u, v) = (u, v)_{\bar{x}}$  and

$$(\delta v, \tilde{u})_* = -(v, \delta^* \tilde{u}), \tag{33}$$

$$(sv, \tilde{u})_* = (v, s^* \tilde{u}). \tag{34}$$

Consider the following space-discrete and time-continuous method for system (7) and (15) in the spatially uniform statement:

$$\partial_t \rho_\alpha + \delta[(s^* \rho_\alpha) u_m] = (-1)^{\alpha+1} \delta[(s^* M) \delta^* \hat{\mu}_{12}] \quad \text{on } \omega_h^*, \quad \alpha = 1, 2, \tag{35}$$

$$\partial_t [(s^* \rho) u] + \delta^* [(s j_m) s u] + (s^* \rho_\alpha) \delta^* \hat{\mu}_\alpha = \delta^* \Pi^{\text{NS}} + \delta^* \Pi^\tau \quad \text{on } \omega_h, \tag{36}$$

where

$$j_m = (s^* \rho) u_m, \quad u_m = u - w, \quad \Pi^{\text{NS}} = \eta \frac{4}{3} \delta u + \zeta \delta u, \tag{37}$$

$$\hat{\mu}_{12} = T^{-1}(\hat{\mu}_1 - \hat{\mu}_2), \quad \Pi^\tau = s[(s^* \rho) u w], \quad w = \tau (s^* \rho)^{-1} [(s^* \rho) u s^* \delta u + (s^* \rho_\alpha) \delta^* \hat{\mu}_\alpha], \tag{38}$$

$$\hat{\mu}_\alpha = \mu_\alpha - \lambda_{\alpha\beta} \delta \delta^* \rho_\beta. \tag{39}$$

The main unknown functions are  $u \in H(\bar{\omega}_h)$  and  $\rho_\alpha \in H(\omega_h^*)$ . In addition,  $\{w, \tau(s^* \rho_1, s^* \rho_2)\} \subset H(\bar{\omega}_h)$  and  $\{\Pi^{\text{NS}}, \mu_\alpha, \hat{\mu}_\alpha, \eta(\rho_1, \rho_2), \zeta(\rho_1, \rho_2), M(\rho_1, \rho_2)\} \subset H(\omega_h^*)$ .

On the boundaries  $x = 0$  and  $x = L$  of the computational domain, we set

$$u_0 = u_N = 0, \quad (\delta^* \rho_\alpha)_0 = (\delta^* \rho_\alpha)_N = 0, \quad (\delta^* \hat{\mu}_\alpha)_0 = (\delta^* \hat{\mu}_\alpha)_N = 0, \quad \alpha = 1, 2. \tag{40}$$

It follows from relations (37)–(39) that for all necessary discrete functions to be determined correctly, the desired functions  $u$  and  $\rho_\alpha$ , as well as  $\mu_\alpha$  and  $\hat{\mu}_\alpha$ , must be continued to wider domains.



To this end, we set  $u \in H(\bar{\omega}_h)$ ,  $\rho_\alpha \in H(\bar{\omega}_h^*)$ , and  $\{\mu_\alpha, \hat{\mu}_\alpha, M\} \subset H(\bar{\omega}_h^*)$ . In this case, for the second and third boundary conditions in (40) to be satisfied, we continue  $\rho_\alpha$  in an *even* manner with respect to the boundary nodes  $x_0$  and  $x_N$ . Note also that (40) implies the lack of the mass flux through the boundary; i.e.,

$$w_0 = w_N = 0, \quad (u_m)_0 = (u_m)_N = 0. \tag{41}$$

By analogy with the continuous case, performing summation of Eqs. (35) over  $\alpha = 1, 2$ , we obtain the discrete complete mass balance equation for the mixture,

$$\partial_t \rho + \delta[(s^* \rho)u_m] = 0. \tag{42}$$

Also note that this discretization obeys the conservation laws for the total mass and the masses of components,

$$(\rho_\alpha, 1)_* = (\rho_{\alpha,0}, 1)_* = \text{const}, \quad \alpha = 1, 2, \quad (\rho, 1)_* = (\rho_{1,0} + \rho_{2,0}, 1)_* = \text{const}. \tag{43}$$

The following difference analog of the corollary of Theorem 1 about the lack of growth in the system total energy holds true.

**Theorem 2.** *For the semidiscrete method (35), (36) one has the relation*

$$\frac{d\mathcal{E}_{\text{tot}}}{dt} = -\frac{4}{3} (\eta(\delta u)^2, 1)_* - (\zeta(\delta u)^2, 1)_* - (T(s^*M)(\delta^* \hat{\mu}_{12})^2, 1) - (\tau w^2, (s^* \rho)^{-1}) \leq 0, \tag{44}$$

where  $\mathcal{E}_{\text{tot}}(t) := (e_{\text{tot}}, 1)_*$  is the discrete analog of the system total energy and

$$e_{\text{tot}} := \frac{1}{2} \rho s u^2 + \psi_0 + \frac{1}{2} \lambda_{\alpha\beta} s [(\delta^* \rho_\alpha) (\delta^* \rho_\beta)]$$

is the discrete analog of the volume density of total energy.

**Proof.** The derivation of relation (44) presented below is based on the proof of Theorem 1 and consists of similar steps.

1. Take the inner product of Eq. (35) by  $\partial_{\rho_\alpha} \psi_0 \equiv \mu_\alpha$ , perform summation over  $\alpha = 1, 2$ , and take the relation  $(\partial_{\rho_\alpha} \psi_0) \partial_t \rho_\alpha = \partial_t \psi_0$  into account to obtain

$$\partial_t (\psi_0, 1)_* + (\mu_\alpha, \delta[(s^* \rho_\alpha)u_m])_* = (\mu_\alpha, (-1)^{\alpha+1} \delta[(s^*M)\delta^* \hat{\mu}_{12}])_*. \tag{45}$$

Considering relations (41), we use formula (33) to transform the second term on the left-hand side in relation (45). We have

$$(\mu_\alpha, \delta[(s^* \rho_\alpha)u_m])_* = -(\delta^* \mu_\alpha, (s^* \rho_\alpha)u_m). \tag{46}$$

Transforming the right-hand side of relation (45) by analogy with (20), we obtain

$$\begin{aligned} (\mu_\alpha, (-1)^{\alpha+1} \delta[(s^*M)\delta^* \hat{\mu}_{12}])_* &= (T\hat{\mu}_{12} + \lambda_{1\beta} \delta \delta^* \rho_\beta - \lambda_{2\beta} \delta \delta^* \rho_\beta, \delta[(s^*M)\delta^* \hat{\mu}_{12}])_* \\ &= -(T(s^*M)(\delta^* \hat{\mu}_{12})^2, 1) + ([\lambda_{1\beta} - \lambda_{2\beta}] \delta \delta^* \rho_\beta, \delta[(s^*M)\delta^* \hat{\mu}_{12}])_*, \end{aligned} \tag{47}$$

where we have used the identity  $\mu_\alpha (-1)^{\alpha+1} \equiv \mu_1 - \mu_2$  and applied formula (33) with allowance for the third condition in (40) when deriving the last expression.

Substituting the expressions (46) and (47) into (45), we arrive at the relation

$$\partial_t (\psi_0, 1)_* - ((s^* \rho_\alpha)u_m, \delta^* \mu_\alpha) = -(T(s^*M)(\delta^* \hat{\mu}_{12})^2, 1) + ([\lambda_{1\beta} - \lambda_{2\beta}] \delta \delta^* \rho_\beta, \delta[(s^*M)\delta^* \hat{\mu}_{12}])_*. \tag{48}$$

2. In what follows, taking the inner product of Eq. (35) by  $-\lambda_{\alpha\beta} \delta \delta^* \rho_\beta$ , we have

$$-(\lambda_{\alpha\beta} \delta \delta^* \rho_\beta, \partial_t \rho_\alpha)_* - (\lambda_{\alpha\beta} \delta \delta^* \rho_\beta, \delta[(s^* \rho_\alpha)u_m])_* = (\lambda_{\alpha\beta} \delta \delta^* \rho_\beta, (-1)^{\alpha+2} \delta[(s^*M)\delta^* \hat{\mu}_{12}])_*. \tag{49}$$

Let us transform the first term on the left-hand side in relation (49) using formula (33), which holds by virtue of the second condition in (40), and taking into account the fact that the coefficients  $\lambda_{\alpha\beta}$  are symmetric,

$$\begin{aligned}
 -(\lambda_{\alpha\beta}\delta\delta^*\rho_\beta, \partial_t\rho_\alpha)_* &= \lambda_{\alpha\beta}(\delta^*\rho_\beta, \delta^*\partial_t\rho_\alpha) \\
 &= \partial_t\left(\frac{1}{2}\lambda_{\alpha\beta}\delta^*\rho_\beta\delta^*\rho_\alpha, 1\right) = \partial_t\left(\frac{1}{2}\lambda_{\alpha\beta}s[\delta^*\rho_\beta\delta^*\rho_\alpha], 1\right)_*, \tag{50}
 \end{aligned}$$

where the penultimate expression was derived using the relation

$$\lambda_{\alpha\beta}(\delta^*\rho_\beta)\partial_t\delta^*\rho_\alpha = \partial_t(\lambda_{\alpha\beta}\delta^*\rho_\beta\delta^*\rho_\alpha/2),$$

similar to (24), and the relation  $\delta^*\partial_t = \partial_t\delta^*$ ; the last expression was derived using formula (34) with allowance for the identities  $1 \equiv s^*1$  and  $\delta^*1 \equiv 0$  and the second condition in (40).

By directly applying formula (33), which holds by virtue of (41), we can reduce the second term on the left-hand side in relation (49) to the form

$$-(\lambda_{\alpha\beta}\delta\delta^*\rho_\beta, \delta[(s^*\rho_\alpha)u_m])_* = ((s^*\rho_\alpha)u_m, \delta^*[\lambda_{\alpha\beta}\delta\delta^*\rho_\beta]). \tag{51}$$

Substituting the expressions (50) and (51) into (49), we obtain

$$\begin{aligned}
 \partial_t\left(\frac{1}{2}\lambda_{\alpha\beta}s[\delta^*\rho_\alpha\delta^*\rho_\beta], 1\right)_* &+ ((s^*\rho_\alpha)u_m, \delta^*[\lambda_{\alpha\beta}\delta\delta^*\rho_\beta]) \\
 &= -([\lambda_{1\beta} - \lambda_{2\beta}]\delta\delta^*\rho_\beta, \delta[(s^*M)\delta^*\hat{\mu}_{12}]), \tag{52}
 \end{aligned}$$

where we have also used the identity  $(-1)^{\alpha+2}\lambda_{\alpha\beta}\delta\delta^*\rho_\beta \equiv -(\lambda_{1\beta} - \lambda_{2\beta})\delta\delta^*\rho_\beta$ .

Adding relations (48) and (52), we have

$$\partial_t\left(\psi_0 + \frac{1}{2}\lambda_{\alpha\beta}s[\delta^*\rho_\alpha\delta^*\rho_\beta], 1\right)_* - ((s^*\rho_\alpha)u_m, \delta^*\hat{\mu}_\alpha) = -(T(s^*M)(\delta^*\hat{\mu}_{12})^2, 1). \tag{53}$$

3. Let us obtain the discrete kinetic energy balance equation for the system. To this end, take the inner product of the momentum balance equation (36) by  $u$ ,

$$(u, \partial_t[(s^*\rho)u]) + (u, \delta^*[(sj_m)su]) + (u, (s^*\rho_\alpha)\delta^*\hat{\mu}_\alpha) = (u, \delta^*\Pi^{NS}) + (u, \delta^*\Pi^\tau). \tag{54}$$

Let us transform the first term on the left-hand side in relation (54). First, note that, by virtue of the relation  $\partial_t s^* = s^*\partial_t$ , formulas (33) and (34), the boundary conditions (40), relations (41), and the discrete total-mass balance equation (42), the following chain of relations holds:

$$\begin{aligned}
 (u^2, \partial_t(s^*\rho)) &= (su^2, \partial_t\rho)_* = -(su^2, \delta j_m)_* = (\delta^*su^2, j_m) \\
 &= (s^*\delta u^2, j_m) = (\delta u^2, sj_m)_* = 2(\delta u, (sj_m)su)_*, \tag{55}
 \end{aligned}$$

where the relations  $s^*\delta = \delta^*s$  and  $\delta u^2 = 2(\delta u)su$  have also been taken into account. Using (34) and (55), we can express the first term on the left-hand side in relation (54) in the form

$$(u, \partial_t[(s^*\rho)u]) = \frac{1}{2}\partial_t(s^*\rho, u^2) + \frac{1}{2}(u^2, \partial_t(s^*\rho)) = \frac{1}{2}\partial_t(\rho, su^2)_* + (\delta u, (sj_m)su)_*. \tag{56}$$

Using the first boundary condition in (40) and formula (33), we write the second term on the left-hand side in relation (54) in the form

$$(u, \delta^*[(sj_m)su]) = -(\delta u, (sj_m)su)_*. \tag{57}$$

Transforming the first and second terms on the right-hand side in relation (54) with the help of formula (33), we have

$$(u, \delta^* \Pi^{\text{NS}}) = -(\delta u, \Pi^{\text{NS}})_* = -\frac{4}{3}(\eta(\delta u)^2, 1)_* - (\zeta(\delta u)^2, 1)_*, \tag{58}$$

$$(u, \delta^* \Pi^\tau) = -(\delta u, \Pi^\tau)_* = -(\delta u, s[us^* \rho])_* = -(us^* \delta u, (s^* \rho) w), \tag{59}$$

where in (59) we have also used formula (34), which holds by virtue of the no-slip conditions (59).

Thus, substituting the expressions (56)–(59) into (54), we obtain the kinetic energy balance equation for the system,

$$\partial_t \left( \rho, \frac{1}{2} s u^2 \right)_* + (u, (s^* \rho) \delta^* \hat{\mu}_\alpha) = -\frac{4}{3}(\eta(\delta u)^2, 1)_* - (\zeta(\delta u)^2, 1)_* - (us^* \delta u, (s^* \rho) w). \tag{60}$$

Adding (53) to (60), we obtain relation (44). The proof of the theorem is complete.

### 6. NONDIMENSIONALIZATION

Let us nondimensionalize system (7), (15) following the paper [11]. For the typical quantities we take

$$\rho^* = \frac{m_2}{3b_2}, \quad p^* = \frac{a_{22}}{27b_2^2}, \quad T^* = \frac{8a_{22}}{27k_B b_2}, \quad L^* = 2b_2^{1/3}, \quad u^* = \sqrt{\frac{p^*}{\rho^*}}.$$

Here  $\rho^*$ ,  $p^*$ , and  $T^*$  correspond to the density, pressure, and temperature at the critical point for the *second* component,  $l^*$  is the typical spatial scale, which is on the order of the thickness of the interface, and  $u^*$  is the typical velocity. The dimensionless variables will be equipped with the symbol “ $\sim$ ” (for example,  $\tilde{\rho}$ ). Thus, we have

$$\begin{aligned} \rho_\alpha &= \rho^* \tilde{\rho}_\alpha, & \mathbf{u} &= u^* \tilde{\mathbf{u}}, & \mathbf{w} &= u^* \tilde{\mathbf{w}}, & \mathbf{x} &= L^* \tilde{\mathbf{x}}, & p &= p^* \tilde{p}, \\ \psi_0 &= p^* \tilde{\psi}_0, & T &= T^* \tilde{T}, & \mu_\alpha &= \frac{p^*}{\rho^*} \tilde{\mu}_\alpha, & t &= \frac{L^*}{u^*} \tilde{t}, & \eta &= \nu_2 \rho^* \tilde{\eta}, \\ M_0 &= \frac{\rho^{*2} u^* L^* T^*}{p^*} \tilde{M}_0, & \mathbf{\Pi}^{\text{NS}} &= \frac{\nu_2 \rho^* u^*}{L^*} \tilde{\mathbf{\Pi}}^{\text{NS}}, & \lambda_{\alpha\beta} &= \frac{L^{*2} p^*}{\rho^{*2}} \tilde{\lambda}_{\alpha\beta}, & D_{\alpha\beta} &= \frac{m^{*2} p^* L^{*2}}{\rho^{*2} k_B T^*} \tilde{D}_{\alpha\beta}. \end{aligned}$$

In what follows, to simplify the notation, we omit the symbol “ $\sim$ ” over all the variables. It is convenient to introduce the following dimensionless variables:

$$m_{21} = \frac{m_2}{m_1}, \quad r_{21} = \frac{a_{21}}{a_{22}}, \quad r_{11} = \frac{a_{11}}{a_{22}}, \quad b_{12} = \frac{b_1}{b_2}, \quad A = \frac{1}{3} \left( \frac{27b_2^{1/3} \hbar^2}{16\pi a_{22} m_2} \right)^{3/2}, \quad \nu_{12} = \frac{\nu_1}{\nu_2}.$$

The relation (4) for the Helmholtz energy acquires the form

$$\begin{aligned} \psi_0(\rho_1, \rho_2) &= T \frac{8}{3} \rho_1 m_{21} \ln \left[ \frac{m_{21}^{5/2} \rho_1 A}{T^{3/2} (1 - \phi)} \right] + T \frac{8}{3} \rho_2 \ln \left[ \frac{\rho_2 A}{T^{3/2} (1 - \phi)} \right] \\ &\quad - 3(r_{11} m_{21}^2 \rho_1^2 + 2r_{21} m_{21} \rho_1 \rho_2 + \rho_2^2) - T \frac{8}{3} (m_{21} \rho_1 + \rho_2), \end{aligned} \tag{61}$$

where  $\phi(\rho_1, \rho_2) = b_{12} \frac{1}{3} m_{21} \rho_1 + \frac{1}{3} \rho_2$ . For system (7), (15), we obtain

$$\begin{aligned} \partial_t \rho_\alpha + \operatorname{div}(\rho_\alpha \mathbf{u}_m) &= (-1)^{\alpha+1} \operatorname{div}(M \nabla \hat{\mu}_{12}), \quad \alpha = 1, 2, \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u}_m \otimes \mathbf{u}) + \rho_\alpha \nabla \hat{\mu}_\alpha &= \frac{1}{\operatorname{Re}} \operatorname{div} \mathbf{\Pi}^{\text{NS}} + \operatorname{div} \mathbf{\Pi}^\tau, \end{aligned}$$

where  $\text{Re} = L^*u^*/\nu_2$  and

$$\begin{aligned} \mathbf{\Pi}^{\text{NS}} &= \eta(\nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^T) + \left(\zeta - \frac{2}{3}\eta\right)(\text{div } \mathbf{u})\mathbf{I}, \quad \mathbf{\Pi}^T = \rho\mathbf{u} \otimes \mathbf{w}, \\ \eta(\rho_1, \rho_2) &= \rho_1\nu_{12} + \rho_2, \quad \mathbf{w} = \frac{\tau}{\rho}[\rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \rho_\alpha \nabla \hat{\mu}_\alpha], \quad \tau = 0.3 \frac{\eta(\rho_1, \rho_2)}{p(\rho_1, \rho_2)}. \end{aligned}$$

### 7. NUMERICAL EXPERIMENT

Let us apply the explicit Euler method to discretize the constructed semidiscrete difference scheme (35), (36) in time  $t$ . To this end, we replace all derivatives with respect to time  $\partial_t f$  with  $\delta_t f := (f^{n+1} - f^n)/\Delta t$ , where  $f$  is the corresponding difference function, the superscript is used for the time layer number, and  $\Delta t$  designates the time step.

To demonstrate the capabilities of the constructed difference scheme, we consider the problem of modeling stratification into different phases of a virtually homogeneous mixture whose component composition is unstable under small perturbations. Such a stratification is often referred to as the spinodal decomposition of the mixture (see, e.g., [13, p. 117]). Modeling this process using system (7), (15) is possible since (i) the homogeneous part of the free energy (61) (respectively, (4)) is nonconvex, a fact that accounts for “stratification”; and (ii) the free energy (3) contains gradient terms that prevent the interface from becoming infinitely thin in the course of stratification (therewith the gradient terms also have a regularizing meaning [5, 9]).

Consider a mixture of components described by the following collection of dimensionless parameters:  $r_{11} = 3.426$ ,  $r_{21} = 1.75$ ,  $b_{12} = 2.028$ ,  $m_{21} = 0.8356$ ,  $T = 0.957$ ,  $\nu_{12} = 10.0$ ,  $\text{Re} = 10.0$ ,  $D_{11} = 12$ ,  $D_{22} = 4$ ,  $D_{12} = D_{21} = 6.9282$ ,  $M_0 = 0.1$ ,  $A = 10^{-5}$ , and  $\zeta = \eta$ .

We take the initial conditions in the form

$$\rho_{1,0}(x_{i+1/2}) = 0.054(1 + \varepsilon(x_{i+1/2})), \quad \rho_{2,0}(x_{i+1/2}) = 1 + \varepsilon(x_i), \quad u_0(x_{i+1/2}) = 0,$$

where  $\varepsilon(x_{i+1/2})$  is a random variable that has a uniform distribution and assumes values in the interval  $[-0.05, 0.05]$ . Consider the domain of size  $L = 200$ . We select the space and time steps to be  $h = L/100$  and  $\Delta t = 2 \cdot 10^{-3}$ , respectively.

Figure 1 presents the dependence  $\mathcal{E}_{\text{tot}}(t) - \mathcal{E}_{\text{tot}}(t_{\text{end}})$ , where  $t_{\text{end}} = 4.93 \cdot 10^4$  is the moment up to which the modeling was carried out. It can be seen that the total energy is nonincreasing in agreement with inequalities (44). Note that a sharp decrease in the total energy is observed at the moment  $t \approx 2.67 \cdot 10^4$ . In this case, the change occurs gradually as clearly demonstrated by the enlarged fragment of the domain  $t \in [26370, 27000]$  (see the bottom of Fig. 1). The kinetic energy  $\mathcal{E}_{\text{kin}}(t) := (\rho, 0.5su^2)_*$  of the system also undergoes a dramatic increase at the same time moment and then starts to drop (Fig. 2).

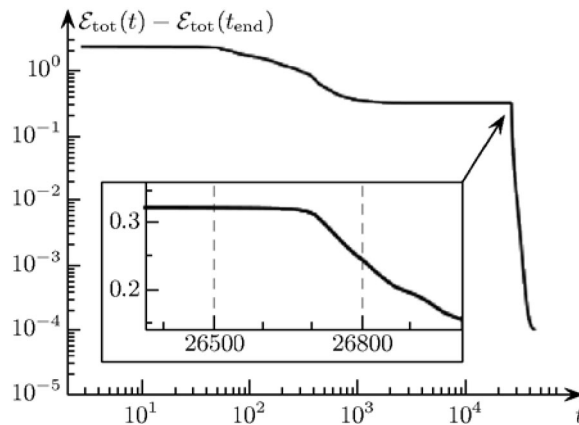
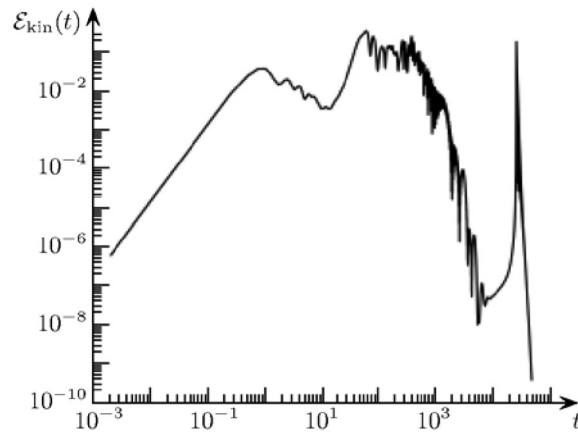
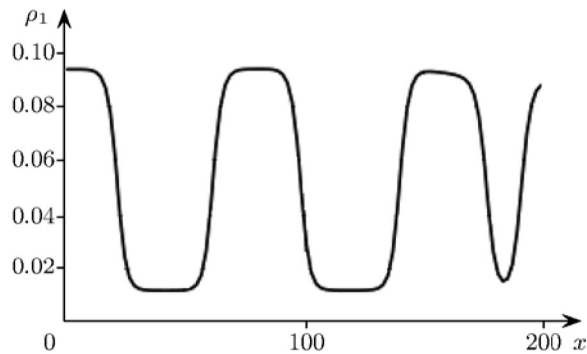


Fig. 1. Evolution of total energy when modeling spinodal decomposition.

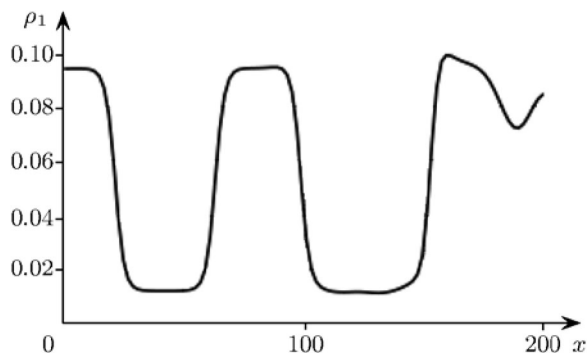


**Fig. 2.** Evolution of kinetic energy when modeling spinodal decomposition.

Such a behavior is explained by the “merger” of two regions of one component composition (“droplets”): four subdomains with  $\rho_1 \approx 0.09$  are observed on the graph of the density distribution  $\rho_1$  at the moment  $t = 26500$  (Fig. 3), while at  $t = 26800$  (Fig. 4) two of them have already virtually “merged.” Figures 5 and 6 show  $\rho_1$  and  $\rho_2$  at the moment  $t = 49 \cdot 10^3$ , when the “merger” has already completed. The number of interphase subdomains (“boundaries”) where  $(\partial_x \rho_\alpha)(\partial_x \rho_\beta) \gg 0$  has decreased, and this has led to an abrupt decrease in the total energy.



**Fig. 3.** Distribution of  $\rho_1$  immediately prior to “merger,”  $t = 26500$ .



**Fig. 4.** Distribution of  $\rho_1$  in the course of “merger,”  $t = 26800$ .

Note that the distributions of  $\rho_1$  and  $\rho_2$  shown in Figs. 5 and 6 are qualitatively very similar while being significantly different quantitatively; namely,  $\rho_1 \in (0.011, 0.092)$  and  $\rho_2 \in (0.49, 1.41)$ . The minimum and maximum values of  $\rho_1$  and  $\rho_2$  agree well with the results in the paper [11].

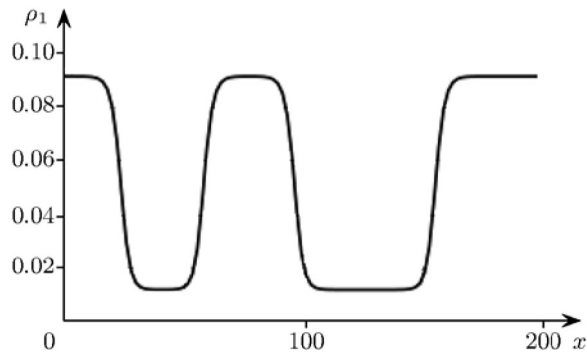


Fig. 5. Distribution of  $\rho_1$ ,  $t = 4.9 \cdot 10^4$ .

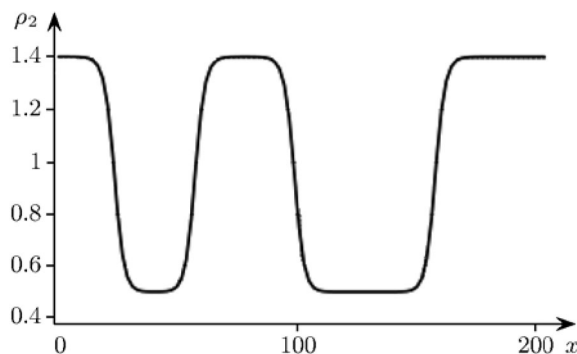


Fig. 6. Distribution of  $\rho_2$ ,  $t = 4.9 \cdot 10^4$ .

It has been checked that the total-mass conservation laws (43) are observed in the computations.

#### REFERENCES

1. Hoang, D.A., Steijn, V., Portela, L.M., Kreutzer, M.T., and Kleijn, C.R., Benchmark numerical simulations of segmented two-phase flows in microchannels using the volume of fluid method, *Comput. Fluids*, 2013, vol. 86, pp. 28–36.
2. Olsson, E. and Kreiss, G., A conservative level set method for two phase flow, *J. Comput. Phys.*, 2005, vol. 210, no. 1, pp. 225–246.
3. Anderson, D., McFadden, G., and Wheeler, A., Diffuse-interface methods in fluid mechanics, *Annu. Rev. Fluid Mech.*, 1998, vol. 30, pp. 139–165.
4. Jamet, D., Torres, D., and Brackbill, J.U., On the theory and computation of surface tension: the elimination of parasitic currents through energy conservation in the second-gradient method, *J. Comput. Phys.*, 2002, vol. 182, no. 1, pp. 262–276.
5. Lowengrub, J. and Truskinovsky, L., Quasi-incompressible Cahn–Hilliard fluids and topological transitions, *Proc. R. Soc. London A*, 1998, vol. 454, pp. 2617–2654.
6. Mauri, R., *Multiphase Microfluidics: The Diffuse Interface Model*, Berlin: Springer, 2012.
7. Favrie, N., Gavriluk, S.L., and Saurel, R., Solid-fluid diffuse interface model in cases of extreme deformations, *J. Comput. Phys.*, 2009, vol. 228, no. 16, pp. 6037–6077.
8. Provatas, N. and Elde, K., *Phase-Field Methods in Material Science and Engineering*, Weinheim: Wiley, 2010.
9. Moelans, N., Blanpain, B., and Wollants, P., An introduction to phase-field modeling of microstructure evolution, *Comput. Coupling Phase Diagrams Thermochem.*, 2008, vol. 32, pp. 268–294.
10. Gelissen, E.J., van der Geld, C.W.M., Baltussen, M.W., and Kuertena, J.G.M., Modeling of droplet impact on a heated solid surface with a diffuse interface model, *Int. J. Multiphase Flow*, 2020, vol. 123, p. 103173.
11. Liu, J., Amberg, G., and Do-Quang, M., Diffuse interface method for a compressible binary fluid, *Phys. Rev. E*, 2016, vol. 93, no. 1, p. 013121.

12. Zhao, X. and Wang, Q., A second order fully-discrete linear energy stable scheme for a binary compressible viscous fluid model, *J. Comput. Phys.*, 2019, vol. 395, pp. 382–409.
13. Dem'yanov, A.Yu., Dinariev, O.Yu., and Evseev, N.V., *Osnovy metoda funktsionala plotnosti v gidrodinamike* (Basics of the Method of Density Functional in Hydrodynamics), Moscow: Fizmatlit, 2009.
14. Dem'yanov, A.Yu. and Dinariev, O.Yu., Applying the method of density functional to modeling the flows of multicomponent multiphase mixtures, *Prikl. Mekh. Tekh. Fiz.*, 2004, vol. 45, no. 5, pp. 68–78.
15. Kudinov, I.V. and Evseev, N.V., Modeling a two-phase flow in a microchannel with the use of the density functional method, *Mat. Model.*, 2010, vol. 22, no. 8, pp. 83–96.
16. Onuki, A., Henry's law, surface tension, and surface adsorption in dilute binary mixtures, *J. Chem. Phys.*, 2009, vol. 130, no. 12, p. 124703.
17. Wheeler, D., Warren, J.A., and Boettinger, W.J., Modeling the early stages of reactive wetting, *Phys. Rev. E.*, 2010, vol. 82, no. 5, p. 051601.
18. Jacqmin, D., Calculation of two-phase Navier–Stokes flows using phase-field modeling, *J. Comput. Phys.*, 1999, vol. 155, no. 1, pp. 96–127.
19. Balashov, V. and Zlotnik, A., An energy dissipative spatial discretization for the regularized compressible Navier–Stokes–Cahn–Hilliard system of equations, *Math. Model. Anal.*, 2020, vol. 25, no. 1, pp. 110–129.
20. Balashov, V.A. and Savenkov, E.B., Thermodynamically consistent spatial discretization of the one-dimensional regularized system of the Navier–Stokes–Cahn–Hilliard equations, *J. Comput. Appl. Math.*, 2020, vol. 372, p. 112743.
21. Chetverushkin, B.N., *Kineticheskie skhemy i kvazigazodinamicheskaya sistema uravnenii* (Kinetic Schemes and Quasihydrodynamic System of Equations), Moscow: MAKS Press, 2004.
22. Elizarova, T.G., *Kvazigazodinamicheskie uravneniya i metody rascheta vyazkikh techenii* (Quasihydrodynamic Equations and Methods for Calculating Viscous Flows), Moscow: Nauchn. Mir, 2007.
23. Sheretov, Yu.V., *Dinamika sploshnykh sred pri prostranstvenno–vremennom osrednenii* (Continuum Dynamics under Spatial–Temporal Averaging), Moscow–Izhevsk: RKhD, 2009.
24. Guermond, J.-L. and Popov, B., Viscous regularization of the Euler equations and entropy principles, *SIAM J. Appl. Math.*, 2014, vol. 74, pp. 284–305.
25. Svärd, M., A new Eulerian model for viscous and heat conducting compressible flows, *Phys. A.*, 2018, vol. 506, pp. 350–375.
26. Elizarova, T.G., Zlotnik, A.A., and Shil'nikov, E.V., Regularized equations for numerical simulation of flows of homogeneous binary mixtures of viscous compressible gases, *Comput. Math. Math. Phys.*, 2019, vol. 59, no. 11, pp. 1832–1847.
27. Balashov, V.A. and Savenkov, E.B., Multicomponent quasi-hydrodynamic model describing multiphase fluid flows with allowance for interphase interaction, *Prikl. Mekh. Tekh. Fiz.*, 2018, vol. 59, no. 3, pp. 57–68.
28. Balashov, V., Zlotnik, A., and Savenkov, E., Analysis of a regularized model for the isothermal two-component mixture with the diffuse interface, *Russ. J. Numer. Anal. Math. Model.*, 2017, vol. 32, no. 6, pp. 347–358.
29. Balashov, V., Savenkov, E., and Zlotnik, A., Numerical method for 3D two-component isothermal compressible flows with application to digital rock physics, *Russ. J. Numer. Anal. Math. Model.*, 2019, vol. 34, no. 1, pp. 1–13.