

## QUASI-HYDRODYNAMIC MODEL OF MULTIPHASE FLUID FLOWS TAKING INTO ACCOUNT PHASE INTERACTION

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**Abstract:** A quasi-hydrodynamic system of equations describing flows of a heat-conducting viscous compressible multiphase multicomponent fluid is constructed taking into account surface effects. The system was obtained by generalizing the methods of obtaining a single-phase quasi-hydrodynamic system and a multicomponent flow model with surface effects based on the concept of microforces and microstresses. The equations are derived using the Coleman–Noll procedure. The results of the simulations show that the constructed model is applicable for modeling multiphase multicomponent flows with allowance for surface effects on the interfaces.

*Keywords:* quasi-hydrodynamic system of equations, multiphase hydrodynamics, diffuse interface.

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### INTRODUCTION

Quasi-gas-dynamic and quasi-hydrodynamic systems of equations are modifications of Navier–Stokes equations that include physically based small dissipative terms [1–3]. In the construction of finite-difference approximations, these terms play the role of regularizers and allow the use of simple central difference approximations to construct corresponding difference schemes.

A quasi-gas-dynamic system was first constructed in the 1980s as a first differential approximation of kinetically matched difference schemes for solving the equations of gas dynamics [1]. This approach is developed in [2, 3]. Later an alternative method for constructing quasi-gas-dynamic equations has been proposed based on averaging the classical equations of hydrodynamics over a small time interval. A quasi-hydrodynamic system has been proposed and studied in detail in [3]. It differs from the quasi-gas-dynamic system in the assumptions used in its derivation.

The objective of this study is to use the quasi-hydrodynamic approach to construct a mathematical model of multiphase multicomponent fluid flows with allowance for the surface properties of phases and phase transitions. Models of the type considered describe the dynamics of interfaces in space and time and physical phenomena due to their presence (surface tension, wettability, phase separation, etc.).

In this paper we construct a model of the type of the diffuse interface model [4–6]. In models of this type, it is assumed that the phases are separated by a thin layer of finite width, in which there is phase interaction which determines the dynamics of the interface. The thickness of the interface is determined by the molecular attraction and repulsion forces acting in the fluid. Such models are widely used, e.g., in the direct modeling of multiphase microflows in rock samples.

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In this paper, the corresponding equations of the model are phenomenologically derived within the framework of the quasi-hydrodynamic approach. The derivation is based on two ideas. First, the spatial phase composition of the fluid in a spatial region (phase distribution) is described by a given continuous field of an order parameter which is taken to be the density of the fluid and (or) the concentration of the phases forming this field. Following [7, 8], it is assumed that micro-forces and microstresses act in the fluid which determine the evolution of order parameters (e.g., phase separation—the formation of cohesive regions (droplets) occupied by one phase). Second, expressions for microforces and additional quasi-hydrodynamic terms are derived in a thermodynamically consistent manner taking into account the second law of thermodynamics and using the Coleman–Noll procedure. Thus, whatever the specific physical meaning of microforces and microstress, the mathematical model does not contradict the basic physical laws (conservation laws of mass, momentum, energy, and angular momentum) and the concepts of phenomenological thermodynamics.

The procedure for constructing the model is similar to the procedure described in [7, 8]. The difference lies in the fact that, in accordance with the quasi-hydrodynamic approach, the mass flux density generally does not coincide with the momentum per unit volume of the medium.

It should be noted that in the model considered, the concept of phase is not explicitly introduced. However, due to the special type of free energy and the presence of terms containing gradients of order parameters, subregions are formed in the flow region which are occupied by a mixture with a composition practically homogeneous in space. This suggests that these regions of space are occupied by a separate phase, which is determined by the corresponding composition (practically homogeneous).

The system of equations derived for two-component phase isothermal flow was used to develop an explicit numerical algorithm. A number of computational experiments have been performed, whose results indicate the validity of the developed model.

## 1. MAIN IDEAS OF THE CONCEPT OF MICROFORCES

The traditional mechanics and thermodynamics of a continuous medium consider macroscopic forces associated with the relative macroscopic motion of points of the medium or a change in its state. Macroscopic forces determine the general behavior of the medium and do not take into account the structure of the medium at the microlevel and the mechanisms of its change.

However, in solving a number of problems, it is necessary to describe the macroscopic level of processes and the corresponding mechanisms associated with the evolution of the microstructure of the medium and not associated with the macroscopic relative motion of material points that make up the body. In this paper, such processes are phase separation in a mixture of fluids with different properties or the merging of droplets of one phase into larger processes due to the presence of surface tension forces at the interface, etc. In this case, the stresses arising in the medium or the thermodynamic forces that cause, e.g., phase separation, are not associated with macroscopic forces. These strains and forces are due to the nature of the interaction of the particles of the medium at the microlevel and manifest themselves even if the body is not affected by external loads.

In the models considered, the microstructure of the medium is given by a certain function (scalar, vector, or tensor), called the order parameter or the phase field. The dynamics of the order parameter is described by a system of microforces and microstress in the same way as the dynamics of macroscopic motion is described by the system of external and internal macroscopic forces acting in the medium. More details of the method of obtaining mathematical models using the concept of microforces and microstress and its applications to construct mathematical models in other fields of physics can be found in [7–10].

## 2. CONSERVATION LAWS IN DIFFERENTIAL FORM

We assume that the fluid consists of  $N$  components and an arbitrarily physically infinitesimal volume can contain any of them. Suppose that a volume of space  $dV$  contains a fluid of mass  $dm$  and that the individual components of mass  $dm_\alpha$  occupy volume  $dV_\alpha$  ( $\alpha = 1, \dots, N$ ). In this case,

$$dV = \sum_{\alpha=1}^N dV_\alpha, \quad dm = \sum_{\alpha=1}^N dm_\alpha.$$

The density of the fluid is given by the formula  $\rho = dm/dV$ . We also introduce the density of a component related to the volume  $dV$  of the fluid as a whole:  $\rho_\alpha = dm_\alpha/dV$ . The parameter  $C_\alpha = \rho_\alpha/\rho$  will be called the mass concentration (mass fraction) of component  $\alpha$ . Then,

$$\sum_{\alpha=1}^N C_\alpha = 1, \quad \rho = \sum_{\alpha=1}^N \rho_\alpha.$$

In accordance with the quasi-hydrodynamic approach, we assume that the mass flux density  $\mathbf{j}_m$  generally differs from the average momentum of unit volume  $\rho\mathbf{u}$ :  $\rho\mathbf{u} - \mathbf{j}_m = \rho\mathbf{w}$ . This expression defines the vector  $\mathbf{w}$ , for which the constitutive relation is obtained below. Thus, for the mass flux density vector, we have

$$\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w}). \quad (1)$$

We denote  $\mathbf{u}_m = \mathbf{j}_m/\rho = \mathbf{u} - \mathbf{w}$ . Further, we assume that a fluid particle moves along the integral line of the differential equation  $d\mathbf{x}/dt = \mathbf{u}_m$ ,  $\mathbf{x}(t_0) = \mathbf{x}_0$ . Here  $d/dt$  is the total time derivative. Then, the formula for the time differentiation of the integral over the moving volume  $V = V(t)$  for the scalar or vector field  $\varphi$  takes the form

$$\frac{d}{dt} \int_{V(t)} \varphi dV = \int_{V(t)} \left[ \frac{\partial \varphi}{\partial t} + \operatorname{div} \left( \frac{\mathbf{j}_m}{\rho} \otimes \varphi \right) \right] dV. \quad (2)$$

The corresponding expression for the total time derivative has the form

$$\frac{d}{dt} (\cdot) = \frac{\partial}{\partial t} (\cdot) + \mathbf{u}_m \cdot \nabla (\cdot). \quad (3)$$

The derivation of the model equations is standard: we first consider conservation laws in integral form, and then, using (2), perform conversion to their differential analogs. This procedure is described in detail in [11].

The law of conservation of mass for component  $\alpha$  has the following form:

$$\frac{\partial}{\partial t} (\rho C_\alpha) + \operatorname{div} (\mathbf{j}_m C_\alpha + \mathbf{h}_\alpha) = \tilde{m}_\alpha, \quad \alpha = 1, \dots, N. \quad (4)$$

Here  $\mathbf{h}_\alpha$  and  $\tilde{m}_\alpha$  is the mass flux density vector of component  $\alpha$  and the bulk density of the sources of mass of component  $\alpha$ , which arises, e.g., due to chemical reactions. We will assume that external flows and sources of mass are absent:

$$\sum_{\alpha=1}^N \mathbf{h}_\alpha = \mathbf{0}, \quad \sum_{\alpha=1}^N \tilde{m}_\alpha = 0.$$

Then, summing Eqs. (4), we obtain the law of conservation of mass for the mixture:

$$\frac{\partial \rho}{\partial t} + \operatorname{div} \mathbf{j}_m = 0.$$

Assuming that the magnitude of the force acting on the boundary  $\partial V(t)$  of the region  $V(t)$  is determined by the stress tensor  $P$ , we have  $\mathbf{p}^{(n)} = \mathbf{n} \cdot P$ , where  $\mathbf{n}$  is the outer unit normal to  $\partial V$ . Consequently,

$$\frac{\partial (\rho\mathbf{u})}{\partial t} + \operatorname{div} (\mathbf{u}_m \otimes \rho\mathbf{u} - P) = \rho\mathbf{f},$$

where  $\mathbf{f}$  is the density of external mass forces. Assuming that the law of conservation of angular momentum is satisfied, we write the stress tensor as

$$P = P^s + \rho\mathbf{u} \otimes \mathbf{w}, \quad (5)$$

where  $P^s$  is a second-rank symmetric tensor [12], which can be represented as the sum of the deviator and the spherical part:  $P^s = P^d + \bar{p}I$  and  $\bar{p} = (\operatorname{tr} P^s)/3$ .

We assume that the vector field of internal microstresses  $\boldsymbol{\xi}$ , the scalar field of internal microforces  $\pi$ , and the scalar field of external microforces  $\gamma$  [7, 10] act in the medium. The term internal means that the values of the corresponding parameters are determined by internal processes in the medium (by a set of constitutive equations relating the microforces and microstress with the order parameter and macroscopic thermodynamic fields), the term external means that the field describes the external impact (its magnitude and nature are not related to the processes and constitutive relations occurring in the medium, and this field can be specified arbitrarily).

This system of microforces and microstress is assumed to satisfy the relations valid for an arbitrary material volume and expressing the balance conditions for microforcess and microstresses, as well as the relations for their work in differential form [7, 10]:

$$\operatorname{div} \boldsymbol{\xi} + \boldsymbol{\pi} + \boldsymbol{\gamma} = 0, \quad \operatorname{div} \boldsymbol{\xi}_\alpha + \boldsymbol{\pi}_\alpha + \boldsymbol{\gamma}_\alpha = 0. \quad (6)$$

Here and below (unless otherwise specified), it is assumed that  $\alpha = 1, \dots, N-1$ .

Taking into account (6), the energy conservation law has the form

$$\begin{aligned} \frac{\partial}{\partial t} (\rho E) + \operatorname{div} (\mathbf{j}_m E) &= \mathbf{j}_m \cdot \mathbf{f} + \operatorname{div} \mathbf{a} - \operatorname{div} \mathbf{q} + \sum_{\alpha=1}^{N-1} \mu_\alpha \tilde{m}_\alpha - \operatorname{div} \left( \sum_{\alpha=1}^{N-1} \mu_\alpha \mathbf{h}_\alpha \right) \\ &+ \sum_{\alpha=1}^{N-1} \left[ \operatorname{div} \left( \frac{dC_\alpha}{dt} \boldsymbol{\xi}_\alpha \right) + \frac{dC_\alpha}{dt} \boldsymbol{\gamma}_\alpha \right] + \operatorname{div} \left( \frac{d\rho}{dt} \boldsymbol{\xi} \right) + \frac{d\rho}{dt} \boldsymbol{\gamma} + \rho r, \end{aligned} \quad (7)$$

where  $E = \varepsilon + \mathbf{u}^2/2$  is the mass density of the total energy,  $r$  is the mass density of energy sources,  $\mathbf{q}$  is the heat flux density,  $\varepsilon$  is the mass density of internal energy,  $\mathbf{a}$  is the vector of the energy flux density, depending on work of internal stresses, and  $\mu_\alpha$  is the generalized chemical potential. The terms with the factors  $\boldsymbol{\xi}_\alpha$ ,  $\boldsymbol{\gamma}_\alpha$ ,  $\boldsymbol{\xi}$ , and  $\boldsymbol{\gamma}$  on the right-hand side of (7) describe the rate of change of energy due to the work of microstresses and external microforces in unit time [7, 10, 11].

The second law of thermodynamics has the form

$$\frac{\partial}{\partial t} (\rho s) + \operatorname{div} \left( s \mathbf{u}_m + \frac{1}{T} \mathbf{q} \right) - \frac{\rho r}{T} \geq 0,$$

where  $s$  is the entropy of unit mass and  $T$  is the temperature.

### 3. DERIVATION OF CONSTITUTIVE RELATIONS

To obtain the dissipative inequality for the free energy of unit mass  $\Psi = \varepsilon - Ts$ , it is reasonable to write all balance relations in Lagrangian form. Further, multiplying the equations of the law of conservation of momentum by  $\mathbf{u}$ , we obtain the kinetic energy balance equation. Then the expression for the law of conservation of mass of a component should be multiplied by  $\mu_\alpha$ , the first relation (6) by  $d\rho/dt$ , and the second relation by  $dC_\alpha/dt$ . Substituting these equations into the energy equation, we obtain the balance equation for internal energy. Using this equation, the second law of thermodynamics, and the relation

$$\frac{d\Psi}{dt} = \frac{d\varepsilon}{dt} + T \frac{ds}{dt} + s \frac{dT}{dt},$$

we obtain the following dissipative inequality for the free energy density:

$$\begin{aligned} \rho \frac{d\Psi}{dt} &\leq -\rho s \frac{dT}{dt} - \mathbf{u} \cdot \operatorname{div} P - \rho \mathbf{w} \cdot \mathbf{f} + \operatorname{div} \mathbf{a} - \sum_{\alpha=1}^{N-1} \mathbf{h}_\alpha \cdot \nabla \mu_\alpha - \frac{\mathbf{q}}{T} \cdot \nabla T \\ &+ \sum_{\alpha=1}^{N-1} \left[ \boldsymbol{\xi}_\alpha \cdot \nabla \left( \frac{dC_\alpha}{dt} \right) - \boldsymbol{\pi}_\alpha \frac{dC_\alpha}{dt} \right] + \left[ \boldsymbol{\xi} \cdot \nabla \left( \frac{d\rho}{dt} \right) - \boldsymbol{\pi} \frac{d\rho}{dt} \right] + \sum_{\alpha=1}^{N-1} \mu_\alpha \rho \frac{dC_\alpha}{dt}. \end{aligned} \quad (8)$$

A detailed derivation of (8) is given in [8, 11].

Next inequality (8) is used to obtain constitutive relations that close the model. This procedure, called the Coleman–Noll procedure [13, 14] allows selection of constitutive relations that make any process described by them allowable.

In accordance with the principle of equipresence [15–17], the mass density of the free energy  $\Psi = \Psi(\mathcal{X})$  depends on the vector of parameters

$$\mathcal{X} = \left\{ \rho, \nabla \rho, \frac{d\rho}{dt}, C_\alpha, \nabla C_\alpha, \frac{dC_\alpha}{dt}, T, \nabla T, \mu_\alpha, \nabla \otimes \mathbf{u} \right\}.$$

Using conservation laws in Lagrangian form, inequality (8) can be written as

$$\begin{aligned}
0 \leq & \frac{dT}{dt} \left( -\rho \frac{\partial \Psi}{\partial T} - \rho s \right) + \frac{d\rho}{dt} \left( -\rho \frac{\partial \Psi}{\partial \rho} - \frac{1}{\rho} \bar{p} - \frac{1}{\rho} \left( \frac{1}{3} \text{tr} Q \right) - \pi \right) \\
& + \frac{d}{dt} (\nabla \rho) \left( -\rho \frac{\partial \Psi}{\partial (\nabla \rho)} + \boldsymbol{\xi} \right) + \sum_{\alpha=1}^{N-1} \frac{dC_\alpha}{dt} \left( -\rho \frac{\partial \Psi}{\partial C_\alpha} - \pi_\alpha + \rho \mu_\alpha \right) \\
& + \sum_{\alpha=1}^{N-1} \frac{d}{dt} (\nabla C_\alpha) \left( -\rho \frac{\partial \Psi}{\partial (\nabla C_\alpha)} + \boldsymbol{\xi}_\alpha \right) - \sum_{\alpha=1}^{N-1} \mathbf{h}_\alpha \cdot \nabla \mu_\alpha - \sum_{\alpha=1}^{N-1} \frac{\mathbf{q}}{T} \cdot \nabla T \\
& + (P^d + Q^d) : L_u^d + Q : S_{u_m} + \Delta_2 + \Delta_3,
\end{aligned} \tag{9}$$

where

$$\begin{aligned}
Q &= \sum_{\alpha=1}^N \nabla C \otimes \nabla \boldsymbol{\xi}_\alpha + \nabla \rho \otimes \boldsymbol{\xi}, & Q^d &= Q - \frac{1}{3} \text{tr} Q; \\
L_u^d &= \frac{1}{2} [(\nabla \otimes \mathbf{u}) + (\nabla \otimes \mathbf{u})^t] - \frac{1}{3} (\text{div} \mathbf{u}) I, & S_u &= \frac{1}{2} [(\nabla \otimes \mathbf{u}) - (\nabla \otimes \mathbf{u})^t], \\
\Delta_2 &= \text{div} (\mathbf{a} - P^d \cdot \mathbf{u} - \bar{p} \mathbf{u}_m - \rho \mathbf{u} (\mathbf{u} \cdot \mathbf{w}) - Q^d \cdot \mathbf{w}) \\
&+ \mathbf{w} \cdot (-\rho \mathbf{f} - \nabla \bar{p} + \rho (\mathbf{u} \cdot \nabla) \mathbf{u} + \text{div} Q^d), \\
\Delta_3 &= \frac{\partial \Psi}{\partial (d\rho/dt)} \frac{d^2 \rho}{dt^2} + \sum_{\alpha=1}^{N-1} \frac{\partial \Psi}{\partial (dC_\alpha/dt)} \frac{d^2 C_\alpha}{dt^2} + \frac{\partial \Psi}{\partial (dT/dt)} \frac{d^2 T}{dt^2} \\
&+ \sum_{\alpha=1}^{N-1} \frac{\partial \Psi}{\partial \mu_\alpha} \frac{d\mu_\alpha}{dt} + \frac{\partial \Psi}{\partial (\nabla \otimes \mathbf{u})} : \frac{d(\nabla \otimes \mathbf{u})}{dt}.
\end{aligned} \tag{10}$$

It is not difficult to show that the conditions presented below make the corresponding terms in (9) non-negative. We assume that the free energy can be expressed as  $\Psi = \Psi(\rho, \nabla \rho, C_\alpha, \nabla C_\alpha, T)$ . Then,  $\Delta_3 = 0$ . Next, suppose that the tensor  $Q$  is symmetric, The entropy is defined by the formula  $s = -\partial \Psi / \partial T$ , and the expressions for microstresses have the form

$$\boldsymbol{\xi} = \rho \frac{\partial \Psi}{\partial (\nabla \rho)}, \quad \boldsymbol{\xi}_\alpha = \rho \frac{\partial \Psi}{\partial (\nabla C_\alpha)}. \tag{11}$$

Relations for  $\pi_\alpha$  and  $\bar{p}$  are written as follows:

$$\bar{p} = -\rho^2 \frac{\partial \Psi}{\partial \rho} - \rho \pi - \frac{1}{3} \text{tr} Q - \zeta \text{div} \mathbf{v}, \quad \pi_\alpha = -\rho \frac{\partial \Psi}{\partial C_\alpha} + \rho \mu_\alpha - B_\alpha \frac{dC_\alpha}{dt} \tag{12}$$

( $\zeta$  and  $B_\alpha$  are non-negative values and  $\mathbf{v}$  is a vector defined below). The constitutive relations for the mass density vectors of the components and the heat flux are written as  $\mathbf{h}_\alpha = -M_\alpha \cdot \nabla \mu_\alpha$  and  $\mathbf{q} = -K \cdot \nabla T$  ( $M_\alpha$  and  $K$  are symmetric non-negative definite tensors of the second rank). The deviator of the tensor  $P^s$  is given by the relation

$$P^d = G : L_u^d - \frac{1}{3} \text{tr} (G : L_u^d) I - Q^d, \tag{13}$$

where  $Q^d = Q - (1/3) \text{tr} Q$  is the deviator tensor  $Q$  and  $G$  is a nonnegative definite fourth-rank tensor which defines the linear mapping of the space of symmetric second-rank tensors into themselves.

Substituting the above relations into the inequality for the free energy (9) and using the equality  $d\rho/dt = -\rho \text{div} \mathbf{u}_m$ , we obtain

$$0 \leq L_u^d : G : L_u^d + \sum_{\alpha=1}^{N-1} B_\alpha \left( \frac{dC_\alpha}{dt} \right)^2 + \sum_{\alpha=1}^{N-1} \nabla \mu_\alpha \cdot M_\alpha \cdot \nabla \mu_\alpha + \nabla T \cdot K \cdot \nabla T + \Theta, \tag{14}$$

where  $\Theta = \Delta_2 - \zeta \text{div} \mathbf{u}_m \text{div} \mathbf{v}$ .

On the right-hand side of (14), all terms other than  $\Theta$  are nonnegative. Therefore, to satisfy the inequality (14), it is sufficient to satisfy the condition  $\Theta \geq 0$  by choosing the form of the constitutive relations. We introduce the following notation:

$$\mathbf{a}^* = P\mathbf{u} - p_0\mathbf{u}_m + \rho\mathbf{u}(\mathbf{u} \cdot \mathbf{w}) + Q^d\mathbf{w}, \quad \mathbf{w}^* = -\rho\mathbf{f} + \nabla p_0 + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} + \text{div } Q^d$$

( $p_0 = -\bar{p} - \zeta \text{div } \mathbf{v}$ ). Then,

$$\Theta = \text{div}(\mathbf{a} - \mathbf{a}^* + \zeta\mathbf{u}_m \text{div } \mathbf{v}) + \mathbf{w} \cdot [\mathbf{w}^* + \nabla(\zeta \text{div } \mathbf{v})] - \zeta \text{div } \mathbf{u}_m \text{div } \mathbf{v}. \quad (15)$$

Expression (15) is equivalent to the expression

$$\Theta = \text{div}(\mathbf{a} - \mathbf{a}^* + \zeta\mathbf{u} \text{div } \mathbf{v}) + \mathbf{w} \cdot \mathbf{w}^* - \zeta \text{div } \mathbf{u} \text{div } \mathbf{v}. \quad (16)$$

There are various types of closure of the system that provide satisfaction of the condition  $\Theta \geq 0$ .

Type 1:

$$\mathbf{v} = -\mathbf{u}_m, \quad \mathbf{a} = \mathbf{a}^* + \zeta\mathbf{u}_m \text{div } \mathbf{u}_m, \quad \mathbf{w} = [\mathbf{w}^* - \nabla(\zeta \text{div } \mathbf{u}_m)]\tau/\rho \quad (17)$$

( $\tau > 0$  is a small parameter which has the dimension of time). It follows from (15) that  $\Theta = |\mathbf{w}^* - \nabla(\zeta \text{div } \mathbf{u}_m)|^2\tau/\rho + \zeta(\text{div } \mathbf{u}_m)^2$ .

Type 2:

$$\mathbf{v} = -\mathbf{u}, \quad \mathbf{w} = \mathbf{w}^*\tau/\rho, \quad \mathbf{a} = \mathbf{a}^* + \zeta\mathbf{u} \text{div } \mathbf{u}.$$

In this case, from (16) we obtain  $\Theta = \Theta^{(2)} = |\mathbf{w}^*|^2\tau/\rho + \zeta(\text{div } \mathbf{u})^2$ .

Type 3:

$$\mathbf{v} = -\mathbf{u}_m, \quad \mathbf{a} = \mathbf{a}^* + \zeta\mathbf{u} \text{div } \mathbf{u}_m + \zeta\mathbf{w} \text{div } \mathbf{u}, \quad \mathbf{w} = [\mathbf{w}^* + \nabla(\zeta \text{div } \mathbf{u})]\tau/\rho.$$

Then, from (16) we obtain  $\Theta = \Theta^{(3)} = (\mathbf{w}^* + \nabla(\zeta \text{div } \mathbf{u}))^2\tau/\rho + \zeta(\text{div } \mathbf{u})^2$ .

It should be noted that expressions (17) are implicit with respect to  $\mathbf{w}$ .

Based on the types of closure 2 and 3, we can construct the family of constitutive relations for  $\mathbf{w}$ . For this, we introduce a parameter  $\beta \in [0, 1]$ . We denote

$$\mathbf{a}_\beta = \beta\mathbf{a}^{(2)} + (1 - \beta)\mathbf{a}^{(3)}, \quad \mathbf{w}_\beta = \beta\mathbf{w}^{(2)} + (1 - \beta)\mathbf{w}^{(3)}, \quad \mathbf{v}_\beta = \beta\mathbf{v}^{(2)} + (1 - \beta)\mathbf{v}^{(3)}. \quad (18)$$

Here the superscripts correspond to the closure number. Substitution of (18) into (16) yields

$$\Theta = \beta\Theta^{(2)} + (1 - \beta)\Theta^{(3)} \geq 0.$$

#### 4. CONSTITUTIVE RELATIONS

We write the expression for the free energy in the form

$$\Psi(\rho, \nabla\rho, C_\alpha, \nabla C_\alpha, T) = \Psi_0(\rho, C_\alpha, T) + \frac{\lambda}{2\rho} |\nabla\rho|^2 + \sum_{\alpha=1}^{N-1} \frac{\lambda_\alpha}{2} |\nabla C_\alpha|^2, \quad (19)$$

where  $\lambda = \lambda(C_\alpha) \geq 0$ ,  $\lambda_\alpha = \text{const} \geq 0$  are specified quantities. This expression of free energy is typical of models of the type considered [4–6, 18] and satisfies the sufficient conditions for inequality (9).

The local part  $\Psi_0$  of the free Helmholtz energy is represented as

$$\Psi_0 = \Psi_{\text{sep}} + \Psi_{\text{mix}}, \quad \Psi_{\text{mix}}(\rho, T) = \sum_{\alpha=1}^N C_\alpha \Psi_\alpha(\rho, T),$$

where  $\Psi_{\text{mix}}$  is the free Helmholtz energy for a homogeneous mixture of two non-interacting components. The term  $\Psi_{\text{sep}}$  describes the phase separation and is given in various forms. In some papers (see, e.g., [19]) for  $N = 2$ , it is assumed that

$$\Psi_{\text{sep}} = A_\psi C_1^2 C_2^2 = A_\psi C^2 (1 - C)^2. \quad (20)$$

For  $N \geq 3$ , we can use the expression [19]

$$\Psi_{\text{sep}} = A_{\psi}^{\alpha,\beta} C_{\alpha}^2 C_{\beta}^2 + \sum_{\alpha=1}^N l_{\alpha}(T) C_{\alpha}^2 (3 - 2C_{\alpha}), \quad (21)$$

where  $A_{\psi}^{\alpha,\beta}$  are some positive constants and  $l_{\alpha}(T)$  are linear functions of temperature.

In the case (20), it is not difficult to show that  $\Psi_{\text{sep}}$  has two local minima at the points  $C = 0$  and  $C = 1$  and one local maximum at the point  $C = 1/2$ . Since the Helmholtz free energy of a fluid particle decreases with time, the state corresponding to  $C = 1/2$  is unstable, and the states corresponding to  $C = 0$  and  $C = 1$  are stable. As a result, phase separation takes place in the system. During the evolution of the system, the distribution of the phases in which one of them (dispersed phase) is collected in droplets located inside the second (dispersive) phase becomes stable.

Taking into account the general constitutive relations for microstresses (11), from (19) we obtain

$$\boldsymbol{\xi} = \lambda \nabla \rho, \quad \boldsymbol{\xi}_{\alpha} = \lambda_{\alpha} \rho \nabla C_{\alpha}, \quad \alpha = 1, \dots, N-1. \quad (22)$$

From (22) and the definition of (10), it follows that

$$Q = \lambda \nabla \rho \otimes \nabla \rho + \rho \sum_{\alpha=1}^{N-1} \lambda_{\alpha} \nabla C_{\alpha} \otimes \nabla C_{\alpha}, \quad \text{tr } Q = \lambda |\nabla \rho|^2 + \rho \sum_{\alpha=1}^{N-1} \lambda_{\alpha} |\nabla C_{\alpha}|^2.$$

Expressing  $\mu_{\alpha}$  from relations (12) and using the balance equation for microforces and microstresses (6) and expressions (22) and (19), we obtain

$$\mu_{\alpha} = \frac{\partial \Psi_0}{\partial C_{\alpha}} - \frac{1}{\rho} \text{div} (\lambda_{\alpha} \rho \nabla C_{\alpha}) + \frac{1}{2\rho} \frac{\partial \lambda}{\partial C_{\alpha}} |\nabla \rho|^2 - \frac{\gamma_{\alpha}}{\rho} + B_{\alpha} \frac{1}{\rho} \frac{dC_{\alpha}}{dt}. \quad (23)$$

Below we assume that  $B_{\alpha} = 0$ ,  $\gamma_{\alpha} = 0$ ,  $\alpha = 1, \dots, N-1$ .

Consider the tensor  $P^d$  defined by relation (13). Assuming that  $[G]_{ijkl} = G_{ijkl} = 2\eta \delta_{ik} \delta_{jl}$  ( $\eta \geq 0$  is the dynamic viscosity and  $\delta_{ij}$  are the components of the second-rank unit tensor) in relation (13), it can be shown that  $P^d = 2\eta L_u^d - Q^d$ . Finally, substituting the obtained relations into expression (5), using (22) and (19), and rearranging the terms, we have

$$P = P_{\text{NS}} - pI + Q_{\text{K}} + Q_c + P_{\text{QHD}}. \quad (24)$$

Here  $P_{\text{NS}} = 2\eta L_u^d + \zeta(\text{div } \mathbf{u})I$  is the tensor of Navier–Stokes viscous stresses;  $p = \rho^2 \partial \Psi_0 / \partial \rho$  is the thermodynamic pressure;  $Q_{\text{K}}$  is the Korteweg stress tensor, which can be related to the capillary forces on the diffuse interface between two phases of the same component and  $Q_c$  is the capillary stress tensor, which can be related to capillary forces on the diffuse interface between different components:

$$Q_{\text{K}} = -\lambda \nabla \rho \otimes \nabla \rho + \left( \rho \text{div} (\lambda \nabla \rho) + \frac{\lambda}{2} |\nabla \rho|^2 + \rho \gamma \right) I, \quad Q_c = -\rho \sum_{\alpha=1}^{N-1} \lambda_{\alpha} \nabla C_{\alpha} \otimes \nabla C_{\alpha};$$

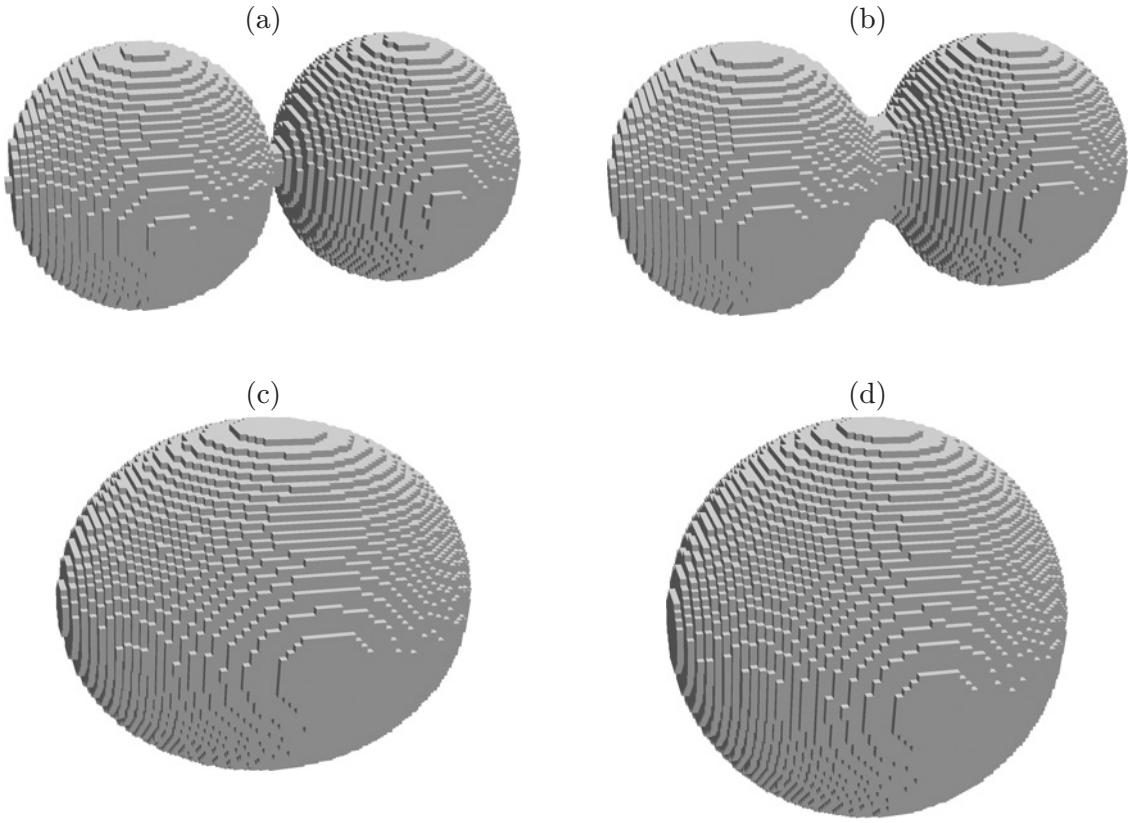
$P_{\text{QHD}}$  is the additional term in the stress tensor relation due to the difference between the mass flow vector and the momentum vector:

$$P_{\text{QHD}} = \rho \mathbf{u} \otimes \mathbf{w} - \zeta(\text{div } \mathbf{w})I.$$

## 5. BASIC EQUATIONS OF THE MODEL

Thus, the resulting system of equations has the following form:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \text{div } \mathbf{j}_m &= 0, \\ \frac{\partial}{\partial t} (\rho C_{\alpha}) + \text{div} (\mathbf{j}_m C_{\alpha} + \mathbf{h}_{\alpha}) &= \tilde{m}_{\alpha}, \quad \alpha = 1, \dots, N-1, \\ \frac{\partial}{\partial t} (\rho \mathbf{u}) + \text{div} (\mathbf{j}_m \otimes \mathbf{u} - P) &= \rho \mathbf{f}, \end{aligned}$$



**Fig. 1.** Stages of coalescence of two spherical droplets for  $t = 0.2 \cdot 10^{-5}$  (a),  $2.4 \cdot 10^{-5}$  (b),  $40.0 \cdot 10^{-5}$  (c), and  $178.0 \cdot 10^{-5}$  s (d).

$$\begin{aligned} \frac{\partial}{\partial t} (\rho E) + \operatorname{div} (\mathbf{j}_m E) &= \mathbf{j}_m \cdot \mathbf{f} + \operatorname{div} \mathbf{a} - \operatorname{div} \mathbf{q} - \operatorname{div} \left( \sum_{\alpha=1}^{N-1} \mu_\alpha \mathbf{h}_\alpha \right) \\ &+ \sum_{\alpha=1}^{N-1} \left[ \operatorname{div} \left( \lambda_\alpha \frac{dC_\alpha}{dt} \rho \nabla C_\alpha \right) + \frac{dC_\alpha}{dt} \gamma_\alpha + \mu_\alpha \tilde{m}_\alpha \right] + \left[ \operatorname{div} \left( \lambda \frac{d\rho}{dt} \nabla \rho \right) + \frac{d\rho}{dt} \gamma \right] + \rho r. \end{aligned}$$

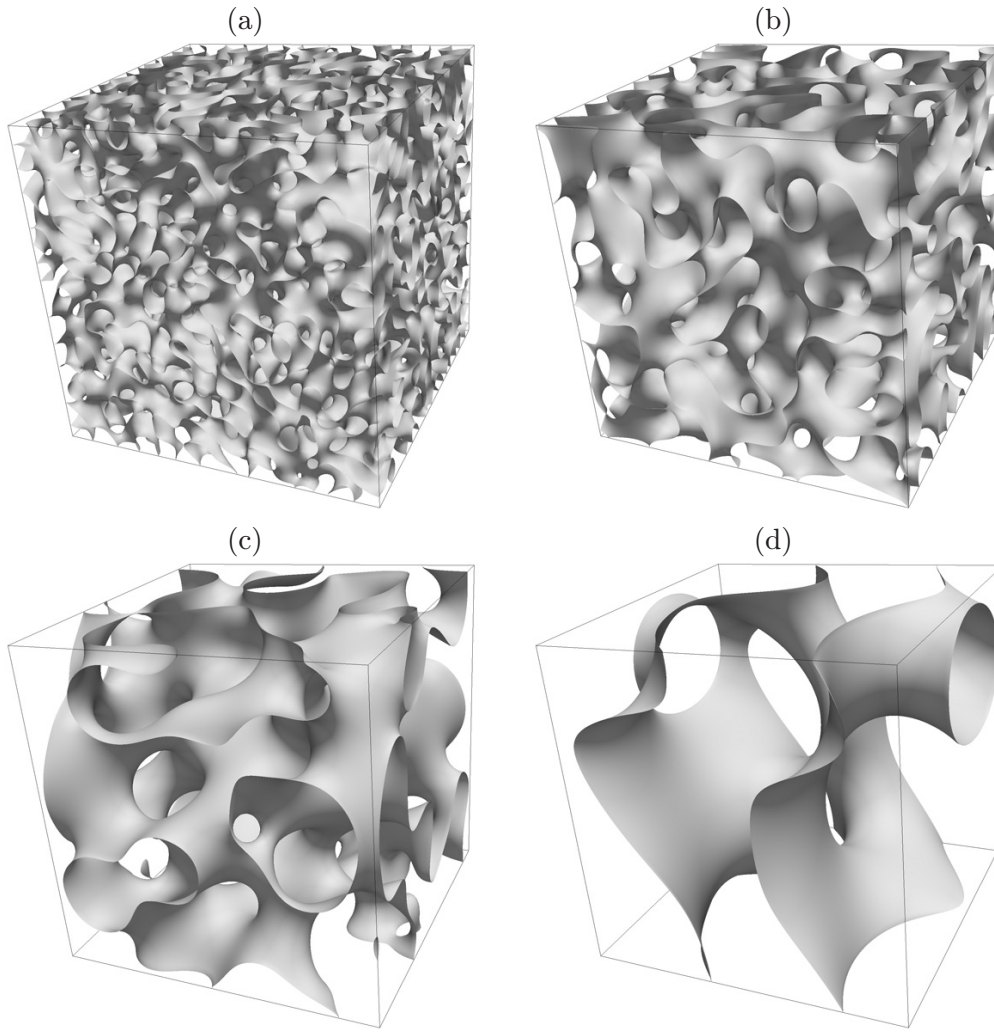
The stress tensor is given by relation (24), the chemical potential  $\mu_\alpha$  by expression (23), the mass flux density is  $\mathbf{j}_m = \rho(\mathbf{u} - \mathbf{w})$ , and the vectors  $\mathbf{w}$  and  $\mathbf{a}$  are given by expression (17) or (18). The quantities  $\gamma$ ,  $\gamma_\alpha$ , and  $B_\alpha$  are usually taken to be zero. Data on surface tension and the thickness of the diffuse interface are used to select the values of  $\lambda$  and  $\lambda_\alpha$  and the coefficients in the expressions for free energy (20) and (21).

## 6. COALESCENCE OF TWO DROPLETS

Below we give the results of simulating the two-component ( $N = 2$  and  $\alpha = 1$ ) two-phase flow describing the coalescence of two closely spaced droplets. The flow is considered isothermal, i.e., the condition  $p = c_s^2 \rho$  is satisfied, where  $c_s$  is the speed of sound. The energy equation is not considered. The explicit difference scheme is used in which the approximation of the capillary stress tensor  $Q$  is similar to that used in [20].

At the initial time, the diffuse boundaries of the droplets begin to blur and their thickness tends to the equilibrium (determined by the model) thickness. At the moment of contact of the boundaries, the surface tension force at the point of contact increase (because at this point, the curvature is great), which leads to coalescence of the droplets. Thus, the droplets merge, on the one hand, due to the blurring of the boundaries, and on the other hand, due to the phase interaction forces acting within the diffuse interface and described in the model by nonlinear terms containing the factor  $\nabla C$ .





**Fig. 2.** Stages of the evolution of the isosurface  $C = 1/2$  for the spontaneous disintegration of a perturbed homogeneous binary mixture for  $t = 0.8 \cdot 10^{-5}$  (a),  $8.0 \cdot 10^{-5}$  (b),  $40.0 \cdot 10^{-5}$  (c), and  $109.2 \cdot 10^{-5}$  s (d).

The boundary conditions are periodic; at the initial time in the computational cells corresponding to the droplets, the concentration  $C = 0.9$ , and in the remaining cells,  $C = 0.1$ . In all cells, zero velocity and unit density are specified. The model parameters have the following values:  $\lambda_1 = 0.0025 \text{ J} \cdot \text{m}^2/\text{kg}$ ,  $A_\psi = 2 \cdot 10^5 \text{ J/kg}$ ,  $M = M_0 C(1 - C)$ ,  $M_0 = 10^{-6} \text{ kg} \cdot \text{s}/\text{m}^3$ ,  $\eta = 0.08 \text{ Pa} \cdot \text{s}$ ,  $\alpha^* = 0.5$ , and  $c_s = 10^3 \text{ m/s}$  ( $\tau = \alpha^* h/c_s$ ).

In the calculation, a  $100 \times 100 \times 100$  computational grid was used. The size of the computational domain is  $L_x = L_y = L_z = 0.01 \text{ m}$ , the time step  $\Delta t = 2 \cdot 10^{-9} \text{ s}$ , and the step in space  $h = L_x/100$ .

Figure 1 shows the stages of the coalescence of two droplets. The interface is the level set  $C = 1/2$ . The cells are shown in which the concentration  $C \in [1/2, 1]$ . It can be seen that at the end of the coalescence process, the droplet takes the form of a sphere. The results of the calculation show that the model and the corresponding numerical algorithm qualitatively describe surface effects.

## 7. SPONTANEOUS DISINTEGRATION OF A HOMOGENEOUS MIXTURE

Below are the results of modeling the spontaneous disintegration of a perturbed homogeneous binary mixture. At the initial time, zero velocity and unit density were specified in each computation cell, and the concentration

value  $C$  was chosen randomly in the interval  $[0.45, 0.55]$ . A  $125 \times 125 \times 125$  grid was used in the simulation. The time step was  $\Delta t = 8 \cdot 10^{-10}$  s, and the step in space  $h = L_x/125$ . The values of the others parameters were the same as in Section 6. We note that the results of a similar simulation for the two-dimensional case are presented in [20].

During the evolution of the mixture, the distribution of  $C$  is first smoothed out, and the components are then gradually separated into two phases (since the minima of the separating free energy are reached at  $C = 0$  and  $C = 1$ , and the free energy decreases during the evolution of the system). After the separation of mixture, the effect of the terms containing the factor  $\nabla C$  increases, which, in turn, determines the action of surface tension forces.

Figure 2 shows the evolution stages of the isosurface  $C = 1/2$ , which is a conditional interface.

## CONCLUSIONS

A quasi-hydrodynamic system of equations describing multiphase multicomponent flows with surface effects was derived. The Coleman–Noll procedure allows the use of several types of closure of this system. For all types of closure, the law of nondecreasing entropy and the inequality for free energy are satisfied.

Setting  $\tau = 0$  in the constructed equations and constitutive relations, we obtain  $\mathbf{w} = 0$ . In this case, the constructed model coincides with well-known models such as the diffuse boundary model, in particular, the Navier–Stokes–Korteweg model (in the case, for one component) and the Navier–Stokes–Cahn–Hilliard model.

Assuming that the number of components  $N = 1$  and the bulk viscosity  $\zeta = 0$  and excluding phase interaction ( $\lambda = \lambda_\alpha = 0$ ) from the model, we obtain the well-known system of quasi-hydrodynamic equations with zero bulk viscosity.

The results of the simulations show that the developed model can be used to simulate multiphase multicomponent flows with surface effects at interfaces.

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