

Modeling of Multicomponent Multiphase Mixture Flows on the Basis of the Density-Functional Method

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Abstract — Examples of numerical calculations of isothermal flows of two-phase two-component mixtures based on the density-functional method are presented. Using this method, the following problems are calculated in the two-dimensional formulation: drop impact on a liquid layer, drop rupture in a Couette flowfield, wetting-angle formation for a drop on a solid surface, development of Rayleigh-Taylor and Kelvin-Helmholtz instability on a gas-liquid interface.

Keywords: density functional, two-phase flow, numerical simulation.

The density-functional method makes it possible to describe a multiphase multicomponent mixture continuously, without introducing density jumps and phase interfaces. This is achieved by introducing the squares of the component density gradients into the expression for the free energy (or entropy) of the mixture [1–5]. The main advantage of this approach is the possibility of finding the spatial phase distribution as one of the results of solving a single problem; there is no need a priori to specify the phase interface surface geometry, to solve the hydrodynamic equations for each phase separately, or to use jump relations. An important feature of the density-functional method is taking the structure of the interphase region into account. This leads to observable effects for fluid flow in a capillary with surface-active walls [6] and for the capillary-gravity wave spectrum [7].

The study of the advantages of the density-functional method for the numerical simulation of multiphase flows has only just begun. Positive results have been obtained for several typical problems. Some of those obtained for plane isothermal viscous two-phase two-component flows are presented below.

In this paper, the basic equations of the theory are given, the numerical algorithms for solving these equations are described, and examples of calculating several typical two-phase flows are presented. The results and further possibilities of the method are discussed.

1. BASIC EQUATIONS OF THE DENSITY-FUNCTIONAL THEORY

We will first recall the basic propositions of the theory for nonisothermal and isothermal flows [3, 4].

Let an M -component mixture (gas or liquid) fill a region D with a piecewise-smooth boundary ∂D corresponding to contact with a stationary solid phase. We introduce the following notation: T is the absolute temperature and n_i is the molar density of the i -component. We will assume that the subscripts i, j , and k run through the values $1, \dots, M$ corresponding to the mixture component numbers and that the indices a, b , and c run through the values $1, 2, 3$ corresponding to the Cartesian coordinates x^a . If not otherwise specified, we assume summation over recurring indices. We will use the following concise notation for derivatives:

$$g_{,T} = \frac{\partial g}{\partial T}, \quad g_{,i} = \frac{\partial g}{\partial n_i}, \quad \partial_a g = \frac{\partial g}{\partial x^a}$$

Nonisothermal case: statics. In accordance with [4], we will specify the entropy of the mixture as the functional

$$S = \int_D \theta dV + \int_{\partial D} s_* dA \quad (1.1)$$

where $\theta = s - \alpha \partial_a T \partial_a T / 2 - \alpha_{ij} \partial_a n_i \partial_a n_j / 2$, $s = s(T, n_i)$ is the entropy of the homogeneous mixture per unit volume, $s_* = s_*(T, n_i)$ is the entropy per unit surface area, $\alpha = \alpha(T, n_i) > 0$, $\alpha_{ij} = \alpha_{ij}(n_k)$ are the coefficients of a positive symmetric matrix, and dV and dA are volume and surface elements.

The energy of the mixture with account for the external gravity field is specified by the functional

$$U = \int_D (u + \rho \varphi) dV + \int_{\partial D} u_* dA \quad (1.2)$$

where $u = u(T, n_i)$ is the internal energy of the homogeneous mixture per unit volume, $u_* = u_*(T, n_i)$ is the energy per unit surface area, $\varphi = \varphi(x^a)$ is the gravity potential, $\rho = m_i n_i$ is the mass density of the mixture, and m_i is the molar mass of the i -component.

The total number of i -component particles is determined by the expression

$$N_i = \int_D n_i dV \quad (1.3)$$

The equilibrium states of the mixture are critical points of the entropy functional (1.1) for fixed values of the energy (1.2) and fixed quantities (1.3). The locally thermodynamically stable points are local constrained maxima of the entropy functional. The globally thermodynamically stable state of the mixture is the point of absolute conditional maximum of the entropy functional.

Thus, the mixture equilibrium states must satisfy the variational principle

$$\delta S - \lambda_0 \delta U + \lambda_i \delta N_i = 0 \quad (1.4)$$

where λ_0 and λ_i are Lagrangian multipliers.

Directly calculating the variation of functional (1.1), we obtain the expression

$$\delta S = \int_D (\phi_0 \delta T + \phi_i \delta n_i) dV + \int_{\partial D} (\phi_{0*} \delta T + \phi_{i*} \delta n_i) dA \quad (1.5)$$

$$\phi_0 = s_{,T} + \frac{1}{2} \alpha_{,T} \partial_a T \partial_a T + \alpha \Delta T$$

$$\phi_i = s_{,i} - \frac{1}{2} \alpha_{,i} \partial_a T \partial_a T - \frac{1}{2} \alpha_{jk,i} \partial_a n_j \partial_a n_k + \alpha_{ij,k} \partial_a n_j \partial_a n_k + \alpha_{ij} \Delta n_j$$

$$\phi_{0*} = s_{*,T} + \alpha l_a \partial_a T, \quad \phi_{i*} = s_{*,i} + \alpha_{ij} l_a \partial_a n_j$$

where l_a is the inward normal to the surface ∂D and $\Delta = \partial_a \partial_a$.

Substituting expression (1.5) in the variational equation (1.4) and using the arbitrariness of the temperature variations and component densities, we obtain the conditions of mixture equilibrium in the form of a system of elliptical equations

$$\phi_0 - \lambda_0 u_{,T} = 0 \quad (1.6)$$

$$\phi_i - \lambda_0 (u_{,i} + m_i \varphi) + \lambda_i = 0 \quad (1.7)$$

and boundary conditions

$$\phi_{0*} - \lambda_0 u_{*,T} = 0 \quad (1.8)$$

$$\phi_{i*} - \lambda_0 u_{*,i} = 0 \quad (1.9)$$

When solving problem (1.6)–(1.9), the $(M + 1)$ Lagrangian multipliers λ_0, λ_i must be found from the specified values (1.2) and (1.3). An analysis of Eq. (1.6) for $T = \text{const}$ shows that $\lambda_0 = T^{-1}$. The requirement for any isothermal state to satisfy the boundary condition (1.8) imposes an additional restriction [4] which will be assumed to hold below:

$$u_{*,T} = T s_{*,T}$$

Nonisothermal case: dynamics. As the basic hydrodynamic equations we will use the traditional equations for the densities, momentum and energy [8]:

$$\partial_t n_i + \partial_a I_{ia} = 0 \tag{1.10}$$

$$\rho(\partial_t v_a + v_b \partial_b v_a) = \partial_b p_{ab} - \rho \partial_a \phi \tag{1.11}$$

$$\partial_t u + \partial_a (v_a u) = p_{ab} \partial_a v_b - \partial_a q_a \tag{1.12}$$

where I_{ia} is the i -component flux vector, $v_a = \rho^{-1} m_i I_{ia}$ is the mean-mass velocity, p_{ab} is the mixture stress tensor, and q_a is the heat flux vector.

We introduce the following auxiliary quantities: $Q_{ia} = I_{ia} - n_i v_a$ — the i -component diffusion flux, q_a^{ex} — the heat flux in the solid phase surrounding the multicomponent mixture considered, $\Sigma_{ab} = (\phi_i n_i - \theta) \delta_{ab} - \alpha \partial_a T \partial_b T - \alpha_{ij} \partial_a n_i \partial_b n_j$, $\Psi_0 = \phi_0 u_{*,T}^{-1}$, and $\Psi_i = \phi_i - \phi_0 u_{*,T}^{-1} u_{*,i}$. The quantity Ψ_0 has inverse temperature dimensionality and is exactly equal to T^{-1} if $T = \text{const}$ or $\alpha = 0$. This gives grounds for introducing the temperature $T_e = \Psi_0^{-1}$ [4] which is generally different from the temperature T . In the hydrodynamic description we will use the following boundary conditions for the dynamic variables: the no-slip condition

$$v_a|_{\partial D} = 0 \tag{1.13}$$

the impermeability condition for the diffusion fluxes:

$$l_a Q_{ia}|_{\partial D} = 0 \tag{1.14}$$

and the balance condition for the surface energy:

$$\partial_t u_* = (q_a^{\text{ex}} - q_a) l_a \tag{1.15}$$

In addition, instead of the boundary conditions (1.8) and (1.9), in the dynamic description we will also use other conditions [4] that do not contain Lagrangian multipliers

$$\phi_{0*} - T_e^{-1} u_{*,T} = 0 \tag{1.16}$$

$$\phi_{i*} - T_e^{-1} u_{*,i} = 0 \tag{1.17}$$

Using relations (1.5), (1.10)–(1.17) and integrating by parts, it is easy to obtain an expression for the derivative of the entropy functional (1.1)

$$\frac{dS}{dt} = \int_{\partial D} T_e^{-1} q_a^{\text{ex}} l_a dA + \int_D \sigma dV \tag{1.18}$$

$$\sigma = \Psi_0 \tau_{ab} \partial_a v_b + q_a \partial_a \Psi_0 + Q_{ia} \partial_a \Psi_i \tag{1.19}$$

$$\tau_{ab} = p_{ab} - \sigma_{ab} \tag{1.20}$$

$$\sigma_{ab} = \Psi_0^{-1} \Sigma_{ab} + (u - u_{*,i} n_i) \delta_{ab} \tag{1.21}$$

The expression for the rate of entropy change (1.18) takes the standard form [9] of the sum of two terms: flow across a surface and entropy production. The hydrodynamic model considered is consistent with the second law of thermodynamics if the entropy production is nonnegative:

$$\sigma \geq 0 \quad (1.22)$$

We note that the expression for the entropy production (1.18) contains a tensor τ_{ab} (1.20) obtained from the stress tensor p_{ab} by subtraction of the tensor σ_{ab} (1.21). The tensor σ_{ab} does not contribute to the entropy production and can be interpreted as the static stress tensor. In the case of an equilibrium homogeneous mixture, this tensor can be reduced to the ordinary stress tensor in an ideal fluid

$$\sigma_{ab} = -p\delta_{ab} \quad (1.23)$$

where $p = (Ts - u + (u_{,i} - Ts_{,i})n_i)$ is the hydrostatic pressure.

To close the hydrodynamic problem (1.10)–(1.17), we need the material relations, that is, expressions for the quantities τ_{ab} , q_a and Q_{ia} which must be compatible with inequality (1.22). Of most interest is the model that gives a minimal generalization of the model of a viscous heat-conducting mixture [8, 9]. For the viscous stress tensor we can use the linearly viscous Navier-Stokes model

$$\tau_{ab} = \left(\mu_v - \frac{2}{3}\mu_s \right) \partial_c v_c \delta_{ab} + \mu_s (\delta_a v_b + \delta_b v_a) \quad (1.24)$$

where μ_v and μ_s are the positive coefficients of bulk and shear viscosity. When formulating the expressions for the heat and diffusion fluxes, it is convenient to denote $Q_{0a} = q_a$. Then, by definition, the quantities $Q_{\alpha a}$ ($\alpha = 0, 1, \dots, M$) include the fluxes q_a and Q_{ia} . Obviously, if the relations

$$Q_{\alpha a} = \mu_{\alpha\beta} \partial_a \Psi_\beta \quad (\alpha, \beta = 0, 1, \dots, M) \quad (1.25)$$

where $\mu_{\alpha\beta}$ is a symmetric nonnegative matrix, hold, then so does the inequality

$$q_a \partial_a \Psi_0 + Q_{ia} \partial_a \Psi_i \geq 0$$

In order to exclude a contradiction between (1.25) and the definition of diffusion fluxes, the transfer coefficient matrix $\mu_{\alpha\beta}$ must satisfy the additional requirement $\mu_{\alpha\beta} a_\beta = 0$, where $a_0 = 0$ and $a_i = m_i$.

Relations (1.24) and (1.25) close the hydrodynamic problem. It can be shown [4] that the hydrodynamic equations are consistent with the static equations (1.6)–(1.9), i. e., the static solution automatically satisfies the hydrodynamic equations and, conversely, the solution of a hydrodynamic problem with the zero component and heat fluxes satisfies the static equations.

Isothermal case: statics. In some cases, a multiphase multicomponent medium can be described in the isothermal approximation. For example, the approximation $T = \text{const}$ can be justified if the thermal conductivity or the heat capacity are high. In the isothermal approximation, the constitutive equations can be obtained by passing to the limit $T = \text{const}$ in the nonisothermal equations. At the same time, the isothermal description can be developed independently on the basis of the principle of minimization of the free energy of the mixture. Then the approaches based on the entropy and free-energy functionals are interrelated.

The free-energy functional can be constructed from the entropy and energy functionals (1.1) and (1.2), respectively:

$$F = U - TS = \int_D \omega dV + \int_{\partial D} f_* dA \quad (1.26)$$

$$\omega = f + \frac{1}{2} v_{ij} \partial_a n_i \partial_a n_j + \rho \varphi$$

where $f = f(T, n_i) = u - Ts$ is the free energy of a homogeneous mixture per unit volume, $f_* = f_*(T, n_i) = u_* - Ts_*$ is the free energy per unit surface area, and $v_{ij} = T\alpha_{ij}(n_k)$.

The mixture equilibrium states are critical points of functional (1.26) at fixed values of (1.3).

Calculating the variation of functional (1.26), we obtain the expression

$$\delta F = \int_D \Phi_i \delta n_i dV + \int_{\partial D} \Phi_{i*} \delta n_i dA \tag{1.27}$$

$$\Phi_i = f_{,i} + m_i \varphi + \frac{1}{2} v_{jk,i} \partial_a n_j \partial_a n_k - v_{ij,k} \partial_a n_j \partial_a n_k - v_{ij} \Delta n_j$$

$$\Phi_{i*} = f_{*,i} - v_{ij} l_a \partial_a n_j$$

The variational equation for equilibrium states with Lagrangian multipliers Λ_i

$$\delta F - \Lambda_i \delta N_i = 0$$

leads to the system of elliptic equations

$$\Phi_i - \Lambda_i = 0 \tag{1.28}$$

and boundary conditions

$$\Phi_{i*} = 0 \tag{1.29}$$

Equations (1.28) correspond to Eqs. (1.7) with $\Lambda_i = T \lambda_i$. The boundary conditions (1.29) correspond to the boundary conditions (1.9).

Isothermal case: dynamics. In the isothermal approximation, the mixture hydrodynamics are described by Eqs. (1.10) and (1.11). We will use the boundary conditions (1.13), (1.14) and (1.29). The latter group of conditions corresponds to conditions (1.17).

Let us denote the functional of the total energy of the system as the sum of the free-energy functional (2.26) and the kinetic energy of the mixture

$$E = F + \frac{1}{2} \int_D \rho v_a v_a dV \tag{1.30}$$

Directly calculating the time derivative of functional (1.30), with account for expression (1.27) and equations (1.10) and (1.11), we arrive at the relation

$$\frac{dE}{dt} = \int_D \Sigma dV \tag{1.31}$$

$$\Sigma = -\tau_{ab} \partial_a v_b + Q_{ia} \partial_a \Phi_i \tag{1.32}$$

As in the nonisothermal case, the viscous stress tensor τ_{ab} and the static stress tensor σ_{ab} are defined by relations (2.20) and (2.21). We note that in the isothermal case the expression for the static stress can be simplified:

$$\sigma_{ab} = (\omega - \Phi_i n_i) \delta_{ab} - v_{ij} \partial_a n_i \partial_b n_j \tag{1.33}$$

To close the hydrodynamic problem, we must specify the expressions for the quantities τ_{ab} and Q_{ia} in such a way as to satisfy the dissipative system condition

$$\Sigma \leq 0 \tag{1.34}$$

It is easy to show that if the material relations (1.24) and (1.25) are assumed, inequality (1.34) is satisfied. We must then use the following relation between the quantities Φ_i and Ψ_i , valid in the isothermal case:

$$\Psi_i = -T^{-1}(\Phi_i - m_i \varphi)$$

The isothermal theory based on functional (1.26) is thus a particular case of the theory based on functional (1.1). It is worth noting that the interrelation between functionals (1.1) and (1.26) leads to a linear temperature dependence of the coefficients v_{ij} .

2. EXAMPLES OF NUMERICAL SIMULATION OF TWO-PHASE FLOWS

As the basic system of equations we will take the component conservation equations (1.10) and the momentum conservation equation (1.11). We will specify the viscous stress tensor by expression (1.24), the static stress tensor by expression (1.33), and the diffusion flux by formula (1.25).

When using the density-functional method for two-phase media, such as liquid-liquid and gas-liquid systems, we must specify the form of the free-energy function, the coefficients of viscosity, diffusion and surface tension on the mixture-solid interface, and the coefficients v_{ij} .

If the deviations of the densities from certain fixed equilibrium values are small, then the free energy of one phase (phase A) can be represented in the form of a quadratic polynomial

$$f_A(n_i) = f_{A0} + f_{Ai}(n_i - n_{iA}) + \frac{1}{2}f_{Aij}(n_i - n_{iA})(n_j - n_{jA}) \quad (2.1)$$

where n_{iA} is the unperturbed molar density of phase A.

The coefficients f_{A0} and f_{Ai} do not enter into the hydrodynamic equations and are used only for calculating the initial unperturbed pressures and chemical potentials.

Therefore, we can assume them to be equal to zero. For hydrodynamic modeling, only the coefficients f_{Aij} are important. We select these coefficients in accordance with the data on the bulk elastic modulus of phase A:

$$E_A = f_{Aij}n_{iA}n_{jA} \quad (2.2)$$

In the case of two-phase flow (phases A and B), the free energy is determined from the expressions for $f_A(n_i)$ and $f_B(n_i)$ as follows:

$$f = \frac{f_A f_B}{f_A + f_B} \quad (2.3)$$

We will assume that the shear and bulk viscosities are known for each phase. For arbitrary component densities, the viscosities can be calculated from the formulas

$$\begin{aligned} \mu_s &= \left(c_A \mu_{sA}^{1/3} + c_B \mu_{sB}^{1/3} \right)^3, & \mu_v &= \left(c_A \mu_{vA}^{1/3} + c_B \mu_{vB}^{1/3} \right)^3 \\ c_A &= \frac{z_B}{z_A + z_B}, & c_B &= \frac{z_A}{z_A + z_B} \\ z_A &= \left(\sum_{i=1}^2 (n_i - n_{iA})^2 \right)^{1/2}, & z_B &= \left(\sum_{i=1}^2 (n_i - n_{iB})^2 \right)^{1/2} \end{aligned} \quad (2.4)$$

In the isothermal case, relations (1.25) lead to the following expression for the diffusion fluxes:

$$Q_{ia} = -D_{ij} \partial_a \Phi_j \quad (2.5)$$

where the symmetric and nonnegative matrix D_{ij} satisfies the condition

$$D_{ij} m_j = 0 \quad (2.6)$$

From (2.5), for $v_{ij} = 0$, there follows the expression for the component concentration flux

$$q_{ia} = n^{-1} Q_{ia} = -n^{-1} D_{ij} \left(\frac{\partial \kappa_j}{\partial c} \right)_n \partial_a c - n^{-1} D_{ij} \left(\frac{\partial \kappa_j}{\partial n} \right)_c \partial_a n$$

where $n = \sum_{i=1}^2 n_i$ is the total density, $c = n_1/n$ is the concentration of component 1, and $\kappa_i = f_{,i}$ is the chemical potential.

Thus, the tabular value of the diffusion coefficient d for component 1 in the mixture is linked with the matrix D_{ij} by the relation

$$d = n^{-1} D_{1j} \left(\frac{\partial \kappa_j}{\partial c} \right)_n \quad (2.7)$$

The diffusion coefficient d can be calculated from the known values of the phase diffusion coefficients d_A and d_B : $d = c_A d_A + c_B d_B$. If the free energy is given (see (2.1)–(2.3)) and the coefficient d is known, then Eq. (2.7) with account for (2.6) unambiguously determines the matrix D_{ij} .

We will assume that the surface tension on the mixture-solid interface is a linear function of the component densities

$$f_* = \xi_{1i} n_i + \xi_0 \quad (2.8)$$

The parameters ξ_0 and ξ_{1i} can be calculated from the known values of the surface tensions on the interfaces between the solid and each phase (A and B):

$$\theta_A = \xi_{1i} n_{iA} + \xi_0, \quad \theta_B = \xi_{1i} n_{iB} + \xi_0 \quad (2.9)$$

The system of linear equations (2.9) always has a solution but this solution is nonunique. The arbitrariness in specifying the dependence (2.8) affects the component distribution near the wall but does not affect the wetting angle.

We will assume the matrix of coefficients v_{ij} to be proportional to the unit matrix. The unknown proportionality coefficient can be fixed from the formula for the surface tension between phases A and B [3]

$$\gamma = \int_0^{+\infty} v_{ij} \partial_r n_i \partial_r n_j dr \quad (2.10)$$

In formula (2.10), the integral is calculated for the static solution of the problem of a phase A drop in phase B or, conversely, of a phase B drop in phase A .

Thus, relations (2.1)–(2.10) make it possible to specify the dimensional parameters of the model. For all the problems considered, we assumed that $\gamma = 0.1$ N/m.

The system of equations (1.10), (1.11), (1.24), (1.33), (2.5) was solved numerically using an explicit conservative difference scheme based on the concept of the method of large particles [10]. In the algorithm developed, the “Lagrangian” stage is completely the same as in [10], while the “Eulerian” stage is constructed starting from the absence of the pressure function from the conservation equations (the terms with the pressure gradient are defined in terms of the derivatives of the free energy f : $p = n_i f_{,i} - f$).

In order to study the opportunities afforded by the density-functional method, we numerically calculated the following model problems: (1) interaction of a liquid drop (phase A) surrounded by another liquid (phase B) with a plane liquid layer (phase A); (2) fragmentation of a liquid drop (phase B) by a liquid flow (phase A); (3) interaction of a liquid drop (phase A) surrounded by another liquid (phase B) with a plane solid wall; (4) development of Rayleigh-Taylor and Kelvin-Helmholtz instability on the interface between two phases.

The problems considered can also be solved by other numerical methods [11–20]. Nevertheless, the density-functional method has at least three advantages: multiphase states can be calculated continuously without the separation of interfaces between the phases; the multiphase states are stable, that is, numerical time steps do not lead to phase “smearing”; all the coefficients used in the algorithm can be calculated on the basis of well-studied experimental data. Other approaches to the description of multiphase flows [11–20] fail to satisfy at least one of these conditions.

We must now consider the choice of a specific class of numerical algorithms [10]. Since at present both experience in numerically solving the above-mentioned system of equations and information on the behavior of the solutions obtained are almost entirely lacking, as the first stage in the development of numerical algorithms for the continuous calculation of multiphase flows it is expedient to use simple difference methods,

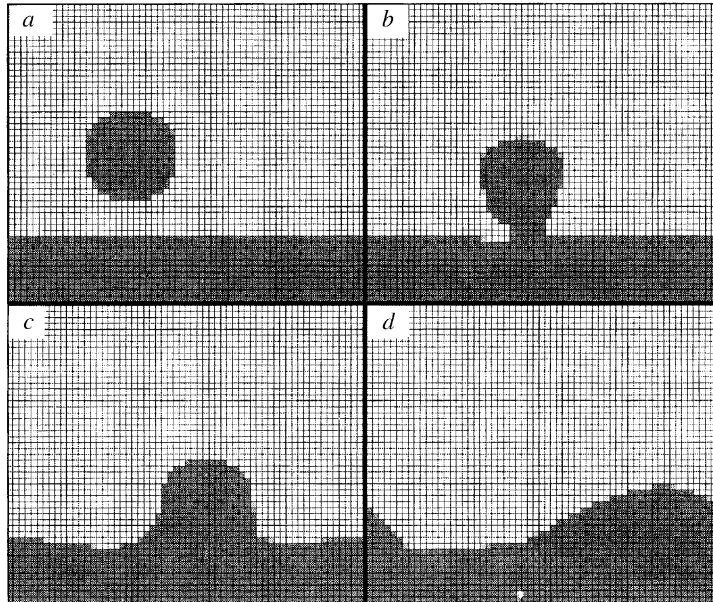


Fig. 1. Drop falling onto a liquid layer

such as the method proposed in [10]. This method is, firstly, simple to realize and efficient and, secondly, has proved its advantages in the calculation of such complex unsteady flows as the Rayleigh-Taylor and Richtmayer-Meshkov instabilities, even in the turbulent mixing stage [11–17]. Moreover, the calculations of the same problems performed on the basis of more complex high-accuracy methods, such as the method of artificial compressibility [13, 17, 19] and the method of [18, 20], have confirmed the high quality of the solution based on the method of [10].

In Figs. 1–4, the shades of grey in the calculation cells reflect the distribution of the concentration of one of the components present, which practically corresponds to the spatial distribution of the corresponding phase.

Problem 1. Initially, the upper half-plane is occupied by a liquid layer (phase B) at rest and the lower half-plane by another liquid layer (phase A). A liquid drop (phase A) moves from the upper into the lower region, at an angle of 30° to the horizontal (see Fig. 1a). The initial velocity of the drop is equal to 10 m/s. The body force field is directed vertically downward. On the upper and lower boundaries, conditions (1.13) and the conditions of vanishing of the component diffusion fluxes (1.14) are assigned. On the left and right boundaries the periodicity conditions are imposed. The following problem parameters are specified: the calculation domain dimensions are 60×50 ; the grid cells are squares with a 0.001 m side; $m_1 = 18$ kg/kmol, $m_2 = 200$ kg/kmol, $\mu_{sA} = 10^{-3}$ Pa·s, $\mu_{sB} = 10^{-2}$ Pa·s, $\mu_v = 10\mu_s$, the phase mass densities $\rho_A = 1000$ kg/m³, $\rho_B = 800$ kg/m³, $E_A = E_B = 10^9$ Pa, and $d_A = d_B = 10^{-9}$ m²/s.

Figure 1a–d shows the process dynamics at successive moments of time. It can be seen that the interaction leads to the formation of a structure with a thin stem of phase A (Fig. 1b) and subsequent liquid “outflow” from the drop into the layer (Fig. 1c) over which perturbations in the form of gravity waves propagate (Fig. 1d).

Similar collision problems have been considered in connection with the need to predict the parameters of jets and sprays formed upon the interaction of various devices with liquids [21]. In simulations, the approximation of high collision velocities, when the viscous and surface-tension effects are negligible, is often used. The problem considered in this paper corresponds to the little studied hydrodynamic phenomena for which the high-velocity approximation is incorrect.

Problem 2. Initially, a liquid drop (phase B) is introduced into an inhomogeneous flow of another liquid (phase A). This is a Couette flow formed by upper and lower boundaries that move at equal velocities

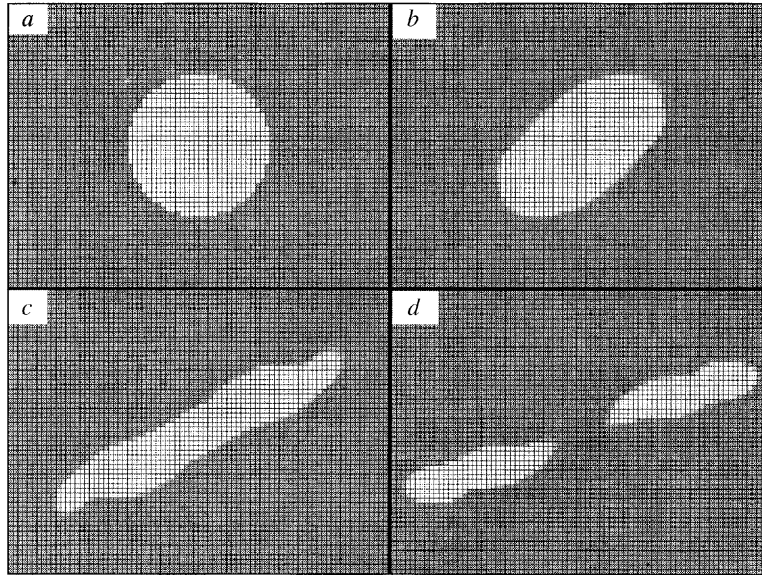


Fig. 2. Liquid drop rupture in shear flow

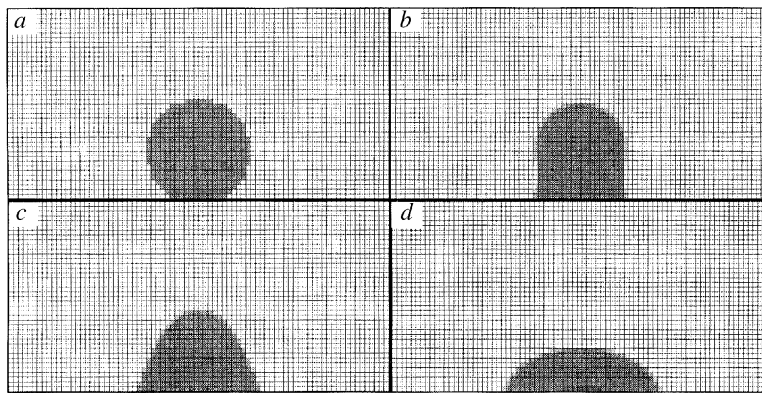


Fig. 3. Spread of a drop over a solid wall

$U = 10$ m/s (in their own planes) in opposite directions (the upper boundary moves from left to right). On the boundaries we assign conditions (1.13) and (1.14) (Fig. 2a). There are no body forces. On the left and right boundaries the periodicity conditions are imposed. The calculation domain is 80×60 and $\mu_s = 10^{-2}$ Pa for both phases; the other problem parameters are the same as in problem 1.

Due to the work done by the viscous forces, the drop begins to change shape (Fig. 2b), elongating in the stream direction. In Fig. 2c, the typical thinning of the middle of the drop can be seen. Then this zone ruptures with the formation of two drops (Fig. 2d).

The phenomena of drop rupture in a liquid flow have been studied experimentally and theoretically [22–26]. Due to the variety of these phenomena, it has proved convenient to combine them into classes. So far, six main fragmentation mechanisms have been distinguished [25, 26]. The problem considered corresponds to the first of these mechanisms (so-called vibrational fragmentation mode). In this case, the drop introduced into the flow is deformed, turning into an elongated ellipsoid, and then disintegrates into two or more droplets. For simulating this process numerically, the Navier-Stokes model, which allows the drop dynamics to be fairly well reproduced up to disintegration, is commonly used. The advantage of the approach proposed in this paper is that it offers the possibility of a unified description of the two-phase system in all stages of drop evolution.

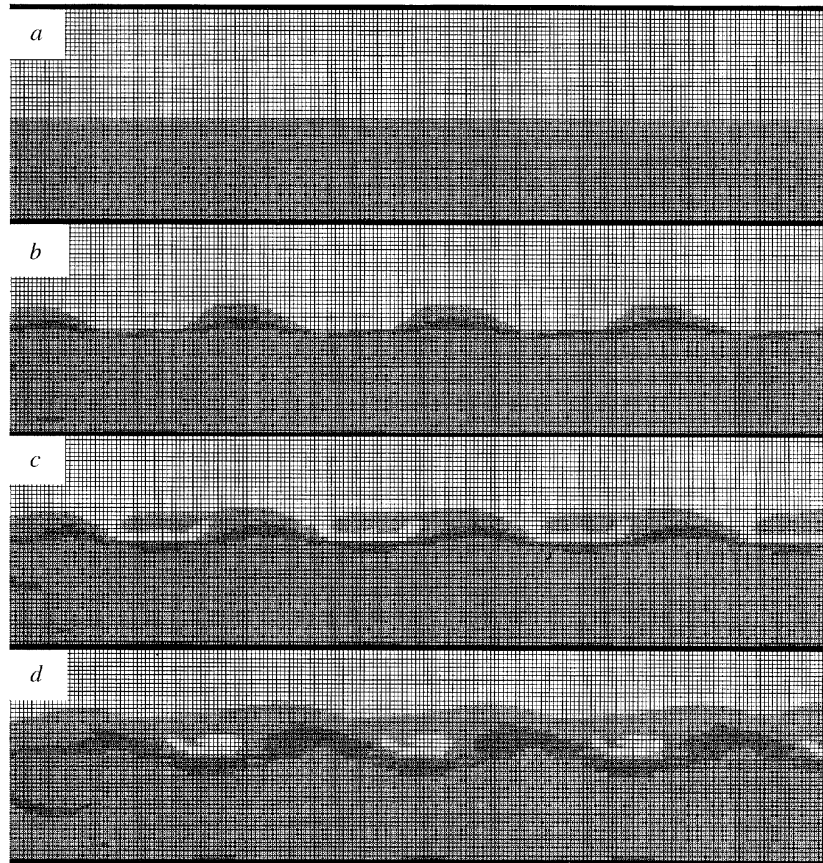


Fig. 4. Development of unstable perturbations on the interface between moving phases

Problem 3. A liquid drop (phase A) at rest, surrounded by a liquid phase B , is initially spherical and touches the lower boundary of the calculation domain (Fig. 3a) which models a solid surface. On the lower boundary, conditions (1.13) and (1.14) for the velocity and the diffusion fluxes and (1.29) for the molar phase densities are assigned. The surface-tension function on the mixture-solid interface is calculated from formula (2.9), where $\theta_B - \theta_A = 0.06$ N/m. On the other boundaries of the calculation domain free-boundary conditions are assigned. There are no body forces. The calculation field dimensions are 80×40 , the side of the square difference-grid cells measures 10^{-4} , and $\mu_s = 10^{-3}$ Pa for phases A and B ; the other problem parameters are the same as in problem 1.

In Fig. 3b–d, we can see the dynamics of establishment of the drop shape on the solid surface with the formation of a sharp wetting angle. The calculation results demonstrate the possibility of using the density functional for the description of the static and dynamic wetting effects. With reference to the present state of experimental and theoretical research in this field (see review [27]), we note two advantages of the approach proposed: (a) the density-functional method is a natural generalization of Cahn's static theory [28] to include the case of multicomponent multiphase viscous mixture flows; (b) the method makes it possible to overcome a certain limitation of the Navier-Stokes model in which, since the particle velocity on the mixture-solid interface is equal to zero (no-slip condition), displacement of the three-phase contact line is forbidden.

Problem 4. Initially (Fig. 4a), the upper half-plane is occupied by a gas phase A moving from right to left at a velocity U and the lower half-plane by a liquid phase B moving in the opposite direction at the same velocity. The body force is perpendicular to the interface and directed into the lighter gas phase. This is a case of Rayleigh-Taylor instability [11]. In the neighborhood of the interface the initial perturbations are specified in the form:

$$v_x = \text{sign}(y)A \sin(kx)e^{-k|y|}, \quad v_y = A \cos(kx)e^{-k|y|}$$

Here, k is the wave number, A is the perturbation amplitude, x is the longitudinal coordinate, and y is the transverse coordinate measured from the interface. On the left boundary, at $y < 0$, the boundary conditions $v_x = U$ and $v_y = 0$ and on the right boundary, at $y \geq 0$, the conditions $v_x = -U$ and $v_y = 0$ are assigned. On the other boundaries of the calculation domain free-boundary conditions are imposed. The problem parameters are as follows: the calculation field dimensions are 200×50 ; the side of the square grid cells measures $4 \cdot 10^{-4}$ m; $m_1 = 2$ kg/kmol, $m_2 = 200$ kg/kmol, $\mu_s = 10^{-5}$ Pa·s for phase A and $\mu_s = 10^{-3}$ Pa·s for phase B, $\mu_v = 10\mu_s$, $\rho_A = 2$ kg/m³, $\rho_B = 800$ kg/m³, $E_A = 10^7$ Pa, $E_B = 10^9$ Pa, $d_A = 10^{-6}$ m²/s, $d_B = 10^{-9}$ m²/s, $U = 5$ m/s, $A = 1$ m/s, and $k = 314$ 1/m.

From an analysis of the dispersion equation for the chosen parameters, it follows [17] that in the neighborhood of the interface Rayleigh-Taylor and Kelvin-Helmholtz instabilities develop, which initially leads to a slight curvature of the interface (Fig. 4b). This process then goes over into a nonlinear stage with a highly deformed interface (Fig. 4c) followed by the formation of separate gas bubbles (Fig. 4d).

This type of hydrodynamic instability has been studied experimentally and theoretically [29, 30] but mainly in the initial stage of the process. Within the framework of linear perturbation theory, the calculations performed on the basis of the density-functional method correspond to the known results [29, 30]. The behavior of the perturbations in the nonlinear stage has still not been sufficiently studied.

Summary. The density-functional method adequately models complex multiphase flows without the use of special techniques for separating the interfaces between phases (the calculation is continuous). This simplifies the algorithm which can easily be adapted for various problem types. In the future, to make the calculations more efficient, it would be desirable to use implicit difference schemes.

The examples of numerical calculations considered show that the density-functional method models the two-phase mixture dynamics quite efficiently in the isothermal approximation. The continuous calculation method proposed is time-saving and can easily be generalized to include both mixtures with more components or phases and three-dimensional problems.

For nonisothermal problems the theory is fairly well developed but the numerical realization of the corresponding system of equations needs further research.

The results were visualized using VR-Geo software (Servis-Nafta Limited).

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