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DESCRIPTION OF VISCOUS-FLUID FLOWS WITH A MOVING SOLID PHASE IN THE DENSITY-FUNCTIONAL THEORY

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The density-functional theory has been extended to the flows of multicomponent multiphase mixtures containing solid bodies. It is proposed to consider these bodies as separate phases of a mixture and the rheology of the indicated bodies as elastic, which enables retention of their shape in the process of motion. This theory allows one to simultaneously describe a flow of a mixture univariately and the phase transformations occurring in it with the participation of the solid phase. Results of numerical simulation of the motion of a solid body with no change of phase and with dissolution in a viscous flow are presented.

Introduction. Every so often it is difficult to describe the dynamics of the interphase boundary in multiphase flows. In many cases, the topology of the interphase boundaries in a flow of a mixture can restructure with a loss of smoothness (coalescence or breakage of drops, formation or disappearance of phases in the process of phase transformations), which makes the formulation of adequate conditions for the case of compression shocks difficult. This problem can be solved with the use of the density-functional theory that allows one to represent the motion of a multicomponent, multiphase mixture as a continuous flow free of compression shocks and interphase boundaries, which is attained by introduction of the squares of the density gradients of the mixture components into the expression for the free energy of the mixture [1–7]. The main advantage of this approach is that the space distribution of the phases in a mixture can be determined from the solution of the unique continuous hydrodynamic problem, which contains information on the structure of the interphase boundary and the interphase transfer of chemical components of the mixture.

In [6, 7], it was shown that the density-functional theory can be used for numerical simulation of two-phase mixtures of the gas–liquid and liquid–liquid types. An important problem of the multiphase hydrodynamics is the description of two-phase flows of the liquid–solid phase type. In the case where the motion of one rigid body in a boundless liquid is considered, a mathematical model is simplified by passing to the reference system related to this body. However, this change accomplishes nothing when the motion of several bodies or the motion of one body in a channel with solid boundaries are considered. The difficulties of mathematical description of the dynamic of the interphase boundaries in a flow of a mixture containing several rigid bodies with mutually movable surfaces are identical to those for gas-liquid mixtures. In particular, the topology of the interphase boundaries in a mixture can change as a result of the coalescence of solid-phase particles or their breakage, the precipitation of the solid phase from the liquid solution, and the dissolution of the solid phase. Since the physical nature of these effects is identical to that of gas-liquid mixtures, it is reasonable to investigate the possibility of extension of the density-functional method to the flows with a solid phase.

In the present work, the possibility of using the density-functional method for simulation of isothermic viscous flows containing solid bodies was investigated. The solid phase is introduced into a model as the liquid or gas phase; the only difference between these cases is that, instead of the Newtonian-liquid rheology, the rheology of an elastic body or, in the general case, the rheology of a viscoelastic body is considered. It is interesting that a change in the rheology causes changes in a number of determining relations of the theory, in particular, in the expressions for chemical potentials and diffusion flows. Below are basic equations of the theory, algorithms of finite-difference realization of these equations, and examples of numerical simulation of typical two-dimensional flows.

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Equations of the Density-Functional Theory for a Mixture Containing a Solid Phase. Let an M-component mixture occupies the area D with a sectionally smooth boundary ∂D corresponding to the contact with an immovable ambient solid body. The mixture can include movable regions in different phase states: gas, liquid, or solid. We will use the following designations: t is time, n_i and m_i are the molar density and molar mass of the ith component, $\rho = m_i n_i$ is the mass density. It is assumed that the indices i, j, and k take values 1, ..., M, corresponding to the numbers of the mixture components; the indices a, b, and c take values 1, 2, and 3 in accordance with the Cartesian coordinates x_a. The summation is performed over recurring indices unless otherwise specified. The following abridged notation is used for derivatives: $g_{,i} = \partial g/\partial n_i$, $\partial_t g = \partial g/\partial t$, and $\partial_a g = \partial g/\partial x_a$. The temperature of the mixture is assumed to be constant; therefore, the temperature dependence of the quantities being considered will be disregarded.

Mixture with a solid phase uneffected by phase transformations. In this case, it is assumed that there exists any initial state of the mixture, in which the solid phase is in the undeformed state. Let x_{a0} be the Cartesian coordinates of a particle of the medium in the initial state and $x_a = x_a(t, x_{b0})$ be the Cartesian coordinates of the same particle at the instant t. In the Euler coordinates, the field of motion of the medium $u_a = u_a(t, x_b)$, related to the mean-mass motion, is defined by the relation

$$u_a = u_a (t, x_b) = x_a - x_{a0} \, . \tag{1}$$

The field of the deformation tensor can be determined, by the field of motion (1), as [8]

$$\varepsilon_{ab} = \varepsilon_{ab} (t, x_c) = 2^{-1} (\partial_b u_a + \partial_a u_b - \partial_a u_c \partial_b u_c) \, . \tag{2}$$

The deformation tensor (2) relates the mass density ρ_0 of the particle at the point x_{a0} in the medium in the initial state to its mass density ρ at the point $x_a = x_a(t, x_{b0})$ at the instant t:

$$\rho = \rho_0 (\det (g_{ab}))^{1/2} \, , \quad g_{ab} = \delta_{ab} - 2\varepsilon_{ab} \, . \tag{3}$$

The velocity field of the medium can be calculated as the time derivative of the current coordinates of the particle of the medium with fixed initial coordinates: $v_a = \partial_t x_a(t, x_{b0})$. In the Euler coordinates, the velocity field is related to the field of motion by the relations following from Eq. (1)

$$\partial_t u_a + v_b \partial_b u_a = v_a \, . \tag{4}$$

Using (2) and (4), one can calculate the time derivative of the deformation tensor

$$\partial_t \varepsilon_{ab} = 2^{-1} (\partial_b v_a + \partial_a v_b) - v_c \partial_c \varepsilon_{ab} - \varepsilon_{ac} \partial_b v_c - \varepsilon_{bc} \partial_a v_c \, . \tag{5}$$

Equation (5) can be used for restoration of the deformation tensor by the known velocity field. It is assumed that the deformation-tensor field of the medium in the initial state is equal to zero.

In the density-functional theory, the free energy of a gas-liquid mixture is determined from the expression including the density-gradient squares of the mixture components [1–7]

$$F_{\text{fl}} = \int_D \omega_{\text{fl}} dV + \int_{\partial D} \theta dA \, , \tag{6}$$

$$\omega_{\text{fl}} = f + \frac{1}{2} \nu_{ij} \partial_a n_i \partial_a n_j \, , \tag{7}$$

where $f = f(n_i)$ is the free energy of a homogeneous mixture per unit volume, $\theta = \theta(n_i)$ is the surface tension at the boundary between the mixture and the immovable ambient solid phase, and $\nu_{ij} = \nu_{ij}(n_k)$ is the positive-definite symmetric matrix related to the interphase-tension coefficient in the case where several phases are present in the mixture

[1, 6, 7]. For example, for the one-dimensional distribution $n_i = n_i(x^1)$, defining the zone of transition from any phase A to the phase B, the interphase-tension coefficient is calculated by the formula

$$\gamma = \int_{-\infty}^{+\infty} \nu_{ij} \partial_1 n_i \partial_1 n_j dx^1 . \tag{8}$$

The energy of the elastic deformation of the solid phase (or phases) present in the mixture is estimated by the functional

$$F_{\mathrm{el}} = \int_D \omega_{\mathrm{el}} dV , \tag{9}$$

$$\omega_{\mathrm{el}} = 2^{-1} \lambda\, (\varepsilon_{aa})^2 + \mu \varepsilon_{ab} \varepsilon_{ab} , \tag{10}$$

where $\lambda = \lambda(n_i)$ and $\mu = \mu(n_i)$ are the Lamé coefficients dependent on the local density of the mixture components. It is assumed that these coefficients are equal to zero for the densities n_i corresponding to the gas and liquid phases. At the same time, in the space occupied by the solid phase (phases), the Lamé coefficients are constant and characterize the elastic properties of the mixture. In the interphase regions, the coefficients $\lambda = \lambda(n_i)$ and $\mu = \mu(n_i)$ change markedly with change in the density n_i.

Expression (9) represents the simplest model of an isotropic elastic solid body [9]. The state of a particle of the medium in the solid phase is determined by the local densities of the mixture components and by the deformation tensor. Consequently, the indicated model takes no account of the possible anisotropy of the solid body or the existence of additional internal degrees of freedom associated with the orientation of the particle and the structural phase transformations. The effects defined by the higher powers in the expansion of the elastic energy in terms of the deformation-tensor components are also disregarded. At the same time, the elastic model being used is geometrically nonlinear because the velocity components in Eq. (5) are not usually small.

The total free energy of the mixture is calculated as the sum of the quantities determined by expressions (6) and (9) and the potential energy of the mixture in the external gravitational field with a potential $\varphi = \varphi(x_a)$:

$$F = \int_D (\omega_{\mathrm{fl}} + \omega_{\mathrm{el}} + \rho\varphi)\, dV + \int_{\partial D} \theta dA . \tag{11}$$

Here, the sum of the quantities determined from (7) and (10) has a physical meaning. The total free energy can be only conditionally divided into the gas-liquid and elastic-solid energies since the set of the densities n_i and the function $f = f(n_i)$ are not independent of the deformations ε_{ab} because of the conditions defined by relation (3). However, the above-described formulation of the model with separation of the components defined by (6) and (9) is convenient to use in practice since the properties of gas-liquid mixtures and solids are frequently investigated independently and by different methods.

We will calculate a variation of functional (11). Let l_a be the internal normal to the surface ∂D. In the process of varying the indicated functional, some variables integrated over the volume are conveniently brought to a surface integral with the use of the Ostrogradskii–Gauss formula

$$\delta F = \int_D (\Phi_i \delta n_i + \chi_{ab} \delta\varepsilon_{ab})\, dV + \int_{\partial D} \Phi_{i*} \delta n_i dA , \tag{12}$$

where

$$\Phi_i = f_{,i} + m_i \varphi + \frac{1}{2} \nu_{jk,i} \partial_a n_j \partial_a n_k - \nu_{ij,k} \partial_a n_j \partial_a n_k - \nu_{ij} \partial_a \partial_a n_j + 2^{-1} \lambda_{,i}\, (\varepsilon_{aa})^2 + \mu_{,i} \varepsilon_{ab} \varepsilon_{ab} ;$$

$$\chi_{ab} = \lambda\varepsilon_{cc}\delta_{ab} + 2\mu\varepsilon_{ab}\ ; \quad \Phi_{i*} = \theta_{,i} - \nu_{ij}l_a\partial_a n_j\ .$$

The hydrodynamics of the mixture is defined by the ordinary conservation equations for the mixture components and momentum [10]

$$\partial_t n_i + \partial_a (n_i v_a + Q_{ia}) = 0\ , \tag{13}$$

$$\rho\ (\partial_t v_a + v_b \partial_b v_a) = \partial_b p_{ab} - \rho\partial_a\varphi\ . \tag{14}$$

Here, Q_{ia} is the vector of the diffusion flow of the ith component and p_{ab} is the stress tensor of the mixture. In accordance with the definition of the mean-mass velocity v_a, the diffusion-flow vector Q_{ia} satisfies the condition $m_i Q_{ia}$ = 0. The quantities Q_{ia} and p_{ab} should be defined with account of the fact that the total energy of the mixture E, including the kinetic and free energies, decreases (11):

$$E = 2^{-1}\int\limits_D \rho v_a v_a dV + F\ . \tag{15}$$

The time derivative of the quantity defined by (15) will be calculated with the use of relations (5), (12)–(14) on condition that

$$v_a \,|\, _{\partial D} = 0\ , \tag{16}$$

$$l_a Q_{ia} \,|\, _{\partial D} = 0\ , \tag{17}$$

$$\Phi_{i*} \,|\, _{\partial D} = 0\ . \tag{18}$$

Condition (16) is an ordinary adhesion condition for viscous flows, (17) is the condition of impenetrability of the boundary for diffusion flows, and expression (18) defines the conditions under which the densities of the mixture components relax instantaneously at the boundary. Now, the time derivative of the quantity E can be easily calculated (15):

$$\frac{dE}{dt} = \int\limits_D \Sigma dV\ , \tag{19}$$

$$\Sigma = -\ \tau_{ab}\partial_a v_b + Q_{ia}\partial_a \Phi_i\ , \tag{20}$$

$$\tau_{ab} = p_{ab} - \sigma_{ab}\ , \tag{21}$$

$$\sigma_{ab} = (\omega_{\text{fl}} + \omega_{\text{el}} - \Phi_i n_i)\ \delta_{ab} - \nu_{ij}\partial_a n_i \partial_b n_j + \chi_{ab} - \chi_{ac}\varepsilon_{cb} - \chi_{bc}\varepsilon_{ca}\ . \tag{22}$$

The functional form of expression (20) allows us to interpret the quantities involved in (21) as components of the viscous-stress tensor and the quantities defined by (22) as components of the static-stress tensor (the stress component independent of the motion). It is easy to show that, for a homogeneous liquid, the static-stress tensor is determined by the hydrostatic pressure p: $\sigma_{ab} = -p\delta_{ab}$, and, in the case where the gas-liquid component defined by (10) is absent, for small deformations the static-stress tensor is equal to the stress tensor of the linear elasticity theory: $\sigma_{ab} = \chi_{ab}$.

In order that the quantity defined by (19) was not positive, it will suffice to require that the following inequality be fulfilled:

$$\Sigma \le 0\,. \tag{23}$$

The determining relations identical to the relations proposed in [1–7] satisfy this condition:

$$\tau_{ab} = \left(\mu_{\mathrm{v}} - \frac{2}{3}\mu_{\mathrm{s}}\right)\partial_c v_c \delta_{ab} + \mu_{\mathrm{s}}\,(\partial_a v_b + \partial_b v_a)\,, \tag{24}$$

$$Q_{ia} = -\,D_{ij}\partial_a \Phi_j\,. \tag{25}$$

Here, $\mu_{\mathrm{v}} = \mu_{\mathrm{v}}(n_i)$, $\mu_{\mathrm{s}} = \mu_{\mathrm{s}}(n_i)$ is the nonnegative coefficients of the volume and shear viscosities, $D_{ij} = D_{ij}(n_k)$ is the nonnegative symmetric diffusion-coefficient matrix obeying the additional condition

$$D_{ij} m_j = 0\,. \tag{26}$$

The determining relations (24) and (25) complete the construction of the model of a multicomponent mixture containing a moving solid phase. In accordance with the above reasonings, all the phases (gas, liquid, solid) are described identically. However, it is assumed that the gas and liquid possess a Newtonian rheology and the solid phase offers an elastic rheology or, if the viscosity coefficient of the slid phase differs from zero, a viscoelastic rheology. The rheologic coefficients of a concrete mixture are determined by the experimental data on its properties.

Mixture with a solid phase participating in phase transformations. If the solid phase participates in phase transformations, the initial state, from which displacements (1) and deformations (2) should be measured, can be difficult to determine. Actually, the solid phase can be absent at the initial moment and be formed in the process of crystallization. For this case, we propose to consider the deformation tensor as not a kinetic variable but as a dynamic characteristic of the medium related to the velocity field by the modified equation (5):

$$\partial_t \varepsilon_{ab} = 2^{-1}\,(\partial_b v_a + \partial_a v_b) - v_c \partial_c \varepsilon_{ab} - \varepsilon_{ac}\partial_b v_c - \varepsilon_{bc}\partial_a v_c - \tau_{\mathrm{r}}^{-1}\varepsilon_{ab}\,. \tag{27}$$

Here, $\tau_{\mathrm{r}} = \tau_{\mathrm{r}}(n_i)$ is a positive quantity with the dimensions of time (relaxation time), dependent on the local composition and characterizing the kinetics of the phase transformations of the solid phase. For example, for a stable solid phase, the quantity τ_{r} can tend to infinity (in this case, Eq. (27) is reduced to Eq. (5)), and, for a gas and a liquid, the value of τ_{r} can be assumed to be close to zero.

The change from Eq. (5) to Eq. (27) changes practically nothing in the above reasonings; in this case, differences appear only in formula (20). A new expression for the quantity Σ has the form

$$\Sigma = -\,\tau_{ab}\partial_a v_b + Q_{ia}\partial_a \Phi_i - \tau_{\mathrm{r}}^{-1}\chi_{ab}\varepsilon_{ab}\,.$$

It is seen that the determining relations (24) and (25) provide the fulfilment of the dissipation condition for model (23). Thus, the model can consistently describe the formation and dissolution of the solid phase.

Numerical Examples of Flows with a Mobile Solid Phase. We will consider two model problems on a two-dimensional flow of a binary mixture ($M = 2$) containing a moving liquid phase A and a moving solid phase B. In the numerical simulation of multiphase, multicomponents flows, it is necessary to calculate a number of phenomenological coefficients and functions, involved in the dynamic equations and determining relations. For this purpose, we will use the computational procedures proposed in [6, 7].

Free energy. If the deviations of the densities from certain fixed equilibrium values are small, the free energy of one phase (phase A) can be defined by the square polynomial

$$f_{\mathrm{A}}\,(n_i) = f_{0\mathrm{A}} + f_{i\mathrm{A}}\,(n_i - n_{i\mathrm{A}}) + 2^{-1} f_{ij\mathrm{A}}\,(n_i - n_{i\mathrm{A}})\,(n_j - n_{j\mathrm{A}})\,,$$

where $n_{i\mathrm{A}}$ is the nondisturbed value of the molar density for the phase A. The coefficients $f_{0\mathrm{A}}$ and $f_{i\mathrm{A}}$ are not involved in the hydrodynamical equation; they are used only for calculating the initial nondisturbed pressures and chemical potentials. These coefficients can be assumed to be equal to zero. For simulation of the fluid dynamics, of importance are only the coefficients $f_{ij\mathrm{A}}$ that are selected in accordance with the data on the modulus of dilatation for the phase A: $E_\mathrm{A} = f_{ij\mathrm{A}} n_{i\mathrm{A}} n_{j\mathrm{A}}$.

In the case of a two-phase flow (phases A and B), the free energy f is determined from the expressions for $f_\mathrm{A}(n_i)$ and $f_\mathrm{B}(n_i)$ in the following way:

$$f = \frac{f_\mathrm{A} f_\mathrm{B}}{f_\mathrm{A} + f_\mathrm{B}} .$$

In the present work, it was assumed that $E_\mathrm{A} = E_\mathrm{B} = 10^9$ Pa.

Viscosity. It is assumed that the shear and volume viscosities of each phase are known. The viscosity of a mixture with arbitrary-density components is determined by empirical formulas that allow one to calculate the viscosity of the mixture by the known viscosities of its components:

$$\mu_\mathrm{s} = \left(c_\mathrm{A} \mu_\mathrm{sA}^{1/3} + c_\mathrm{B} \mu_\mathrm{sB}^{1/3} \right)^3 , \quad \mu_\mathrm{v} = \left(c_\mathrm{A} \mu_\mathrm{vA}^{1/3} + c_\mathrm{B} \mu_\mathrm{vB}^{1/3} \right)^3 ,$$

$$c_\mathrm{A} = \frac{z_\mathrm{B}}{z_\mathrm{A} + z_\mathrm{B}} , \quad c_\mathrm{B} = \frac{z_\mathrm{A}}{z_\mathrm{A} + z_\mathrm{B}} ,$$

$$z_\mathrm{A} = \left(\sum_{i=1}^{2} (n_i - n_{i\mathrm{A}})^2 \right)^{1/2} , \quad z_\mathrm{B} = \left(\sum_{i=1}^{2} (n_i - n_{i\mathrm{B}})^2 \right)^{1/2} .$$

It was assumed that $\mu_\mathrm{sA} = 10^{-3}$ Pa·sec, $\mu_\mathrm{vA} = 10^{-2}$ Pa·sec, and $\mu_\mathrm{vB} = \mu_\mathrm{sB} = 0$.

Diffusion. We will calculate the matrix D_{ij} from the relation for the concentration flow of the mixture components following from (25) at $\nu_{ij} = 0$:

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

where $n = \sum_{i=1}^{2} n_i$ is the total density, $c = \frac{n_1}{n}$ is the concentration of the first component, and $\kappa_i = f_{,i}$ is the chemical potential. Thus the table diffusion coefficient d of the first mixture component is related to the matrix D_{ij} by the relation

$$d = n^{-1} D_{1j} \left(\frac{\partial \kappa_j}{\partial c} \right)_n . \tag{28}$$

If the free energy f is prescribed for a two-component mixture, the matrix D_{ij} can be uniquely determined by the coefficient d defined by Eq. (28) on condition (26). The diffusion matrix of the mixture is calculated by the known values of the diffusion matrix for the phases $D_{ij\mathrm{A}}$ and $D_{ij\mathrm{B}}$: $D_{ij} = c_\mathrm{A} D_{ij} + c_\mathrm{B} D_{ij\mathrm{B}}$.

The following values of the parameters being considered were used.

The diffusion coefficient of the second component in the phase A is equal to 10^{-4} m^2·sec^{-1} and this coefficient of the first component in the phase B is 10^{-10} m^2·sec^{-1}.

The surface tension at the mixture–solid wall interface is equal to zero: $\theta = 0$.

The matrix coefficients ν_{ij} are constants proportional to the unit-matrix coefficients: $\nu_{ij} = \nu\delta_{ij}$. The unknown coefficient ν is determined from the expression for the surface tension coefficient (8) of the interface between the phases A and B in the case of static solution of the problem; it is equal to $\gamma = 0.05$ N/m.

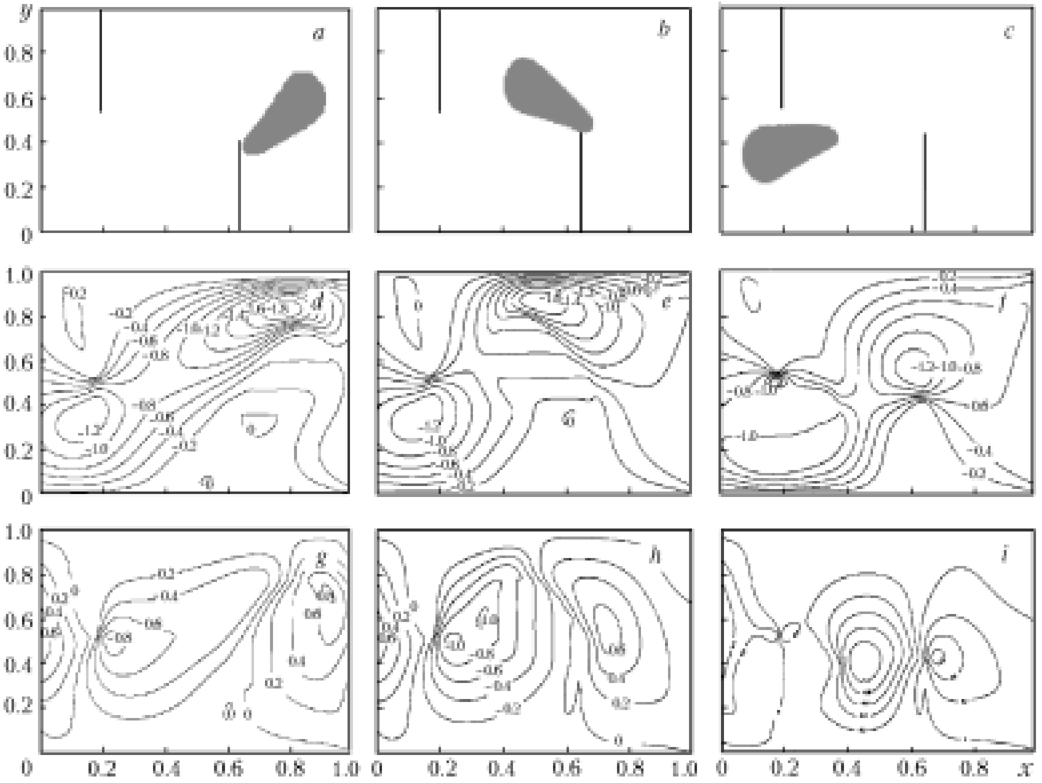

Fig. 1. Concentration fields of the solid component (a–c), the longitudinal velocity v_1 (d–f), and the transverse velocity v_2 (g–i) at the instant of time $t = 0.041$ sec (a, d, g), 0.074 sec (b, e, f), and 0.135 sec (c, f, i). v_1, v_2, m/sec; x, y, m.

The Lamé coefficients are calculated by the formulas $\lambda = \lambda_0 c_B^2$ and $\mu = \mu_0 c_B^2$, where $\lambda_0 = \mu_0 = 10^6$ Pa. It should be noted that, since the coefficient μ has a relatively small value, shear deformations of the phase B took place in the calculations.

The other parameters of the model had the following values: $\rho_1 = 1000$ kg/m^3, $\rho_2 = 1500$ kg/m^3, $m_1 = 18$ kg/mole, and $m_2 = 50$ kg/mole.

In both problems, the motion of a solid body, formed by the phase B, in a flow of a viscous fluid representing the phase A was considered. In the first problem, the solid phase does not experience phase transformations, and, in the second problem, this phase is subjected to such transformations (it is dissolved). A mixture flows in a channel containing two immobile partitions serving as the guides for the mixture flow. The upper and lower walls of the channel are impenetrable. At these walls and at the partitions, the boundary conditions (16)–(18) are fulfilled. The fluid consisting of the pure first component flows into the channel with a velocity $u_0 = -0.55$ m/sec on its right side, and, on the left side of the channel, the mixture is removed with a rate necessary for the retention of a medium pressure in the channel. The computational region is approximated with the use of 200 × 100 square cells with sides of length $5 \cdot 10^{-4}$ m. An explicit computational scheme of the second order of accuracy with nodes positioned in staggered rows [11] is used. At the initial instant of time, a part of the computational region is occupied by the first component (fluid), and the other part, representing the initial position of the solid body, is occupied by the second component. The initial velocity of the flow is equal to zero.

Problem 1. *Flow of a mixture with a moving solid phase with no change of phase.* It is assumed that the liquid phase A contains 100 percent of the first component and the solid phase B contains 100 percent of the second component.

Figure 1 shows the computational-grid cells (Fig. 1a–c) occupied by the solid phase and the isolines of the fields of the longitudinal v_1 (Fig. 1d–f) and transverse v_2 (Fig. 1g–i) velocity components at different successive instants of time. The straight lines in Fig. 1a–c denote the impenetrable partitions. As is seen from the figures, the solid body moves along the curvilinear trajectory, bends around the partitions and, in doing so, conserves its initial

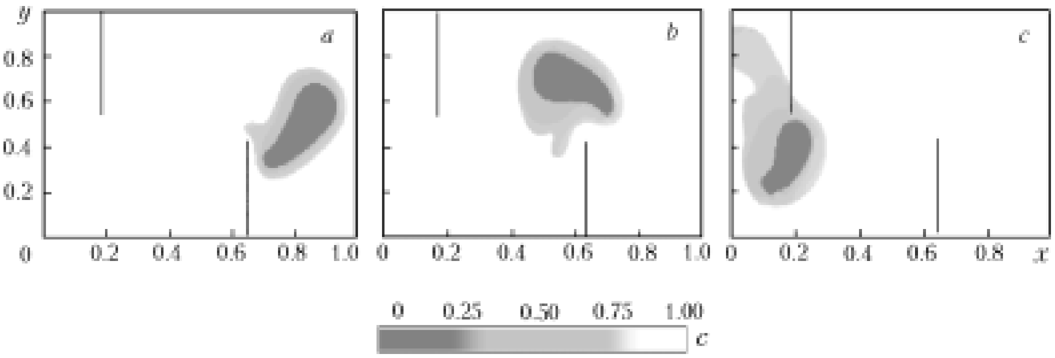

Fig. 2. Concentration fields of the solid component in problem 2 at the instant of time $t = 0.057$ (a), 0.093 (b), and 0.219 sec (c). x, y, m.

shape. The fluid motion is coordinated with the solid motion: the velocity field is continuous. Moreover, the isolines of the longitudinal velocity inside the body are always parallel to the horizontal walls of the channel, and the transverse-velocity isolines are always perpendicular to them, which is characteristic of the motion of solid bodies. In accordance with the boundary conditions (16), both velocity components are equal to zero at the upper and lower sides of the model.

Problem 2. *Flow of a mixture with a moving solid phase experiencing phase transformations.* It is assumed that the phase A in equilibrium contains 90 percent of the first component and the solid phase B contains 100 percent of the second component. Since the liquid phase in the initial state is insufficiently saturated, the solid body is dissolved. In Fig. 2, the concentration fields of the second component at three successive instants of time are shown by the grey-colored gradations. In this case, once the solid body begins to move, it is dissolved and its shape is changed. At the instant of time $t = 0.219$ sec, only about one-half its initial volume is remained. It should be noted that the trajectories of the solid body in this problem and in the previous one are different. This is explained by the fact that all the fields calculated are interdependent and the change in the concentration field leads in the end to a change in the velocity field determining the trajectory of the body. It should be also noted that the rapid dissolution of the body is due to the large diffusion coefficient, characteristic of dense gases, used for the liquid phase.

Conclusions. The results of our numerical simulation show that viscous flows containing solid bodies can be adequately described using equations of the density-functional theory. These equations allow one to perform a unified description of the solid and liquid phases without formulation of the conditions of contact at the liquid–solid body interface. Moreover, one and the same system of equations is used for description of flows with change of phase and flows with no such a change.

In the present work, only the isothermic flows were considered. However, the theory can be extended to the nonisothermic case as was done earlier for the gas-liquid mixtures [2, 7].

NOTATION

c, concentration of the first component; c_A, c_B, subsidiary variables; D, space region; d, diffusion coefficient of the first component, m^2/sec; d_A, surface element, m^2; ∂D, boundary of a space region; dV, volume element, m^3; D_{ij}, $D_{ij\mathrm{A}}$, and $D_{ij\mathrm{B}}$, matrices of the diffusion coefficients of the mixture and the phases A and B, respectively, sec·mole^2/(m^3·kg); E, total energy of the mixture, J; E_A and E_B, modulus of dilatation of the phases A and B, respectively, Pa; F, total free energy of the mixture, J; f, free energy of the homogeneous mixture per unit volume, Pa; f_A and f_B, total free energy of the phases A and B respectively, Pa; $f_{0\mathrm{A}}$, $f_{i\mathrm{A}}$, and $f_{ij\mathrm{A}}$, coefficients of the zero-, first-, and second-power square polynomials of the phase free energy, Pa, kg·m^2/(sec·mole) and kg·m^5/(sec·mole); F_el, contribution of the energy of the solid-phase elastic deformations to the free energy, J; F_fl, free energy of the gas-liquid mixture, J; g, arbitrary subsidiary function; g_{ab}, metric tensor; l_a, internal normal to the surface; m_i, molar mass of the ith component, kg/mole; n, total molar density of the mixture, mole/m^3; n_i, molar density of the ith component, mole/m^3; $n_{i\mathrm{A}}$, $n_{i\mathrm{B}}$, nondisturbed molar density of the ith component of the phases A and B respectively, mole/m^3; p, pressure, Pa; p_{ab}, stress tensor of the mixture, Pa; Q_{ia}, diffusion-flow vector of the ith component, mole/(sec·m^2); t, time, sec; u_0, velocity of the first-component flow, m/sec; u_a, displacement of a particle of the medium along the Cartesian coordinate x_a relative to its initial position, m; v, mean-mass velocity, m/sec; x, y, Cartesian coordinates, m; z_A, z_B, subsidiary variables, mole/m^3; γ, coefficient of interphase surface tension, N/m; δ_{ab}, unit matrix; ε_{ab}, deformation tensor; θ, surface tension at the interface between the mixture and the immovable ambient solid phase, Pa·m; κ_i, chemical potential of the ith component, kg·m^2/(sec·mole); λ and μ, first and second Lame coefficients of the mixture, Pa; λ_0 and μ_0, first and second Lamé coefficients of the solid phase, Pa; μ_s, shear-viscosity coefficient, Pa·sec; μ_{vA} and μ_{vB}, volume-viscosity coefficients; μ_{sA} and μ_{sB}, shear-viscosity coefficients of the phases A and B respectively, Pa·sec; μ_v, volume-viscosity coefficient of the phases A and B respectively, Pa·sec; ν_{ij}, coefficients of the symmetric positive-definite matrix, kg·m^7/(sec^2·mole^2); ρ, mass density of the mixture, kg/m^3; ρ_0,mass density of the mixture in the initial state, kg/m^3; Σ, subsidiary function, Pa/sec; σ_{ab}, static-stress tensor of the mixture, Pa; τ_{ab}, viscous-stress tensor of the mixture, Pa; τ_r, relaxation time, sec; φ, gravitational potential; m^2/sec^2; Φ_i and Φ_{i*}, generalized chemical potentials of the ith component of the mixture in the bulk and at the surface, kg·m^2/(sec·mole) and kg·m^3/(sec·mole); χ_{ab}, subsidiary tensor, Pa; ω_{el}, contribution of the elastic-deformation energy of the solid phase to the free energy per unit volume, Pa; ω_{fl}, free energy of the gas-liquid mixture per unit volume, Pa. Subscripts: el, elastic; fl, gas-liquid mixture; r, relaxation; v, volume; s, shear; a, b, c, for Cartesian coordinates; i, j, k, for mixture components.

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