

MODEL OF THE MOTION OF A TWO-COMPONENT LIQUID WITH ALLOWANCE OF CAPILLARY FORCES

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In this study we consider the familiar mathematical hydrodynamics problem of determining the motion of two immiscible viscous liquids, with surface tension at their interface. In the classical formulation the existence of surface tension means that the condition [1-3]

$$[P \cdot n] = \sigma kn,$$

is satisfied at the interface Γ ; here, P is the stress tensor; n is the vector of the normal to Γ ; k is the average curvature of the surface Γ ; σ is a constant; and $[\cdot]$ denotes a jump in the function as it passes through Γ .

The solvability of the given problem has been proved only "in the small," i.e., either for a fairly small interval of time or in the neighborhood of the exact solution. In view of this, the use of the classical formulation in numerical simulation can lead to misunderstandings. It makes sense to look for formulations that would be close to the classical from the mechanical, and possibly the mathematical, point of view and would admit a solution "as a whole." This is the goal of our study.

The model proposed takes into account the interdiffusion of the liquids as well as the effect of the surface tension, even though the interface "becomes softer."

1. Derivation of the model. Suppose that a volume Ω contains two incompressible liquids. For simplicity we set the density of both liquids equal to unity. The distribution of the components of the mixture in the volume will be defined by giving their concentrations. Suppose that φ is the concentration of one of the liquids. Following [4, 5], we define the free-energy density as

$$f = f(T, \varphi, \nabla\varphi) = w(T, \varphi) + \frac{\alpha}{2} |\nabla\varphi|^2. \quad (1.1)$$

Here T is the temperature; $w(T, \varphi)$ is the free-energy density of a homogeneous liquid; and α is a positive constant.

We assume that the process is isothermal and so T acts as a parameter. Nevertheless, it is important to choose a value of T . The point is that in real solutions w is a convex function in φ if the temperature is higher than a critical value T_c . If $T < T_c$ part of the function is nonconvex [5-7]. The diffusion coefficient is negative for concentrations from that part and so-called ascending diffusion occurs, with the components of the mixture tending to separate.

The term $\alpha/2 |\nabla\varphi|^2$ introduces a surface tension of sorts into the system. Suppose that a particle of liquid occupies a region $V_1 = \{0 \leq x_k \leq 1, k = 1, 2, 3\}$ and that the concentration φ depends only on x_1 , i.e., the vector $\nabla\varphi$ is directed along the x_1 axis. We stretch the particle twofold along the x_2 axis, keeping its volume constant. Suppose that

$$F_i = \int_{V_i} f dx_1 dx_2 dx_3 \quad (i = 1, 2)$$

is the free energy of the liquid before and after deformation and $V_2 = \{0 \leq x_1 \leq 1/2, 0 \leq x_2 \leq 2, 0 \leq x_3 \leq 1\}$ is the region occupied by the liquid after deformation. Then

$$F_1 = \int_{V_1} \left(w(\varphi(x)) + \frac{\alpha}{2} |\nabla_x \varphi|^2 \right) dx_1 dx_2 dx_3 = \int_0^{1/2} \int_0^2 \int_0^1 \left(w(\varphi(y)) + \frac{\alpha}{8} |\nabla_y \varphi|^2 \right) dy_1 dy_2 dy_3,$$

$$F_2 = \int_0^2 \int_0^2 \int_0^1 \left((\varphi(y)) + \frac{\alpha}{2} |\nabla_y \varphi|^2 \right) dy_1 dy_2 dy_3.$$

We see that $F_2 > F_1$, i.e., the free energy increases as the particle is stretched along the concentration isolines and the system should "resist" this.

Let us proceed to describe the model. Within the framework of the one-velocity treatment φ should satisfy the equation

$$\frac{\partial \varphi}{\partial t} + \mathbf{v} \cdot \nabla \varphi = \operatorname{div} \mathbf{j}, \quad (1.2)$$

where \mathbf{v} is the velocity of the macroscopic motion of the liquid; and \mathbf{j} is the vector of the diffusion flow. According to the Cahn–Hillar theory [5-7], the diffusion flow is proportional to the gradient of the generalized chemical potential θ ,

$$\mathbf{j} = \beta \nabla \theta, \quad (1.3)$$

which in turn is a functional derivative of the free energy:

$$\theta = -\alpha \Delta \varphi + w'(\varphi) \quad (1.4)$$

(the prime denotes the derivative with respect to the argument).

The incompressibility condition for the liquid presumes that

$$\operatorname{div} \mathbf{v} = 0. \quad (1.5)$$

Finally, the momentum equation is written in the standard way:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = \operatorname{div} P + \mathbf{g}. \quad (1.6)$$

Here \mathbf{g} is the vector of the external mass force.

The form of the stress tensor still has to be taken into account. We do this by the virtual power method. First we assume that there are no viscous forces. Suppose that ω is an arbitrary volume of the liquid, $\mathbf{u}(\mathbf{x})$ is a vector field in ω (field of virtual velocity) such that $\operatorname{div} \mathbf{u} = 0$, $\mathbf{u}|_{\partial\omega} = 0$. Then for rather small $t > 0$ the mapping $\mathbf{h}_t(\mathbf{x}) = \mathbf{x} + \mathbf{t}\mathbf{u}(\mathbf{x})$ gives an internal strain of a liquid particle ω . The power of the stresses causing that strain, at $t = 0$, can be calculated in two ways:

$$N(\mathbf{u}) = - \int_{\omega} P_0 : D(\mathbf{u}) d\mathbf{x}$$

(P_0 is stress tensor without viscosity, $D(\mathbf{u})$ is the strain-rate tensor with the components $D_{ij}(\mathbf{u}) = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$);

$$\begin{aligned} N(\mathbf{u}) &= \frac{d}{dt} \int_{\omega} \left(w(\varphi(\mathbf{h}_t(\mathbf{x}))) + \frac{\alpha}{2} |\nabla(\varphi(\mathbf{h}_t(\mathbf{x})))|^2 \right) d\mathbf{x} \Big|_{t=0} \\ &= \int_{\omega} (w'(\varphi) \nabla \varphi \cdot \mathbf{u} + \alpha \nabla \varphi \cdot \nabla(\nabla \varphi \cdot \mathbf{u})) d\mathbf{x} = \int_{\omega} \alpha (\nabla \varphi \otimes \nabla \varphi) : D(\mathbf{u}) d\mathbf{x}. \end{aligned}$$

Since the function \mathbf{u} is arbitrary, when we equate the two expressions for the power we obtain

$$\operatorname{div} P_0 = \operatorname{div} (-\alpha (\nabla \varphi \otimes \nabla \varphi) + S)$$

(S is an arbitrary spherical tensor, which arises because $\operatorname{div} \mathbf{u} = 0$). It is convenient to take $S = -p\mathbf{I} + \alpha |\nabla \varphi|^2 \mathbf{I}$, where \mathbf{I} is a unit tensor and p is the pressure. Since only the divergence of the stress tensor appears in Eq. (1.6), we can assume that

$$P_0 = -\alpha (\nabla \varphi \otimes \nabla \varphi) + S.$$

Adding the viscous stress to P_0 , we obtain

$$P = -pI + 2\mu D(v) + \alpha(|\nabla\varphi|^2 I - \nabla\varphi \otimes \nabla\varphi) \quad (1.7)$$

(μ is the viscosity).

The last term in (1.7) is the operator of projection onto the tangential plane to the surface of the level of the function φ . This term is responsible for the surface tension.

Equations (1.2)-(1.7) form a closed model. As for the function w , its dependence on φ is determined by the properties of the specific medium chosen. It is convenient to assume henceforth that φ is not the concentration but a phase function, which depends linearly on the concentration and is equal to -1 if the concentration is zero and 1 if the concentration is equal to 1 . The form of the equations does not change. We consider the system at a below-critical temperature, i.e., when $w(\varphi)$ is a nonconvex function. The motivation for this choice is given below. For definiteness we assume that

$$w(\varphi) = \gamma^{-1}W(\varphi) = \gamma^{-1}(\varphi^2 - 1)^2, \quad (1.8)$$

where γ is a constant that characterizes the miscibility of the two liquids. If the free energy F of the liquid in the volume Ω is limited by the constant C , then

$$\gamma^{-1} \int_{\Omega} W(\varphi) dx \leq C.$$

Hence it follows that the measure of the set $D_k = \{x \in \Omega: W(\varphi(x)) > k\}$ is evaluated as

$$\text{mes}D_k \leq C\gamma/k$$

for any constant $k > 0$. We see that $\text{mes}D_k \rightarrow 0$ as $\gamma \rightarrow 0$, i.e., the measure of the set where $|\varphi| \neq 1$ tends to zero as $\gamma \rightarrow 0$. For near-zero values of γ , therefore, the liquids virtually do not mix. Accordingly, since we want to construct a model that gives an approximate description of the motion of immiscible liquids, the choice of the function w in the form (1.8) is justified.

Remark. Generally speaking, W is defined only on the segment $[-1, 1]$. It can be assumed to be equal to $+\infty$ outside that segment. This complicates matters somewhat because of the differentiation of the function. We assume that W has the form (1.8) on the entire number axis. This is not a very big assumption if γ is sufficiently small.

Models similar to the one proposed here have already been studied for describing pure diffusion without transfer [7] and for describing phase transitions [8-11].

2. Let us carry out a formal asymptotic analysis of the proposed model. We write the system (1.2)-(1.8) in dimensionless variables. Characteristic scales of length and velocity, l and V , are assumed to exist in the motion under study. We introduce new independent variables

$$x' = l^{-1}x, \quad t' = l^{-1}Vt$$

and new unknown functions

$$v' = V^{-1}v, \quad p' = l(V\mu)^{-1}p, \quad \theta' = l(V\mu)^{-1}\theta.$$

Then the equations become

$$\begin{aligned} \text{Re} \left(\frac{\partial v'}{\partial t'} + (v' \cdot \nabla') v' \right) &= -\nabla' p' + \Delta' v' + A \text{div}(|\nabla\varphi|^2 I - \nabla\varphi \otimes \nabla\varphi) + g, \\ \text{div} v' &= 0, \quad \frac{\partial \varphi}{\partial t'} + (v' \cdot \nabla') \varphi = B \Delta' \theta', \\ -A \Delta' \varphi + C^{-1} W'(\varphi) - \theta' &= 0, \end{aligned}$$

where $Re = \nu\mu^{-1}$; $A = \alpha(I\nu\mu)^{-1}$; $B = \beta\mu\Gamma^{-1}$; $C = \gamma\nu\mu\Gamma^{-1}$.

Suppose that ε is a positive small parameter. Setting $Re = 1$, $A = B = \varepsilon$, $C = c\varepsilon$ (c is a constant), we rewrite the system as

$$\begin{aligned} \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v} &= \operatorname{div}T + \varepsilon \operatorname{div}(|\nabla\varphi|^2 I - \nabla\varphi \otimes \nabla\varphi) + \mathbf{g}, \\ T &= -pI + 2D, \operatorname{div}v = 0, \frac{\partial\varphi}{\partial t} + \mathbf{v} \cdot \nabla\varphi = \varepsilon\Delta\theta, \\ -\varepsilon\Delta\varphi + \frac{c}{\varepsilon}W'(\varphi) - \theta &= 0. \end{aligned} \quad (2.1)$$

We assume that a solution of this problem exists and that all functions that form that solution are differentiable the required number of times.

Let us consider the case of two spatial variables, since the dimensionality is of no particular consequence.

We define the curve $\Gamma(t) = \{(x, y): \varphi(x, y, t) = 0\}$ (x, y are the Cartesian coordinates in the plane). We assume that $\Gamma(t)$ is sufficiently smooth. In the neighborhood of the curve $\Gamma(t)$ we can define the function

$$r(x, y, t) = \operatorname{signdist}((x, y), \Gamma(t)),$$

i.e., r is the distance from a point to $\Gamma(t)$, taken with the minus sign on one side of Γ and a plus sign on the other side. Then $|\nabla r| = 1$, $\Delta r = k$ (k is the mean curvature of the level line of the function r).

We represent all of the functions in the model as power-series expansions of ε , using different expansion inside and outside a neighborhood of the curve $\Gamma(t)$ and then glue them together.

The external expansions have the form

$$\begin{aligned} \varphi(x, y, t, \varepsilon) &= \varphi_0(x, y, t) + \varepsilon\varphi_1(x, y, t) + \varepsilon^2 \dots, \\ \theta(x, y, t, \varepsilon) &= \theta_0(x, y, t) + \varepsilon\theta_1(x, y, t) + \varepsilon^2 \dots, \\ \mathbf{v}(x, y, t, \varepsilon) &= \mathbf{v}_0(x, y, t) + \varepsilon\mathbf{v}_1(x, y, t) + \varepsilon^2 \dots, \\ T(x, y, t, \varepsilon) &= T_0(x, y, t) + \varepsilon T_1(x, y, t) + \varepsilon^2 \dots, \\ p(x, y, t, \varepsilon) &= p_0(x, y, t) + \varepsilon p_1(x, y, t) + \varepsilon^2 \dots \end{aligned} \quad (2.2)$$

The internal expansions. Into the neighborhood of $\Gamma(t)$ we introduce the local coordinates (r, s) , where s is the arc length measured along $\Gamma(t)$ from a fixed point. We stretch this neighborhood, replacing r with a new coordinate $\rho = r/\varepsilon$. Then

$$\begin{aligned} \varphi(x, y, t, \varepsilon) &= \Phi(\rho, s, t, \varepsilon) = \Phi_0 + \varepsilon\Phi_1 + \varepsilon^2 \dots, \\ \theta(x, y, t, \varepsilon) &= \Xi(\rho, s, t, \varepsilon) = \Xi_0 + \varepsilon\Xi_1 + \varepsilon^2 \dots, \\ \mathbf{v}(x, y, t, \varepsilon) &= \mathbf{V}(\rho, s, t, \varepsilon) = \mathbf{V}_0 + \varepsilon\mathbf{V}_1 + \varepsilon^2 \dots, \\ T(x, y, t, \varepsilon) &= \Lambda(\rho, s, t, \varepsilon) = \Lambda_0 + \varepsilon\Lambda_1 + \varepsilon^2 \dots, \\ p(x, y, t, \varepsilon) &= \Psi(\rho, s, t, \varepsilon) = \Psi_0 + \varepsilon\Psi_1 + \varepsilon^2 \dots \end{aligned} \quad (2.3)$$

Substituting the expansions (2.2) into the system (2.1) and separating the terms of order $O(1)$, we obtain

$$\frac{\partial\varphi_0}{\partial t} + \mathbf{v}_0 \cdot \nabla\varphi_0 = 0; \quad (2.4a)$$

$$W'(\varphi_0) = 0; \quad (2.4b)$$

$$\frac{\partial\mathbf{v}_0}{\partial t} + (\mathbf{v}_0 \cdot \nabla)\mathbf{v}_0 = \operatorname{div}T_0 + \mathbf{g}; \quad (2.4c)$$

$$\operatorname{div}\mathbf{v}_0 = 0; \quad (2.4d)$$

$$T_0 = -p_0I + 2D_0. \quad (2.4e)$$

Here

$$D_{0,j} = \frac{1}{2} \left(\frac{\partial u_{0j}}{\partial x_j} + \frac{\partial u_{0j}}{\partial x_j} \right).$$

It follows from (2.4b) that φ_0 can assume the values ± 1 and 0 . But $\varphi_0 \neq 0$ since if $\varphi_0 = 0$ at some point, then that point belongs to $\Gamma(t)$ and the expansions (2.2) were calculated outside the neighborhood of $\Gamma(t)$.

Let us now consider the internal expansions. We write (2.1) in the neighborhood of $\Gamma(t)$ in local coordinates:

$$\begin{aligned} & \varepsilon \mathbf{V}_t + \mathbf{V}_\rho(r_t + \mathbf{V} \cdot \nabla r) + \varepsilon \mathbf{V}_s(s_t + \mathbf{V} \cdot \nabla s) \\ & = \Lambda_\rho \nabla r + \varepsilon \Lambda_s \nabla s - \Phi_\rho^2 \operatorname{div}(\nabla r \otimes \nabla r) \\ & - \varepsilon \Phi_\rho \Phi_s \operatorname{div}(\nabla r \otimes \nabla s + \nabla s \otimes \nabla r) - (\Phi_\rho \Phi_s)_\rho \nabla s \\ & - \varepsilon (\Phi_\rho \Phi_s)_s \nabla r - \varepsilon^2 \Phi_s^2 \operatorname{div}(\nabla s \otimes \nabla s) \\ & - \varepsilon^2 (\Phi_s^2)_s |\nabla s|^2 \nabla s + (\Phi_\rho^2)_s \nabla s \\ & + \varepsilon (\Phi_s^2)_\rho |\nabla s|^2 \nabla r + (\Phi_s^2)_\rho |\nabla s|^2 \nabla s + \varepsilon \mathbf{g}; \end{aligned} \quad (2.5)$$

$$\varepsilon^2 \Phi_t + \varepsilon \Phi_\rho(r_t + \mathbf{V} \cdot \nabla r) + \varepsilon^2 \Phi_s(s_t + \mathbf{V} \cdot \nabla s) = \Xi_{\rho\rho} + \varepsilon \Xi_\rho \nabla r + \varepsilon^2 |\nabla s|^2 \Xi_s + \varepsilon^2 \Delta s \Xi_s; \quad (2.6)$$

$$-\varepsilon \Xi = \Phi_{\rho\rho} + \varepsilon \Delta r \Phi_\rho + \varepsilon^2 |\nabla s|^2 \Phi_s + \varepsilon^2 \Delta s \Phi_s - cW'(\Phi); \quad (2.7)$$

$$\varepsilon \Lambda = -\varepsilon \Psi I + 2(\mathbf{V}_\rho \otimes \nabla r + \nabla r \otimes \mathbf{V}_\rho) + 2\varepsilon(\mathbf{V}_s \otimes \nabla s + \nabla s \otimes \mathbf{V}_s). \quad (2.8)$$

We denote $\mathbf{u} = r_t$, $\mathbf{n} = \nabla r$, $\tau = \nabla s$, and $k = \Delta r$ and expand those functions in power series of r ,

$$\begin{aligned} u(r,s) &= u_0(s) + \varepsilon u_1(s)\rho + \varepsilon^2 \dots, \\ \mathbf{n}(r,s) &= \mathbf{n}_0(s) + \varepsilon \mathbf{n}_1(s)\rho + \varepsilon^2 \dots, \\ \tau(r,s) &= \tau_0(s) + \varepsilon \tau_1(s)\rho + \varepsilon^2 \dots, \\ k(r,s) &= k_0(s) + \varepsilon k_1(s)\rho + \varepsilon^2 \dots \end{aligned} \quad (2.9)$$

(u_0, \mathbf{n}_0, k_0 are the velocity in the direction of the normal, the normal, and the average curvature of the surface $r = 0$).

We substitute the expansions (2.3) and (2.9) into Eqs. (2.5)-(2.8) and retain terms of order $O(1)$:

$$\begin{aligned} \mathbf{V}_{\varphi_0}(u_0 + \mathbf{V}_0 \cdot \mathbf{n}_0) &= \Lambda_{\varphi_0} \cdot \mathbf{n}_0 - \Phi_{\varphi_0}^2 k_0 \mathbf{n}_0 - (\Phi_{\varphi_0} \Phi_{\varphi_0})_\rho \tau_0 + (\Phi_{\varphi_0}^2)_s \tau_0; \\ \Xi_{\varphi_0\rho} &= 0; \end{aligned} \quad (2.10)$$

$$\Phi_{\varphi_0\rho} - cW'(\Phi_0) = 0; \quad (2.11)$$

$$\mathbf{V}_{\varphi_0} \otimes \mathbf{n}_0 + \mathbf{n}_0 \otimes \mathbf{V}_{\varphi_0} = 0. \quad (2.12)$$

Here we have taken into account the fact that $\operatorname{div}(\nabla r \otimes \nabla r) = \Delta r \nabla r$, since $|\nabla r| = 1$.

From (2.12) it follows that

$$\mathbf{V}_{\varphi_0} = 0. \quad (2.13)$$

Now we use the condition for gluing the asymptotic expansions:

$$\Phi_0|_{\rho = \pm \infty} = \varphi_0(\Gamma_\pm); \quad (2.14a)$$

$$\Lambda_0|_{\rho = \pm \infty} = T_0(\Gamma_{\pm}); \quad (2.14b)$$

$$\mathbf{V}_0|_{\rho = \pm \infty} = \mathbf{v}_0(\Gamma_{\pm}) \quad (2.14c)$$

[$f(\Gamma_{\pm})$ denotes the trace of the function f on the surface Γ to the left and right]. From (2.4b) and (2.14a) we can conclude that

$$\Phi_0|_{\rho = \pm \infty} = \pm 1. \quad (2.15)$$

Solving Eq. (2.11) with the conditions at infinity (2.15), we obtain

$$\Phi_0 = \text{th}(\rho\sqrt{2c}). \quad (2.16)$$

Moreover, we find that Φ_0 does not depend on s ; this circumstance, along with (2.10) and (2.13), gives

$$\Lambda_{\varphi} \mathbf{n}_0 - \Phi_{\varphi}^2 k_0 \mathbf{n}_0 = 0.$$

Integrating this equation with respect to ρ for $-\infty$ to $+\infty$, we obtain

$$(\Lambda_0|_{\rho = +\infty} - \Lambda_0|_{\rho = -\infty}) \mathbf{n}_0 = \sigma k_0 \mathbf{n}_0,$$

where

$$\sigma = \int_{-\infty}^{+\infty} \Phi_{\varphi}^2 d\rho = 1/(3\sqrt{2c}).$$

Using (2.14b), from the last equation we have

$$(T_0(\Gamma_+) - T_0(\Gamma_-)) \mathbf{n}_0 = \sigma k_0 \mathbf{n}_0. \quad (2.17)$$

Here σ is the surface tension. It depends on the properties of the specific medium taken (in our case, on the form of the function w).

According to (2.13), \mathbf{V}_0 does not depend on ρ and so

$$\mathbf{V}_0|_{\rho = +\infty} - \mathbf{V}_0|_{\rho = -\infty} = 0,$$

and, as follows from (2.14c),

$$\mathbf{v}_0(\Gamma_+) - \mathbf{v}_0(\Gamma_-) = 0. \quad (2.18)$$

At the interface Γ the system of equations (2.4), along with the conditions (2.17) and (2.18), gives the classical formulation of the problem of the motion of two immiscible liquids, separated by a surface having surface tension.

Our asymptotic analysis shows that the classical formulation of the problem is a zeroth approximation of the model (2.1). The discussions of this point are in no way rigorous, but they do give reason to hope that the model (2.1) can be used with sufficient accuracy in practical problems.

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