

Flows of two slightly miscible fluids in porous media: two scale numerical modelling

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Abstract

We address the two-scale homogenization of the Navier-Stokes and Cahn-Hilliard equations in the case of a weak miscibility of a two-component fluid. To this end a notion of the miscibility strength is formulated on the basis of a correlation between the upscaling parameter and the surface tension. As a result, a two-scale model is derived. Macro-equations turn out to be a generalization of the Darcy law enjoying cross-coupling permeability tensors. It implies that the Darcy velocity of each phase depends on pressure gradients of both the phases. Micro-equations serve for determination both of the permeability tensors and the capillary pressure. An example is constructed by analytical tools to describe capillary displacement of oil by mixture of water with Carbon dioxide in a system of hydrophobic parallel channels.

Keywords: Multicomponent multiphase fluids, Phase field model, Two-scale homogenization, Cross-coupling permeability

1 Introduction

A number of laboratory experiments and related digital 3D core processing demonstrate the reliability of the application of mathematical models of multiphase flows based on the concept of a phase field, the Navier-Stokes and Cahn-Hilliard equations [1]. However, predicting flows in large volumes of a porous medium faces computational difficulties due to the multiplicity and complexity of microchannels. Therefore, the development of methods for averaging the Navier-Stokes and Cahn-Hilliard equations is an urgent task. As regards averaging the flow equations in a heterogeneous medium, the most well-known approach is the two-scale homogenization method [2]. It is natural to use such a method when there is a scale separation between the processes occurring at the scale of pores and at the scale, for example, of the wellbore zone. The Darcy law was derived from the Navier-Stokes flow equations in [3]. Attempts to perform two-scale homogenization of the Navier-Stokes and Cahn-Hilliard equations encounter the difficulty of decoupling micro and macro-equations [4]. However, it was proved in [5] that the decoupling of macro and micro equations is possible in the case of strong miscibility, when fluid phases are separated by a diffuse boundary of finite width, independent of the scale ratio. The goal of the present paper is to perform upscaling the Navier-Stokes and Cahn-Hilliard equations in the case of weak miscibility.

2 Basic equations

For equilibrium reversible processes of a two-component fluid, the thermodynamic Gibbs identity has the form [6]

$$dE = \theta dS + \mu_0 d\rho + \mu d(\rho c), \quad (1)$$

where E is the internal energy per unit volume, θ is the absolute temperature, S is the entropy per unit volume, ρ is the total density of the mixture, μ_0 is the chemical potential of the mixture, c is the mass concentration of the supplied component and μ is the chemical potential of this component. Since thermodynamic pressure is the derivative of energy with respect to volume, it follows from equation (1) that pressure satisfies the following representation formula [6]:

$$p = -E + \theta S + \mu_0 \rho + \mu \rho c. \quad (2)$$

The value $\varphi = \rho c$ has the meaning of the partial density of the second component, i.e. $\varphi = \bar{\rho}_2 \phi_2$, where $\bar{\rho}_i$ and ϕ_i are the true density and the volume concentration of the phase i . Due to equations (1) and (2), the chemical potential μ satisfies the equality

$$\mu = \frac{\partial f}{\partial \varphi}, \quad f = E + p - \theta S.$$

with f standing for the Gibbs free energy.

According to the Cahn-Hilliard theory, the chemical potential for dissipative processes in two-component mixtures is defined as the variational derivative $\mu = \delta f / \delta \varphi$ of the Ginzburg-Landau free energy

$$f = \gamma w(\varphi) + \frac{\alpha}{2} |\nabla \varphi|^2,$$

composed of a hydrophobic bulk component $\gamma w(\varphi)$ and a hydrophilic surface component $\alpha |\nabla \varphi|^2 / 2$. Hence,

$$\mu = \gamma w'(\varphi) - \alpha \Delta \varphi, \quad \text{where} \quad w'(\varphi) = \frac{dw}{d\varphi}. \quad (3)$$

The dimensional constants γ and α are inversely and directly proportional to the interfacial layer width. We consider the bulk free energy component as a double well potential [4]

$$\omega(\varphi) = \varphi_2^2 (1 - \varphi_2)^2 = \frac{\varphi^2 (\bar{\rho}_2 - \varphi)^2}{\bar{\rho}_2^4}. \quad (4)$$

Let η_i be the viscosity of the phase i . For the mixture, the density and viscosity are described by the linear approximations

$$\rho = \rho_1 + \rho_2 = \frac{\bar{\rho}_1 (\bar{\rho}_2 - \varphi) + \bar{\rho}_2 \varphi}{\bar{\rho}_2}, \quad \tilde{\eta} = \frac{\eta_1 (\bar{\rho}_2 - \varphi) + \eta_2 \varphi}{\bar{\rho}_2} \equiv \eta_1 \phi_1 + \eta_2 \phi_2.$$

The concentration satisfies the mass conservation law

$$\frac{\partial \varphi}{\partial t} + (\mathbf{v} \cdot \nabla) \varphi + \operatorname{div} \mathbf{j} = 0.$$

The concentration flux \mathbf{j} obeys Fick's law

$$\mathbf{j} = -\beta \nabla \mu,$$

where β is the mobility [6]. As for the velocity vector \mathbf{v} , it is governed by the Navier-Stokes equation

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + \operatorname{div} \tau + \rho \mathbf{g}.$$

Here \mathbf{g} is the acceleration due to gravity and τ is the dissipative part of the stress tensor:

$$\tau = 2\tilde{\eta} D^v + \alpha S, \quad S = \frac{1}{3} |\nabla \varphi|^2 \cdot I - \nabla \varphi \otimes \nabla \varphi, \quad (\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j. \quad (5)$$

The matrix D^v is the symmetric part of the velocity gradient $\nabla \mathbf{v}$, i.e. $2D^v = \nabla \mathbf{v} + (\nabla \mathbf{v})^*$. The representation formulas (5) were first proved in [7] (see also [5] for their

derivation). Observe that the parameter α in equation (5) is the same as in equation (3). If the fluid is incompressible i.e.

$$\operatorname{div} \mathbf{v} = 0,$$

the deviatoric part of the tensor τ is equal to zero due to the presence of the term with the identity matrix I in equation (5). This is important for the pressure to be determined correctly.

Let us pass to dimensionless variables

$$\mathbf{x}' = \frac{\mathbf{x}}{H}, \quad \mathbf{v}' = \frac{\mathbf{v}}{V}, \quad V = \frac{H}{T}, \quad p' = \frac{Hp}{V\eta_1}, \quad \mu' = \frac{\bar{\rho}_1 H \mu}{V\eta_1}, \quad \mathbf{j}' = \frac{\mathbf{j}}{\bar{\rho}_1 V}, \quad \varphi' = \frac{\varphi}{\bar{\rho}_2} \equiv \phi_2,$$

$$Re = \frac{\bar{\rho}_1 H V}{\eta_1}, \quad Fr = \frac{gH}{V^2}, \quad \Lambda = \frac{\alpha \bar{\rho}_2^2}{\eta_1 V H}, \quad B = \frac{\beta \eta_1}{\bar{\rho}_1^2 H^2}, \quad \Gamma = \frac{\gamma H \bar{\rho}_1}{\bar{\rho}_2 V \eta_1},$$

with H, V, T standing for the reference values. Thus, we arrive at the following model

$$\mu' = \Gamma \frac{dw(\varphi')}{d\varphi'} - \Lambda \Delta' \varphi', \quad \omega(\varphi') = \varphi'^2 (1 - \varphi')^2,$$

$$\mathbf{j}' = -B \nabla' \mu', \quad \frac{\rho}{\bar{\rho}_1} = \varphi' R + 1 - \varphi', \quad R = \bar{\rho}_2 / \bar{\rho}_1,$$

$$R \left(\frac{\partial \varphi'}{\partial t'} + (\mathbf{v}' \cdot \nabla') \varphi' \right) + \operatorname{div}' \mathbf{j}' = 0,$$

$$\frac{\rho}{\bar{\rho}_1} \operatorname{Re} \left(\frac{\partial \mathbf{v}'}{\partial t'} + (\mathbf{v}' \cdot \nabla') \mathbf{v}' \right) = -\nabla' p' + \operatorname{div}(2\eta(\varphi') D') - \frac{\rho}{\bar{\rho}_1} \operatorname{Fr} \cdot \operatorname{Re} \mathbf{e}_z +$$

$$\Lambda \operatorname{div}' \left(\frac{1}{3} |\nabla' \varphi'|^2 \cdot I - \nabla' \varphi' \otimes \nabla' \varphi' \right), \quad \eta(\varphi') = \varphi' \eta_2 / \eta_1 + 1 - \varphi',$$

$$\operatorname{div}' \mathbf{v}' = 0,$$

where $\mathbf{e}_z = \mathbf{e}_3$ is a unit vector directed against gravity. We note that φ' has the meaning of the volume fraction of the phase 2 i.e. $\varphi' = \phi_2$.

If we omit the primes and make the assumption that the Reynolds number is small, then the equations take the form

$$\mu = \Gamma w'(\varphi) - \Lambda \Delta \varphi, \tag{6}$$

$$\mathbf{j} = -B \nabla \mu, \tag{7}$$

$$R \left(\frac{\partial \varphi}{\partial t} + (\mathbf{v} \cdot \nabla) \varphi \right) + \operatorname{div} \mathbf{j} = 0, \tag{8}$$

$$0 = -\nabla p + 2 \operatorname{div}(\eta(\varphi) D) + \Lambda \operatorname{div} \left(\frac{1}{3} |\nabla \varphi|^2 \cdot I - \nabla \varphi \otimes \nabla \varphi \right), \tag{9}$$

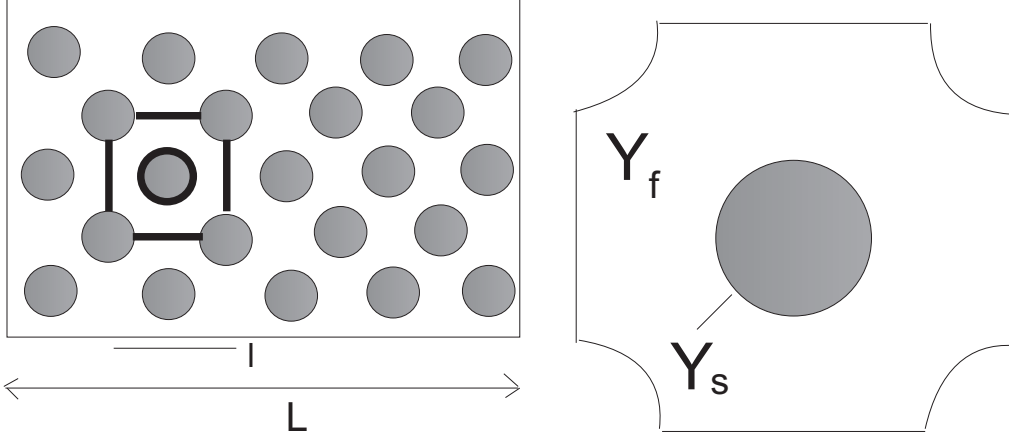


Fig. 1 $\varepsilon = l/L$. (a) The dimensionless domain Ω consists of fluid (white) and solid (grey) subdomains Ω_f^ε and Ω_s^ε . (b) Fluid domain Y_f .

$$\operatorname{div} \mathbf{v} = 0. \quad (10)$$

From the point of view of mathematical correctness, suitable boundary conditions on impenetrable boundaries are the following:

$$\mathbf{v} = 0, \quad \frac{\partial \varphi}{\partial n} = 0, \quad \mu = 0 \quad \left(\text{or } \frac{\partial \mu}{\partial n} = 0 \right). \quad (11)$$

The condition $\partial \varphi / \partial n = 0$ corresponds to a wetting angle of 90 degrees.

3 Miscibility

Here we give a mathematical definition of the miscibility strength. We consider flows in a perforated domain Ω_f^ε enjoying a periodical structure, Fig. 1(a). Given the unit cube $Y = (0, 1)^n$, $n = 2, 3$, we describe such a structure as follows. The periodicity cell Y consists of the fluid and solid domains Y_f and Y_s , Fig. 1(b). If Ω is an area in \mathbb{R}^n , then its perforated part $\Omega_f^\varepsilon = \cup_{z \in \mathbb{Z}^n} \varepsilon(Y_f + z) \cap \Omega$ is a fluid domain, where $Y_f + z$ is the shift of the region Y_f by the vector z and $\varepsilon(Y_f + z)$ is its contraction by a factor of ε . The parameter ε is the ratio of the size l of the periodic cell εY to the size L of the region Ω , $\varepsilon = l/L$.

Let us discuss some properties of problem (6)-(11). First, we note that the following energy equality holds:

$$\frac{d}{dt} \int_{\Omega_f^\varepsilon} \frac{\Gamma w(\varphi)}{\Lambda} + \frac{|\nabla \varphi|^2}{2} dx + \int_{\Omega_f^\varepsilon} \frac{B|\nabla \mu|^2}{\Lambda R} + \frac{2\eta|\nabla \mathbf{v}|^2}{\Lambda} dx = 0. \quad (12)$$

Indeed, due to equation (8), one can write the derivative of energy as follows:

$$\frac{\Gamma}{\Lambda} \frac{d}{dt} \int_{\Omega_f^\varepsilon} w(\varphi) dx = \frac{\Gamma}{\Lambda} \int_{\Omega_f^\varepsilon} w'(\varphi) \varphi_t dx = -\frac{\Gamma}{\Lambda} \int_{\Omega_f^\varepsilon} w'(\varphi) (R^{-1} \operatorname{div} \mathbf{j} + \mathbf{v} \cdot \nabla \varphi) dx.$$

By equation (7), we conclude that

$$\frac{\Gamma}{\Lambda} \frac{d}{dt} \int_{\Omega_f^\varepsilon} w(\varphi) dx = \frac{\Gamma B}{R\Lambda} \int_{\Omega_f^\varepsilon} w'(\varphi) \Delta \mu dx - \frac{\Gamma}{\Lambda} \int_{\partial \Omega_f^\varepsilon} w \mathbf{v} \cdot \mathbf{n} d\sigma = \frac{\Gamma B}{R\Lambda} \int_{\Omega_f^\varepsilon} w'(\varphi) \Delta \mu dx. \quad (13)$$

On the other hand, if we multiply equation (8) by $\Delta \varphi$ and integrate by parts, we get the equality

$$\frac{d}{dt} \int_{\Omega_f^\varepsilon} \frac{|\nabla \varphi|^2}{2} dx + \int_{\Omega_f^\varepsilon} \frac{B|\nabla \mu|^2}{R\Lambda} dx = -\frac{\Gamma B}{R\Lambda} \int_{\Omega_f^\varepsilon} w'(\varphi) \Delta \mu dx + \int_{\Omega_f^\varepsilon} (\mathbf{v} \cdot \nabla \varphi) \Delta \varphi dx. \quad (14)$$

The last integral in the above formula can be written as

$$\int_{\Omega_f^\varepsilon} (\mathbf{v} \cdot \nabla \varphi) \Delta \varphi dx = - \int_{\Omega_f^\varepsilon} \frac{2\eta |\nabla \mathbf{v}|^2}{\Lambda} dx.$$

Summation of equalities (13) and (14) results in formula (12). Its consequence is the following inequality:

$$\int_{\Omega_f^\varepsilon} w(\varphi(x, t)) dx \leq \int_{\Omega_f^\varepsilon} w(\varphi_0) dx + \frac{\Lambda}{2\Gamma} \int_{\Omega_f^\varepsilon} \frac{|\nabla \varphi_0|^2}{2} dx, \quad \varphi_0(x) = \varphi|_{t=0}. \quad (15)$$

In view of (4), the equality

$$\int_{\Omega_f^\varepsilon} w(\varphi(x, t)) dx = 0$$

is possible only in the absence of miscibility, i.e. when φ is either 0 or 1. Therefore, the condition for the initial concentration

$$\int_{\Omega_f^\varepsilon} w(\varphi_0(x)) dx \leq \delta, \quad \varphi_0 = \varphi|_{t=0} \quad (16)$$

implies weak initial miscibility provided δ is small. Given a constant c_0 , we restrict ourselves to the following class of initial data:

$$\int_{\Omega_f^\varepsilon} |\nabla \varphi_0|^2 dx \leq c_0. \quad (17)$$

It follows from (15)–(17) that

$$\int_{\Omega_f^\varepsilon} w(\varphi(x, t)) dx \leq 2\delta \quad (18)$$

provide the ratio Λ/Γ is small enough. Thus, small values of Λ/Γ insure weak miscibility.

Let ε_0 be the dimensionless interface thickness. In a number of papers [8] it is assumed that $\Gamma \sim 1/\varepsilon_0$ and $\Lambda \sim \varepsilon_0$. Therefore $\Lambda/\Gamma \sim \varepsilon_0^2$. The introduced mathematical criterion of weak miscibility (18) is consistent with the condition of small interface thickness.

4 Two-scale homogenization

The case of strong miscibility was considered in [5]. Here we are interested in weak miscibility. Let us return to the dimensional parameters γ and α . In a number of papers [8] it is assumed that

$$\gamma = \gamma_0 \sigma / \delta, \quad \alpha = \alpha_0 \sigma \delta,$$

where $\alpha_0[\text{cm}^6 \cdot \text{g}^{-2} \cdot \text{c}^{-1}]$ and $\gamma_0[\text{c}^{-1}]$ are dimensional multipliers, $\sigma[\text{g}/\text{c}]$ is the surface tension, $\delta[\text{cm}]$ is the interface thickness. Let us assume that the surface tension and interface thickness are related to the homogenization parameter ε as follows:

$$\sigma = \tilde{\sigma} \varepsilon, \quad \delta = \tilde{\delta} \varepsilon \implies \gamma = \gamma_0 \tilde{\sigma} / \tilde{\delta}, \quad \alpha = \tilde{\alpha} \varepsilon^2, \quad \tilde{\alpha} = \alpha_0 \tilde{\sigma} \tilde{\delta},$$

with $\tilde{\sigma}, \tilde{\delta}, \tilde{\alpha}$ not depending on ε . In dimensionless variables, these hypotheses have the form

$$\Gamma(\varepsilon) = \tilde{\Gamma}, \quad \Lambda(\varepsilon) = \tilde{\Lambda} \varepsilon^2 \quad \text{while} \quad \varepsilon \rightarrow 0, \quad \text{where} \quad \tilde{\Gamma} = \frac{\gamma_0 H \bar{\rho}_1 \tilde{\sigma}}{\bar{\rho}_2 V \eta_1 \tilde{\delta}}, \quad \tilde{\Lambda} = \frac{\bar{\rho}_2^2 \tilde{\alpha}}{\eta_1 V H}.$$

As for the dimensionless mobility, we assume that

$$B = \tilde{B} \varepsilon^3 \quad \text{while} \quad \varepsilon \rightarrow 0.$$

Note that the parameters $\tilde{\Gamma}, \tilde{\Lambda}$ and \tilde{B} are assumed to be independent of ε . Instead of the time variable t , we introduce the slow time τ and the fast time t' related to the scaling parameter ε as follows:

$$\tau = \varepsilon^2 t, \quad t' = \varepsilon t \quad \text{while} \quad \varepsilon \rightarrow 0.$$

It is easy to check that

$$\frac{\partial f(t'(t), \tau(t))}{\partial t} = \varepsilon f_{t'}(t, \tau) + \varepsilon^2 f_\tau(t, \tau), \quad \text{i.e.} \quad \frac{\partial}{\partial t} = \varepsilon \frac{\partial}{\partial t'} + \varepsilon^2 \frac{\partial}{\partial \tau},$$

for any function $f(t', \tau)$.

In accordance with the two-scale homogenization approach, we are looking for a solution \mathbf{v}^ε , φ^ε , p^ε , μ^ε of problem (6)-(11) as asymptotic series

$$\mathbf{v}^\varepsilon(x) = \varepsilon^2 \mathbf{v}^0(x, y) + \varepsilon^4 \mathbf{v}^1(x, y) + \cdots, \quad y = x/\varepsilon,$$

$$p^\varepsilon(x) = p^0(x, y) + \varepsilon p^1(x, y) + \cdots, \quad y = x/\varepsilon,$$

$$\varphi^\varepsilon(x) = \varphi^0(x, y) + \varepsilon^2 \varphi^2(x, y) + \cdots, \quad y = x/\varepsilon,$$

$$\mu^\varepsilon(x) = \mu^0(x, y) + \varepsilon \mu^1(x, y) + \cdots, \quad y = x/\varepsilon,$$

$$\mathbf{j}^\varepsilon(x) = \varepsilon^2 \mathbf{j}^0(x, y) + \varepsilon^3 \mathbf{j}^1(x, y) + \cdots, \quad y = x/\varepsilon.$$

It is assumed that the coefficients $f^i(x, y)$ in these formulas are defined in $\Omega \times Y$ and they are Y -periodic in y .

Below, we use the following differentiation formula

$$\frac{\partial f(x, x/\varepsilon)}{\partial x_i} = \left(\frac{\partial f(x, y)}{\partial x_i} + \frac{1}{\varepsilon} \frac{\partial f(x, y)}{\partial y_i} \right) \Big|_{y=x/\varepsilon}.$$

Calculations reveal that

$$\frac{\partial \mathbf{v}^\varepsilon(x)}{\partial x_j} = \varepsilon^2 \sum_{i=0} \varepsilon^i \frac{\partial \mathbf{v}^i(x, y)}{\partial x_j} + \varepsilon \sum_{i=0} \varepsilon^i \frac{\partial \mathbf{v}^i(x, y)}{\partial y_j},$$

$$\operatorname{div}(\eta^\varepsilon D^\varepsilon) = \operatorname{div}_y(\eta^0 D_y^0) + O(\varepsilon), \quad \eta^0 = \eta(\varphi^0), \quad 2(D_y^0)_{ij} = \frac{\partial v_i^0}{\partial y_j} + \frac{\partial v_j^0}{\partial y_i},$$

$$\frac{\partial \varphi^\varepsilon(x)}{\partial x_j} = \sum_{i=0, i \neq 1} \varepsilon^i \left(\frac{\partial \varphi^i(x, y)}{\partial x_j} + \frac{1}{\varepsilon} \frac{\partial \varphi^i(x, y)}{\partial y_j} \right),$$

$$\frac{\partial^2 \varphi^\varepsilon(x)}{\partial x_k \partial x_j}$$

$$= \sum_{i=0, i \neq 1} \varepsilon^i \left(\frac{\partial^2 \varphi^i(x, y)}{\partial x_k \partial x_j} + \frac{1}{\varepsilon^2} \frac{\partial^2 \varphi^i(x, y)}{\partial y_k \partial y_j} + \frac{1}{\varepsilon} \frac{\partial^2 \varphi^i(x, y)}{\partial x_k \partial y_j} + \frac{1}{\varepsilon} \frac{\partial^2 \varphi^i(x, y)}{\partial y_k \partial x_j} \right),$$

$$\Delta \varphi^\varepsilon(x) = \sum_{i=0, i \neq 1} \left(\varepsilon^i \Delta_x \varphi^i(x, y) + \varepsilon^{i-2} \Delta_y \varphi^i(x, y) + 2\varepsilon^{i-1} \sum_k \frac{\partial^2 \varphi^i(x, y)}{\partial y_k \partial x_k} \right),$$

where $y = x/\varepsilon$. According to the theory of two-scale homogenization, the variables x and y on the right-hand side of these formulas are considered independent variables

when the derivatives are substituted into the equations. For example, equation (6) becomes

$$\sum_{i=0} \varepsilon^i \mu^i(x, y) = \tilde{\Gamma} \omega'(\xi) - \varepsilon^2 \tilde{\Lambda} \sum_{i=0, i \neq 1} \left(\varepsilon^i \Delta_x \varphi^i(x, y) + \varepsilon^{i-2} \Delta_y \varphi^i(x, y) + 2\varepsilon^{i-1} \sum_k \frac{\partial^2 \varphi^i(x, y)}{\partial y_k \partial x_k} \right),$$

with

$$\xi = \sum_{i=0, i \neq 1} \varepsilon^i \varphi^i(x, y).$$

One can write this equation in the form

$$(\dots)_0 + \varepsilon(\dots)_1 + \varepsilon^2(\dots)_2 + \dots = 0.$$

According to the method of asymptotic expansions, the coefficients $f^i(x, y)$ in the series are determined from the equations $(\dots)_k = 0$. In particular, the equalities $(\dots)_0 = 0$ and $(\dots)_1 = 0$ imply that the following micro and macro equations are valid:

$$\mu^0 = \tilde{\Gamma} \omega'(\varphi^0) - \tilde{\Lambda} \Delta_y \varphi^0, \quad (x, y) \in \Omega \times Y_f, \quad (19)$$

$$\mu^1 = -\tilde{\Lambda} [\operatorname{div}_y(\nabla_x \varphi^0) + \operatorname{div}_x(\nabla_y \varphi^0)], \quad (x, y) \in \Omega \times Y_f. \quad (20)$$

Substituting the series into the momentum equation (9) and equating to zero the coefficients at the powers ε^0 and ε^{-1} leads to the macro and micro equations

$$\nabla_x p^0 + \nabla_y p^1 = 2 \operatorname{div}_y(\eta^0 D_y^0) + \frac{\tilde{\Lambda}}{3} [\nabla_x |\nabla_y \varphi^0|^2 + 2 \nabla_y(\nabla_y \varphi^0 \cdot \nabla_x \varphi^0)] \quad (21)$$

$$-\tilde{\Lambda} \operatorname{div}_y(\nabla_x \varphi^0 \otimes \nabla_y \varphi^0 + \nabla_y \varphi^0 \otimes \nabla_x \varphi^0) - \tilde{\Lambda} \operatorname{div}_x(\nabla_y \varphi^0 \otimes \nabla_y \varphi^0),$$

$$\nabla_y p^0 = \frac{\tilde{\Lambda}}{3} \nabla_y(\nabla_y \varphi^0 \cdot \nabla_y \varphi^0) - \tilde{\Lambda} \operatorname{div}_y(\nabla_y \varphi^0 \otimes \nabla_y \varphi^0). \quad (22)$$

Similarly, substituting the series into equation (8) and equating to zero the coefficients at the powers ε and ε^2 leads to the micro and macro equations

$$R \left(\frac{\partial \varphi^0}{\partial t'} + \mathbf{v}^0 \cdot \nabla_y \varphi^0 \right) = \tilde{B} \operatorname{div}_y(\nabla_y \mu^0), \quad (23)$$

$$R \left(\frac{\partial \varphi^0}{\partial \tau} + \mathbf{v}^0 \cdot \nabla_x \varphi^0 \right) = \tilde{B} \operatorname{div}_x(\nabla_y \mu^0) + \tilde{B} \operatorname{div}_y(\nabla_x \mu^0 + \nabla_y \mu^1). \quad (24)$$

Finally, we derive from (10) the following micro and macro equations:

$$\operatorname{div}_y \mathbf{v}^0 = 0, \quad \operatorname{div}_x \mathbf{v}^0 = 0. \quad (25)$$

The boundary conditions for the micro-equations are

$$\mathbf{v}^0 = 0, \quad \nabla_y \varphi^0 \cdot \mathbf{n} = 0, \quad \nabla_y \mu^0 \cdot \mathbf{n} = 0 \quad \forall (x, y) \in \Omega \times \partial Y_f.$$

The macro-equations enjoy the following boundary conditions:

$$\nabla_x \varphi^0 \cdot \mathbf{n} = 0, \quad (\nabla_x \mu^0 + \nabla_y \mu^1) \cdot \mathbf{n} = 0 \quad \forall (x, y) \in \partial \Omega \times Y_f.$$

Thus a two-scale mathematical model is derived. It consists of the macro and micro-equations (19)-(25) which are strongly coupled.

5 Generalization of the Darcy law and the cross-coupling mobilities

In this section we derive a simplified two-scale model with the macro and micro-equations almost decoupled.

5.1 Stabilization with respect to the fast time t'

Let us first consider some properties of the micro-equations. Like in Section 3, multiplying equation (23) by $\Delta_y \varphi^0$ and integrating over Y_f leads to the energy equality

$$\frac{d}{dt'} \int_{Y_f} \frac{R}{2} |\nabla_y \varphi^0|^2 + \frac{R\tilde{\Gamma}}{\Lambda} \omega dy + \int_{Y_f} \frac{\tilde{B}}{\Lambda} |\nabla_y \mu^0|^2 dy = 0.$$

Hence, after stabilization with respect to the fast time t' up to the settling time $t'_*(x)$, the solution acquires the property

$$\int_{Y_f} |\nabla_y \mu^0|^2 dy = 0 \quad \implies \nabla_y \mu^0 = 0,$$

implying that μ^0 evolve towards a state characterized by the condition $\nabla_y \mu^0 = 0$. This property is of importance for the numerical treatment of the model, as it provides a stopping criterion for the evolution of the microscopic problems. Such an idea is borrowed from [8]. In what follows, our numerical calculations prove that stabilization occurs very quickly.

5.2 Derivation of a generalized Darcy law

Taking into account formula (19), the condition $\nabla_y \mu^0 = 0$ and the identity

$$\operatorname{div}_y (\nabla_y \varphi \otimes \nabla_y \varphi) = \nabla_y |\nabla_y \varphi|^2 / 2 + \Delta_y \varphi \nabla_y \varphi,$$

one can rewrite equation (22) as

$$\nabla_y P = 0, \quad \text{where} \quad P = p^0 + \frac{\tilde{\Lambda}}{6} |\nabla_y \varphi^0|^2 + \tilde{\Gamma} \omega - \mu^0 \varphi^0. \quad (26)$$

It implies that the function P does not depend on the micro-variable y .

The macro-equation (21) for \mathbf{v}^0 is equivalent to

$$\frac{\partial P}{\partial x_i} + \varphi^0 \frac{\partial \mu^0}{\partial x_i} = 2 \frac{\partial}{\partial y_j} (\eta^0 D_{y,i,j}^0) - \frac{\partial}{\partial y_i} (p^1 + \frac{\tilde{\Lambda}}{3} \nabla_x \varphi^0 \cdot \nabla_y \varphi^0) - \quad (27)$$

$$\mathbf{e}_i \cdot 2\tilde{\Lambda} \nabla_y \varphi^0 \operatorname{div}_y (\nabla_x \varphi^0), \quad 2D_{y,i,j}^0 = \frac{\partial v_i^0}{\partial y_j} + \frac{\partial v_j^0}{\partial y_i}.$$

We look for a solution in the form

$$\mathbf{v}^0 = \frac{\partial P}{\partial x_i} \mathbf{W}^i + \frac{\partial \mu^0}{\partial x_i} \mathbf{U}^i + \mathbf{w}, \quad (28)$$

with unknown vector functions \mathbf{W}^i , \mathbf{U}^i and \mathbf{w} , which are Y -periodic with respect to the fast variable y . Equality (27) is certain to be true when these functions solve the following problems in the cell Y_f :

$$\operatorname{div}_y (2\eta^0 D_y \mathbf{W}^i) - \nabla_y q_i^p = \mathbf{e}_i, \quad \operatorname{div}_y \mathbf{W}^i = 0, \quad \mathbf{W}^i|_{\partial Y_f} = 0,$$

$$\operatorname{div}_y (2\eta^0 D_y \mathbf{U}^i) - \nabla_y q_i^\mu = \varphi^0 \mathbf{e}_i, \quad \operatorname{div}_y \mathbf{U}^i = 0, \quad \mathbf{U}^i|_{\partial Y_f} = 0,$$

$$\operatorname{div}_y (2\eta^0 D_y \mathbf{w}) - \nabla_y q = \mathbf{G}, \quad \operatorname{div}_y \mathbf{w} = 0, \quad \mathbf{w}|_{\partial Y_f} = 0,$$

where

$$\mathbf{G} = 2\tilde{\Lambda} \nabla_y \varphi^0 \operatorname{div}_y (\nabla_x \varphi^0) + \frac{\tilde{\Lambda}}{3} \nabla_y (\nabla_x \varphi^0 \cdot \nabla_y \varphi^0).$$

Note that the function $p^1(x, y)$ satisfies the equation

$$0 = \frac{\partial}{\partial y_i} \left(-p^1 + q_j^p \frac{\partial P}{\partial x_j} + q_j^\mu \frac{\partial \mu}{\partial x_j} + q \right).$$

By the linearization argument, one can assume that $\mathbf{G} = 0$. Hence, $\mathbf{w} = 0$ and formula (28) becomes

$$\mathbf{v}^0 = \frac{\partial P}{\partial x_i} \mathbf{W}^i + \frac{\partial \mu^0}{\partial x_i} \mathbf{U}^i. \quad (29)$$

For convenience, we denote $\chi_1(x, y, \tau, t') = 1 - \varphi^0$ and $\chi_2(x, y, \tau, t') = \varphi^0$. The functions χ_1 and χ_2 can be considered as regularized phase indicators since they become the characteristic functions in case of a sharp interface. We introduce porosity and phase saturations as follows:

$$\xi = \int_{Y_f} dy = |Y_f|, \quad S_k(x, \tau, t') = |Y_f|^{-1} \int_{Y_f} \chi_k dy.$$

Similarly, we define the Darcy velocities and phase pressures

$$\mathbf{v}^{(k)}(x, \tau, t') = \int_{Y_f} \mathbf{v}^0(x, y, \tau, t') \chi_k(x, y, \tau, t') dy,$$

$$p_k(x, \tau, t') = \int_{Y_f} p^0(x, \tau, t') \chi_k(x, \tau, t') dy.$$

Now, it follows from (29) that the Darcy velocities satisfy the equations

$$\mathbf{v}^{(k)} = C^{(k)}(x) \nabla_x P + E^{(k)}(x) \nabla_x \mu^0, \quad k = 1, 2, \quad (30)$$

where the mobilities are given by the formulas

$$C^{(k)}(x, \tau, t') = \int_{Y_f} \chi_k \mathbf{W}^i \otimes \mathbf{e}_i dy, \quad E^{(k)}(x, \tau, t') = \int_{Y_f} \chi_k \mathbf{U}^i \otimes \mathbf{e}_i dy.$$

The component form of these equations is determined by the equalities

$$C_{nm}^{(k)} = \int_{Y_f} \chi_k W_n^m dy, \quad E_{nm}^{(k)} = \int_{Y_f} \chi_k U_n^m dy.$$

Equalities (30) can be reformulated in terms of phase pressures by excluding the functions P and μ^0 . Indeed, multiplying equation (26) by χ_k and integrating over Y_f , we obtain the formulas

$$\xi P S_k + \mu^0 c_k = p_k + \nu_k, \quad c_k(x, \tau, t') = \int_{Y_f} \varphi^0 \chi_k dy,$$

$$\nu_k(x, \tau, t') = \int_{Y_f} \chi_k \left(\frac{\tilde{\Lambda}}{6} |\nabla_y \varphi^0|^2 + \tilde{\Gamma} \omega(\varphi^0) \right) dy.$$

Hence we obtain that

$$\xi P = -(l_1^p(x) \tilde{p}_1 - l_2^p(x) \tilde{p}_2), \quad \mu^0 = l_1^\mu(x) \tilde{p}_1 - l_2^\mu(x) \tilde{p}_2,$$

where $\tilde{p}_i = p_i + \nu_i$ and

$$l_1^p = \frac{c_2}{c_1 S_2 - c_2 S_1}, \quad l_2^p = \frac{c_1}{c_1 S_2 - c_2 S_1}, \quad l_1^\mu = \frac{S_2}{c_1 S_2 - c_2 S_1}, \quad l_2^\mu = \frac{S_1}{c_1 S_2 - c_2 S_1}.$$

Observe that

$$c_1 S_2 - c_2 S_1 = -|Y_f| S_1 S_2 \neq 0,$$

provided $\chi_j(y)$ are characteristic functions and $S_1 S_2 \neq 0$. In applications, the condition $S_1 S_2 \neq 0$ is always satisfied due to the presence of residual saturations. Moreover, in approximate calculations one can always assume that $\delta < S_i < 1 - \delta$ for small δ .

It follows from (30) that

$$\mathbf{v}^{(k)} = -\xi^{-1} C^{(k)} \nabla_x (l_1^p \tilde{p}_1 - l_2^p \tilde{p}_2) + E^{(k)} \nabla_x (l_1^\mu \tilde{p}_1 - l_2^\mu \tilde{p}_2), \quad k = 1, 2. \quad (31)$$

Let us introduce the reduced pressures

$$\Pi_1 = l_1^p \tilde{p}_1 - l_2^p \tilde{p}_2 \equiv -\xi P, \quad \Pi_2 = -(l_1^\mu \tilde{p}_1 - l_2^\mu \tilde{p}_2) \equiv -\mu^0.$$

Then equation (29) becomes

$$\mathbf{v}^0(x, y) = -\frac{\mathbf{W}^i}{\xi} \frac{\partial \Pi_1}{\partial x_i} - \mathbf{U}^i \frac{\partial \Pi_2}{\partial x_i},$$

and

$$\tilde{p}_1 = \frac{\Pi_1 l_2^\mu + \Pi_2 l_2^p}{l_2^\mu l_1^p - l_1^\mu l_2^p}, \quad \tilde{p}_2 = \frac{\Pi_1 l_1^\mu + \Pi_2 l_1^p}{l_2^\mu l_1^p - l_1^\mu l_2^p}.$$

Observe that

$$l_2^\mu l_1^p - l_1^\mu l_2^p = -\frac{1}{c_1 S_2 - c_2 S_1} \neq 0$$

in case of a sharp interface. In terms of reduce pressures, the Darcy law (31) becomes

$$\mathbf{v}^{(k)} = -N_{kj} \nabla_x \Pi_j, \quad (32)$$

where

$$N_{11} = \xi^{-1} C^{(1)}, \quad N_{12} = E^{(1)}, \quad N_{21} = \xi^{-1} C^{(2)}, \quad N_{22} = E^{(2)}. \quad (33)$$

It is a principal feature of the Darcy law (32) that it contains the cross-coupling mobility tensors. Empirical arguments in favor of the cross-coupling coefficient are discussed in [9].

5.3 Macro-equations for the phase saturations S_1, S_2 and the reduced pressures Π_1, Π_2

Integrating equation (24) over the fluidic domain Y_f and applying equations (25) provides the macro-equations

$$\frac{\partial(\xi \bar{\rho}_k S_k)}{\partial \tau} + \operatorname{div}_x(\bar{\rho}_k \mathbf{v}^{(k)}) = 0, \quad k = 1, 2. \quad (34)$$

Excluding velocities brings these equations to the form

$$\frac{\partial(\xi \bar{\rho}_k S_k)}{\partial \tau} - \operatorname{div}_x(\bar{\rho}_k N_{kj} \nabla_x \Pi_j) = 0, \quad S_1 + S_2 = 1, \quad k = 1, 2. \quad (35)$$

In our considerations we substituted the variables $\mathbf{v}^0(x, y)$, $p^0(x, y)$ and $\varphi^0(x, y)$ by the macro-variables $\mathbf{v}^{(k)}(x)$, $p_k(x)$ and $S^k(x)$, ($k = 1, 2$). The payment for such doubling of variables is the lack of macro-equations. To complete the system of macro-equations (35) for the functions S_2, Π_1 and Π_2 , we introduce the capillary pressure p_c as a function of the variable S_2 . Then the equality

$$p_c(S_2) = p_2 - p_1 \quad (36)$$

holds. It is generally accepted that phase 1 is more wetting if $p_c > 0$ and $p_c(S_1)$ is a decreasing function of the saturation S_1 [10]. Let us write equation (36) in terms of the reduced pressures Π_1 and Π_2 :

$$\tilde{p}_c = (S_1 - S_2)\Pi_1 + \Pi_2(c_1 - c_2), \quad \tilde{p}_c = p_c(S_2) + \nu_{2,1}, \quad \nu_{2,1} = \nu_2 - \nu_1. \quad (37)$$

Since $S_1 + S_2 = 1$ and $c_1 + c_2 = \xi S_2$, equality (37) is equivalent to

$$p_c(S_2) + \nu_{2,1} = (1 - 2S_2)\Pi_1 + (\xi S_2 - 2c_2)\Pi_2. \quad (38)$$

Here p_c and $\nu_{2,1}$ are the equilibrium and non-equilibrium parts of the capillary pressure. Fig. 2 clarifies the meaning of these pressures. It shows the infinitesimal part of the pore channel associated with the spatial variable x . Phases 1 and 2 are separated by an interfacial layer L . If S_2 is the saturation of the phase 2 at the point x , then $p_c(S_2) = p(B) - p(A)$, where A and B are points at the boundary of the interfacial layer L . The non-equilibrium part of the capillary pressure $\nu_{2,1}$ is calculated on the basis of the micro-equations.

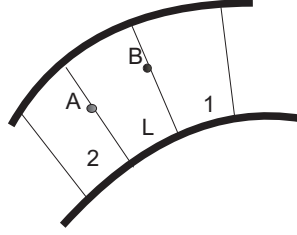


Fig. 2 Equilibrium part of the capillary pressure $p_c = p(B) - p(A)$.

The system of macro-equations (35), (38) for the functions S_2, Π_1 and Π_2 is coupled with the following system of micro-equations for the functions $\varphi^0, \mu^0, \mathbf{W}^i, q_i^p, \mathbf{U}^i, q_i^\mu$ in the cell Y_f :

$$\mu^0 = \tilde{\Gamma}\omega'(\varphi^0) - \tilde{\Lambda}\Delta_y\varphi^0, \quad (39)$$

$$R \left(\frac{\partial\varphi^0}{\partial t} + \mathbf{v}^0 \cdot \nabla_y\varphi^0 \right) = \tilde{B}\operatorname{div}_y(\nabla_y\mu^0), \quad (40)$$

$$\operatorname{div}_y(2\eta^0 D_y \mathbf{W}^i) - \nabla_y q_i^p = \mathbf{e}_i, \quad \operatorname{div}_y \mathbf{W}^i = 0, \quad \mathbf{W}^i|_{\partial Y_f} = 0, \quad (41)$$

$$\operatorname{div}_y(2\eta^0 D_y \mathbf{U}^i) - \nabla_y q_i^\mu = \varphi^0 \mathbf{e}_i, \quad \operatorname{div}_y \mathbf{U}^i = 0, \quad \mathbf{U}^i|_{\partial Y_f} = 0, \quad (42)$$

where

$$\mathbf{v}^0(x, y) = -\frac{\mathbf{W}^i}{\xi} \frac{\partial \Pi_1}{\partial x_i} - \mathbf{U}^i \frac{\partial \Pi_2}{\partial x_i}, \quad \eta^0 = \frac{\varphi^0 \eta_2}{\eta_1} + 1 - \varphi^0. \quad (43)$$

The micro-equations (39)–(43) are to be solved on a time interval $0 < t' < t'_*(x)$ determined by the stabilization criterion (26). In our numerical calculations the fast time variable t' in macro-equations (35) and (38) is fixed to be equal to the stabilization time $t'_*(x)$. Generally, equation (38) does not define S_2 uniquely by values of Π_1 and Π_2 since $\nu_{2,1}$ and c_2 are defined by the micro-equations.

It follows from (34) that the total velocity $\mathbf{v} = \mathbf{v}^{(1)} + \mathbf{v}^{(2)}$ satisfies the equation

$$\operatorname{div}_x \mathbf{v} = 0.$$

Hence,

$$\operatorname{div}_x ((N_{11} + N_{21}) \nabla_x \Pi_1 + (N_{12} + N_{22}) \nabla_x \Pi_2) = 0.$$

6 Example

Here, we perform an analysis of the two scale model under the assumption of slow micro-convection. It implies that we neglect the term $\mathbf{v}^0 \cdot \nabla_y \varphi^0$ in equation (40). Consider an example of a synthetic porous medium, which consists of isolated horizontal channels of constant cross section, see Fig. 3(a). For a problem with such a geometry, the macro-equations will be one-dimensional for a flow along the horizontal axis x . Phase velocities and phase pressures are found by solving 1D-equations on the interval $0 < x < x_*$. But the kinetic coefficients depend on the volume fraction φ^0 which is to be determined by solving the evolutionary 2D-equation in the domain Y_f , see Fig. 3(b):

$$Y_f = \{(y_1, y_2) : 0 < y_1 < 1, \quad r_1 < y_2 < r_2\},$$

where $0 < r_1 < r_2 < 1$. For simplicity we set $x_* = 1$.

Let us illustrate the numerical algorithm on the example of a special displacement problem, when the boundary condition $S = S_- = \text{const}$ for the concentration of the second component is maintained on the left boundary, and the initial concentration of this component is given as in Fig. 4, i.e. $S = S_-$ for $0 < x < \sigma$ and $S = S_+ = \text{const}$ for $\sigma < x < 1$. Let us consider the first slow time interval $0 < \tau < \tau_1$. In what follows, we write φ instead of φ^0 and μ instead of μ^0 .

Step 1. 2D-problem for the Cahn-Hilliard equations in the periodicity cell. We start from the initial conditions $S_k(x, \tau)|_{\tau=0} = S_{k0}(x)$, $k = 1, 2$. Given x , we chose initial values of $\varphi(y, t') = \chi_2(y, t')$ such that

$$\frac{1}{|Y_f|} \int_{Y_f} \chi_k dy = S_{k0}(x) \quad \text{at } t' = 0, \quad k = 1, 2. \quad (44)$$

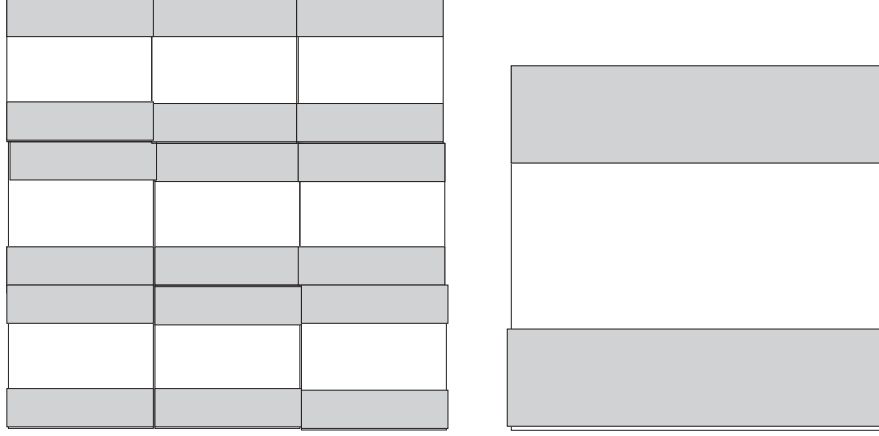


Fig. 3 (a) System of isolated horizontal channels of invariable cross-section. Domain Ω consists of fluid (white) and solid (grey) subdomains Ω_f^z and Ω_s^z . (b) Periodicity cell Y with the fluid zone Y_f (white color).

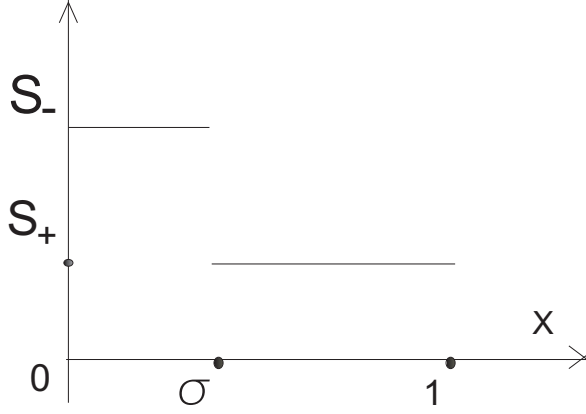


Fig. 4 Profile of initial saturation of the second component

Given numbers $\delta > 0$, $0 < a < 1/2$, $a + \delta < \zeta < 1 - a - \delta$, we introduce the set $A_\zeta^{(a)}$:

$$A_\zeta^{(a)} = \{(y_1, y_2) \in Y_f : |y_1 - \zeta| < a\}.$$

On Fig. 5, this set is marked by 2. According to Fig. 4 and Fig. 5, we choose the initial function $\varphi|_{t'=0} = \varphi_{\zeta a \delta}(y, t')|_{t'=0}$ to be the piecewise linear one corresponding to a drop:

$$\varphi_{\zeta, a, \delta}(y, t')|_{t'=0} = \begin{cases} 1 & \text{if } y \in A_\zeta^{(a)} \\ 0 & \text{if } y \notin A_\zeta^{(a+\delta)} \\ \alpha_1 y_1 + \beta_1 & \text{if } \zeta - a - \delta < y_1 < \zeta - a \\ \alpha_2 y_1 + \beta_2 & \text{if } \zeta + a < y_1 < \zeta + a + \delta, \end{cases} \quad (45)$$

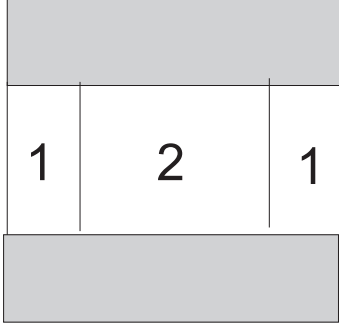


Fig. 5 Phase distribution at $t' = 0$ in case when $0 < S_{20} < 1$.

where

$$\alpha_1 = \frac{1}{\delta}, \quad \alpha_2 = -\alpha_1, \quad \beta_1 = 1 - \frac{\zeta - a}{\delta}, \quad \beta_2 = 1 + \frac{\zeta + a}{\delta}.$$

Observe that equality (44) does not define the initial profile (45) uniquely. To fulfill condition (44), it is possible to choose the function $\varphi_{\zeta, a, \delta}(y, t')|_{t'=0}$ by variation of a only. With such a choice of initial data, we define the function $\varphi(x, y, t', \tau)|_{\tau=0}$ as a solution of the following micro-equations with periodic boundary conditions:

$$R \frac{\partial \varphi}{\partial t'} = \tilde{B} \Delta_y (\tilde{\Gamma} \omega'(\varphi) - \tilde{\Lambda} \Delta_y \varphi), \quad (46)$$

$$\varphi(y, t')|_{y_1=0} = \varphi(y, t')|_{y_1=1}, \quad \mu(y, t')|_{y_1=0} = \mu(y, t')|_{y_1=1}, \quad (47)$$

$$\frac{\partial \varphi}{\partial n} \Big|_{\partial Y_f} = 0, \quad \frac{\partial \mu}{\partial n} \Big|_{\partial Y_f} = 0, \quad (48)$$

on the interval $0 < t' < t'_*(x)$, obeying the condition

$$\nabla_y \mu = 0 \quad \text{in } Y_f, \quad \text{where } \mu = \tilde{\Gamma} \omega'(\varphi) - \tilde{\Lambda} \Delta_y \varphi. \quad (49)$$

On the first interval $0 < \tau < \tau_1$, we define

$$\varphi(x, y, t', \tau) = \varphi(x, y, t', \tau)|_{\tau=0}, \quad \chi_k(x, y, t', \tau) = \chi_k(x, y, t', \tau)|_{\tau=0}, \quad (50)$$

where $k = 1, 2$. Due to boundary conditions, the functions χ_k do not depend on the variable y_2 . The unique solution of (46)-(48) is

$$\varphi = 1 \quad \text{if } S_{20}(x) = 1 \quad (\text{or } \varphi = 0 \quad \text{if } S_{20}(x) = 0). \quad (51)$$

Step 2. 2D-problems for the Stokes equations in the periodicity cell. For each $0 < x < 1$ and $0 < \tau < \tau_1$, the function $\varphi(y_1, t')$ is assumed to be known. Let us

consider two periodic problems for the Stokes equations for $(\mathbf{W}^{(i)}, q_i^p)$ and $(\mathbf{U}^{(i)}, q_i^\mu)$:

$$\operatorname{div}_y(2\eta D_y \mathbf{W}^{(i)}) - \nabla_y q_i^p = \mathbf{e}_i, \quad \operatorname{div}_y \mathbf{W}^{(i)} = 0, \quad \mathbf{W}^{(i)}|_{\partial Y_f} = 0, \quad (52)$$

$$\operatorname{div}_y(2\eta D_y \mathbf{U}^{(i)}) - \nabla_y q_i^\mu = \varphi \mathbf{e}_i, \quad \operatorname{div}_y \mathbf{U}^{(i)} = 0, \quad \mathbf{U}^{(i)}|_{\partial Y_f} = 0, \quad (53)$$

$$\mathbf{W}^{(i)}|_{y_1=0} = \mathbf{W}^{(i)}|_{y_1=1}, \quad \mathbf{U}^{(i)}|_{y_1=0} = \mathbf{U}^{(i)}|_{y_1=1}, \quad (54)$$

$$q_i^p|_{y_1=0} = q_i^p|_{y_1=1}, \quad q_i^\mu|_{y_1=0} = q_i^\mu|_{y_1=1}, \quad (55)$$

with $\eta = \eta(\varphi) = 1 - \varphi + \varphi\eta_2/\eta_1$. Assume for simplicity that $\eta_2 = \eta_1$. Hence $\eta = 1$.

One can verify easily that problems (52), (54), (55) have the following periodic solutions in the variable y_1 :

$$W_1^{(1)} = \frac{(y_2 - r_1)(y_2 - r_2)}{2}, \quad W_2^{(1)} = 0, \quad q_1^p = \text{const},$$

$$W_1^{(2)} = 0, \quad W_2^{(2)} = 0, \quad q_2^p = -y_2.$$

As for problem (53), (54), (55) with $i = 1$, a periodic solution is given by the formulas

$$U_1^{(1)} = \frac{(y_2 - r_1)(y_2 - r_2)}{2} \int_0^1 \chi_2(y_1) dy_1, \quad U_2^{(1)} = 0,$$

$$q_1^\mu = y_1 \int_0^1 \chi_2(y_1) dy_1 - \int_0^{y_1} \chi_2(y_1) dy_1.$$

Step 3. Averaging in the micro-variable. Now, the mobility tensors and the kinetic coefficients are defined as follows:

$$C^{(k)}(x, \tau, t') = \int_{Y_f} \chi_k \mathbf{W}^i \otimes \mathbf{e}_i dy, \quad (56)$$

$$E^{(k)}(x, \tau, t') = \int_{Y_f} \chi_k \mathbf{U}^i \otimes \mathbf{e}_i dy, \quad (57)$$

$$S_k(x, \tau, t') = \frac{1}{|Y_f|} \int_{Y_f} \chi_k dy, \quad (58)$$

$$c_k(x, \tau, t') = \int_{Y_f} \varphi^0 \chi_k dy, \quad c_1 + c_2 = \xi S_2, \quad (59)$$

$$\nu_k(x, \tau, t') = \int_{Y_f} \chi_k \left(\frac{\tilde{\Lambda}}{6} |\nabla_y \varphi^0|^2 + \tilde{\Gamma} \omega(\varphi^0) \right) dy. \quad (60)$$

We denote

$$A = \frac{1}{\xi} \int_{r_1}^{r_2} W_1^{(1)}(y_2) dy_2 = -\frac{\xi^2}{12}, \quad \xi = r_2 - r_1.$$

It follows from solutions of the Stokes problems that

$$C_{11}^{(k)} = \int_{Y_f} \chi_k W_1^{(1)} dy = \xi S_k A, \quad C_{11}^{(1)} + C_{11}^{(2)} = \xi A, \quad (61)$$

$$E_{11}^{(k)} = \int_{Y_f} \chi_k U_1^{(1)} dy = \frac{A}{\xi} \left(\int_{Y_f} \chi_k dy \right) \left(\int_{Y_f} \chi_2 dy \right) = A \xi S_k S_2, \quad (62)$$

$$C_{ij}^{(k)} = \int_{Y_f} \chi_k W_i^{(j)} dy = 0, \quad (i, j) \neq (1, 1), \quad (63)$$

$$E_{21}^{(k)} = \int_{Y_f} \chi_k U_2^{(1)} dy = 0. \quad (64)$$

Clearly,

$$E_{11}^{(1)} + E_{11}^{(2)} = \xi A S_2. \quad (65)$$

With χ_k independent of y_2 , the function c_k and ν_k are given by the formulas

$$c_k(x, \tau, t') = \xi \int_0^1 \chi_2 \chi_k dy_1, \quad (66)$$

$$\nu_k(x, \tau, t') = \xi \int_0^1 \chi_k \left(\frac{\tilde{\Lambda}}{6} \left(\frac{\partial \chi_2}{\partial y_1} \right)^2 + \tilde{\Gamma} \omega(\chi_2) \right) dy_1. \quad (67)$$

Note that the fast variable t' in (56)-(67) is taken to be equal to $t'_*(x)$.

Step 4. Solution of the macro-equations. We address the one-dimensional macro-equations and look for a solution (S_2, Π_1, Π_2) depending on τ and the variable $x = x_1$. Since $C_{21}^{(k)} = 0$ and $E_{21}^{(k)} = 0$, we derive from the representation formulas (32) and (33) that the velocities $\mathbf{v}^{(k)}$ are directed along the x -axis, i.e. $\mathbf{v}^{(k)} = (v_1^{(k)}, 0)$.

System (35)-(38) admits a one-dimensional solution $S(\tau, x)$, $\Pi_1(\tau, x)$, $\Pi_2(\tau, x)$, where $S = S_2$. The equation $\text{div}(\mathbf{v}^{(1)} + \mathbf{v}^{(2)}) = 0$ becomes

$$\frac{\partial}{\partial x} (v_1^{(1)} + v_1^{(2)}) = 0, \quad \text{i.e.} \quad v_1^{(1)} + v_1^{(2)} = V.$$

Passing to pressures, we obtain that

$$-\xi C \frac{\partial \Pi_1}{\partial x} - E \frac{\partial \Pi_2}{\partial x} = V(\tau). \quad (68)$$

where

$$C = C_{11}^{(1)} + C_{11}^{(2)}, \quad E = E_{11}^{(1)} + E_{11}^{(2)}.$$

Due to (61) and (62), equation (68) is equivalent to

$$-A \left(\frac{\partial \Pi_1}{\partial x} + \xi S \frac{\partial \Pi_2}{\partial x} \right) = V. \quad (69)$$

The macro-equation (35) for $S = S_2$ can be formulated as

$$\frac{\partial(\xi S)}{\partial \tau} + \frac{\partial}{\partial x} \left(-\xi^{-1} C_{11}^{(2)}(x, \tau) \frac{\partial \Pi_1}{\partial x} - E_{11}^{(2)}(x, \tau) \frac{\partial \Pi_2}{\partial x} \right) = 0. \quad (70)$$

Due to (61) and (62), equation (70) admits the form

$$\frac{\partial(\xi S)}{\partial \tau} - \frac{\partial}{\partial x} \left(AS \left(\frac{\partial \Pi_1}{\partial x} + \xi S \frac{\partial \Pi_2}{\partial x} \right) \right) = 0. \quad (71)$$

It follows from (69) that equation (71) becomes

$$\frac{\partial(\xi S)}{\partial \tau} + V \frac{\partial S}{\partial x} = 0. \quad (72)$$

This macro equation describes a displacement with a discontinuity front, when at the initial moment of time on the interval $0 < x < 1$, the function S takes the value S_+ , $0 \leq S_+ \leq 1$, and the boundary condition $S = S_-$, $S_+ \leq S_- \leq 1$ is kept at the input boundary $x = 0$:

$$S|_{t=0} = S_+, \quad S|_{x=0} = S_-.$$

The functions S, Π_1, Π_2 satisfy the following macro-problem

$$\frac{\partial(\xi S)}{\partial \tau} - \frac{\partial}{\partial x} \left(AS \frac{\partial \Pi_1}{\partial x} + A \xi S^2 \frac{\partial \Pi_2}{\partial x} \right) = 0, \quad (73)$$

$$\frac{\partial}{\partial x} \left(\frac{\partial \Pi_1}{\partial x} + \xi S \frac{\partial \Pi_2}{\partial x} \right) = 0, \quad (74)$$

$$\Pi_1 + \frac{(\xi S - 2c_2(\cdot))}{1 - 2S} \Pi_2 = \frac{\tilde{p}_c}{1 - 2S}, \quad \tilde{p}_c = p_c(S) + \nu_{2,1}(\cdot), \quad \nu_{2,1} = \nu_2 - \nu_1, \quad (75)$$

where the notation $f(\cdot)$ implies that the function f depends not only on the macro-variables (x, τ) , but on the micro-equations (46)-(50) as well. The fast time t' in

equations (73)-(75) is set to be equal to the stabilization time $t'_*(x)$. Due to the properties (51), the macro-equations admit a solution given by constants:

$$S = 1, \quad \Pi_1 = -p_c(1), \quad \Pi_2 = \text{const},$$

and

$$S = 0, \quad \Pi_1 = p_c(0), \quad \Pi_2 = \text{const}.$$

We look for a piecewise continuous solution to problem (73) for equations (73)-(75) with the discontinuity front $x = \sigma(t)$. Equation (74) is equivalent to the system of equations (69) and (72). We introduce the jump $[S]_\sigma$ of the discontinuous function $S(x)$ at the line of discontinuity $x = \sigma(\tau)$:

$$[S]_\sigma = \lim_{\delta \rightarrow 0} S(\sigma(\tau) + \delta, \tau) - \lim_{\delta \rightarrow 0} S(\sigma(\tau) - \delta, \tau).$$

By the Hugoniot condition [11]

$$\xi[S]_\sigma \dot{\sigma} = V[S]_\sigma,$$

it results from the scalar conservation law (72) that the front satisfies the equation

$$\xi \dot{\sigma} = V, \quad \dot{\sigma} \equiv \frac{d\sigma}{d\tau}.$$

Following the method of [11] we introduce the self-similar variable $\zeta = x/\sigma(\tau)$ and look for a solution in the form of a centered wave $S(x, \tau) = S(\zeta)$ behind the front. In the domain $0 < x < \sigma(\tau)$, equation (72) becomes

$$(-\zeta \dot{\sigma} + V) S' = 0, \quad S' \equiv \frac{dS}{d\zeta}, \quad 0 < \zeta < 1.$$

The equality $S = \text{const} = S_-$ holds behind the front. Before the front, i.e. in the domain $x > \sigma(\tau)$, we assume that $S = \text{const} = S_+$.

To simplify calculations, the data Π_i^0, Π_i^1 ($i = 1, 2$) in the boundary conditions

$$\Pi_i|_{x=0} = \Pi_i^0, \quad \Pi_i|_{x=1} = \Pi_i^1, \quad i = 1, 2,$$

are assumed to satisfy the special restrictions

$$\Pi_1^0 + \xi \Pi_2^0 S|_{x=0} = 0, \quad \Pi_1^0 + \Pi_2^0 \frac{\xi S - 2c_2}{1 - 2S} \Big|_{x=0} = \frac{\tilde{p}_c}{1 - 2S} \Big|_{x=0}, \quad (76)$$

$$\Pi_1^1 + \xi \Pi_2^1 S|_{x=1} = 0, \quad \Pi_1^1 + \Pi_2^1 \frac{\xi S - 2c_2}{1 - 2S} \Big|_{x=1} = \frac{\tilde{p}_c}{1 - 2S} \Big|_{x=1}. \quad (77)$$

We integrate equations (69) over the intervals $0 < x < \sigma$ and $\sigma < x < 1$ paying attention that the reduced pressures Π_1 and Π_2 are continuous. As a result, we obtain the equalities

$$\Pi_1^\sigma + \xi S_- \Pi_2^\sigma = -\frac{V\sigma}{A}, \quad \Pi_1^\sigma + \xi S_+ \Pi_2^\sigma = \frac{V(1-\sigma)}{A}, \quad (78)$$

where Π_i^σ is the value of Π_i at $x = \sigma$. It follows from (78) that

$$\Pi_1^\sigma = -\frac{V(S_- + \sigma[S]_\sigma)}{A[S]_\sigma}, \quad \xi \Pi_2^\sigma = \frac{V}{A[S]_\sigma}. \quad (79)$$

Let us calculate the jumps of the capillary curve (75):

$$\Pi_2^\sigma \left[\frac{\xi S - 2c_2}{1 - 2S} \right]_\sigma = \left[\frac{\tilde{p}_c}{1 - 2S} \right]_\sigma.$$

Taking into account formula (79), we arrive at the following equation for the front velocity:

$$V \left[\frac{\xi S - 2c_2}{1 - 2S} \right]_\sigma = \xi A[S]_\sigma \left[\frac{\tilde{p}_c}{1 - 2S} \right]_\sigma, \quad A = -\frac{\xi^2}{12}. \quad (80)$$

The assumption that the phase velocities behind the front and ahead of the front do not depend on the spatial coordinate makes it possible to determine these velocities. Indeed, applying (61) and (62) we conclude that

$$v_1^{(1)} = -AS_1 \frac{\partial \Pi_1}{\partial x} - A\xi S_1 S_2 \frac{\partial \Pi_2}{\partial x}, \quad (81)$$

$$v_1^{(2)} = -AS_2 \frac{\partial \Pi_1}{\partial x} - A\xi S_2^2 \frac{\partial \Pi_2}{\partial x}. \quad (82)$$

We integrate equation (81) for $v_1^{(1)}$ over the intervals $0 < x < \sigma$ and $\sigma < x < 1$, keeping in mind formula (79). As a result, we obtain

$$\sigma v_1^{(1)} = -A(1 - S_-)\Pi_1^\sigma - A\xi(1 - S_-)S_- \Pi_2^\sigma = \sigma V(1 - S_-),$$

$$(1 - \sigma)v_1^{(1)} = A(1 - S_+)\Pi_1^\sigma + A\xi(1 - S_+)S_+ \Pi_2^\sigma = (1 - \sigma)V(1 - S_+).$$

Hence,

$$v_1^{(1)} = \begin{cases} V(1 - S_-) & \text{if } x < \sigma(\tau) \\ V(1 - S_+) & \text{if } x > \sigma(\tau), \end{cases} \quad v_1^{(2)} = \begin{cases} VS_- & \text{if } x < \sigma(\tau) \\ VS_+ & \text{if } x > \sigma(\tau). \end{cases} \quad (83)$$

Because of (69), one can derive from (81) and (82) the equality $S_2 v_1^{(1)} = S_1 v_1^{(2)}$. It implies that

$$v_1^{(i)} = S_i V, \quad 0 < x < 1. \quad (84)$$

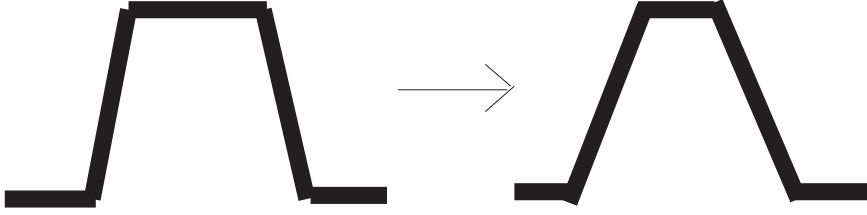


Fig. 6 Dynamics of a drop in the cell. The scheme of profiles of $\chi_2(y_1)$ at the initial and final moments.

Formulas (83) and (84) are equivalent.

The saturation is given by the formula

$$S(x, \tau) = \begin{cases} S_- & \text{if } x < \sigma(\tau), \\ S_+ & \text{if } x > \sigma(\tau). \end{cases}$$

Let us determine the reduced pressures. Integration of equation (69) over the interval $0 < x < \sigma$, taking into account the boundary conditions (76), (77) leads to the equalities

$$\Pi_1 + \xi S \Pi_2 = -\frac{Vx}{A}, \quad \Pi_1 + \Pi_2 \frac{\xi S - 2c_2}{1 - 2S} = \frac{\tilde{p}_c}{1 - 2S},$$

which allow to find Π_i on the interval $0 < x < \sigma$. As for the interval $\sigma < x < 1$, these pressures solve the system

$$\Pi_1 + \xi S \Pi_2 = \frac{V(1-x)}{A}, \quad \Pi_1 + \Pi_2 \frac{\xi S - 2c_2}{1 - 2S} = \frac{\tilde{p}_c}{1 - 2S}.$$

Let us find the front velocity in the degenerate case when $S_+ = 0$ and $S_- = 1$. One can easily verify that problem (46)-(50) with the initial data $S_0(x) = 0$ has the solution $\varphi = 0$. Similarly, the function $\varphi = 1$ is the solution for the initial data $S_0(x) = 1$. Hence, $\nu_i(\cdot) = 0$, $c_2^+ = 0$, $c_2^- = \xi$. Thus, the front satisfies the equation

$$V = A(p_c(0) + p_c(1)) = \text{const}, \quad \xi \sigma(\tau) = V\tau.$$

Remark 1. *In our case, the second phase is water with the gas CO_2 dissolved in it, and phase 1 is oil. Carbon dioxide is highly soluble in oil and mixes well with it. It serves to reduce the surface tension at the phase boundary. Water allows us to use the assumption of the incompressibility of the entire mixture as a whole. We assume hydrophobicity, so $p_c \equiv p_2 - p_1 < 0$. According to Leverett's hypothesis, the capillary pressure p_c as a function of the variable S_2 is increasing and $p_c = 0$ at $S_2 = 1$. Further, for simplicity, we will assume that $p_c = S_2 - 1$. In view of the incompressibility, it does not seem strange that, according to formula (83), all oil ahead of the front moves at the same speed in the positive direction of the x_1 axis. The injection of water with gas at the point $x_1 = 0$ is ensured by maintaining the boundary condition $S^- = \text{const}$. Since $A = -\xi^2/12$, the hydrophobicity condition ensures the inequality $V > 0$.*

Let us find the approximate front velocity analytically in the case when $1/2 > S_+ > 0$ and $1/2 < S_- < 1$. Calculations show that for large values of the parameter $\tilde{\Gamma}$ the initial drop is “smeared”, i.e. the interfacial layer will increase while remaining compact, see Fig. 6. The final stabilization time t'_* turns out to be small (10^{-2}) and does not depend on x , it is chosen from the condition $\int_{Y_f} |\nabla_y \mu|^2 \leq 10^{-4}$.

Let us approximate the solution $\varphi_*(y_1) = \varphi(y_1, t'_*)$ at the final moment t'_* by the piecewise linear function $\varphi_{\zeta, a_*, \delta_*}(y_1)$ of the form (45), taking $a_* < a$ and $\delta_* > \delta$ instead of a and δ . The first approximation criterion is the equality

$$\int_0^1 \varphi_*(y_1) dy_1 = \int_0^1 \varphi_{\zeta, a_*, \delta_*}(y_1) dy_1. \quad (85)$$

In this case, the center ζ of the drop-like function $\varphi_{\zeta, a_*, \delta_*}$ remains in place and the size of the interface δ_* depends only on t'_* . Note that the solutions of (46)-(50) satisfy the conservation law

$$\frac{d}{dt'} \int_{Y_f} \varphi(y, t') dy = 0,$$

implying that

$$\int_0^1 \varphi(y_1, t') dy_1|_{t'=0} = \int_0^1 \varphi_{\zeta, a_*, \delta_*} dy_1 \equiv S_*. \quad (86)$$

Equality (86) is equivalent to

$$2a^\pm + \delta^\pm = 2a_*^\pm + \delta_*^\pm = S^\pm.$$

It is not difficult to verify that the non-equilibrium part $\nu_{2,1}^*$ of the capillary pressure at the final moment of fast time, defined by formulas (67) and (75), is identically zero for the piecewise linear function $\varphi_{\zeta, a_*, \delta_*}$. As for the parameter c_{2*} , determined by the piecewise linear function $\varphi_{\zeta, a_*, \delta_*}$, it is not difficult to establish the formula

$$c_{2*}^\pm = 2\xi(a_*^\pm + \delta_*^\pm/3) = \xi(S^\pm - \delta_*^\pm/3). \quad (87)$$

This equality is the second criterion for constructing the function $\varphi_{\zeta, a_*, \delta_*}(y_1)$. The criteria (85) and (87) make it possible to determine the parameters a_*^\pm and δ_*^\pm uniquely, since S^\pm and c_{2*}^\pm are independent of ζ when calculated by the function $\varphi_{\zeta, a_*^\pm, \delta_*^\pm}^{pm}$. With the use of the piecewise linear function $\varphi_{\zeta, a_*, \delta_*}$, formula (80) takes the form

$$V \left[\frac{S - 2\delta_*/3}{1 - 2S} \right]_\sigma = -A[S]_\sigma \left[\frac{p_c(S)}{1 - 2S} \right]_\sigma, \quad A = -\frac{\xi^2}{12}. \quad (88)$$

Applicability of equality (88) is determined by the inequalities $1/2 < S^- < 1$, $0 < S^+ < 1/2$. It is for such cases that the velocity V is positive in the hydrophobic case provided the quantities δ_*^\pm are small enough. Indeed, equation (88) reduces to

$$\frac{12V}{\xi^2} = p_c(S^+)(1 - 2S^-) - p_c(S^-)(1 - 2S^+) > 0.$$

when $\delta_*^\pm = 0$. By continuity, the sign of the velocity is preserved at small δ_*^\pm . The required small values can be achieved by varying the coefficients in the micro-problem (46)-(48). In particular, formula (88) becomes

$$V = \frac{\xi^2 \{p_c(S^+)(1 - 2S^-) - p_c(S^-)(1 - 2S^+)\}}{12(1 - 4\delta_*/3)}, \quad (89)$$

if $\delta_*^+ = \delta_*^- = \delta_*$. Hence, $V > 0$ provided

$$1/2 < S^- < 1, \quad 0 < S^+ < 1/2, \quad \delta_* < 3/4.$$

The above analytical considerations were based on a piecewise linear approximation of the final concentration $\varphi^*(y_1)$. Now, we calculate the front velocity directly without involving such approximations. To this end, we fix data as follows:

$$\tilde{\Lambda} = 1, \quad \tilde{\Gamma} = 10^3, \quad \tilde{B} = 1, \quad \xi = 0.2, \quad R = 1.2, \quad S^- = 0.6, \quad S^+ = 0.4, \quad L = 1.$$

Here, L is a given positive constant in the equation $p_c = L(S - 1)$ which describes the hydrophobic capillary pressure curve qualitatively. One can write equation (80) in the form

$$V \left\{ \frac{\xi S^+ - 2c_2^+}{1 - 2S^+} - \frac{\xi S^- - 2c_2^-}{1 - 2S^-} \right\} = -\frac{\xi^3(S^+ - S^-)}{12} \left\{ \frac{\nu_{2,1}^+}{1 - 2S^+} - \frac{\nu_{2,1}^-}{1 - 2S^-} \right\} \quad (90)$$

$$-\frac{\xi^3(S^+ - S^-)}{12} \left\{ \frac{p_c(S^+)}{1 - 2S^+} - \frac{p_c(S^-)}{1 - 2S^-} \right\},$$

where

$$c_2^\pm = \xi \int_0^1 (\varphi_*^\pm)^2 dy_1, \quad \int_0^1 \varphi_*^\pm dy_1 = S^\pm,$$

$$\nu_{2,1}^\pm = \xi \int_0^1 (2\varphi_*^\pm - 1) \left(\frac{\tilde{\Lambda}}{6} \left| \frac{\partial \varphi_*^\pm}{\partial y_1} \right|^2 + \tilde{\Gamma} \omega(\varphi_*^\pm) \right) dy_1.$$

Here, $\varphi_*^\pm(y_1)$ is the solution of problem (46)-(48) at the final fast moment with the initial data satisfying the condition

$$\int_0^1 \varphi^\pm|_{t=0} dy_1 = S^\pm. \quad (91)$$

Fig. 7 and Fig. 8 depict results of numerical solution of problem (46)-(48) at the final moment of the fast time for the piecewise linear initial data (45) corresponding to different positions and sizes of the initial drop. We apply FreeFem++. Details are presented in Appendix A. The stabilization time turned out to be $3 \cdot 10^{-2}$ with the time step equal to $5 \cdot 10^{-3}$. Recall that the parameters of the initial drop (ζ, a, δ) are consistent with saturation according to formula (91). The same is true for the

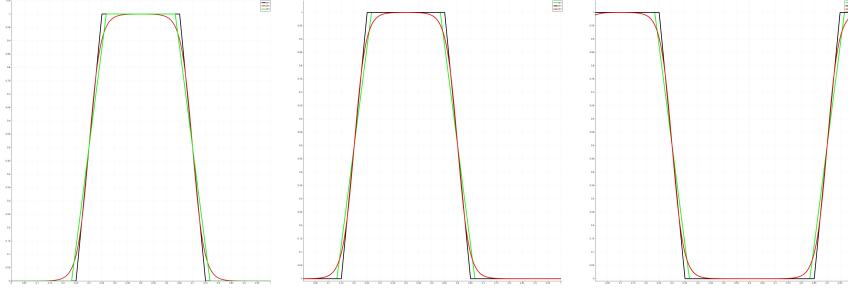


Fig. 7 Profiles of concentration for $S = 0.4$. Black and green curves correspond to initial data and piecewise linear approximation of the final concentration. Red curve is the final profile of concentration. The symmetry center ζ is equal to 0.5, 0.4, 0.1 in (a), (b), (c) respectively.

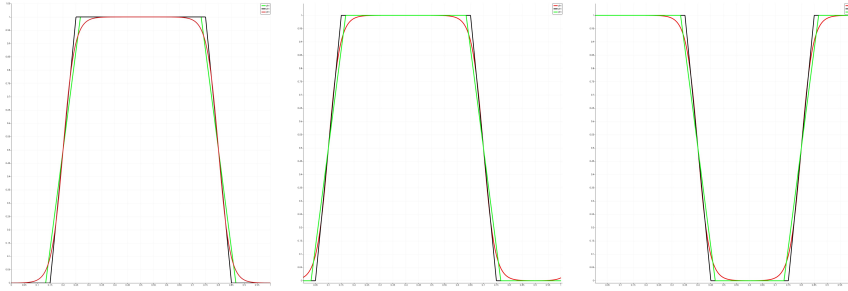


Fig. 8 Profiles of concentration for $S = 0.6$. Black and green curves correspond to initial data and piecewise linear approximation of the final concentration. Red curve is the final profile of concentration. The symmetry center ζ is equal to 0.5, 0.4, 0.1 in (a), (b), (c) respectively.

sizes (ζ, a_*, δ_*) of the final droplet approximation. Here are the numerical results for saturation $S = 0.4$:

$$a = 0.15, \delta = 0.1, a_* = 0.132937, \delta_* = 0.134125, c_2 = 0.0710583.$$

For $S = 0.6$ we have

$$a = 0.25, \delta = 0.1, a_* = 0.232937, \delta_* = 0.134125, c_2 = 0.111058.$$

As for the parameter $\nu_{2,1}$, it takes the value $2 \cdot 10^{-6}$ both for $S = 0.4$ and $S = 0.6$. The small values of the parameter $\nu_{2,1}$ and the front width δ_* justify the applicability of formula (89). If we calculate the velocity using it, we get $V = 8.11852940 \cdot 10^{-4}$. Calculating the velocity directly using formula (90) leads to the value $V = 8.118485611 \cdot 10^{-4}$.

Step 5. The process is repeated on the interval $\tau_1 < \tau < \tau_2$. In this case, the initial function $\varphi(y, t')|_{t'=0}$ is calculated according to the rule (45) if we replace the function

$S_0(x)$ to $S(x, \tau_1)$. Since the function $S(x, \tau_1)$ still takes only two values S^- and S^+ , the velocity V remains the same as on the interval $0 < \tau < \tau_1$.

7 Conclusion

We studied the two-scale homogenization of a phase-field model for flows in porous media with surface tension effects. The pore-scale equations consist of a strongly coupled system of the Navier-Stokes and the Cahn-Hilliard equations. The fluid phases are separated by an evolving diffusive layer of a finite width. We introduced a notion of the miscibility strength which is generally correlated with the scaling parameter. The case of weak miscibility is studied corresponding to a thin diffusive interface layer. Under some hypotheses, the two-scale mathematical model is proved to reduce to a Darcy-like laws with the cross-coupling permeability tensors which are not introduced empirically but are determined through a solution of the micro-equations. The cross-coupling effect implies that each phase has its own pressure and the seepage velocity of each phase depends on the pressure gradients of both the phases. Numerically, the macro and micro-equations can be decoupled. To this end an example is constructed for the seepage flow in the system of parallel hydrophobic channels. Such a flow can be treated as a capillary displacement of oil by injection of mixture of water with Carbon dioxide.

Declarations

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- The authors declare no conflict of interest.
- Ethics approval. Not applicable.

Appendix A Evolution of a droplet

All our numerical calculations for the Cahn-Hilliard equations are performed with the use of FreeFem++. To tackle nonlinearity, the Newton-Raphson iteration procedure is employed. As for the temporal discretization, an explicit in time method is applied with the time step equal to 5×10^{-3} . The code was validated by applying it to the problem concerning the evolution of a droplet initially located in the center of the domain and having the form of a quadrat, i.e. $\varphi = 1$ inside the quadrat and $\varphi = 0$ outside it when $t = 0$ [12]. The boundary of the droplet is slightly “blurred”. It is clear that the droplet ultimately should take the spherical form [13] due to gradient of chemical potential. In the domain

$$Y = \{0 < y_1 < 1, 0 < y_2 < 1\},$$

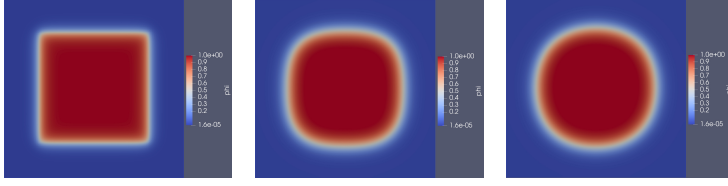


Fig. A1 Initial quadrat becomes a circle with smeared boundary. The number of steps are equal to 0(a), 20(b) and 40(c).

we consider the following initial boundary value problem

$$R \frac{\partial \varphi}{\partial t} = \tilde{B} \Delta \mu, \quad \mu = \tilde{\Gamma} \omega'(\varphi) - \tilde{\Lambda} \Delta \varphi,$$

$$\frac{\partial \varphi}{\partial n} \Big|_{\partial Y_f} = 0, \quad \frac{\partial \mu}{\partial n} \Big|_{\partial Y_f} = 0, \quad \varphi|_{t=0} = \varphi_0(y),$$

where

$$\varphi_0(y) = 0.5(1 + \tanh(b(a - \max\{|y_1 - 0.5|, |y_2 - 0.5|\}))).$$

We use the following data:

$$\tilde{\Lambda} = 1, \quad \tilde{\Gamma} = 10^3, \quad R = 1.2, \quad B = 1, \quad b = 10^6, \quad a = 0.3.$$

Calculations reveal that the initial quadrat becomes a circle, Fig. A1.

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