A model for multiphase, multicomponent, and thermal flow in neutrally wetting porous media, built on the diffuse-interface assumption ☆

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ABSTRACT

A model is presented that describes the simultaneous flow of maximally three fluid phases in a neutrally wetting porous medium.

The model is based on the diffuse interface framework that, unlike traditional models, requires neither relative permeabilities nor flash calculations. It describes the phases as different manifestations of one and the same fluid where density changes rapidly but continuously inside layers of finite thickness between phases (the diffuse interfaces).

The fluid is assumed to be a mixture of non-reacting chemical species. These are limited in number and nature by the requirement that the mixture's viscosity, thermal conductivity, and Helmholtz free energy are obtainable through existing theories. This applies to most hydrocarbons and to water.

The model has been presented earlier (Papatzacos, 2010) and illustrated with isothermal applications. A temperature equation is developed in the present paper and an application with a production well and a cold water injector well is considered. The numerical results of the application confirm earlier results showing the movements of the fluid and of its interfaces. In addition, the application focuses on the numerical problems inherent to the temperature equation. These are related to the smallness of the thermal conductivity, and to the thinness of the diffuse interfaces. It is shown that a careful application of boundary and initial conditions effectively solves these problems. Density and temperature maps for various times, including velocities, are shown. Production curves are provided, showing no instability at water breakthrough.

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1. Introduction

This paper presents an alternative model to existing thermal compositional models for flow in porous media (FPM). It avoids the use of relative permeabilities, and the assumption of instantaneous phase separation, two characteristic features of existing models.

It results from an averaging of the equations of general fluid flow (GFF) valid inside the pores. The diffuse-interface (DI) assumption is an essential constituent, whereby interfaces between phases do not exist as surfaces but as transition regions of finite thickness.

This introductions is organized as follows: Section 1.1 is a brief description of the main features of the DI assumption; Section 1.2 gives an overview of the model construction; Section 1.3 compares the present model to other compositional models; Section 1.4 lists the particular problems that arise with the present model; Section 1.5 lists the notational conventions used.

The rest of the paper is organized as follows. The balance equations for mass, momentum, and entropy are derived in Section 2. Information concerning the two important components of the model, the Helmholtz free energy density and the transport coefficients, is given in Sections 3.1 and 3.2, respectively. The differential equations of the model, i.e., the balance equations in dimensionless form, are given in Section 4. Some special considerations concerning the initial and boundary conditions, relating to unfamiliar features of the differential equations and to the problems connected to the temperature equation, are outlined in Section 5. A numerical example is described in Section 6, where the situation considered is one of injection and production at different temperatures.

1.1. A brief introduction to the diffuse interface formalism

The DI formalism can be traced back to two works by van der Waals: his thesis (van der Waals, 1873) and a paper published in 1893. The thesis introduced the now well known equation of state (EOS) for a fluid consisting of a single chemical species,

$$P = \frac{nR_G T}{V - nb} - \frac{an^2}{V^2}, \tag{1}$$

giving the pressure P in terms of the number of moles n, the volume V and the temperature T; R_G is the gas constant while a and b are two constants depending on the chemical species considered (see for example chapter 3 in Firoozabadi, 1999).

This EOS predicts that, for $T < T_c$ where T_c is the critical temperature, a transition will occur from a one-phase to a two-phase state. There is a saturated liquid at volume V^ℓ and pressure P_e, and a saturated gas at volume V^g and pressure P_e. The values of V^ℓ, V^g, and P_e can be calculated by Maxwell's equal area rule. For $T < T_c$, and $V^\ell < V < V^g$, then $P(V, T)$ given by Eq. (1) is the pressure of a metastable or an unstable fluid state, depending on whether dP/dV is negative or positive. Any such state will go to a corresponding stable two-phase state with the same values of V and T but with pressure $P = P_e$.

The 1893 paper concerns the theory of capillarity for a one component fluid. The English version, due to Rowlinson (1979) is referred to here. Anticipating modern theories, van der Waals calculated the Helmholtz free energy of a pure fluid as

$$\psi(V, T) = - \int P \, \mathrm{d}V, \tag{2}$$

using Eq. (1) for P. He could then show that, for a given $T < T_c$, then $\psi = L + W$, where, as functions of V, L is linear and W is W-like, i.e., W has two minima, both of value 0, and a maximum in between. The minima occur for the volumes V^ℓ and V^g given by Maxwell's rule, and the values of $\psi(V, T)$ for $V^\ell < V < V^g$ correspond to metastable or unstable fluid states. The straight line connecting the minima is a line of constant chemical potential containing the stable two-phase states to which the unstable or metastable states go to.

The *essential postulate* (Rowlinson, 1979 and Rowlinson and Widom, 1982, Chapter 3) of the 1893 paper, later to be called the diffuse interface assumption, is as follows: in a single-component fluid where two phases coexist, there are thin regions between the phases where the density changes rapidly but continuously. The derivatives of the density are then important, and are accordingly added to the list of state variables, usually restricted to density ρ and temperature T. Thus the free energy density of the whole fluid can be denoted $\Psi(\rho, T, \nabla\rho, \nabla^2\rho, \ldots)$. The Taylor expansion of Ψ reduces to

$$\Psi = \psi(\rho, T) + \frac{1}{2}\lambda|\nabla\rho|^2, \tag{3}$$

when it is assumed (i) that the fluid is isotropic, and (ii) that the lowest non-zero order in the expansion in terms of the derivatives is sufficient (Cahn and Hilliard, 1958). It is additionally assumed that λ is a constant. In Eq. (3), ψ is the free energy density given by Eq. (2), now expressed in terms of variables ρ and T. It is in the sequel called the free energy density of the "bulk fluid", referring to that part of the fluid which is far from the regions between the phases, and thus does not depend on the derivatives of the density.

DI models for two-phase GFF (Anderson et al., 1998) connect the mechanics of the fluid to its thermodynamics, through a van der Waals type EOS, and through a modification to the pressure brought about by expression (3). The differential equations for mass, momentum, and energy balance give a complete description of both flow and phase behavior. For an analysis of the mechanisms involved, see Novick-Cohen and Segel (1984). Basically, the existence of unstable fluid states mentioned above causes the fluid to gradually (in time) segregate into phases. It can be shown (see Papatzacos, 2002, Appendix B.2.1) that, in a one component fluid, the thickness of the interface region is proportional to $\sqrt{\lambda}$.

The DI models for FPM that have appeared after 2000 use the same connection between mechanics and thermodynamics. The averaged balance equations are formally the same as in GFF so that the same techniques apply. Since the present paper treats many-component fluids, a generalization of the basic equations of the DI formalism is required: a generalization of Eq. (1) is provided by the Redlich–Kwong EOS (see Section 3.1), and a generalization of (3) is obtained by using a sum over the squared gradients of the component densities, each multiplied by its own constant Λ^α (see Eq. (9)).

It must finally be mentioned that a modern advance in the DI framework relates to Eq. (3). Its derivation is based on the assumption that the density gradient is small, i.e., physically, that the fluid is near the critical point. Using the DI method away from the critical point needs therefore to be justified. This has been done in several works since the 1980s: See Anderson et al. (1998), and Ganesan and Brenner (2000).

1.2. Overview of the model construction

An overview of the model construction follows. The assumptions are listed, then the construction steps are given, showing in particular the simplifications that are introduced. For details, see Papatzacos (2002, 2008, 2010).

Marle's method of averaging (Marle, 1982) has been used, with the following general assumptions:

1. Solid rigidity: the porous medium is perfectly rigid.
2. Validity of the Navier–Stokes equations inside the pores. This assumption establishes what is called the Navier–Stokes level (alternatively the pore level) below. Pore space is filled with molecules belonging to ν chemical species (also referred to as chemical components) that do not chemically react with each other.
3. DI assumption at the Navier–Stokes level: if there are many fluid phases inside the pores, then there are finite thickness interfaces between any two of them.
4. Identity between averaged fluid and pore level fluid: after averaging, see step ii below, it is meaningful to speak of an *averaged fluid* consisting of ν chemical components and obeying the same thermodynamical laws as the fluid at the Navier–Stokes level. In particular, the equation of state (EOS) is the same. Differences between the local temperatures of the solid and of the fluid are negligible.
5. DI assumption at the Darcy level: the properties of the averaged fluid are continuous in space and time. In the finite thickness interfaces, gradients of densities are important, and the Helmholtz free energy depends on the squared gradients of these densities. This dependence is written as an addition to the Hlmholtz free energy in the form of a linear combination of the squared density gradients.

The model construction is performed by the following steps:

i. Mass, momentum, and energy balance equations are written, for the fluid inside the pores, at the pore surfaces, and for the rock. Because of the DI assumption (see 3 above), there are no surface-like interfaces, and no balance equations for such interfaces (Papatzacos, 2002, 2008, 2010).