PORE-SCALE PHASE FIELD MODEL OF TWO-PHASE FLOW IN POROUS MEDIUM

Igor Bogdanov[1*], Sylvain Jardel[1], Anis Turki[1], Arjan Kamp[1]
[1]Open & Experimental Centre for Heavy Oil, University of Pau, Pau, France
*Corresponding author: igor.bogdanov@univ-pau.fr

Abstract: Pore-scale modeling of multiphase flow through porous media is addressed most frequently to improve our understanding of flow and transport phenomena in such settings. Besides, it can be used to obtain macro-scale constitutive equations, to provide multiphase flow properties for large scale models, to predict how these properties may vary with rock type, wettability, etc.

The description of a physical interface separating different phases inside a pore volume is a problem of crucial importance for such a modeling. Instead of using a regularization technique to capture the interface, which may affect the results in non-trivial way, the diffuse interface method is based on thermodynamic treatment of phase transition (or phase mixing) zone. As a result, it is a good choice for a numerical technique, handling the morphological changes of the interface.

We have used systematically the diffuse interface model (or equivalently, the field phase model) of two-phase immiscible stable and unstable flow for 2D and 3D computations in a porous medium. We compared numerical solutions to analytical solutions for simple geometries (parallel flat plates and a cylindrical tube) and calculated subsequently phase flows between regular arrays of cylinders or spheres.

In all cases to check a flow regime we calculated phase relative permeabilities. The impact of flow stability, wettability and capillary number on the flow pattern and models computational performance are also presented and discussed.

Keywords: pore scale flow, phase field, surface tension, wettability, capillary number.

1. Introduction

The underlying relation of the theory of multiphase flow through porous media – the generalized Darcy's law – applies to great variety of laminar (law local Reynold's number) flow cases (see *eg* Bear (1972), ch.5). The few known extensions to it - for lower and higher Reynold's number (Brinkman, Forchheimer etc. formulations) - just "prove the rule". In many petroleum and environmental applications, however, the Darcy's law is used not because it perfectly suits a flow problem but rather due to the absence of other general and more precise description of a fluid flow inside pores. For example, one of the problems which seem to be beyond the conventional theory framework is the so-called viscous fingering or in other words, a case of Saffman-Taylor instability observed in porous medium at heavy oil displacement by a more mobile fluid (*eg* water). The other examples are emulsion, foamy oil and so-called pre-Darcy flow still waiting for an adequate general model. Numerous attempts which have been made in the past decades to improve the understanding of mass transfer in porous media demonstrated that a pore scale description provides fruitful details of fluids transfer and distribution (*eg* Kalaydjan (1990), Whitaker (1986)).

So methodologically, the detailed flow description can be used to obtain macro-scale constitutive equations, to assign multiphase flow properties in large scale models, to predict how these properties may vary with rock type, wettability, etc.

Numerically speaking, the additional problems arise mainly from the phase dynamic boundary (interface) model which is a problem of crucial importance for a pore scale modeling. However available methods for modeling an interface separating fluids and possessing arbitrary configuration are limited.

Instead of applying a regularization technique to capture the interface, which may affect the results in non-trivial way, the diffuse interface method exploits a thermodynamic treatment of phase transition (or mixing) zone. As a result, physically justified approach is a good choice for a numerical technique, handling the morphological changes of the interface.

We present in current paper our recent work on diffuse interface approach application to two-phase flow problem. Our main purpose is to develop efficient 3D diffuse interface model which will allow us both to study the flow regimes and to evaluate its main parameters for the realistic pore space geometries.

2. Main physical factors of two-phase flow problem

Besides the pore space geometry which normally is oversimplified (and yet without proper argumentation - like in current work), the most important among the factors affecting the flow regimes on pore scale seem to be wettability, viscosity ratio and capillary number. The wettability together with the interfacial tension contributes to phase distribution equilibrium; the dynamic viscosity ratio (hereinafter $M=\mu_r/\mu_i$, i.e. recovered or initial to injected phase viscosity ratio) provides the conditions for stable or unstable displacement both at drainage and imbibitions. Finally, the capillary number characterizes the degree of deviation from equilibrium in a capillary dominating environment. The contact angle θ is wettability parameter giving the phase interface orientation with respect to grain surface (see model below). This parameter indicates wetting phase and defines the phase distribution inside pore space (Bear (1972), ch.9).

By conventional definition the capillary number characterizes the viscous to capillary (forces) ratio via following relation

$$Ca=\mu u/\sigma , \qquad (1)$$

which also can be interpreted, for instance, like ratio of pressure drop by viscous fluid flow to pressure drop by interfacial tension across the phases separating interface. Here μ is typical dynamic viscosity [Pa·s], u fluid velocity [m/s] and σ surface tension [N/m]. For the sake of simplicity we'll use in our estimations the value of capillary number at initial time: $Ca=Ca(t=0)= \mu_r\ u_t(t=0)/\sigma$, where u_t is total fluid volumetric flow, μ_r.viscosity of oil (recovered fluid).

Three other model parameters which usually arise during dimensional analysis – Reynold's, diffusive Peclet and Cahn numbers – have been kept within standard variations for the problems of interest, i.e. $Re<1$, $Cn<<1$, $Pe>1$.

3. Phase field model for COMSOL *Multiphysics* applications

Below is presented only the brief description of Cahn-Hilliard model. For more details of the theory and its formalism see Jacqmin (1999), Badalassi et al. (2003), Fichot et al. (2007). The second gradient theory assumes that free energy of a system is a functional of an order parameter φ, its gradient $\nabla\varphi$ and the temperature T:

$$F = F(\varphi, \nabla\varphi, T). \qquad (2)$$

In the case of an isothermal binary fluid, a free energy can be defined for flow configurations where the system is not in equilibrium as:

$$F(\varphi, \nabla\varphi) = \alpha\int_\Omega f\ dV = \alpha\int_\Omega \frac{1}{2}\left(|\nabla\varphi|^2 + g(\varphi)\right)\, dV \qquad (3)$$

where Ω is the region of space occupied by the system and φ is a dimensionless phase-field variable which serves to identify the two fluids with volume fraction $(1+\varphi)/2$ and $(1-\varphi)/2$. The chemical potential is defined as:

$$\nu = \alpha\ f'_\varphi\ , \qquad (4)$$

where α is the mixing energy density [N]. The fourth order partial differential equation describing the evolution of φ is the convective Cahn-Hilliard equation:

$$\frac{\partial\varphi}{\partial t} + (\mathbf{u}\cdot\nabla)\ \varphi - \nabla\cdot\left(M(\varphi)\nabla\mu\right) = 0\,. \qquad (5)$$

For $g(\varphi)$ a following double potential form is chosen:

$$g(\varphi) =(1/4\xi^2)\cdot(\varphi^2-1)^2, \qquad (6)$$

where ξ is a capillary width, [m], that scales with the thickness of the diffuse interface. Finally, from (4) it follows that the chemical potential can be written as:

$$\nu = \frac{\alpha}{\xi^2}\left[\varphi(\varphi^2-1) - \xi^2\nabla^2\varphi\right], \qquad (7)$$

while for the mobility the chosen expression is:

$$M(\varphi) =M_c\ (1-\gamma\varphi^2)\ \xi^2 \qquad (8)$$

where $0 \le \gamma \le 1$. At $\gamma\to 0$ the phase separation dynamics is controlled by bulk diffusion; in the opposite case $\gamma\to 1$, the phase separation dynamics is controlled by interface diffusion. Combining (5),(7) and the *modified* Navier-Stokes equations for incompressible fluid, the system of model equations to be solved reads as:

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\ \mathbf{u}\right) + \nabla p = \nabla\cdot\left[\mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)\right] + \nu\cdot\nabla\varphi$$

$$\nabla\cdot\mathbf{u} = 0$$

$$+\text{eq.}(5)\ +\text{eq.}(7) \qquad (9)$$

The equilibrium profile is obtained by minimizing the free-energy functional, with respect to the variations of the function φ, solving for

$\nu \equiv \delta F/\delta\varphi = 0$.

In the case of one-dimensional interface the solution is (cf. Jacqmin (1999))

$$\varphi = \pm\tanh[x/(\sqrt{2}\xi)]. \qquad (10)$$

In all calculations presented below the equation (10) has been used to give initial phase field over model region. The surface tension is introduced through the integral of the free-energy density across the interface; it can be shown that it relates two above defined model parameters α and ξ via the following relation:

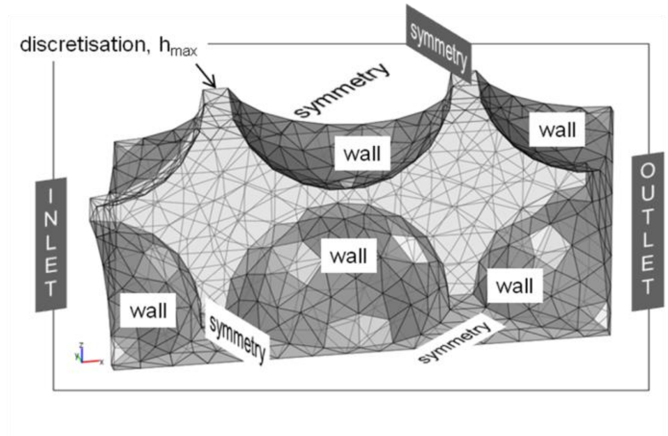
$$\sigma = (2\sqrt{2}/3)\cdot(\alpha/\xi). \qquad (11)$$

4. Boundary conditions

For the great majority of presented computations the boundary conditions are given in a way to impose a fixed pressure drop over the limits along a flow direction and extending a region geometry in lateral direction(s) via giving symmetry boundary conditions in a consistent way (cf. Figure 1a). The former just means that both normal phase diffusive and normal convective fluid flux disappear on the lateral boundaries. Standard wall conditions are used for the grain surfaces with no-slip and no phase diffusion flux given. Particular and specific conditions for different cases under consideration will be specified in due place during their description.

5. Results and discussion

As the main purpose of current work is the development of 3D model of two-phase flow and its systematic application to heavy oil displacement problems, let's start with the very



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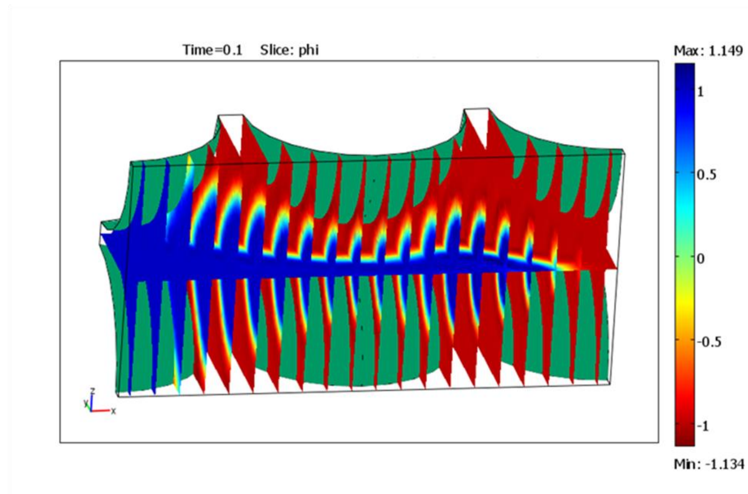

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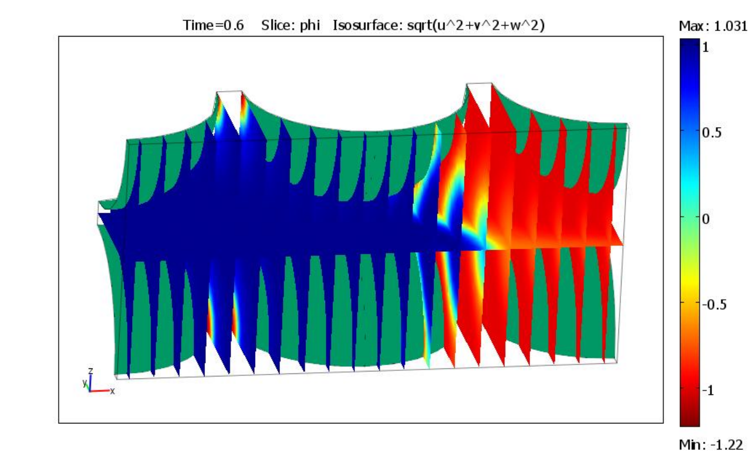


Figure 1. 3D model geometry and boundary conditions (a), viscous limit case phase field, *Ca*=0.15 (b) and intermediate case phase field, *Ca*=$2\cdot 10^4$ (c).

first results obtained recently using 3D COMSOL phase field model of the flow.

5.1 Results of 3D model

The model including few spherical grains in a regular packing is illustrated in Figure 1a. Symmetry conditions imposed on all lateral sides allows to complete the geometrical characterization of a medium in lateral directions (Figure 1a). The phase field variable is illustrated in Figure 1b,c for case of drainage of low viscous fluid for two different capillary numbers *Ca*. For relatively small *Ca* the distribution of φ only slightly depends on viscosity ratio *M*. Within the framework of this model we can't see classical fingers because their typical size exceeds the single pore size. Instead the local "finger" of injected fluid can be distinguished easily along the axis of flow channel – Figure 1b. Such a phenomenon which can be characterized as a simultaneous segregated flow of both phases in pores, was a starting point for modeling stationary segregated flow patterns in 3D and 2D systems and to further evaluate the (stationary) phase relative permeabilities (see below).

At higher *Ca*, however, the displacement becomes more complete, the "finger" of injected fluid disappears and volume of trapped oil decreases – Figure 1c. Becoming more and more important, the capillary force which is inversely proportional to pore/throat size constrains the fluids to occupy the medium pore space according to their size. This shows unambiguously the variation of flow pattern and therefore the phase permeability dependency on capillary number, at least.

5.2 Stationary segregated flow in channels

Before passing to determination of the transport medium properties let's have a look at analytical results for simple cases of segregated Hagen-Poiseuille flow in 2D two-phase systems. Making use of classical solution for single incompressible fluid and assuming that in two-phase case

(1) wetting fluid occupies the layer close to channel wall;

(2) the share stress in continuous throughout the fluid -

one arrives at "generalized" analytical solution which exists, evidently, both for linear (2D cartesian) and axisymmetrical (2D cylindrical) cases. This immediately leads to analytical closed form expressions for relative phase permeabilies illustrated in Figure 2 evaluated at different viscosity ratios (the only solution parameter). In this Figure the difference between numerical (symbols) and analytical (solid lines) solutions is due to the finite interface thickness ξ in numerical model. This difference tends regularly to zero at $\xi \to 0$. Note that at $M>1$ the non-wetting phase relative permeability shown in Fugure 2 exceeds 1 or in other words, demonstrates "non-darcian" behavior. As non-wetting occupies the channel space along a symmetry axis (or plane) where the flow velocity takes maximum value while wetting phase covers a wall and forms a kind of lubrication film for non-wetting phase "jet", a significantly augmented debit can be obtained. This lubrication effect at viscous phase drainage may locally take place in natural porous media and contribute to flow deviation from Darcy's law. The question is to which extent the segregated flow pattern is representative for a particular case of two phase flow in natural porous medium.

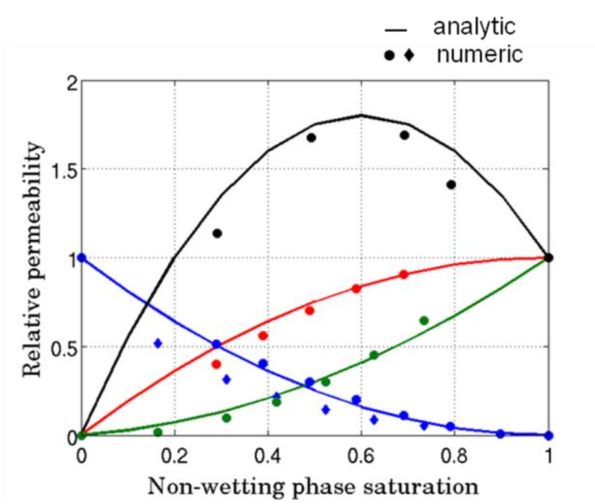


Figure 2. Phase relative permeabilities: numerical (symbols) and analytical (solid lines) results for wetting (blue) and non-wetting phase at M=0.1 (green); 1 (red); 10 (black).

5.3 Segregated flow in a synthetic 2D/3D media

Following the same reasoning the stationary segregated flow patterns have been studied for the simple models of 2D granular medium with grains represented by regular array of circles (cf. Figure 3) and of equivalent 3D media presented above in the subsection 5.1 (Figure 1). The lubrication effect takes place at M>1 in both cases. At the same time, being greater than 1 the maximum value of phase permeability in 2D and 3D is significantly less for 1D (analytical) case. The effect of more complex flow geometry is favorable for conventional Darcy's law based theory.

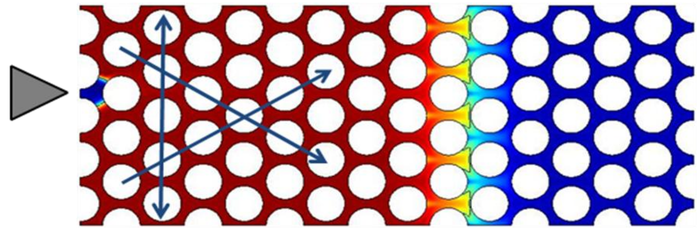
5.4 Pore scale models of viscous fingering

The viscous fingering effect is a particular case of Rayleigh-Taylor instability well-known in fluid mechanics. It takes place in case of displacement of less mobile (more viscous) liquid by more mobile (less viscous) one. In other words, the fingering normally occurs at M>1. This phenomenon occurs independently of medium properties and results in dynamic flow pattern which is sensitive to local variation of properties and may have a stabilized quasi-steady state.

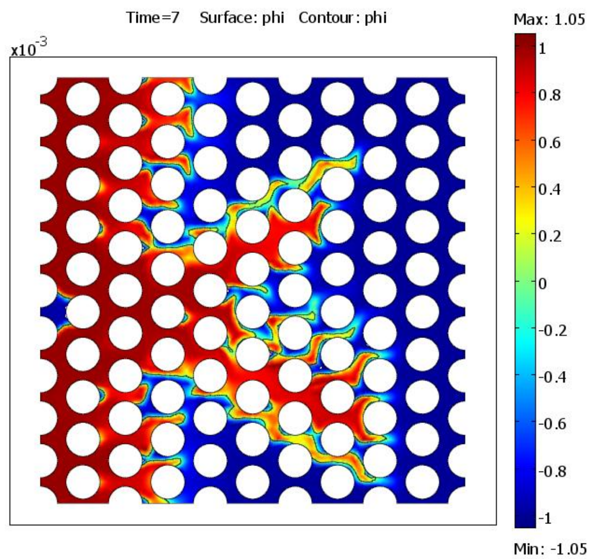
A uniform slightly anisotropic medium presented in Figure 3a was chosen for modeling of growing fingers at different viscosity ratio and capillary numbers. To accelerate the fingers development small initial flow perturbation (no-flow boundary condition) indicated by gray triangle in Figure 3a has been imposed. At viscosity ratio M<1 , however, it doesn't help to disturb plane displacement front.

At relatively high capillary numbers (viscous limit) the flow pattern depends on viscosity ratio only, the growing fingers following local properties variation related mainly to grain size/shape and perhaps, wettabily variations. At pore scale the typical porous material of oil reservoir is never homogeneous like it can be at Darcy scale (REV), so viscous fingering always faces and passes through local preferential flow paths. This aspect of fingering-channeling interaction can be seen in Figure 3b where two primary fingers follows main directions of anisotropic medium.

In the opposite limit of locally dominating capillary forces the interfacial tension effectively blocks the throats with radius below (at drainage) or above (at imbibition) certain critical value. For example, at drainage conditions this results in typical singular rivulet-like flow pattern



(a)



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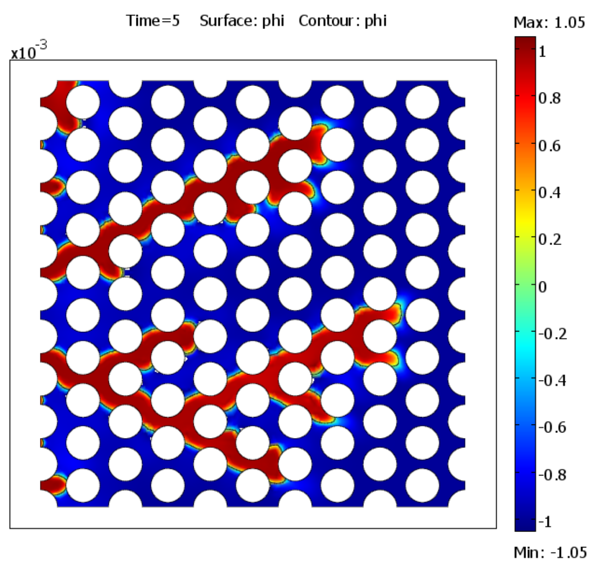

(c)

Figure 3. Stable drainage flow at M=0.1 in uniform anisotropic medium (a); unstable drainage flow at M=300 (viscous limit) (b); same case as (b) at capillary limit (c).

shown in Figure 3c. Note that local medium heterogeneities also plays important role here.

5.5 Topics for nearest future

The locally dominating capillary forces at pore scale are responsible for mass exchange by capillary imbibition which is important mechanism in many practical applications. Modeling this process in its dynamics in pores may provide better understanding of mass transfer from both qualitative and quantitative viewpoints. Realistic geometry of pores becomes one of key factors for such a modeling.

It seems possible that nothing but complex interplay between pore geometry, fluids wetting and viscous properties, interfacial tension and hydraulic potential contributes equally to the validity of existing theoretical approach. Then any more or less important simplification may lead to a deviation from "equilibrium" and even to degenerate behavior. From this viewpoint the pore scale models can be ultimately useful because of explicit description of all important physical mechanisms.

6. Conclusions

Promising first results have been obtained for 3D two-phase flow model based on diffuse interface approach. Flow regimes at viscous and capillary limits, for drainage and imbibitions, at favorable and unfavorable to viscous fingering viscosity ratio. Analysis of results expressed in terms of phase relative permeabilities allows to distinguish classical (Darcy's law based) and "non-classical" flow behavior which generally takes place, at least, locally during stable and unstable displacement.

Additional efforts are needed to extend the application field for 3D diffuse interface COMSOL model of two-phase pore scale flow.

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8. Acknowledgements

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