PHYSICAL REVIEW E VOLUME 58, NUMBER 5 NOVEMBER 1998

Dynamics of wetting fronts in porous media

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(Received 22 April 1998; revised manuscript received 4 September 1998)

We propose a phenomenological approach for describing the dynamics of wetting front propagation in porous media. Unlike traditional models, the proposed approach is based on the dynamic nature of the relation between capillary pressure and medium saturation. We choose a modified phase-field model of solidification as a particular case of such a dynamic relation. We show that in the traveling wave regime the results obtained from our approach reproduce those derived from the standard model of flow in porous media. In a more general case, the proposed approach reveals the dependence of front dynamics upon the flow regime. [S1063-651X(98)51411-0]

PACS number(s): 47.55.Mh, 47.55.Kf, 68.45.Gd, 87.22.As

The dynamics of fluids in porous media has been a subject of numerous theoretical and experimental studies because of its importance for engineering and environmental applications [1–3]. Among the most challenging problems in this area is modeling fluid flow through a partially saturated medium, in particular the propagation of wetting (or drying) fronts. This has been addressed on both ''microscopic'' (or pore-scale) and ''macroscopic'' (on scales larger than pore-size) levels. The fluid dynamics in the pore networks has been studied by numerous authors both theoretically [4] and experimentally [5,6]. These studies on the microscopic scale provide valuable insight into the underlying mechanisms of fluid transport in porous media. A microscopic description requires the detailed information of the pore structure and pore-size distribution. When this information is not available, as often happens for large domains, one has to rely upon a macroscopic description. This description is useful for determining such integral characteristics as the width and propagation velocity of moving wetting fronts, the influence of its curvature on the dynamics, etc.

The subject of the present work is the dynamics of wetting fronts in porous media when a liquid phase (water) displaces air. A straightforward description of this process consists of treating wetting fronts as sharp interfaces, which separates completely wet and dry regions [5,7]. However, in many realistic cases the structure of the transitional zone (wherein water saturation varies gradually) cannot be neglected. One can either describe the dynamics of the liquid and air phases separately, or noting that air pressure is close to atmospheric, consider only the dynamics of the liquid phase. These two approaches generally produce similar results (Ref. [8], p. 213). The latter approach seems to be more attractive due to its simplicity.

Within the framework of the chosen approach water flow is described by Darcy's law which, similarly to Ohm's law for electric current, stipulates the proportionality between the flux and gradient of a potential (see, e.g., [7]). For flow through porous media a water pressure, averaged over many pore sizes, plays the role of the potential. Richards [9] has empirically generalized Darcy's law onto flow in partially saturated porous media (PSPM) by letting the proportionality coefficient depend on saturation θ of the medium ($0<\theta<1$). Coupled with the mass conservation law, the generalized Darcy's law constitutes the existing macroscopic description of the fluid dynamics in PSPM. To complete this description, one needs to specify a relation between θ and capillary pressure (normalized by the product of fluid density ρ and gravitational acceleration g) ψ. Traditionally this relation is assumed to be algebraic [1,10]. However, this contradicts the numerous experimental evidences revealing the dependence of the θ-ψ relation upon the conditions of the experiment. In particular, this relation exhibits *hysteresis* for wetting and drying of a medium [1,10,11].

In the present Rapid Communication we propose a phenomenological approach to describe the propagation of wetting fronts in porous media, which is based on a *dynamic* θ-ψ relation. Our description consists of two dynamic equations for θ and ψ coupled by nonlinear sources. This implies that the traditional algebraic θ-ψ correspondence is replaced by a nonlocal (integro-differential) relationship. The proposed model is an application of the well-known ''phase-field'' approach used to describe solidification, electrodeposition, and other physical problems [12–17]. We show that, under certain conditions, dynamics of the wetting front in our approach reproduce that in the traditional approach. The same is true for the pressure profiles associated with the wetting fronts obtained from both models. We demonstrate that, under different conditions, this equivalence breaks down, with our model revealing a dynamic nature of the θ-ψ relation.

The generalized Darcy's law for flux $\mathbf{q}$ through PSPM has a form $\mathbf{q}=-K(\theta)\boldsymbol{\nabla}(\psi-x_3)$, where K is the saturation-dependent conductivity of the medium and x_3 is the vertical coordinate (positive downward) that stands for the gravitational component of pressure (normalized by ρg). Here ψ is measured relative to the ambient atmospheric pressure, so that $\psi<0$ for the partially saturated and $\psi\geqslant 0$ for the fully saturated medium. Combined with the mass conservation law, $\partial\theta/\partial t = -\boldsymbol{\nabla}\cdot\mathbf{q}$, this leads to the equation introduced by Richards [9]

$$\frac{\partial\theta}{\partial t} = \boldsymbol{\nabla}\cdot[K(\theta)\boldsymbol{\nabla}(\psi - x_3)]. \tag{1}$$

Over the years a number of algebraic θ-ψ and $K(\theta)$ relations have been proposed empirically (see, e.g., [18–20]). The Richards equation (RE) (1) combined with such a relation constitutes the traditional approach to describe flow in PSPM. Since algebraic relations are not supported by experimental data, in what follows we propose an approach with a dynamic θ-ψ relation.

To describe flow in PSPM, we modify the phase-field model (PFM) from [12]

$$\frac{\partial\psi}{\partial t} = D\nabla^2\psi - \frac{1}{S}\frac{\partial\theta}{\partial t} - D\frac{\partial\theta}{\partial x_3}, \tag{2}$$

$$\tau\frac{\partial\theta}{\partial t} = W^2\nabla^2\theta + [2\theta - 1 - \lambda(\psi - \psi_f)\theta(1-\theta)]\theta(1-\theta), \tag{3}$$

where $D = K_s/S$ is the diffusion coefficient, K_s is the conductivity of a fully saturated medium, S is the specific storage (measure of compressibility of the fluid and medium), τ is a characteristic time scale of the saturation dynamics, and W is the width of a moving wetting front. The model parameter λ will be determined as a function of macroscopic parameters K_s, W, and τ. The constant ψ_f is the normalized capillary pressure along the moving front in the sharp-interface limit. We will demonstrate below that ψ_f coincides with the pressure in the dry medium far ahead of the wetting front. Since the width of the capillary zone, associated with the localized wetting fronts, is much smaller than the typical scale of the pressure variation, the following holds: $W^2/\tau \ll D$. We have added the last term in Eq. (2) to PFM [12], to account for the gravitational force.

Our model is phenomenological in the sense that presently we do not provide a rigorous physical motivation for the nonlinear source term on the right-hand side of Eq. (3). Nevertheless, the model captures the main features of the wetting fronts' propagation in porous media. In particular, numerous experiments [21,22] have shown that under certain conditions the wetting fronts remain localized and propagate in a self-similar manner. The medium is fully saturated ($\theta = 1$) behind the front region and completely dry ($\theta = 0$) ahead of the front. The cubic polynomial in Eq. (3) provides for such a structure of the wetting front (similar to the PFM for solidification). The fact that the liquid moves in the direction opposite to the pressure gradient is accounted for by the term proportional to $(\psi - \psi_f)$ in Eq. (3), since its presence makes the depths of the two minima of the corresponding potential energy different.

Equations (2) and (3) have to be supplemented by a constraint to ensure conservation of mass. The specific storage is related to the compressibility of the fluid and porous medium as $S = \rho g \omega(\beta_f - \beta_s + \beta_p)$ (Ref. [8], p. 108). Here ω is the medium porosity (fraction of pore volume in the total volume v of the medium), and β_f, β_m, and β_p are the compressibility coefficients of the fluid, solid grains, and pores, respectively. The total mass of the fluid is given by $M = \int_v \omega\,\rho\,\theta\,d\mathbf{x}$. For incompressible fluids and media ($S = 0$), since $D = K_s/S$, Eq. (2) reads $\partial\theta/\partial t = K_s(\nabla^2\psi - \partial\theta/\partial x_3)$, which conserves mass. For compressible fluids and media $dM/dt = Q$, where Q is the total mass flux through the medium, provides the global constraint on the system [Eqs. (2) and (3)].

Since S is the *specific* storage of a medium, the effect of the compressibility of fluids and media on flow dynamics is characterized by the dimensionless parameter SL, where L is a typical domain size. For many practical applications, such as the flow of water through low porosity rocks, $S \sim 10^{-5} - 10^{-7}\ \mathrm{m}^{-1}$ and $L \sim 10^{-1} - 10^3$ m. Thus $SL \ll 1$, and the fluid and medium are virtually incompressible.

We consider propagation of one-dimensional (1D) wetting fronts in a slightly compressible medium with $SL \ll 1$. The dynamics of these fronts is described by 1D Eqs. (2),(3), and the mass conservation constraint is satisfied automatically. Two different situations exist: horizontal (gravity-free) and vertical front propagation. To maintain propagation of a self-similar front, we choose the constant flux condition $\partial(\psi - x_3)/\partial x_i = -q/K_s$ at $x_i = 0$, and the no-flux condition for capillary force $\partial\psi/\partial x_i = 0$ at $x_i = L$. Here $i = 1$ or $i = 3$ for horizontal or vertical flow, respectively, and q is an external velocity flux. At the boundary behind the front, $x_i = 0$, the medium is fully saturated ($\theta = 1$), and at the boundary ahead of the front, $x_i = L$, the medium is dry ($\theta = 0$).

Let us apply a traveling wave ansatz $z = x_i - Vt$, for a front moving with velocity V, to 1D Eqs. (2) and (3). Relations $W \sim V\tau$ and $W^2/\tau \ll D$ give rise to a small parameter Pe$\ll 1$, where Pe$=VW/D$ is the Péclet number. The perturbation analysis around Pe$=0$, similar to that performed in [12], gives a front moving with velocity $V = q$, and saturation and capillary pressure profiles

$$\theta(z) = \frac{1}{2}\left[1 - \tanh\left(\frac{z}{2\sqrt{2}W}\right)\right] + O(\mathrm{Pe}), \tag{4}$$

$$\psi(z) = \psi_f + J\left\{W\sqrt{2}\ln 2 - \frac{z}{2} + W\sqrt{2}\ln\left[\cosh\left(\frac{z}{2\sqrt{2}W}\right)\right]\right\} + O(\mathrm{Pe}^2). \tag{5}$$

Here J is an absolute value of the capillary pressure gradient at the boundary. It is given by $J = q/K_s$ for a horizontally propagating front, and by $J = (q/K_s - 1)$ for a vertically propagating front. A vertical wetting front does not exist when $q \leqslant K_s$, i.e., when the external flux is not large enough to compensate for the effect of the gravity force, and thus develop a saturated zone.

The saturation profile (4) is evaluated in the zeroth order in Pe, since, for the localized wetting fronts, saturation varies in the narrow region $W \ll \sqrt{D\tau}$. Hence the higher order corrections to θ influence the nonlocal pressure profile (5) only in the second order. The solvability condition for the equation for θ in the first order (similar to [12]) yields $\tau/\lambda \approx -0.313 W^2 J/q$.

We now compare our approach with the traditional (Richards) approach. One of the most widely used examples of

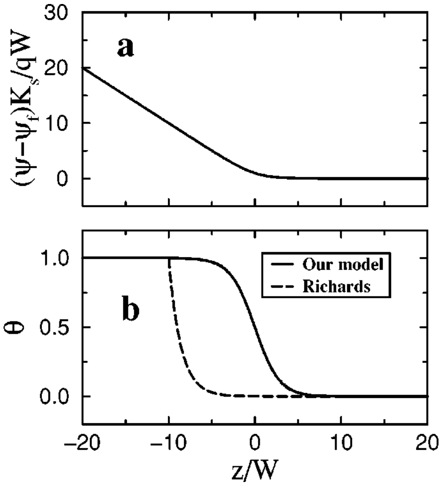

FIG. 1. (a) Normalized capillary pressure $(\psi-\psi_f)K_s/qW$ and (b) saturation profiles in the traveling wave coordinate. In (b) normalized capillary pressure in a dry medium is taken, $\psi_f K_s/qW = -10$.

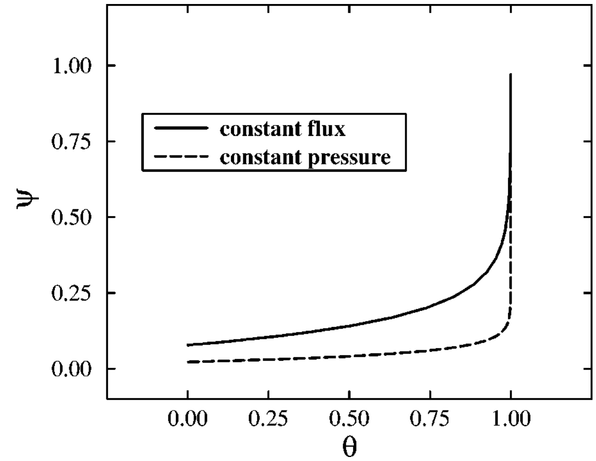

FIG. 2. Dynamic θ-ψ relation for both the traveling wave and non-traveling-wave regimes. Parameters of the simulations are $D=1$, $W=0.1$, $S=0.005$, $\tau=1$. For the traveling wave regime $q=K_s$. The value of λ is calculated according to the selection result $\tau/\lambda \approx -0.313W^2J/q$. System size $L=10$ and number of grid points is 201. Time step $dt=0.001$.

algebraic functions $\theta(\psi)$ and $K(\theta)$, complementary to RE (1), has been proposed by Gardner [10,18],

$$\theta(\psi)=e^{\alpha\psi}, \quad K(\theta)=K_s\theta, \tag{6}$$

where α is the pore-size distribution parameter. The first equation in Eq. (6) is valid for $\psi<0$ (when the medium is partially saturated) while, for $\psi\geqslant 0$ (for a fully saturated medium), $\theta\equiv 1$. The same boundary conditions as before are used. Substituting Eq. (6) into 1D Eq. (1), and applying the traveling wave ansatz gives, after a series of transformations, the solution for the pressure profile

$$\psi(z)=\frac{\ln 2}{\alpha}+\psi_L-\frac{Jz}{2}+\frac{1}{\alpha}\ln\left[\cosh\left(\frac{\alpha J}{2}z\right)\right], \tag{7}$$

where ψ_L is a large negative number corresponding to the pressure in the dry medium far ahead of the front.

Comparing Eq. (7) with Eq. (5) we find that the pressure profiles obtained from both models coincide, provided that the relations between the parameters $\sqrt{2}WJ=\alpha^{-1}$ and $\psi_f=\psi_L$ hold. Figure 1(a) shows the resulting pressure profile from both models. Substituting Eq. (7) into the first relation in Eq. (6) we obtain the saturation profile for the Richards model. The result is compared with the saturation profile (4) in Fig. 1(b). Although the saturation profiles differ within the capillary zone, this difference occurs on the very small scale W. An unphysical sharp kink that appears in the Richards model for $\theta(z)$ is absent in our model. Comparing Fig. 1(b) with the experimental data presented in Figs. 2–5 of Ref. [22] shows that the saturation profile obtained by our model agrees with the experiments.

Though in the traveling wave regime our model reproduces the results obtained from the Richards model, it is also capable of capturing the dynamic θ-ψ relation in different regimes, without adjusting the parameters. This is not the case for the Richards model, where one needs to adjust the parameter α in Eq. (6) to different experimental regimes. To demonstrate the dynamic nature of the θ-ψ relation in our model, we have performed the numerical simulations of 1D Eqs. (2),(3) under several boundary conditions. We solved the system [Eqs. (2),(3)] using finite differences. Note that though in our simulations $SL\ll 1$, we keep the term $S\partial\psi/\partial t$ in Eq. (2). Despite being small, this term provides a relaxational feature to a numerical solution of Eq. (2), which stabilizes the numerical algorithm. Figure 2 shows $\theta(\psi)$ obtained from these simulations for horizontal flow. The solid line in the figure corresponds to the traveling wave regime, resulting from the previously described boundary conditions. The dashed line represents $\theta(\psi)$ at time $t=1000$ corresponding to the wetting with the constant pressure at $x_1=0$ and the same no-flux condition at $x_1=L$.

Note that in the limit of the narrow capillary zone, $W\to 0$, our model describes the dynamics of sharp interface, which separates completely wet $(\theta=1)$ and completely dry $(\theta=0)$ regions. This is in analogy with the PFM of solidification that reduces to the free-boundary problem [12]. It follows from Eq. (5) that in this limit $\psi(0)=\psi_f$ and $\psi_z(0)=-J$. Moreover, Eq. (2) reduces to a diffusion equation, which is commonly used to describe flow in saturated media.

In conclusion, we have proposed an approach to describe the dynamics of wetting fronts in porous media. Unlike the traditional approach, our phenomenological approach reflects the dynamic nature of the relationship between capillary pressure and saturation of a medium. We have found that this relationship varies with the flow regimes, which is supported by experimental data. We have demonstrated that, in the traveling wave regime, the proposed model reproduces the results obtained from the standard approach. We plan to extend our approach to two- and three-dimensional media, incorporating in the description the front curvature and anisotropy of the medium. We expect to develop experimental support for the proposed approach by measuring quantitative features of the wetting fronts in porous media, such as the dependence of the front width on external flux.

We are grateful to R. Camassa, G. Forest, M. Hyman, S.-Y. Chen, and J. Glazier for fruitful and clarifying discussions.

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