

# Percolation as a Basic Concept for Macroscopic Capillarity

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Received: 12 November 2008 / Accepted: 6 February 2009  
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**Abstract** The concepts of relative permeability and capillary pressure are crucial for the accepted traditional theory of two phase flow in porous media. Recently, a theoretical approach was introduced that does not require these concepts as input (Hilfer, *Physica A*, 359:119–128, 2006a; *Phys. Rev. E*, 73:016307, 2006b). Instead it was based on the concept of hydraulic percolation of fluid phases. This paper presents the first numerical solutions of the coupled nonlinear partial differential equations introduced in Hilfer (*Phys. Rev. E*, 73:016307, 2006b). Approximate numerical results for saturation profiles in one spatial dimension have been calculated. Long time limits of dynamic time-dependent profiles are compared to stationary solutions of the traditional theory. The initial and boundary conditions are chosen to model the displacement processes that occur when a closed porous column containing two immiscible fluids of different density is raised from a horizontal to a vertical position in a gravitational field. The nature of the displacement process may change locally in space and time between drainage and imbibition. The theory gives local saturations for nonpercolating trapped fluids near the endpoint of the displacement.

**Keywords** Capillarity · Hysteresis · Residual saturation · Multiphase flow · Porous media · Immiscible displacement

## 1 Introduction

Almost all accepted and applied theories of multiphase flow in porous media are based on generalized Darcy laws and the concurrent concept of relative permeabilities (Wyckoff and Botset 1936). Despite the fact that Wyckoff and Botset (1936) strongly emphasized the variation of hydraulically disconnected fluid regions (Jamin 1860), almost all subsequent applications of the relative permeability concept treat the residual nonwetting (or irreducible wetting) saturations as material constants (Bear 1972; Collins 1961; Dullien 1992; Helmig 1997; de Wiest 1969; Scheidegger 1957; Marsily 1986)

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Modern theories of multiphase flow in porous media often resort to microscopic models (e.g., network models) (Bear et al. 1987; Blunt et al. 1992; Bryant et al. 1993; Dias and Payatakes 1986; van Dijke and Sorbie 2002; Fatt 1956; Ferer et al. 2003; Hidajat et al. 2001; Hilfer 1996; Jerauld and Salter 1990; Payatakes and Neira 1977). An important motivation is the need to derive or estimate macroscopic relative permeabilities from pore scale parameters. It was emphasized in Wyckoff and Botset (1936), however, that the “*possibility of determining the overall dynamical behavior of nonhomogeneous fluids from a study of microscopic details*” is remote (Wyckoff and Botset 1936, p. 326). One should instead consider saturation, velocities, and pressure gradient “*to derive therefrom the overall or macroscopic behavior of the system*” (Wyckoff and Botset 1936). Rather surprisingly, the authors of (Wyckoff and Botset 1936) emphasize the important difference between “*continuous moving*” fluids and “*stationary or locked*” fluids in their introduction, but later cease to distinguish between them in the main body of the paper. Experimentally, the volume fraction of stationary, locked, trapped, or nonpercolating fluid phases varies strongly with time and position (Abrams 1975; Avraam and Payatakes 1995; Taber 1969; Wyckoff and Botset 1936). Modeling such variations of trapped or nonpercolating fluid phases explicitly is the main objective of this paper.

Dispersed droplets, bubbles, or ganglia of one fluid phase obstruct the motion of the other fluid phase. Extensive experimental and theoretical studies of this simple phenomenon exist (Avraam and Payatakes 1999; Gardescu 1930; Jamin 1860; McKellar and Wardlaw 1982; Øren et al. 1992; Oxaal 1991; Oxaal et al. 1991; Payatakes 1982). It is, therefore, surprising that the concept of hydraulic percolation has been neglected in the modeling of two phase flow until 10 years ago (Hilfer 1998).

Given that the basic concept of hydraulic percolation for macroscopic capillarity has been discussed extensively in (Hilfer 2006a, b, c) our objective in this paper is to find approximate numerical solutions of the mathematical model. Let us, therefore, begin the discussion by formulating a set of mathematical equations for the hydraulic percolation approach in Sect. 2. One also needs to specify initial and boundary conditions representing a realistic experiment. Raising a closed column from a horizontal to a vertical orientation causes simultaneous imbibition and drainage processes inside the medium as emphasized already in Hilfer (2006b). In this paper, we report approximate numerical results for the full time evolution of such simultaneous imbibition and drainage processes. As expected, the resulting equilibrium saturations depend strongly on the initial conditions. Moreover, they differ significantly from the equilibrium profiles of the traditional theory.

## 2 Formulation of the Model

### 2.1 Balance Laws

Consider a one-dimensional, homogeneous, isotropic, and incompressible porous column filled with two immiscible Newtonian fluids. In a one-dimensional model transversal variations and column thickness are neglected. Let  $S_{\mathbb{W}} = S_{\mathbb{W}}(x, t)$  denote the saturation of wetting fluid (called water), and  $S_{\mathbb{O}} = S_{\mathbb{O}}(x, t)$  the saturation of nonwetting fluid (called oil). Here, time is  $t \geq 0$ , and  $x \in [0, L]$  is the position in a column of length  $L$ . Each of the two fluid phases is considered to consist of a continuous, mobile, percolating subphase, and of a discontinuous, isolated, trapped, or nonpercolating subphase as discussed in Hilfer (1998); Hilfer and Besserer (2000a); Hilfer (2006a, b, c). Following the notation of Hilfer (2006b), the percolating phase of water is indexed by  $i = 1$  and its nonpercolating phase is

indexed by  $i = 2$ . The water saturation is then  $S_{\mathbb{W}} = S_1 + S_2$ . The percolating oil phase is indexed as  $i = 3$  and its nonpercolating phase by  $i = 4$ . The oil saturation is  $S_{\mathbb{O}} = S_3 + S_4$ . The volume fraction  $\phi_i$  of phase  $i$  is defined as  $\phi_i = \phi S_i$ , where the volume fraction of the pore space, also called porosity, is  $\phi$ . The volume fraction of the solid matrix is denoted as  $\phi_5 = 1 - \phi$ . Volume conservation requires

$$\phi_1 + \phi_2 + \phi_3 + \phi_4 + \phi_5 = 1 \tag{1a}$$

$$S_1 + S_2 + S_3 + S_4 = 1 \tag{1b}$$

to hold.

The mass balance of fluid phase  $i$  can be expressed in differential form as

$$\frac{\partial(\phi_i \varrho_i)}{\partial t} + \frac{\partial(\phi_i \varrho_i v_i)}{\partial x} = M_i, \tag{2}$$

where  $\varrho_i(x, t)$ ,  $\phi_i(x, t)$ ,  $v_i(x, t)$  are mass density, volume fraction and velocity of phase  $i$  as functions of position  $x \in \mathbb{S} = [0, L] \subset \mathbb{R}$ , and time  $t \in \mathbb{R}_+$ .  $M_i$  is the mass transfer rate from all other phases into phase  $i$ .

The momentum balance is written as ( $i = 1, 2, 3, 4$ )

$$\phi_i \varrho_i \frac{D^i}{Dt} v_i - \phi_i \frac{\partial \Sigma_i}{\partial x} - \phi_i F_i = m_i - v_i M_i, \tag{3}$$

where  $\Sigma_i$  is the stress tensor in the  $i$ th phase,  $F_i$  is the body force per unit volume acting on the  $i$ th phase,  $m_i$  is the momentum transfer into phase  $i$  from all the other phases, and  $D^i/Dt = \partial/\partial t + v_i \partial/\partial x$  denotes the material derivative for phase  $i$ . The stress tensor for the nonpercolating phases is defined as the momentum flux across surfaces in the three-dimensional continuum (see [Hilfer and Besserer \(2000b\)](#) for more discussion).

### 2.2 Constitutive Assumptions

For a macroscopically homogeneous porous medium

$$\phi(x) = \phi = \text{const} \tag{4}$$

is assumed. Incompressible fluids are assumed, so that their densities

$$\varrho_1(x, t) = \varrho_{\mathbb{W}} \tag{5a}$$

$$\varrho_2(x, t) = \varrho_{\mathbb{W}} \tag{5b}$$

$$\varrho_3(x, t) = \varrho_{\mathbb{O}} \tag{5c}$$

$$\varrho_4(x, t) = \varrho_{\mathbb{O}} \tag{5d}$$

are independent of  $x, t$ .

The percolating and the nonpercolating phases are able to exchange mass through breakup and coalescence of droplets, ganglia, and clusters. The mass transfer rates must depend on rates of saturation change. They are, here, assumed to be

$$M_1 = -M_2 = \eta_2 \phi \varrho_{\mathbb{W}} \left( \frac{S_2 - S_2^*}{S_{\mathbb{W}}^* - S_{\mathbb{W}}} \right) \frac{\partial S_{\mathbb{W}}}{\partial t} \tag{6a}$$

$$M_3 = -M_4 = \eta_4 \phi \varrho_{\mathbb{O}} \left( \frac{S_4 - S_4^*}{S_{\mathbb{O}}^* - S_{\mathbb{O}}} \right) \frac{\partial S_{\mathbb{O}}}{\partial t}, \tag{6b}$$

where  $\eta_2, \eta_4$  are constants. The parameters,  $S_{\text{W}}^*, S_{\text{O}}^*, S_2^*$ , and  $S_4^*$ , are defined by

$$S_{\text{W}}^* = (1 - S_{\text{O}r})\Theta(\partial_t S_{\text{W}}) + S_{\text{Wi}}[1 - \Theta(\partial_t S_{\text{W}})] \tag{7a}$$

$$S_{\text{O}}^* = 1 - S_{\text{W}}^* \tag{7b}$$

$$S_2^* = S_{\text{Wi}}[1 - \Theta(\partial_t S_{\text{W}})] \tag{7c}$$

$$S_4^* = S_{\text{O}r}\Theta(\partial_t S_{\text{W}}), \tag{7d}$$

where  $S_{\text{Wi}}, S_{\text{O}r}$  are limiting saturations for  $S_2, S_4$ . In Eq. 7, the shorthand  $\partial_t = \partial/\partial t$  is used and

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x \leq 0 \end{cases} \tag{8}$$

denotes the Heaviside unit step function. Equation (7) follows from the form used in Hilfer (2006b) for small rates of saturation change. The mass exchange depends on the sign of  $\partial_t S_{\text{W}}$ . The sign determines the type of process. It can switch locally between drainage and imbibition. This results in hysteresis. The structure of the mass exchange term was chosen with hindsight such that theoretical results obtained in the residual decoupling approximation agree with experimental measurements of capillary pressure. The mass exchange terms have recently been further generalized to reproduce not only capillary pressure but also experimental capillary desaturation curves (Hilfer 2009).

Turning to the momentum balance, note first that the inertial term will not be neglected in this paper. The stress tensor for the four phases are specified as

$$\Sigma_1 = -P_1 \tag{9a}$$

$$\Sigma_2 = -P_3 + \gamma P_2^* S_2^{\gamma-1} \tag{9b}$$

$$\Sigma_3 = -P_3 \tag{9c}$$

$$\Sigma_4 = -P_1 + \delta P_4^* S_4^{\delta-1}, \tag{9d}$$

where  $P_1$  and  $P_3$  are the fluid pressures in the percolating phases. The constants  $P_2^*, P_4^*$ , and exponents  $\gamma, \delta$  are constitutive parameters. The assumptions for the nonpercolating phases reflect their modified pressure. This phenomenon seems to have been observed in experiment (Ataie-Ashtiani et al. 2003, Fig. 1, p. 233).<sup>1</sup> In applications, the parameters  $P_2^*, P_4^*$ , and  $\gamma, \delta$  are determined by measuring capillary pressure curves (see below). The body forces are assumed to be given by gravity and capillarity. They are specified as

$$F_1 = \varrho_1 g \sin \vartheta \tag{10a}$$

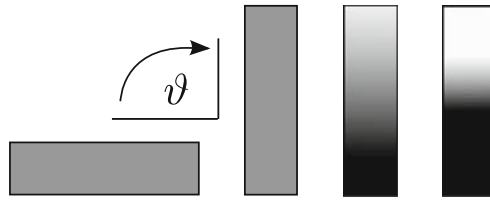
$$F_2 = \varrho_2 g \sin \vartheta + \Pi_a \frac{\partial S_1^{-\alpha}}{\partial x} \tag{10b}$$

$$F_3 = \varrho_3 g \sin \vartheta \tag{10c}$$

$$F_4 = \varrho_4 g \sin \vartheta + \Pi_b \frac{\partial S_3^{-\beta}}{\partial x} \tag{10d}$$

with constitutive constants  $\Pi_a, \Pi_b$ , and exponents  $\alpha, \beta > 0$ . The angle  $0 \leq \vartheta \leq \pi/2$  is the angle between the direction of the column and the direction of gravity with  $\vartheta = \pi/2$

<sup>1</sup> Figure 2 in Ataie-Ashtiani et al. (2003) shows that the pressure measured by the pore pressure transducers PPT3 and PPT4 rebounds after the end of the infiltration, i.e., when the DNAPL has passed and the transducers measure the pressure of water and residual PCE.



**Fig. 1** Raising a closed column according to the protocol of (14). Initially, the column is oriented horizontally and the saturations are constant. Regions of high water saturation are indicated in darker shade, and regions of high oil saturation are indicated in lighter shade. The last two columns illustrate the simultaneous imbibition (lower part of column) and drainage (upper part of column) processes that finally result in the formation of a capillary fringe

corresponding to alignment. In applications, the parameters  $\Pi_a$ ,  $\Pi_b$ , and  $\alpha$ ,  $\beta$  are determined by measuring capillary pressure curves. The capillary body forces in Eq. 10 reflect the wetting properties of the medium. They oppose gravity and reduce buoyancy driven flows of the disconnected phases. This is illustrated in the figures below.

Finally, the momentum transfer terms are assumed to be given by linear viscous drag characterized by constitutive resistance coefficients  $R_{ij}$  through the equations

$$m_1 = R_{13}(v_3 - v_1) + R_{14}(v_4 - v_1) - R_{15}v_1 \tag{11a}$$

$$m_2 = R_{23}(v_3 - v_2) + R_{24}(v_4 - v_2) - R_{25}v_2 \tag{11b}$$

$$m_3 = R_{31}(v_1 - v_3) + R_{32}(v_2 - v_3) - R_{35}v_3 \tag{11c}$$

$$m_4 = R_{41}(v_1 - v_4) + R_{42}(v_2 - v_4) - R_{45}v_4, \tag{11d}$$

where  $R_{12} = 0$  and  $R_{34} = 0$  was used because there is no common interface and hence, no direct viscous interaction between these phase pairs. Remember that the index  $i = 5$  represents the rock matrix. For more details on these constitutive assumptions the reader is referred to the original papers (Hilfer 2006a, b, c).

The balance laws (1b), (2), and (3) combined with the constitutive assumptions given above provide 9 equations for the 10 unknowns  $S_i$ ,  $v_i$ ,  $P_1$ ,  $P_3$  with  $i = 1, 2, 3, 4$ . To close the system of equations the conditions  $v_2 = 0$  or  $v_4 = 0$  could be used. These conditions apply when the nonpercolating phases are immobile as it is often observed in experiment. It turns out, however, that there exists a less restrictive and, in our opinion, more natural self-consistent closure.

The self-consistent closure condition used in this paper follows naturally from many limiting cases. One such limit is the residual decoupling approximation close to hydrostatic equilibrium described in detail in (Hilfer 2006b, Sect. 5, p.216ff). A second, more general limiting case is the limit of vanishing velocities, i.e.,  $v_i \rightarrow 0$  for  $i = 1, 2, 3, 4$ . Here, we formulate the self-consistent closure condition in its most general form as

$$\begin{aligned} 0 = & \left( \frac{R_{13}}{\phi_1} + \frac{R_{14}}{\phi_1} + \frac{R_{15}}{\phi_1} + \frac{R_{31}}{\phi_3} - \frac{R_{41}}{\phi_4} + \frac{M_1}{\phi_1} \right) v_1 + \varrho_1 \frac{D^1}{Dt} v_1 \\ & + \left( -\frac{R_{23}}{\phi_2} - \frac{R_{24}}{\phi_2} - \frac{R_{25}}{\phi_2} + \frac{R_{32}}{\phi_3} - \frac{R_{42}}{\phi_4} + \frac{M_1}{\phi_2} \right) v_2 - \varrho_2 \frac{D^2}{Dt} v_2 \\ & + \left( -\frac{R_{13}}{\phi_1} + \frac{R_{23}}{\phi_2} - \frac{R_{31}}{\phi_3} - \frac{R_{32}}{\phi_3} - \frac{R_{35}}{\phi_3} - \frac{M_3}{\phi_3} \right) v_3 - \varrho_3 \frac{D^3}{Dt} v_3 \\ & + \left( -\frac{R_{14}}{\phi_1} + \frac{R_{24}}{\phi_2} + \frac{R_{41}}{\phi_4} + \frac{R_{42}}{\phi_4} + \frac{R_{45}}{\phi_4} - \frac{M_3}{\phi_4} \right) v_4 + \varrho_4 \frac{D^4}{Dt} v_4. \end{aligned} \tag{12}$$

This condition follows self-consistently from the constitutive theory. It expresses the experimental observation that the pressure difference  $P_3 - P_1$  depends more strongly on saturations than on velocities, and that it remains nonzero even for vanishing velocities. Adding Eq. 3 for  $i = 2$  and  $i = 3$  and subtracting Eq. 3 with  $i = 1$  and  $i = 4$  from the result gives

$$\frac{\partial P_3}{\partial x} = \frac{\partial P_1}{\partial x} + \frac{\partial}{\partial x} \left[ \Pi_a S_1^{-\alpha} - \Pi_b S_3^{-\beta} + \gamma P_2^* S_2^{\gamma-1} - \delta P_4^* S_4^{\delta-1} \right]. \tag{13}$$

In this form, the self-consistent closure has been used in the numerical calculation below.

The mathematical model defined above was introduced and discussed in Hilfer (2006a, b, c). It was recently extended to include surface tension (Hilfer 2009). Notation and model formulation in this paper follow (Hilfer 2006b). Approximations and analytical solutions for some special cases were given in Hilfer (2006a, b, c). Here, the system of equations will be solved by numerical methods. To this end, initial and boundary conditions are needed and will be discussed next.

### 3 Initial Conditions, Boundary Conditions, and Model Parameters

Consider a cylindrical column containing a homogeneous, isotropic, and incompressible porous medium. The column is closed at both ends and filled with two immiscible fluids. Assume that the surface and interfacial tensions are such that the capillary fringe is much thicker than the column diameter, so that a one-dimensional description is appropriate.

The experimental situation considered here is that of raising a closed column as described in (Hilfer 2006b, p. 223). It is illustrated in Fig. 1. Initially, at instant  $t = 0$ , both fluids are at rest. The column is oriented horizontally ( $\vartheta = 0$ ), i.e., perpendicular to the direction of gravity. The displacement processes are initiated by rotating the column into a vertical position. The time protocol for rotating the column may be written as

$$\vartheta(t) = \arcsin \left\{ \frac{1}{2} \left[ \tanh \left( \frac{t - t_*}{t_{**}} \right) + 1 \right] \right\}, \tag{14}$$

where  $t_*$  is the instant of most rapid rotation and  $t_{**}$  is the inverse rate of the rotation.

The constitutive equations yield the following system of 10 coupled nonlinear partial differential equations

$$\frac{\partial S_1}{\partial t} + \frac{\partial(S_1 v_1)}{\partial x} = \eta_2 \left( \frac{S_2 - S_2^*}{S_{\text{W}}^* - S_{\text{W}}} \right) \frac{\partial S_{\text{W}}}{\partial t} \tag{15a}$$

$$\frac{\partial S_2}{\partial t} + \frac{\partial(S_2 v_2)}{\partial x} = -\eta_2 \left( \frac{S_2 - S_2^*}{S_{\text{W}}^* - S_{\text{W}}} \right) \frac{\partial S_{\text{W}}}{\partial t} \tag{15b}$$

$$\frac{\partial S_3}{\partial t} + \frac{\partial(S_3 v_3)}{\partial x} = \eta_4 \left( \frac{S_4 - S_4^*}{S_{\text{O}}^* - S_{\text{O}}} \right) \frac{\partial S_{\text{O}}}{\partial t} \tag{15c}$$

$$\frac{\partial S_4}{\partial t} + \frac{\partial(S_4 v_4)}{\partial x} = -\eta_4 \left( \frac{S_4 - S_4^*}{S_{\text{O}}^* - S_{\text{O}}} \right) \frac{\partial S_{\text{O}}}{\partial t} \tag{15d}$$

$$\begin{aligned} \rho_{\text{W}} \frac{D^1}{Dt} v_1 + \frac{\partial P_1}{\partial x} - \rho_{\text{W}} g \sin \vartheta \\ = \sum_{j=1}^5 \frac{R_{1j}}{\phi S_1} (v_j - v_1) - \frac{\eta_2 v_1}{S_1} \left( \frac{S_2 - S_2^*}{S_{\text{W}}^* - S_{\text{W}}} \right) \frac{\partial S_{\text{W}}}{\partial t} \end{aligned} \tag{15e}$$

$$\begin{aligned} & \varrho_{\mathbb{W}} \frac{D^2}{Dt} v_2 + \frac{\partial}{\partial x} (P_3 - \gamma P_2^* S_2^{\gamma-1} - \Pi_a S_1^{-\alpha}) - \varrho_{\mathbb{W}} g \sin \vartheta \\ &= \sum_{j=1}^5 \frac{R_{2j}}{\phi S_2} (v_j - v_2) + \frac{\eta_2 v_2}{S_2} \left( \frac{S_2 - S_2^*}{S_{\mathbb{W}}^* - S_{\mathbb{W}}} \right) \frac{\partial S_{\mathbb{W}}}{\partial t} \end{aligned} \tag{15f}$$

$$\begin{aligned} & \varrho_{\mathbb{O}} \frac{D^3}{Dt} v_3 + \frac{\partial P_3}{\partial x} - \varrho_{\mathbb{O}} g \sin \vartheta \\ &= \sum_{j=1}^5 \frac{R_{3j}}{\phi S_3} (v_j - v_3) - \frac{\eta_4 v_3}{S_3} \left( \frac{S_4 - S_4^*}{S_{\mathbb{O}}^* - S_{\mathbb{O}}} \right) \frac{\partial S_{\mathbb{O}}}{\partial t} \end{aligned} \tag{15g}$$

$$\begin{aligned} & \varrho_{\mathbb{O}} \frac{D^4}{Dt} v_4 + \frac{\partial}{\partial x} (P_1 - \delta P_4^* S_4^{\delta-1} - \Pi_b S_3^{-\beta}) - \varrho_{\mathbb{O}} g \sin \vartheta \\ &= \sum_{j=1}^5 \frac{R_{4j}}{\phi S_4} (v_j - v_4) + \frac{\eta_4 v_4}{S_4} \left( \frac{S_4 - S_4^*}{S_{\mathbb{O}}^* - S_{\mathbb{O}}} \right) \frac{\partial S_{\mathbb{O}}}{\partial t} \end{aligned} \tag{15h}$$

$$S_1 + S_2 + S_3 + S_4 = 1 \tag{15i}$$

$$\frac{\partial P_3}{\partial x} = \frac{\partial P_1}{\partial x} + \frac{\partial}{2\partial x} \left[ \Pi_a S_1^{-\alpha} - \Pi_b S_3^{-\beta} + \gamma P_2^* S_2^{\gamma-1} - \delta P_4^* S_4^{\delta-1} \right], \tag{15j}$$

where  $v_5 = 0$ ,  $R_{12} = 0$ ,  $R_{34} = 0$ , and the quantities  $S_{\mathbb{W}}^*$ ,  $S_{\mathbb{O}}^*$ ,  $S_2^*$ ,  $S_4^*$  are defined in Eq. 7. This system of 10 equations is reduced to a system of only 9 equations by inserting Eq. 15j into Eqs. 15f and 15g to eliminate  $\partial P_3/\partial x$ . The remaining 9 unknowns are  $S_i$ ,  $v_i$ , ( $i = 1, 2, 3, 4$ ) and  $P_1$ .

The system (15) has to be solved subject to initial and boundary data. No flow boundary conditions at both ends require

$$v_i(0, t) = 0, \quad i = 1, 2, 3, 4 \tag{16a}$$

$$v_i(L, t) = 0, \quad i = 1, 2, 3, 4. \tag{16b}$$

The fluids are incompressible. Hence, the reference pressure can be fixed to zero at the left boundary

$$P_1(0, t) = 0. \tag{17}$$

The saturations remain free at the boundaries of the column.

Initially, the fluids are at rest and their velocities vanish. The initial conditions are ( $i = 1, 2, 3, 4$ )

$$v_i(x, 0) = v_i^0(x) = 0 \tag{18a}$$

$$P_1(x, 0) = P_1^0(x) = 0 \tag{18b}$$

$$S_i(x, 0) = S_i^0(x) = S_i^0. \tag{18c}$$

In the present study, the initial saturations will be taken as constants, i.e., independent of  $x$ .

The model parameters are chosen largely identical to the parameters in Hilfer (2006b). They describe experimental data obtained at the Versuchseinrichtung zur Grundwasser- und Altlastensanierung (VEGAS) at the Universität Stuttgart (Sheta 1999). The model parameters are  $\varrho_{\mathbb{W}} = 1,000 \text{ kg m}^{-3}$ ,  $\varrho_{\mathbb{O}} = 800 \text{ kg m}^{-3}$ ,  $\phi = 0.34$ ,  $S_{\mathbb{W}i} = 0.15$ ,  $S_{\mathbb{O}r} = 0.19$ ,  $\eta_2 = 4$ ,  $\eta_4 = 3$ ,  $\alpha = 0.52$ ,  $\beta = 0.90$ ,  $\gamma = 1.5$ ,  $\delta = 3.5$ ,  $\Pi_a = 1,620 \text{ Pa}$ ,  $\Pi_b = 25 \text{ Pa}$ ,  $P_2^* = 2,500 \text{ Pa}$ , and  $P_4^* = 400 \text{ Pa}$ . In Hilfer (2006b), only stationary and quasistationary solutions were considered, and the viscous resistance coefficients remained unspecified. In order to

find realistic values remember that  $R_{31} + R_{41} + R_{15} = 2\mu_{\text{w}}\phi^2/k$  (Hilfer 2006a, b). Realistic values for the viscosity and permeability are  $\mu_{\text{w}} = 0.001\text{kg m}^{-1}\text{s}^{-1}$  and  $k = 10^{-12}\text{m}^2$ . Based on these orders of magnitude, the viscous resistance coefficients are specified as  $R_{13} = R_{31} = R_{14} = R_{41} = R_{23} = R_{32} = R_{24} = R_{42} = R_{15} = R_{35} = 1.7 \times 10^8 \text{kg m}^{-3}\text{s}^{-1}$ , and  $R_{25} = R_{45} = 1.7 \times 10^{16} \text{kg m}^{-3}\text{s}^{-1}$ .

The column is filled with water having total saturation  $S_{\text{w}} = 0.45$  and oil with saturation  $S_{\text{o}} = 0.55$ . Two different initial conditions will be investigated that differ in relative abundance of the nonpercolating phase. The saturations for initial condition A and B are in obvious notation given as

$$S_1^{0A} = 0.449, \quad S_1^{0B} = 0.302 \quad (19a)$$

$$S_2^{0A} = 0.001, \quad S_2^{0B} = 0.148 \quad (19b)$$

$$S_3^{0A} = 0.377, \quad S_3^{0B} = 0.549 \quad (19c)$$

$$S_4^{0A} = 0.173, \quad S_4^{0B} = 0.001. \quad (19d)$$

These phase distributions can be prepared experimentally by an imbibition process for A or by a drainage process for initial condition B. The values for the nonpercolating saturations were chosen from the nonpercolating saturations predicted within the residual decoupling approximation. They can be read off from Fig. 5 in Hilfer (2006b). The values for the percolating phases follow from the requirement that the total water saturation is 0.45. The time scales for raising the column are chosen as  $t_* = 50,000 \text{ s}$ ,  $t_{**} = 10,000 \text{ s}$  corresponding to roughly 3 h.

## 4 Numerical Implementation

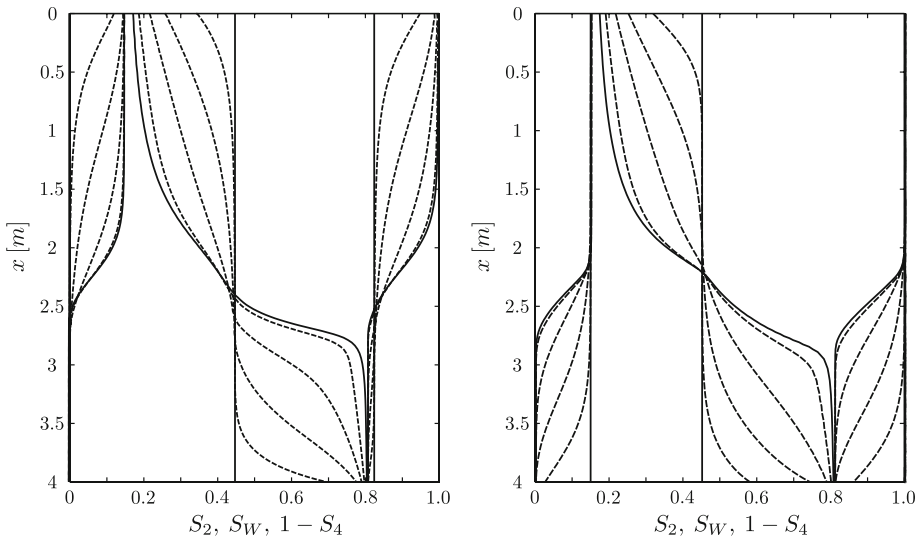
The coupled system of nonlinear partial differential and algebraic equations is solved numerically using an adaptive moving grid solver (Zegeling and Blom 1992; Blom and Zegeling 1994; Dam and Zegeling 2006). Its FORTRAN implementation was described in Blom and Zegeling (1994). Space is discretized by finite differences. The time integration within this algorithm is performed using the public domain differential algebraic solver DASSL, which is a higher order implicit backward Euler scheme.

The mathematical model does not fit exactly the structure of the solver. The following reformulations and adaptations had to be imposed: Elimination of time derivatives, regularization of saturation, flux symmetrization, and pressure stabilization using the pressure projection method (Chorin 1967). In addition, an adaptive algorithm contains parameters regulating the spatial smoothing or the adaptivity of the moving grid. Details of the numerical implementation will be given elsewhere (Doster et al. 2009). Although a thorough sensitivity analysis with respect to all artificial parameters shows that the solutions are insensitive to the parameters over a wide range, it is clear that the numerical solutions presented below are approximate at best. They are given mainly to illustrate qualitatively the differences between the present theory and the accepted traditional theory.

## 5 Results

Figure 2 shows the time evolution of the saturation profile starting from initial conditions A (left figure) and B (right figure). Time instants shown are  $t = 0 \text{ s}$ ,  $t = 6 \times 10^6 \text{ s}$  (solid

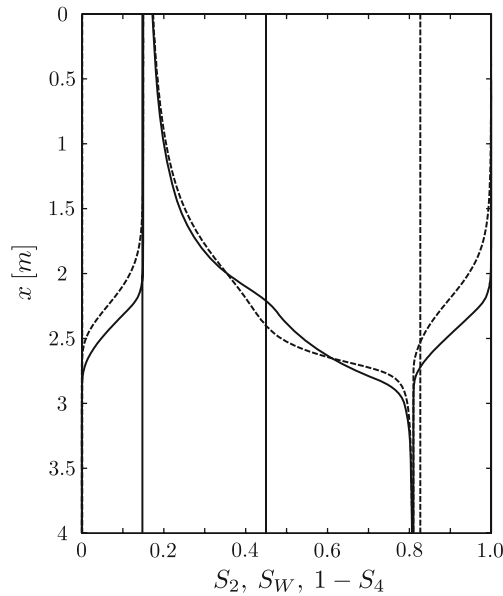




**Fig. 2** Approximate numerical solutions of Eq. 15 showing time evolution of saturation profiles  $S_2(x, t)$ ,  $S_W(x, t)$ , and  $1 - S_4(x, t)$  at times  $t = 0$  s,  $t = 6 \times 10^6$  s (solid lines), and  $t = 10^5$ ,  $2.5 \times 10^5$ ,  $5 \times 10^5$ ,  $7.5 \times 10^5$  s (dashed lines), respectively, when raising a closed column of length  $L = 4$  m from a horizontal to a vertical orientation. The left figure shows the time evolution starting from initial condition A in Eq. 19, the right figure for initial condition B. Solid vertical lines correspond to  $t = 0$  when the column is horizontal. Dashed lines correspond to intermediate times. The first dashed line corresponding to instant  $t = 10^5$  s is the time when the column has just reached a vertical orientation. Solid curves show the quasistationary solution for  $t = 6 \times 10^6$  s. While the upper part of the column is drained, imbibition takes place simultaneously in the lower part. Near  $x = 2.5$  m, drainage takes place initially but is later followed by imbibition

lines) as well as  $t = 10^5$  s,  $t = 2.5 \times 10^5$  s,  $t = 5 \times 10^5$  s, and  $t = 10^6$  s (dashed lines). Gravity is oriented downward along the ordinate. A complete saturation profile consists of three curves. The leftmost curve of a triple is  $S_2(x, t)$ , the middle curve is  $S_W(x, t)$ , and the rightmost curve is  $1 - S_4(x, t)$ . From these curves the saturations are easily read off using Eq. 1b. Namely, at fixed height  $x$ , the distance from the ordinate to the first curve of a triple represents  $S_2(x)$ , the distance between the first and the second curve represents  $S_1(x)$ , the distance between the second and the third represents  $S_3(x)$ , and the distance between the third curve and 1 represents  $S_4(x)$ . The initial saturations at  $t = 0$  correspond to vertical straight lines. Subsequent profiles at  $t = 10^5$ ,  $2.5 \times 10^5$ ,  $5 \times 10^5$ , and  $7.5 \times 10^5$  s are represented by four triples of dashed curves. The final quasistationary profile at  $t = 6 \times 10^6$  s is represented by one triple of solid curves.

At  $t = 0$  the column is oriented horizontally and at  $t = 10^5$  s the column has just reached its vertical position. As the water begins to imbibe the lower part of the column the upper part is simultaneously drained. As the oil rises upward it merges with the residual oil and creates irreducible water (left figure). Equivalently, the process may be viewed as leaving behind residual oil (see the lower right corner of the right figure). Similarly, the water falling to the bottom may be viewed as leaving behind irreducible water (see the upper left corner of the left figure), or as merging with the irreducible water thereby creating residual oil as seen in the right figure. Note also that in the region around  $x = 2.5$  m the process can change with time from drainage to imbibition. Therefore, in the process of raising a closed column the nature of the displacement (imbibition vs. drainage) is not only position but also time-dependent.



**Fig. 3** Initial ( $t = 0$ ) and quasistationary ( $t = 6 \times 10^6$  s) saturation profiles  $S_i(x, t)$  as a function of height  $x$  after raising a closed column of length  $L = 4$  m. Two triples of curves (solid and dashed) are shown. In each triple, the leftmost curve shows  $S_2(x)$ , the center curve shows  $S_W(x)$ , and the rightmost curve shows  $1 - S_4(x)$ . The triple of dashed vertical straight lines represents the saturation profile at  $t = 0$  for initial condition A in Eq. 19, while the triple of solid vertical lines represents initial condition B (the rightmost solid line and leftmost dashed line coincide almost with the bounding box). Note that the dashed and solid lines at  $S = 0.45$  coincide. The triple of dashed curves represents the quasistationary saturation profile for  $t \rightarrow \infty$  resulting from initial condition A, while the triple of solid curves represents the stationary saturation profile for  $t \rightarrow \infty$  resulting from initial condition B. The figure illustrates that the quasistationary profiles depend strongly on the initial condition

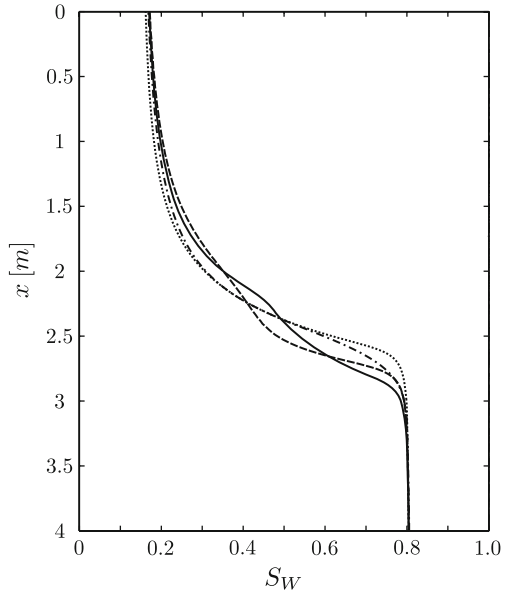
Figure 3 compares the quasistationary ( $t = 6 \times 10^6$  s) saturation profiles for different initial conditions. Dashed lines and curves correspond to initial condition A in Eq. 19, while solid lines and curves show results for initial condition B. The straight vertical line at 0.45 is a double line. It represents the initial water saturation of 0.45 for both initial conditions. Figure 3 shows a strong dependence on the initial distribution of nonpercolating fluids. In particular, the nonpercolating nonwetting fluid depends strongly on the initial condition. Initial condition A represents a fluid distribution that could ensue after an imbibition, while initial condition B could be realistic after a drainage.

Figure 4 illustrates the differences between the present theory and the traditional theory. It shows the two quasistationary profiles (solid and dashed middle curves) as in Fig. 3 calculated dynamically from the present theory and compares them to stationary solutions of the traditional theory based on the capillary pressure concept. In the traditional theory, the water saturation in hydrostatic equilibrium in a vertical column is given as (Bear 1972)

$$S_W(x) = P_c^{-1}(C + (\rho_{\text{O}} - \rho_{\text{W}})gx), \tag{20}$$

where  $P_c$  is the capillary pressure and  $C$  is an integration constant. In view of the boundary conditions (closed column), the integration constant is fixed such that

**Fig. 4** Comparison of the quasistationary water saturation curves shown in Fig. 3 with the traditional theory for two phase flow. The dashed and solid curves are identical to the corresponding curves in Fig. 3. The dashed-dotted curve shows the hydrostatic equilibrium calculated from Eq. 20 using the appropriate secondary drainage capillary pressure function obtained in the residual decoupling approximation with the same parameters in Hilfer (2006b). The dotted curve shows the hydrostatic equilibrium water saturation profile calculated from Eq. 20 using the secondary imbibition capillary pressure function



$$\int_0^L S_W(x) dx = 0.45L \tag{21}$$

is the total water volume. The dash-dotted curve in Fig. 4 is obtained in this way by specifying for  $P_c$  the appropriate secondary drainage curve for the porous medium. This secondary drainage curve was obtained in Hilfer (2006b) and can be seen in Fig. 1 of Hilfer (2006b). The dotted curve in Fig. 4 is obtained by specifying for  $P_c$  the secondary imbibition curve for the medium. This imbibition curve can be seen also in Fig. 1 of Hilfer (2006b). The comparison shows that the quasistationary solutions obtained from Eq. 15 differ significantly in the region of the capillary fringe from the equilibrium profiles predicted by the traditional theory.

### 6 Conclusion

Numerical solutions were calculated for the coupled system (15) of nonlinear partial differential equations obtained by macroscopic constitutive modeling of two phase flow. The equations are based on the concept of hydraulic percolation of fluid phases. The results illustrate the ability of the new theory to describe drainage and imbibition occurring simultaneously within the same sample, or sequentially at the same position inside a porous medium. Stationary solutions are compared to predictions from the traditional theory and significant differences are found. We emphasize that the numerical solutions are approximate. We encourage experimental groups to measure residual fluid distributions during or after immiscible displacement. Such measurements would allow us to test our theoretical predictions against experiment.

**Acknowledgements** The authors thank P. Zegeling for many fruitful discussions. They are grateful to the Deutsche Forschungsgemeinschaft and the International Research and Training Group on Nonlinearities and Upscaling (IRTG NUPUS) for financial support.

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