On the porous-continuum modeling of gravity-driven fingers in unsaturated materials: Extension of standard theory with a hold-back-pile-up effect

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[1] The traditional Richards equation (RE) in combination with standard monotonic properties (constitutive relations and hysteretic equations of state) has been shown to lack critical physics required to model gravity-driven fingering (GDF). We extend the RE with an experimentally observed hold-back-pile-up (HBPU) effect not captured in the standard porous-continuum RE formulation. We postulate the HBPU effect is tied to wetting front sharpness and can be mathematically formulated in a variety of ways to include hypodiffusive, hyperbolic, and mixed spatial-temporal forms involving respectively a Laplacian, a second-order derivative in time, and a Laplacian of a first-order derivative in time of the state variables. For each, we can infer an extended flux relation comprised of the Darcy-Buckingham flux plus an additional component due to the HBPU effect. Extended flux relations that are mathematically similar to each can be found in the single-phase and multiphase flow literature, however, all with very different underlying conceptualizations of the possible physics. *INDEX TERMS:* 1866 Hydrology: Soil moisture; 1875 Hydrology: Unsaturated zone; 1829 Hydrology: Groundwater hydrology; *KEYWORDS:* wetting front instability, gravity-driven fingers, nonmonotonicity, extended porous media theory, hypodiffusive and hyperbolic flux relations, dynamic capillary pressure

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1. Introduction

[2] Over the last 40 years, gravity-driven fingering (GDF) within water-wettable porous materials has been observed and studied in many laboratory and field experiments [e.g., *Palmquist and Johnson*, 1960, 1962; *Tabuchi*, 1961; *Peck*, 1965; *Hill and Parlange*, 1972; *Raats*, 1973; *White et al.*, 1976, 1977; *Diment and Watson*, 1985; *Glass et al.*, 1988, 1989a, 1989d, 1990; *Baker and Hillel*, 1990; *Selker et al.*, 1992a, 1992c; *Lu et al.*, 1994; *Liu et al.*, 1994a, 1994b; *Nicholl et al.*, 1994; *Babel et al.*, 1995; *Hendrickx and Yao*, 1996; *Yao and Hendrickx*, 1996; *Selker and Schroth*, 1998; *Wang et al.*, 1998a, 1998b; *Nissen et al.*, 1999; *Geiger and Durnford*, 2000; *Sililo and Tellam*, 2000; *Yao and Hendrickx*, 2001]. Additionally, a number of investigations have focused on theoretical aspects of this phenomenon and its simulation using a variety of approaches [e.g., *Philip*, 1975; *Parlange and Hill*, 1976; *Diment et al.*, 1982; *Diment and Watson*, 1983; *Tamai et al.*, 1987; *Hillel and Baker*, 1988; *Glass et al.*, 1989b, 1989c, 1991; *Selker et al.*, 1992b; *Chang et al.*, 1994; *Chen and Neuman*, 1996; *Neumann and Chen*, 1996; *Glass and Yarrington*, 1996; *Nieber*, 1996; *Kapoor*, 1996; *Babel et al.*, 1997; *Kacimov and Yakimov*, 1998; *Wang et al.*, 1998c; *Geiger and Durnford*, 2000; *Ursino*, 2000; *Benson*, 2001; *Du et al.*, 2001].

[3] A recent comprehensive discussion of the physics of GDF, including theoretical relations, laboratory and field observations, as well as a number of complicating factors, such as media heterogeneity, that modify GDF behavior or limit its formation, is presented by *Glass and Nicholl* [1996]. They argue that in texturally homogenous porous materials, the parameters that control the intrinsic nature of GDF are the initial moisture content, θ_i, the applied surface flux, q_s [L T^{-1}], and the porous media nonlinearity (e.g., Figure 1). In general, the physical conditions that allow the wetting front (WF) to become unstable, and ultimately render a fingered response, entail a specific intersection of the θ_i, q_s, and material nonlinearity parameter spaces. We ordinarily find GDF to occur when the applied flux is less than the medium's saturated conductivity (K_s [L T^{-1}]), the initial moisture content is low (i.e., $\theta_i \sim 0$), and the material nonlinearity is high (e.g., see $n = 15$ curves in Figure 1). On the other hand, we do not find GDF when $q_s \geq K_s$, $\theta_i \gg 0$, and material nonlinearity is low (e.g., soils or $n = 1.5$ in Figure 1). Recent experiments conducted by *Yao and Hendrickx* [1996] also indicate that GDF does not occur for very small surface flux (i.e., $q_s \ll K_s$). However, for all these parameters, it is not presently known exactly where the transition from "no fingers" to "fingers" occurs as a combination of θ_i, q_s, and material nonlinearity.

[4] A signature characteristic of GDF is the presence of saturated finger tips that drain at a distance behind, thus yielding nonmonotonic structures within the pressure and saturation fields [e.g., *Glass et al.*, 1989c]. Recently, we have shown that the Richards Equation (RE) along with standard relative permeability [e.g., *Mualem*, 1976] and pressure-saturation [e.g., *van Genuchten*, 1980] relations, all com-

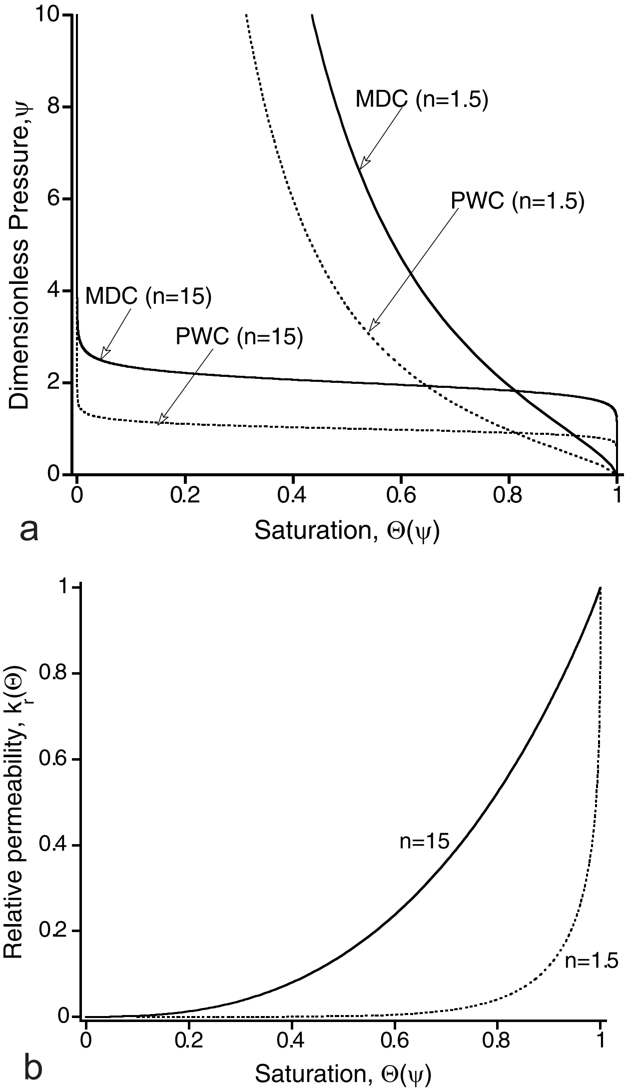


Figure 1. Standard monotonic properties as typically measured for unsaturated porous materials. (a) Hysteretic pressure-saturation relations for primary wetting (PWC) and main drainage (MDC) for material where gravity-driven fingering (GDF) is typically observed to occur (i.e., curves denoted by $n = 15$) as well as material that does not exhibit GDF (i.e., curves denoted by $n = 1.5$). (b) Relative permeability as a function of saturation for $n = 15$ and $n = 1.5$ materials. The pressure-saturation curves are developed using the *van Genuchten* [1980] model (13a) for dimensionless $\alpha = 1$ for PWC and $\alpha = 0.5$ for MDC [see *Eliassi and Glass*, 2001a, 2001b]. Here we assume PWC and MDC are scaled to have the same maximum saturation value of 1 (i.e., we are not considering the effects of air and water entrapment on PWC and MDC, respectively). The relative permeability versus saturation, which normally does not display a hysteretic response, is evaluated using the *Mualem* [1976] model.

monly considered valid for unsaturated flow through unsaturated porous media, cannot generate GDF or its nonmonotonic signature for situations where it is found to occur [*Eliassi and Glass*, 2001a]. As an illustration, Figure 2a compares a nonmonotonic profile as found along a single finger with a monotonic profile as calculated using the one-dimensional vertical RE with hydraulic properties measured for a material that exhibits GDF (i.e., $n = 15$ curves in Figure 1). We see that the WF for the finger profile is held behind the monotonic RE solution, and, while the saturation far behind the WFs are the same at an asymptotic saturation value, Θ_A (controlled by the applied flux and the hydraulic conductivity), the behaviors at the WF are quite different. Figure 2b traces the pressure-saturation history at a point for both profiles in context of the hysteretic pressure-saturation relations for the medium. While the monotonic RE solution wets only to Θ_A along the primary wetting curve, the finger profile pushes beyond and then reverses to follow a drainage curve behind. Thus, in comparison with the monotonic profile simulated by RE, when GDF occurs, infiltrating water first experiences a ''hold-back'' and a ''pile-up'' across the WF and then undergoes a hysteretic reversal.

[5] The RE combined with standard monotonic hydraulic properties is a simple conceptual-mathematical model developed in context of a volume averaged, porous-continuum approach. The RE simply combines the continuity of mass (assuming no mass transfer between phases and incompressibility of water phase) with a flux relation. The flux is considered as a simple gradient law with water driven by water phase pressure (assuming resistance of the air phase is negligible) and gravity forces. The constant of proportionality in the flux relation is given by the hydraulic conductivity that monotonically increases with moisture content from zero to its saturated value (e.g., Figure 1b). Water pressure under unsaturated conditions is considered to be less than that in the air phase due to capillary forces (water is wetting) and monotonically increases with moisture content on wetting while exhibiting hysteresis on drainage (e.g., Figure 1a). When monotonic hydraulic properties (relative permeability and pressure-saturation relations) are measured in context of this porous-continuum conceptualization, the RE has demonstrated predictive capability under many unsaturated flow conditions. Because of this success, the RE based approach is often extrapolated as valid in all porous materials where capillary and gravity forces are thought to be the critical drivers [e.g., *Hillel*, 1980, p. 21]. Interestingly, we see that the textbook case of initially dry, narrow size distribution sands where capillary and gravity forces should dominate, yields GDF with its nonmonotonic signature, a notably aberrant behavior uncharacteristic of the RE.

[6] As a step toward development of a more comprehensive unsaturated flow theory, we consider the extension of the standard porous-continuum approach to allow the modeling of GDF. In this paper, we incorporate the experimentally observed hold-back-pile-up (HBPU) effect as an additional term within the porous-continuum governing equation for flow through unsaturated media. By induction, we postulate this term as a function of state variables in three different ways and then recover the underlying extended flux relations for each. The behaviors of these three different forms are illustrated with a simple analytical approximation near the WF. We also examine the behavior of one formulation by varying the critical control parameters (i.e., θ_i, q_s, and material nonlinearity) and illustrate that the term's magnitude at the WF depends directly on these control parameters.

Finally, we consider a variety of extended theories from the single and multiphase flow literature to give possible support for our hypothesized terms. Interestingly, we find that each form has its parallel but arising from very different conceptualizations of possible underlying physics.

2. Formulation of the Hold-Back-Pile-Up Effect

[7] Traditional unsaturated flow theory combines the mass conservation equation with the Darcy-Buckingham (DB) flux relation to yield the Richards Equation (RE) [e.g., *Hillel*, 1980, p. 21]. Assuming water is incompressible and in absence of any sinks and/or sources, conservation of mass is given by

$$\frac{\partial\theta(\psi)}{\partial t} = -\vec{\nabla}\cdot\vec{q} \qquad (1)$$

where t [T] is the time, $\theta(\psi)$ [L^3 L^{-3}] is the hysteretic volumetric moisture content relation (i.e., the equation of state), ψ [L] is the capillary pressure head, $\vec{\nabla}$ [L^{-1}] is the gradient operator vector, and $\vec{q}$ [L T^{-1}] is the linear momentum flux vector. The DB flux, which simply considers the pressure head and gravitational potentials, is given by [e.g., *Sposito*, 1986]:

$$\vec{q}_{DB} = -K(\theta)\vec{\nabla}(\psi + z) \qquad (2)$$

where we use the notation $\vec{q}_{DB}$ [L T^{-1}] as a reference to the standard DB flux vector, $K(\theta)$ [L T^{-1}] is the hydraulic conductivity function and z [L] refers to the vertical distance. Thus letting $\vec{q} = \vec{q}_{DB}$, direct substitution of (2) into (1) yields the standard form of the RE, i.e., the standard equation governing flow through unsaturated porous materials:

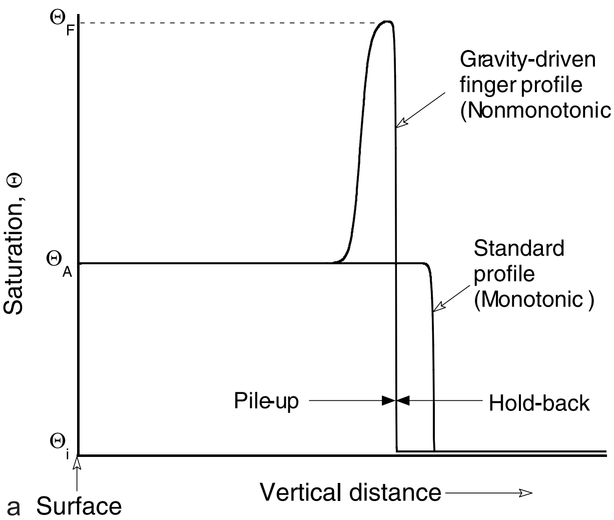
$$\frac{\partial\theta(\psi)}{\partial t} = \vec{\nabla}\cdot\left[K(\theta)\vec{\nabla}\psi\right] + \frac{\partial K(\theta)}{\partial z} \qquad (3)$$

The functional forms for $\theta(\psi)$ and $K(\theta)$, have been measured for a wide variety of materials from mildly nonlinear soils to highly nonlinear, narrow grain size distribution sands where GDF is found (Figure 1). In general, these relations have been found to be monotonic during wetting, that is, as pressure increases, the saturation and permeability always increase.

[8] To yield the nonmonotonic behavior demonstrated in Figure 2a, we consider inclusion of an additional term into the RE that mathematically models the HBPU effect introduced in Section 1. We write an extended governing equation with the additional component, $R(\theta)$ [T^{-1}]:

$$\frac{\partial\theta(\psi)}{\partial t} = \vec{\nabla}\cdot\left[K(\theta)\vec{\nabla}\psi\right] + \frac{\partial K(\theta)}{\partial z} + R(\theta) \qquad (4)$$

Figure 3 illustrates the general behavior of $R(\theta)$ with a negative minimum ahead of the WF as the "hold-back,"



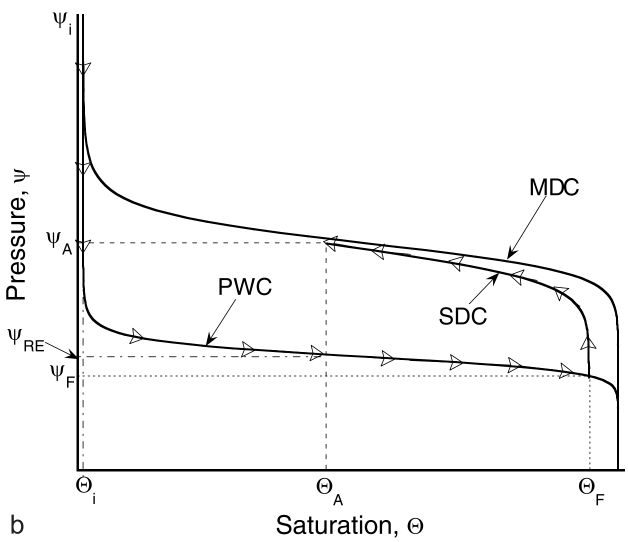


Figure 2. (opposite) Graphical illustration of the nonmonotonic signature of gravity-driven fingering (GDF). (a) A nonmonotonic saturation profile as found experimentally along a finger is compared to a one-dimensional solution of the vertical Richards equation (RE) with standard monotonic properties (Figure 1) as measured on media exhibiting GDF. Laboratory experiments reveal that slow constant applied surface flux ($R_s = q_s/K_s < 1$) into an initially dry ($\Theta_i \sim 0$) and highly nonlinear porous material ($n = 15$) yields a nonmonotonic signature with a saturation at the front, Θ_F, that is near or at $\Theta = 1$ and drains a distance behind. Yet numerical solution using the standard form of RE can only admit a monotonic profile with a maximum saturation of Θ_A, where $\Theta_A < \Theta_F$. Here Θ_A is the asymptotic saturation value such that, $R_s = K(\Theta_A)/K_s$, with $K(\Theta_A)$ being the hydraulic conductivity function evaluated at Θ_A. (b) Hysteretic pressure-saturation curves bounded by the primary wetting curve (PWC) and the main drainage curve (MDC) are used to illustrate the advancement history at a point in Figure 2a as the WF profile advances. The zone immediately ahead of the WF is at the initial condition, (ψ_i, Θ_i) and resides on the PWC. As the WF passes, the RE solution reaches an asymptotic value of (ψ_{RE}, Θ_A) and then stops. For the finger the pressure and saturation continue to rise to the maximum value of (ψ_F, Θ_F). The pressure then reverses forcing the point to follow a scanning drainage curve (SDC) and eventually drains to the asymptotic value (ψ_A, Θ_A). The difference between these two solutions identifies the hold-back-pile-up (HBPU) effect.

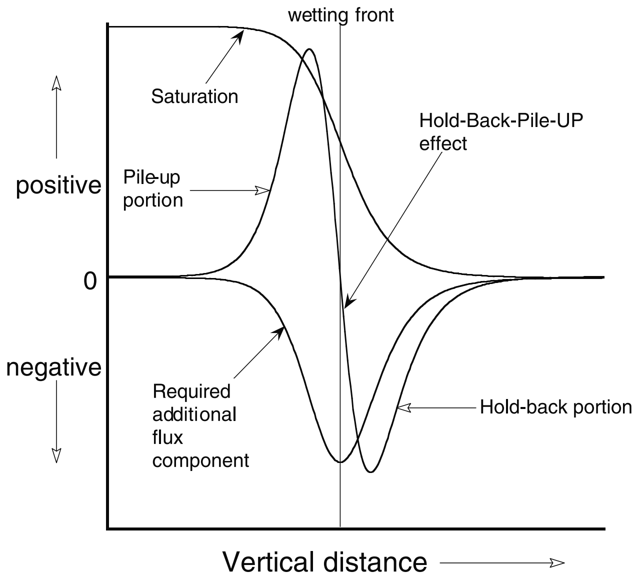


Figure 3. Representation of the hold-back-pile-up (HBPU) effect. Across the wetting front (WF), where the pressure and saturation gradients are greatest, the HBPU effect must have a negative minimum (hold-back) ahead of the WF to counter diffusion and a positive maximum (pile-up) behind the WF to increase the pressure and saturation. Within the flux relation the functional form of the HBPU effect yields an additional flux component that opposes flow as it crosses the WF.

and a positive maximum behind the WF as the "pile-up." As also shown in this figure, the HBPU effect yields a negative flux component that opposes the capillary driven flux at the WF.

[9] For the combination of θ_i, q_s, and material nonlinearity where GDF occurs, the magnitude of the HBPU must be large enough to result in an over-pressurization and thus over-saturation immediately behind the WF. Conversely, for those parameter combinations where GDF does not occur, the HBPU must be negligible. Since θ_i, q_s, and material nonlinearity ultimately define the "sharpness" of the WF and the sharper the WF, the greater the tendency for GDF to occur, we postulate the magnitude of the HBPU should depend directly on the WF sharpness. Considering this required behavior, we may write a variety of mathematical representations for the HBPU effect. The simplest forms contain second-order spatial or temporal differential operators of state variables θ and/or ψ. For example, consider:

$$R_{hdiff}(\theta) = \vec{\nabla} \cdot \left[F(\theta)\vec{\nabla}\theta(\psi)\right] \tag{5}$$

$$R_{hyper}(\theta) = -\frac{\partial}{\partial t}\left[T(\theta)\frac{\partial}{\partial t}\theta(\psi)\right] \tag{6}$$

where we refer to $R_{hdiff}(\theta)$ and $R_{hyper}(\theta)$ as the hypodiffusive and hyperbolic forms of the HBPU, respectively. As we will see in Section 4, terms with these forms can be found in the literature within extended continuum theory applied to porous media. Higher-order differential operators could also be used; however, they will yield additional swings across the WF beyond the HBPU pair shown in Figure 3. For example, consider the third order mixed spatial-temporal differential operator:

$$R_{mix}(\theta) = \vec{\nabla} \cdot \left\{L(\theta)\vec{\nabla}\left[\frac{\partial}{\partial t}\theta(\psi)\right]\right\} \tag{7}$$

where we refer to $R_{mix}(\theta)$ as the mixed form of the HBPU. While many other third- and higher-differential operators can be appropriately formulated, we will see that a form of (7) can also be traced within the context of previously proposed extended theory (see Section 4).

[10] The functions $F(\theta)$ [L^2 T^{-1}], $T(\theta)$ [T], and $L(\theta)$ [L^2] represent new phenomenological coefficients (i.e., new constitutive properties) within each form of the HBPU. It is important to note that in all cases, $R(\theta)$ must be formulated such as to oppose the capillary component ahead and increase the pressure and saturation behind the WF. Thus given the moisture content and pressure head behaviors at the WF, $F(\theta)$ must be an intrinsically negative function, while $T(\theta)$ must be intrinsically positive. As we will see in Section 3, the sign required of $L(\theta)$ is less straightforward because $R_{mix}(\theta)$ contains an additional swing across the WF. Finally, we note that $R(\theta)$ could be formulated as a combination of hypodiffusive, hyperbolic, and mixed forms, and could in principle be hysteretic.

[11] To infer the extended flux relations that would result in governing equation (4) in combination with HBPU terms in (5), (6) and (7), let us consider the flux to be a simple combination of the DB flux (2) plus an additional component, or:

$$\vec{q} = \vec{q}_{DB} + \vec{q}_i, \qquad \text{with } i = \text{hdiff, hyper, and/or mix} \tag{8}$$

where $\vec{q}_i$ is the additional flux component that arises from each HBPU formulation. By taking the negative inverse divergence of each form of $R(\psi)$, we can easily find $\vec{q}_i$ for each form.

[12] For the hypodiffusive form of the HBPU, we have:

$$\vec{q}_{hdiff} = -F(\theta)\vec{\nabla}\theta(\psi) \tag{9}$$

The hypodiffusive flux, $\vec{q}_{hdiff}$, implies the existence of a process that acts oppositely to that of the capillary component.

[13] For the hyperbolic form of the HBPU, one can show (refer to *Eliassi* [2001] for details):

$$\vec{q}_{hyper} = -T(\theta)\frac{\partial\vec{q}}{\partial t} - \vec{\nabla}^{-1} \cdot \left[\frac{\partial T(\theta)}{\partial t}\vec{\nabla}\cdot\vec{q} - \frac{\partial\vec{q}}{\partial t}\cdot\vec{\nabla}T(\theta)\right] \tag{10}$$

The hyperbolic flux, $\vec{q}_{hyper}$, now introduces a dynamic memory effect with $T(\theta)$ being the moisture content dependent time required for the effect to vanish.

[14] Finally, for the mixed form of the HBPU, we have

$$\vec{q}_{mix} = -L(\theta)\vec{\nabla}\left[\frac{\partial}{\partial t}\theta(\psi)\right] \tag{11}$$

At the WF where θ varies sharply in both time and space, $\vec{q}_{mix}$ introduces a dynamic effect which is further accentuated by its spatial gradient.

3. Analytical Illustration of HBPU Effect

[15] To illustrate the general behavior of the three forms of the HBPU effect in (5), (6), and (7), we assume a simple functional form of the pressure profile that allows us to conceptually vary the influences of initial moisture, applied flux, and material properties. For this purpose, we choose a travelling waveform for the pressure profile, in one-dimension (1D), as

$$\psi(\chi) = (\psi_B - \psi_i)\left[e^{-\left(\frac{\chi}{\chi_{WF}}\right)^{\omega}} - 1\right] + \psi_B \qquad (12)$$

where $\chi = z - v_0 t$ [L] is a similarity variable, v_0 [L T^{-1}] is the propagation speed, ψ_B [L] and ψ_i [L] respectively refer to the pressure behind and ahead of the WF (roughly representing the boundary and initial conditions, respectively), ω is a positive exponent that sharpens the WF as its value increases, and χ_{WF} [L] is a parameter that can be used to shift the WF position in the χ direction.

[16] With an equation of state (i.e., pressure-saturation) relationship, we can then obtain a saturation profile as a function of χ. For these purposes, we use the standard model introduced by *van Genuchten* [1980], e.g., the relation used to evaluate curves in Figure 1a:

$$\Theta(\psi) \equiv \frac{\theta(\psi) - \theta_r}{\theta_s - \theta_r} = \left[1 + (\alpha_w|\psi|)^n\right]^{-m} \qquad (13a)$$

where $\Theta(\psi)$ is the saturation as a function of capillary pressure, ψ, θ_r [L^3 L^{-3}] and θ_s [L^3 L^{-3}] are respectively the residual and satiated (i.e., contains entrapped air) moisture content values, α_w [L^{-1}] is the representative inverse capillary pressure of the wetting curve, and n defines the nonlinearity of the porous media with $m = 1 - (1/n)$. Substituting (12) into (13a) and scaling lengths (i.e., ψ, χ, ψ_B, ψ_i, χ_{WF}, and z) by α_w, v_0 by K_s, and t by $\alpha_w K_s$, the dimensionless saturation profile is given by:

$$\Theta(\chi) = \left\{1 + \left(\left|(\psi_B - \psi_i)\left[e^{-\left(\frac{\chi}{\chi_{WF}}\right)^{\omega}} - 1\right] + \psi_B\right|\right)^{n}\right\}^{-m} \qquad (13b)$$

where all variables in (13b) are now redefined to be dimensionless.

[17] Figure 4 shows the saturation profiles as a function of Θ_i, Θ_B, and ω, obtained from (13b). Here $\Theta_i \equiv \Theta(\psi_i)$ represents the initial saturation (i.e., saturation ahead of the WF), and $\Theta_B \equiv \Theta(\psi_B)$ refers to the saturation behind the WF (and roughly represents the influence of applied flux, q_s). Figure 4a shows for given Θ_B and ω values, as Θ_i increases, the WF sharpness (i.e., the gradient) decreases. Conversely, for fixed Θ_i and ω values, as Θ_B decreases (Figure 4b), the saturation behind the WF reduces which naturally decreases the WF sharpness. Finally, the effect of varying ω (for fixed values of Θ_B and Θ_i) is presented in Figure 4c, where as ω decreases the WF becomes less steep. Since Θ_B, Θ_i, and ω all control sharpness of the WF, we can use their variation to illustrate the behavior of HBPU effect with respect to the critical control parameters q_s, θ_i, and material nonlinearity.

[18] Provided that the functional forms of $F(\theta)$, $T(\theta)$, and $L(\theta)$ are available, we can substitute pressure profile (12) into the 1D representations of (5), (6), and (7) and use the chain-rule to explicitly evaluate $R_{hdiff}(\theta)$, $R_{hyper}(\theta)$, and $R_{mix}(\theta)$, in terms of χ. For illustration's sake, we only consider constant values where, $F(\theta) = F_0 = -1$, $T(\theta) = T_0 = 1$, and $L(\theta) = L_0 = -1$. For this choice of values, both $R_{hdiff}(\theta)$ and $R_{hyper}(\theta)$ yield identical responses across the WF. Figure 5 depicts the normalized profiles for $R_{hdiff}(\theta)$, $R_{hyper}(\theta)$, and $R_{mix}(\theta)$ plotted along with a saturation profile, near the WF (i.e., where the gradients are largest). Clearly, all three forms of $R(\theta)$ comply with the required form of the HBPU in Figure 3. They all display first a negative minimum and then a positive maximum across the WF, respectively. However, because $R_{mix}(\theta)$ involves a third-order derivative, this form yields an additional negative swing (i.e., another hold-back) behind the HBPU. Conversely, if we choose $L(\theta)$ to be a positive function, (e.g., $L_0 = 1$), there will be a positive swing at the leading edge of the WF before the HBPU. Whether the HBPU will be effective when combined with either additional swing is unclear and likely dependent on the functional behavior of $L(\theta)$.

[19] To illustrate the variations of the HBPU effect as a function of WF sharpness, we now use $R_{hdiff}(\theta)$ with $F_0 = -1$ and change the WF sharpness through variables Θ_i, Θ_B, and ω, as we did in Figure 4. Based on Figures 6a and 6b, as the WF becomes less sharp through either an increase in Θ_i, or a decrease in Θ_B, magnitude of $R_{hdiff}(\theta)$ near the WF is systematically reduced. To consider media nonlinearity (i.e., variations of n in (13a)), not only will ω increase as n increases, but the functional response of $\Theta(\psi)$ is influenced by n as well. To remove this additional complexity, we ignore the effect of n on $\Theta(\psi)$ and qualitatively demonstrate the effect of material nonlinearity by simply changing ω (i.e., we let n have the same value as in the other cases considered so far). Figure 6c depicts the $R_{hdiff}(\theta)$ profiles as a function of ω values. As ω is decreased and the WF becomes less sharp, the magnitude for the resulting $R_{hdiff}(\theta)$ also reduces. We note that in all cases, as the WF becomes less sharp, not only is the magnitude of $R_{hdiff}(\theta)$ reduced but its waveform also spreads over a greater zone across the WF. Thus as the WF becomes sharper, not only the magnitude of $R_{hdiff}(\theta)$ grows, it is also more tightly focused.

[20] $R_{hdiff}(\theta)$ yields a response with variation of Θ_i, Θ_B, and ω that is consistent with the way initial and boundary conditions and material nonlinearity influence GDF. Using this simple analytic approach, $R_{hyper}(\theta)$ can also be shown to yield behavior consistent with GDF but we are less certain in regards to $R_{mix}(\theta)$. Because full behavior will arise only in context of the other nonlinear terms of the flow equation, we can only truly evaluate the intrinsic differences among the various forms of the HBPU term through numerical solution of the respective governing equations.

4. Similarity to Other Existing Theories

[21] The mathematical representations of the HBPU effect, presented in section 2, have been postulated by induction. That is, we know the behavior we wish to model and simply include the necessary terms in the governing equation from which we infer extended flux relations. However, many

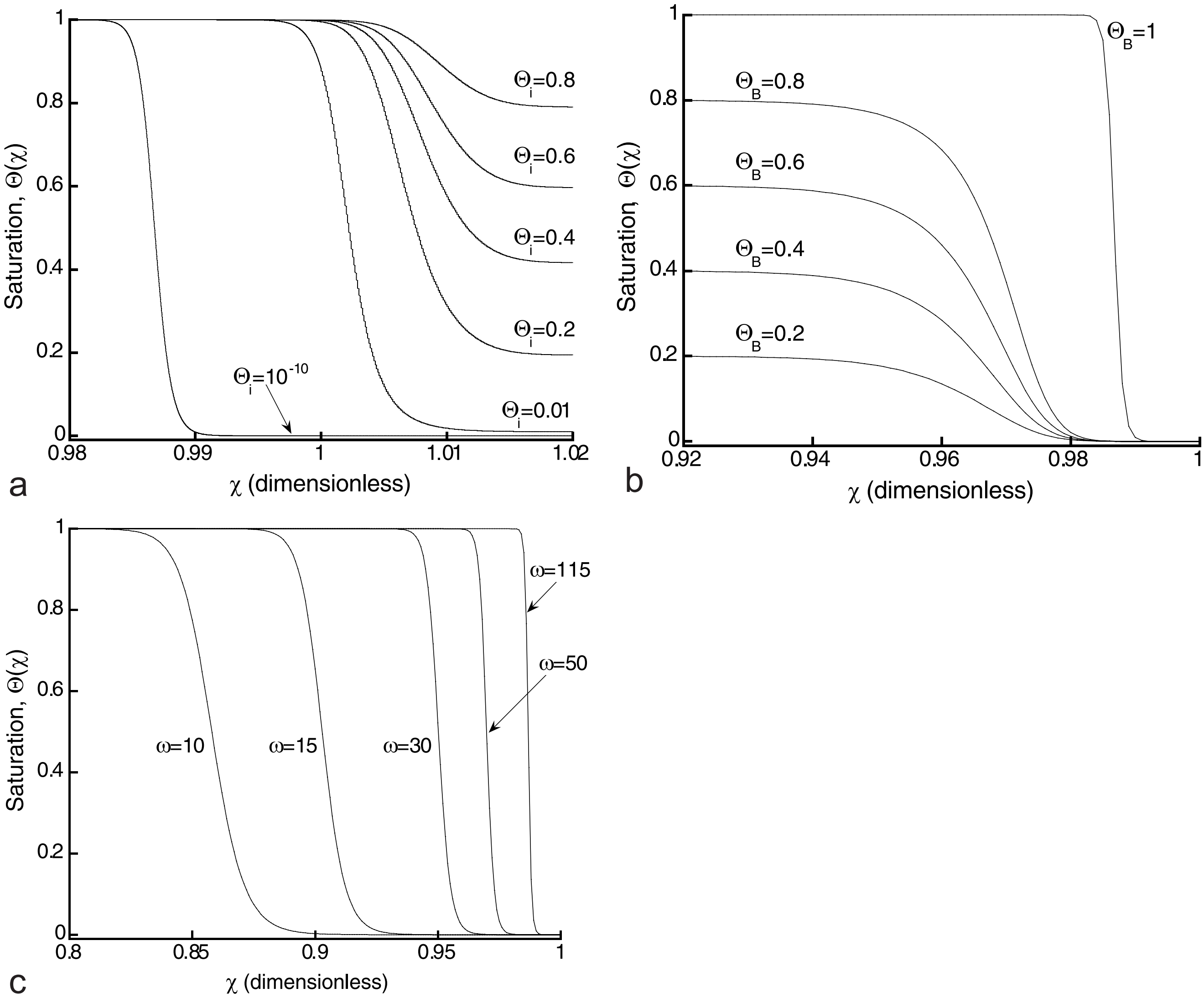


Figure 4. Saturation profiles, evaluated using (13b), are focused near the WF to illustrate the effects of (a) initial saturation Θ_i for $\omega = 115$ and $\Theta_B = 1$, (b) boundary saturation Θ_B for $\omega = 115$ and $\Theta_i = 10^{-10}$, and (c) media nonlinearity through the sharpness factor ω for $\Theta_i = 10^{-10}$ and $\Theta_B = 1$. To obtain the various Θ_i values, we use the dimensionless form of (13a) with dimensionless initial pressure values $\psi_i = -5.18$, -1.39, -1.11, -1.03, -0.98, and -0.92. Similarly, we find Θ_B values using dimensionless boundary pressure values $\psi_B = -1.11$, -1.03, -0.98, -0.92, and 0. Other dimensionless values include $v_0 = 1$, $t = 0$, $\chi_{WF} = 1$, and $n = 15$.

investigators working from first principles have also suggested a variety of extensions to the DB flux relation such as can be developed from the Navier-Stokes momentum equation [e.g., *Raats and Klute*, 1968; *Gray and O'Neill*, 1976; *Sposito*, 1978], or from alternative single and multiphase flow theories [e.g., *Marle*, 1982; *Kalaydjian*, 1987; *Pavone*, 1989; *Hassanizadeh and Gray*, 1990; *del Rio and Lopez de Haro*, 1991; *Hilfer*, 1998]. We note that some of these theories consist of many equations with many unknowns, and all contain new parameters and constitutive relations, few of which have been measured. However, with the forms of our hypothesized additional flux components in mind, we are able to find parallels for each from across these extended theories. Whether any of these parallel terms correctly embody the physics of the HBPU effect is an open question.

[22] As illustration, we have selected three theories that yield flux relations similar to our postulated hypodiffusive, hyperbolic, and mixed form fluxes. We first consider the theory of *Hassanizadeh and Gray* [1990] and identify terms similar to the hypodiffusive flux. We next present the theory of *del Rio and Lopez de Haro* [1991] for unsaturated flows as well as the standard simplification of the Navier-Stokes momentum flux, each of which yield hyperbolic flux relations. Finally, we consider the proposed dynamic capillary pressure equation of *Hassanizadeh and Gray* [1993a] and show it can yield a flux relation that is mathematically similar to the mixed form flux.

4.1. A Parallel for the Hypodiffusive Flux Relation

[23] Starting from the volume averaging theorems, *Hassanizadeh and Gray* [1990] discuss the thermodynamic basis of multiphase flow through porous media. Ultimately, they derive alternative representations of the conservation equations and constitutive relations that are more compre-

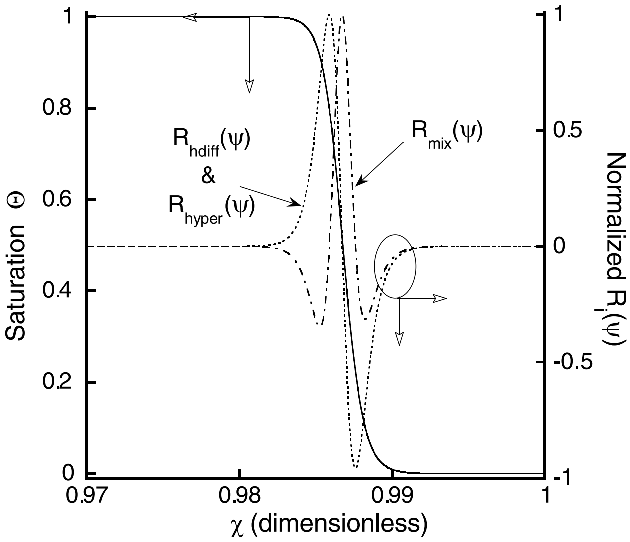


Figure 5. Normalized representations of the hypodiffusive, $R_{hdiff}(\theta)$, hyperbolic, $R_{hyper}(\theta)$, and the mixed, $R_{mix}(\theta)$, forms of the hold-back-pile-up (HBPU) effect (right-hand vertical axis) is plotted along with a hypothetical saturation profile (left-hand vertical axis) focused near the wetting front. The profiles for $R_{hdiff}(\theta)$, $R_{hyper}(\theta)$, and $R_{mix}(\theta)$ show their basic response complies with the required behavior of the HBPU effect in Figure 3. Here we let $\psi_i = -5.2$, $\psi_B = 0$, $v_0 = 1$, $t = 0$, $\chi_{WF} = 1$, $\omega = 115$, $n = 15$, $F(\theta) = -1$, $T(\theta) = 1$, $L(\theta) = -1$, and to obtain a better representation each $R_i(\theta)$ is normalized by its positive maximum value. Note that for this combination of parameter values, $R_{hdiff}(\theta)$ and $R_{hyper}(\theta)$ yield identical responses.

hensive than the traditional multiphase flow equations. In the Hassanizadeh and Gray's (HG) theory, the complete set of flow equations (including bulk phases and interfaces) encompass 30 conservation equations and 35 primary unknowns, which altogether require constitutive relations for 111 quantities [*Gray et al.*, 1999]. However, *Gray and Hassanizadeh* [1991a] and *Hassanizadeh and Gray* [1993b] discuss a variety of physical situations where their theory can be simplified to yield more tractable representation of the flux relations for single- and multiphase porous media flow.

[24] To start with, we consider the quasi-equilibrium assumption [*Gray and Hassanizadeh*, 1991b], i.e., we assume the porous media flow is slow enough to neglect the transient and advective terms. If we further assume the water phase is incompressible, flow is isothermal, porosity is constant, porous medium remains rigid and is isotropic, and neglect the contribution of air phase dynamics, the water phase flux relation becomes (i.e., further simplification of equation (23) of *Hassanizadeh and Gray* [1993b]):

$$\varepsilon S^w \vec{v}^w = -\frac{kk_r^w}{\mu^w}\left\{\left(\vec{\nabla}p^w - \rho^w\vec{g}\right) + \rho^w\left[\frac{\partial A^w}{\partial a^{wa}}\vec{\nabla}a^{wa} + \frac{\partial A^w}{\partial a^{ws}}\vec{\nabla}a^{ws} + \frac{\partial A^w}{\partial S^w}\vec{\nabla}S^w\right]\right\} \quad (14)$$

where ε is the porosity, S^w is the water saturation, $\vec{v}^w$ [L T^{-1}] is the water phase velocity vector, k [L^2] is the isotropic intrinsic permeability, k_r^w is the relative permeability function, μ^w [M L^{-1} T^{-1}] is the viscosity of water, p^w [M L^{-1} T^{-2}] is the water pressure, ρ^w [M L^{-3}] is the water density, $\vec{g}$ [L T^{-2}] is the gravitational vector, A^w [L^2 T^{-2}] is the macroscopic Helmholtz free energy per unit mass of the water phase, and a^{wa} [L^{-1}] and a^{ws} [L^{-1}] are the specific interfacial areas for the water-air and water-solid interfaces, respectively.

[25] As stated in (14), the variations of the free energy, A^w, as a function of saturation as well as water-solid and air-water interfacial areas, provide three additional gradients that are normally unaccounted for in the standard two-phase theory. However, to fully define A^w, we must introduce additional conservation equations for a^{wa} and a^{ws} [e.g., see *Gray and Hassanizadeh*, 1991a, 1991b; *Hassanizadeh and Gray*, 1990, 1993a, 1993b]. We can avoid this additional complexity if we assume A^w is a constitutive property, where A^w is a general function of S^w, a^{wa}, and a^{ws}, or

$$A^w = A^w(a^{wa}, a^{ws}, S^w) \quad (15)$$

We should be clear that A^w could also depend on several other independent variables [*Gray and Hassanizadeh*, 1991a, 1991b] and additionally, it may be hysteretic. Next, we can attain closure by either simply assuming that a^{wa} and a^{ws} have negligible effects on the bulk fluid motion, or by allowing a^{wa} and a^{ws} to be defined with additional constitutive relations that are functions of water saturation, e.g., $a^{wa} = a^{wa}(S^w)$ and $a^{ws} = a^{ws}(S^w)$. Considering such an approach, A^w reduces to only a function of saturation, S^w, and (14) can be cast into:

$$\varepsilon S^w \vec{v}^w = -\frac{kk_r^w}{\mu}\left[\left(\vec{\nabla}p^w - \rho^w\vec{g}\right) + \rho^w\frac{\partial A^w}{\partial S^w}\vec{\nabla}S^w\right] \quad (16)$$

[26] Rewriting (16) in terms of the flux vector, $\vec{q}$, pressure head, ψ, and moisture content, θ, we then have

$$\vec{q} = -\left[K(\theta)\vec{\nabla}(\psi + z) + F(\theta)\vec{\nabla}\theta(\psi)\right] \quad (17a)$$

where $\vec{q} = \varepsilon S^w \vec{v}^w$ is the flux vector, $K(\theta) = K_s k_r^w$ is the hydraulic conductivity function, $\psi = p^w/(\rho^w g)$ is the pressure head, g [L T^{-2}] is the acceleration of gravity, $\theta = \varepsilon S^w$ is the moisture content, and $F(\theta)$ [L^2 T^{-1}] is a general function of the form

$$F(\theta) = \frac{K(\theta)}{g}\left(\frac{\partial A^w}{\partial\theta}\right) \quad (17b)$$

The term involving the gradient of $\theta(\psi)$, on the right-hand side (RHS) of (17a), is similar to the form of $\vec{q}_{hdiff}$ in (9). For (17a) to yield the appropriate HBPU effect, $F(\theta)$ must be intrinsically negative. *Hassanizadeh and Gray* [1993a, 1993b] state that during the imbibition process, for the saturation of a wetting phase fluid to increase, the free energy of the system must decrease. That is, if we interpret the free energy functional, $A^w(\theta)$, to be greatest when water content is low and let it monotonically decrease as the water content increases, $\partial A^w/\partial\theta$ and thus $F(\theta)$ in (17b) will be intrinsically negative.

4.2. Two Parallels for the Hyperbolic Flux Relation

[27] The classical form of the thermal diffusion equation (i.e., the Fourier's heat flux relation) has the unphysical

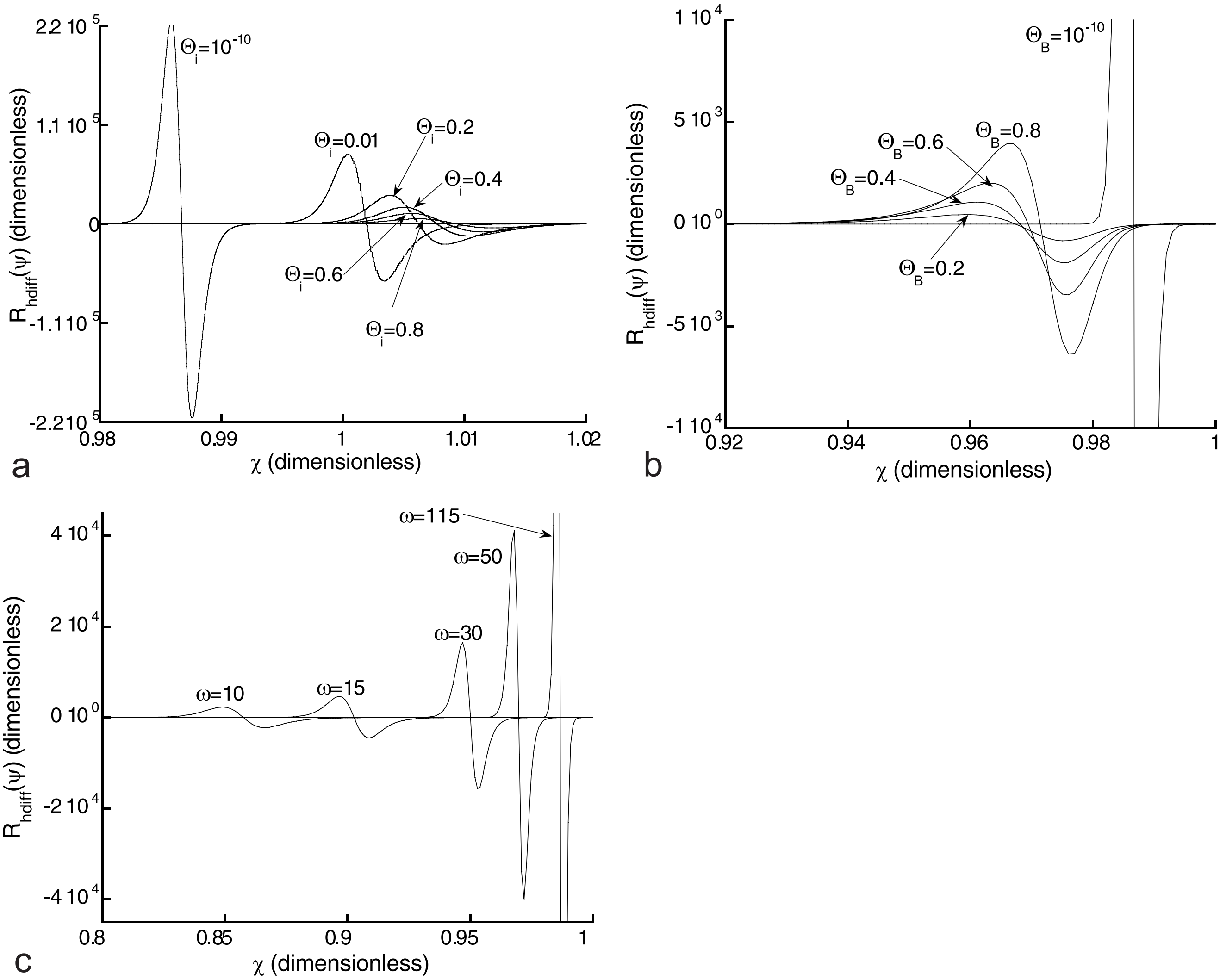


Figure 6. Response of the hypodiffusive form of the hold-back-pile-up (HBPU) effect, as a function of the initial saturation Θ_i, boundary saturation Θ_B, and media nonlinearity through the sharpness factor ω. Since Θ_i, Θ_B, and ω control the wetting front sharpness, they also directly influence the magnitude of the HBPU effect as (a) Θ_i, (b) Θ_B, and (c) ω values are systematically varied. The values for all variables are the same as those in Figures 4 and 5. However, unlike Figure 5, the various $R_{hdiff}(\theta)$ profiles are not normalized by their positive maximum values.

property of transmitting heat at an infinite propagation speed [e.g., see *Joseph and Preziosi*, 1989]. In other words, a sudden temperature change at any point within a conducting medium is instantly felt everywhere, even though the effect is at a much lower amplitude at distant points. One remedy for this shortcoming of the Fourier's law is to use a hyperbolic form of heat conduction equation where heat is not transmitted by diffusion but rather in the form of waves resulting in the notion of "heat waves" or "second sound" [e.g., see *Joseph and Preziosi*, 1989]. However, there appears to be some debate over the physical appropriateness of the hyperbolic form of the Fourier's flux relation [e.g., see *Mandelis*, 2001].

[28] The basic rationale for choosing a hyperbolic extension over a simple gradient relation is then to ensure that perturbations propagate at a finite velocity. The importance of hyperbolic transport within the contexts of moisture and mass transport can be found in several recent works [e.g., *del Rio and Lopez de Haro*, 1991; *Hassanizadeh*, 1996; *Vazquez et al.*, 1997; *Sobolev*, 1997]. Hyperbolic transport equations, derived from first principles, are mostly based on Extended Irreversible Thermodynamics (EIT) [e.g., see *Vazquez et al.*, 1997]. Simply put, equations with hyperbolic transport incorporate an additional inertial-like or acceleration term into the standard form of the flux multiplied by a relaxation time.

[29] With regards to unsaturated flow, *del Rio and Lopez de Haro* [1991] have employed EIT to formally derive the following hyperbolic form of the flux relation for unsaturated flows:

$$\vec{q} = -K(\theta)\vec{\nabla}(\psi + z) - \tau\frac{\partial\vec{q}}{\partial t}, \tag{18a}$$

where τ [T] is the relaxation time assumed to be a function of state variables. Clearly, the second term on the RHS of (18a) mathematically resembles the first term on the RHS of $\vec{q}_{hyper}$, stated in (10). The transient (i.e., the inertia-like) portion of the flux in (18a) accounts for the fluctuations far from equilibrium [e.g., see *Vazquez et al.*, 1997]. Such fluctuations, of course, may last for a much shorter period than the intrinsic time of the process in the full domain, and depends directly on the functional form and magnitude of $\tau(\theta)$. *del Rio and Lopez de Haro* [1991] derive an expression for the relaxation time, τ, which as a function of moisture content, θ, can be stated as

$$\tau(\theta) = \alpha_{20}\left[\frac{K(\theta)\theta(\psi)\gamma}{(\psi + z) + \gamma\theta(\psi)}\right] \tag{18b}$$

where α_{20} [T^2 L^{-1}] is a phenomenological scalar that must be determined experimentally and $\gamma = \gamma(\psi) = [\partial\psi/\partial\theta(\psi)]$ [L]. *del Rio and Lopez de Haro* [1991] present no guidance as how to evaluate the functional form or how to experimentally determine the magnitude of α_{20} and suggest to simply assume τ is a constant, say τ_0, or (18a) becomes

$$\vec{q} = -K(\theta)\vec{\nabla}(\psi + z) - \tau_0\frac{\partial\vec{q}}{\partial t} \tag{19a}$$

If we also treat $T(\theta)$ as a constant, say T_0, the form of $\vec{q}_{hyper}$ in (10) simplifies to

$$\vec{q}_{hyper} = -T_0\frac{\partial\vec{q}}{\partial t} \tag{19b}$$

which makes the form of $\vec{q}_{hyper}$ in (19b) similar to the second term on the RHS of (19a). Since the relaxation time, τ, is a positive quantity [*del Rio and Lopez de Haro*, 1991], $\vec{q}_{hyper}$ in (19a) can yield the appropriate HBPU effect.

[30] We can find another basis for the hyperbolic flux relation if we consider the Navier-Stokes (NS) momentum conservation equation. For example, the NS momentum conservation equation, specialized for the incompressible fluid flow in unsaturated materials, can be stated as [e.g., *Raats and Klute*, 1968; *Gray and O'Neill*, 1976; *Sposito*, 1978]:

$$\frac{\partial\vec{q}}{\partial t} + \vec{\nabla}\cdot\left(\theta^{-1}\vec{q}^{\,2}\right) = -g\left[\vec{\nabla}(\psi + z) + \frac{\vec{q}}{K(\theta)}\right] + \nu\vec{\nabla}^2\vec{v} \tag{20a}$$

where ν [L^2 T^{-1}] is the kinematic viscosity and $\vec{v}$ [L T^{-1}] is the velocity vector. On the left-hand side of (20a), the first and second terms respectively define the accumulation and advective components, the first term on the RHS is the total pressure drop in the porous media, the second term defines the momentum due to the porous material resistance, and the third term accounts for the viscous dissipation. Multiplying both sides of (20a) with [$K(\theta)/g$] and rearranging, we obtain

$$\vec{q} = -K(\theta)\vec{\nabla}(\psi + z) - \frac{K(\theta)}{g}\left[\frac{\partial\vec{q}}{\partial t} + \vec{\nabla}\cdot\left(\theta^{-1}\vec{q}^{\,2}\right) - \nu\vec{\nabla}^2\vec{v}\right] \tag{20b}$$

Neglecting the advective and viscous dissipation terms, which is a quite reasonable assumption for slow flows in porous materials, we have

$$\vec{q} = -K(\theta)\vec{\nabla}(\psi + z) - \frac{K(\theta)}{g}\frac{\partial\vec{q}}{\partial t} \tag{20c}$$

Clearly, (20c) is mathematically similar to (18a) and the second term on the RHS of (20c) is akin to $\vec{q}_{hyper}$ in (19b). Note that, the factor $K(\theta)/g$ on RHS of (20c) can be interpreted as the (positive) relaxation time for the hyperbolic NS equation.

4.3. A Parallel for the Mixed Form Flux Relation

[31] Another extension to the standard unsaturated flow theory suggested by *Hassanizadeh and Gray* [1993a] involves the concept of dynamic capillary pressure [see also *Marle*, 1982; *Kalaydjian*, 1987; *Pavone*, 1989]. *Hassanizadeh and Gray* [1993a] argue that the common definition of capillary pressure, p^c, i.e., $p^c = p^a - p^w$, where p^a is the air pressure, must be viewed as an equilibrium force balance and not a definition for the capillary pressure. Alternatively, they suggest the following formulation for the capillary pressure:

$$L^w\frac{\partial S^w}{\partial t} = p^c(S^w) - (p^a - p^w) \tag{21a}$$

where L^w [M L^{-1} T^{-1}] is a nonnegative material coefficient. If we allow $p^a = 0$, (21a) reduces to

$$p^w = L^w\frac{\partial S^w}{\partial t} - p^c(S^w) \tag{21b}$$

Considering the standard form of the Darcy flux for the water phase and substituting for p^w from (21b), we then have the following flux relation:

$$\varepsilon S^w\vec{v}^w = -\frac{kk_r^w}{\mu}\left[\vec{\nabla}\left(-p^c + L^w\frac{\partial S^w}{\partial t}\right) - \rho^w\vec{g}\right] \tag{22}$$

[32] In terms of the flux vector, $\vec{q}$, pressure head, ψ, moisture content, θ, and letting $\psi = -\psi^c$, we can write the following form of the flux relation:

$$\vec{q} = -K(\theta)\vec{\nabla}(\psi + z) - \left[L(\theta)\vec{\nabla}\frac{\partial\theta(\psi)}{\partial t}\right] \tag{23}$$

where $L(\theta) = [K(\theta)(L^w/\rho^w g)]$ [L^2] and the second group of terms on the RHS of (23), is similar to $\vec{q}_{mix}$, stated in (11). According to *Hassanizadeh and Gray* [1993a], L^w is a nonnegative property, thus making $L(\theta)$ a positive function. As we discussed in Section 3, when L is positive, an additional swing is introduced before the HBPU. This swing will be positive and thus diffusive in nature. Whether this additional diffusion will be removed through the functional behavior of $L(\theta)$ is uncertain.

5. Concluding Remarks

[33] We have extended the standard Richards Equation (RE) with a term that embodies a porous-continuum level representation of the hold-back-pile-up (HBPU) effect, where the hold-back (HB) operates at the forward edge of the wetting front (WF) to prevent over-spreading due to capillary diffusion and the pile-up (PU) operates behind to increase the pressure and thus the water saturation of a finger tip. In combination with capillary hysteresis, the HBPU should lead to a pressure reversal immediately behind the WF and ultimately yield a nonmonotonic signature such as found in GDF. Considering the limited data

presented in the literature, the critical conditions manifesting GDF are an intersection of porous media properties, initial dryness, and applied surface flux that yield a sharp WF. For this reason, we tie the HBPU effect to WF sharpness and formulate it as dependent on the spatial and/or temporal variations of the state variables such that its action is focused by steep gradients and/or rates of change. We present three possible mathematical representations of the HBPU effect with associated extended flux relations, referred to as the hypodiffusive, hyperbolic, and mixed spatial-temporal, their names indicative of their forms within the extended governing equation. However, we note that we are not limited to these particular three forms, as others can be constructed to yield the HBPU as well.

[34] Our approach to obtain mathematical representations of the HBPU effect is grounded in inductive reasoning, i.e., we are guided by the experimentally observed macroscopic behavior of GDF and suggest various mathematical forms that will yield this behavior. Considering extended theories for single-phase and multiphase flow built from first principles, if we once again reason with our end in mind, we can find parallels for each of the forms for the HBPU we have presented. For instance, a hypodiffusive flux relation can be distilled from the generalized two-phase flow theory of *Gray and Hassanizadeh* [1991a] considering the concept of the Helmholtz free energy of the water phase as influenced by the interfacial areas of the three phases (i.e., water, air, and solid). Within the context of extended irreversible thermodynamics, *del Rio and Lopez de Haro* [1991] derive a hyperbolic flux relation containing an inertial-like term with a relaxation time function that imparts memory. Simplification of the standard form of the Navier-Stokes equation also yields a hyperbolic flux relation with an inertial relaxation time that is a function of hydraulic conductivity. Finally, using the dynamic capillary pressure concept of *Gray and Hassanizadeh* [1991a], where the capillary pressure is comprised of both static and time-dependent portions, a mixed form flux can be derived.

[35] It is important to note that, at present, it is not known whether any of these theories based on first principles are appropriate for the purpose of modeling GDF. Indeed, not only is their more general validity still in question, but the respective constitutive properties within these theories have yet to be fully defined, parameterized, or measured. This clearly emphasizes the need for further theoretical development in conjunction with physical experiments specifically designed to study such phenomena as the free energy, relaxation time, and dynamic capillary pressure. From our analytical study, we do know that at least two postulated HBPU forms yield the behavior, at least in isolation, which we argue is necessary to model GDF at a porous-continuum level. However, as a WF develops and advances into the domain, there will be significant feedback between all components (capillary, gravity, and HBPU). Thus, to fully consider the ability of the HBPU to model GDF, we must conduct direct numerical simulations using the various forms of the extended governing equation.

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