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Dynamic Capillary Pressure Mechanism for Instability in Gravity-Driven Flows; Review and Extension to Very Dry Conditions

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Abstract. Several alternative mathematical models for describing water flow in unsaturated porous media are presented. These models are based on an equation for conservation of mass of water, and a generalized linear law for water flux (Darcy's law) containing a term called the dynamic capillary pressure. The distinct form of each alternative model is based on the specific form of expression used to describe the dynamic capillary pressure. The conventional representation arises when this pressure is set equal to the equilibrium pressure given by the capillary pressure – saturation function for unsaturated porous media, and this conventional approach leads to the Richards equation. Other models are derived by representing the dynamic capillary pressure by a rheological relationship stating that the pressure is not given directly by the capillary pressure – saturation function. Two forms of rheological relationship are considered in this manuscript, a very general non-equilibrium relation, and a more specific relation expressed by a first-order kinetic equation referred to as a relaxation relation. For the general non-equilibrium relation the system of governing equations is called the general Non-Equilibrium Richards Equation (NERE), and for the case of the relaxation relation the system is called the Relaxation Non-Equilibrium Richards Equation (RNERE). Each of the alternative models was analyzed for flow characteristics under gravity-dominant conditions by using a traveling wave transformation for the model equations, and more importantly the flow described by each model was analyzed for linear stability. It is shown that when a flow field is perturbed by infinitesimal disturbances, the RE is unconditionally stable, while both the NERE and the RNERE are conditionally stable. The stability analysis for the NERE was limited to disturbances in the very low frequency range because of the general form of the NERE model. This analysis resulted in what we call a low-frequency criterion (LFC) for stability.

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This LFC is also shown to apply to the stability of the RE and the RNERE. The LFC is applied to stability analysis of the RNERE model for conditions of initial saturation less than residual.

1. Introduction

The instability of unsaturated flows during infiltration or redistribution of water within soils and the vadose zone has been identified to be one form of preferential flow through which fast transport of contaminants might reach ground water resources (Glass *et al.*, 1988; Nieber, 2001). Due to the recognition of the importance of this process, much effort has been expended in the experimental and mathematical analyses of gravity-driven unstable flows in unsaturated porous media with the idea that the development of a complete theory and parameterization of unstable flows should provide important components of soil hydrology and solute transport models.

The importance of gravity-driven unstable flows in unsaturated soils was first recognized upon the publication of the first definitive study of gravity-driven fingering in layered porous media in the paper by Hill and Parlange (1972). Several earlier reports of gravity-driven fingering had been reported by other investigators (e.g. Tabuchi, 1961; Smith, 1967) but those studies were not definitive enough with relation to gravity-driven fingering to capture the interest of soil physics and soil hydrology researchers. The work of Hill and Parlange did indeed capture that interest and motivated extensive experimental and theoretical work. A number of experimental studies of gravity-driven fingering followed, using two-dimensional slab chambers filled with porous media packed either as two homogeneous layers of different texture (Diment and Watson, 1985; Glass *et al.*, 1989a,c; Baker and Hillel, 1990; Wang *et al.*, 1998a, b), as completely homogeneous systems (Selker *et al.*, 1992a; Liu *et al.*, 1994b; Bauters *et al.*, 2000; Deinert *et al.*, 2002), or as heterogeneous systems (Sililo and Tellam, 2000). The first definitive experimental study for fingering in field soils was given by Starr *et al.* (1978).

Experimental data quantifying unstable flow have been derived using visual observations of finger width and velocity, flow within individual fingers, water pressure measurements within individual fingers (Selker *et al.*, 1992b), and water saturation distributions within fingers using either light transmission (Glass *et al.*, 1989a), gamma-ray attenuation (Bauters *et al.*, 2000), or neutron radiography (Deinert *et al.*, 2002). One point that comes out of all of these studies is that fingers are observed to occur when the initial saturation is below the residual. For conditions where the initial saturation is above residual, fingers of width less than the width of the experimental chamber are not observed to occur, at least by the methods of observation utilized to date.

The first mathematical analysis of gravity-driven unstable flow was formulated by Raats (1973) wherein he used the Green-Ampt model of infiltration, a sharp front model, as the basis for his analysis. The same basic model was used in the linear stability analysis presented by Philip (1975a, b) for gravity-driven flows. Philip's analysis was similar to that presented by Saffman and Taylor (1958) and Chuoke *et al.* (1959) for viscous fingering, and showed that flows become unstable when the pressure gradient opposes the flow. His spectral analysis provided expressions to calculate the critical perturbation wavelength and estimates of finger widths, but the derived expressions contained properties related to Hele-Shaw cells and not to real soils. Philip (1975a) explained that the Green-Ampt approximation has significant limitations as the basis for the stability analysis of infiltrating flows in real soils, and argued the need to perform analysis of flow instability for the conditions where the wetting front is not sharp. As explained by Philip (1975a) this would mean a stability analysis of the Richards equation, which he stated would prove to be difficult. This need was partially met by the work of Parlange and Hill (1976) wherein the stability analysis of the Green-Ampt type of model was extended to real soils by imposing a diffuse structure to the wetting front. Their analysis provided expressions for estimates of finger width as a function of imposed flow, saturated hydraulic conductivity of the soil, initial moisture content, and sorptivity. The analysis of Parlange and Hill has had a lasting impact as many formulae for estimating finger size have been derived based on their original work (Wang *et al.*, 1989a; Glass *et al.*, 1989b; Liu *et al.*, 1994a; deRooij and Cho, 1999).

The first stability analysis to the full Richards equation was presented by Diment *et al.* (1982). In their analysis the basic equation of flow was given by the Richards equation, and the pressure for the flow field was perturbed. The form of their resulting perturbation equation was not tractable to analytical solution, so a numerical solution was sought instead and results were reported by Diment and Watson (1983). For the limited cases considered they concluded that flows governed by the Richards equation are stable to infinitesimal perturbations. But their results were based on a numerical solution and therefore it was not possible to provide a general result for all conditions wherein linear stability analysis would apply.

Kapoor (1996) presented an analytical solution to the perturbed steady-state Richards equation and concluded that steady-state flows governed by the Richards equation are unconditionally stable for the exponential form of the hydraulic conductivity – pressure function and conditionally stable for other forms such as the Brooks and Corey (1964) and van Genuchten (1980) forms of the hydraulic conductivity – pressure function. Ursino (2000) performed a similar analysis to that of Kapoor except in her case time-dependent flows were considered. She showed that for the exponential form of the hydraulic conductivity – pressure function, Richards' equation is unconditionally stable, and therefore concluded that flow instabilities must originate from some pore-scale process not included in the conventional upscaling of the flow equation.

In the most recent published analyses the saturation flow field governed by the saturation form of the Richards equation has been subjected to stability analysis by Du *et al.* (2001) and Egorov *et al.* (2002, 2003). The resulting perturbed flow equation was evaluated analytically by Du *et al.* but due to it complex nature their analysis was incomplete, leading them to the conclusion that the Richards equation is conditionally stable. One important feature of the work by Egorov *et al.* was that it provided a complete analytical result for the perturbed flow equation and the results led to the conclusion that the Richards equation is unconditionally stable. Their result is consistent with the nonlinear stability analysis given by Otto (1996, 1997), which concluded that the Richards equation is unconditionally stable to all perturbations (infinitesimal and finite) in homogeneous unsaturated porous media. Egorov *et al.* (2003) extended the nonlinear analysis of Otto by showing that the Richards equation is unconditionally stable to all perturbations even for heterogeneous porous media.

These final results point to the fact that flow instabilities that occur in gravity-driven flows must result from a flow process not included (explicitly or implicitly) in the Richards equation, and therefore we must conclude that the flow process is not described adequately by the conventional Darcy law. In line with the conclusion of Ursino (2000), we conclude that the process that causes flows to become unstable must arise from pore-scale phenomena not included in the conventional governing equations. Going further and following the work of Hassanizadeh and Gray (1993) we would postulate that one possible pore-scale process that could cause instabilities is the process described by dynamic capillary pressure – saturation relations. The results presented to date in Egorov *et al.* (2002, 2003) seem to support this postulate.

This manuscript will provide an overview of the current state of understanding from a mathematical analyses standpoint, of gravity-driven flow instabilities in unsaturated porous media. The presentation will review the results presented to date by Egorov *et al.* (2002, 2003) with respect to the unconditional stability of the Richards equation, and the conditional stability of flows described by models that include the dynamic capillary pressure effect. In addition, we will present some new results that relate to the extension of the models of Egorov *et al.* to the (dry) range of saturations below residual saturation.

2. Overview of Selected Governing Equations for Unsaturated Flow

The three-dimensional mass balance equation is written in non-dimensional form as

$$\frac{\partial s}{\partial t} - \nabla \cdot (K(s)\nabla p) - \frac{\partial K(s)}{\partial z} = 0, \tag{1}$$

where s is the effective saturation equal to $(S - S_r)/(1 - S_r)$, S is the water saturation, S_r is the residual saturation, p is the water pressure, $K(s)$ is the unsaturated hydraulic conductivity, and z is the z-coordinate taken positive upward opposite to the direction of gravity, and t is the time. This equation is based on the substitution of Darcy's law into the equation for conservation of mass. Different forms of the mass balance equation can be obtained depending on the form of the pressure function p. The forms available to define the pressure function are numerous. The first one is based on a conventional formulation and thereby leads to the Richards Equation (RE) and is given by

$$p = P(s). \tag{2}$$

This equation describes the conventional equilibrium relation between water pressure and water saturation, and can be non-hysteretic or hysteretic. The substitution of p from relation (2) into equation (1) yields the conventional RE given by

$$\frac{\partial s}{\partial t} - \nabla \cdot (K(s)\nabla P(s)) - \frac{\partial K(s)}{\partial z} = 0 \tag{3}$$

or in saturation form the equation is

$$\frac{\partial s}{\partial t} - \nabla \cdot (D(s)\nabla s) - \frac{\partial K(s)}{\partial z} = 0, \tag{4}$$

where $D(s) = K(s)P'(s)$. Substitution of relation (2) into Darcy's law ($\boldsymbol{q} = -K(s)\nabla p - K(s)\boldsymbol{e}_z$) gives

$$\boldsymbol{q} = -K(s)\nabla P(s) - K(s)\boldsymbol{e}_z, \tag{5}$$

where $\boldsymbol{e}_z$ is the unit vector in the vertical.

A more general form of the pressure function is given by the relation

$$F\left(s, p, \frac{\partial s}{\partial t}, \frac{\partial p}{\partial t}, \ldots\right) = 0. \tag{6}$$

This equation indicates a non-equilibrium relation between water pressure and saturation. The dependence of the pressure on the saturation and temporal derivatives of the saturation and the pressure are indicated by the terms included in the argument of the function. The idea for non-equilibrium relations for water pressure and saturation is based on experimental evidence presented in various studies (Kirkham and Feng, 1949; Nielsen *et al.*, 1962; Rawlins and Gardner, 1963; Topp *et al.*, 1967; Smiles *et al.*, 1971; Wildenschild *et al.*, 2001) and theoretical considerations (Hassanizadeh and Gray, 1993; Hassanizadeh *et al.*, 2002; Dahle *et al.*, 2002). Since this function has a generalized form it is not possible to introduce it directly into the mass balance equation and thereby provide a distinct equation. But an analysis of Equation (1) coupled with relation (6) is possible as will be shown in Section 3. The combination of equations (1) and (6) will hereafter be referred to as the NERE model.

A specific form of relation (6) that we will spend a significant part of the next sections describing is given by the relaxation equation

$$\tau(s,p)\frac{\partial s}{\partial t} = p - P(s), \tag{7}$$

where $\tau(s,p)$ is a relaxation parameter in the kinetic rheological relation for non-equilibrium capillary pressure – saturation relations. Substitution of function p from relation (7) into Equation (1) leads to

$$\frac{\partial s}{\partial t} - \nabla\cdot(K(s)\nabla P(s)) - \nabla\cdot\left(K(s)\nabla\left(\tau(s,p)\frac{\partial s}{\partial t}\right)\right) - \frac{\partial K(s)}{\partial z} = 0 \tag{8}$$

and into Darcy's law we get

$$q = -K(s)\nabla P(s) - K(s)\nabla\left(\tau(s,p)\frac{\partial s}{\partial t}\right) - K(s)\boldsymbol{e}_z. \tag{9}$$

The equations given by equation (1) and relation (7) or alternatively Equation (8) will hereafter be referred to as the RNERE model. In relation (9) we have the usual gradient of the equilibrium pressure term, but also the gradient of the relaxation term which contains the temporal rate of change of saturation.

For most of the analyses to follow we consider conditions where the saturation falls in the range $0 < s < 1$, however, in Section 4.2.2 we consider the case where the initial saturation is less than residual.

3. Review of Stability Analyses of the RE

Linear stability analyses of the RE have been presented by Diment and Watson (1983), Ursino (2000), Kapoor (1996), Du *et al.* (2001) and Egorov *et al.* (2002, 2003). Diment and Watson, Ursino, and Kapoor all started with the pressure-based form of the RE, while Du *et al.* and Egorov *et al.* utilized the saturation-based form of the RE.

Starting with the saturation-based form of the RE the traveling wave equation is derived using the transformation variables

$$s = s(\xi), \quad \xi = z + Vt \tag{10}$$

subject to the boundary conditions

$$s(-\infty) = s_-, \quad s(+\infty) = s_+, \qquad 0 < s_- < s_+ < 1, \tag{11}$$

where the velocity V of the traveling wave is given by

$$V = \frac{K(s_-) - K(s_+)}{s_- - s_+}. \tag{12}$$

Applying these variables to equation (4) yields the traveling wave form of the RE,

$$V\frac{\mathrm{d}s}{\mathrm{d}\xi} - \frac{\mathrm{d}}{\mathrm{d}\xi}\left(D(s)\frac{\mathrm{d}s}{\mathrm{d}\xi}\right) - \frac{\mathrm{d}K(s)}{\mathrm{d}\xi} = 0. \tag{13}$$

The solution for equation (13) subject to the boundary conditions at infinity ($\xi = +\infty$) is given as (Philip, 1957)

$$\xi(s) - \xi_* = \int_{s_*}^{s} \frac{D(s)\mathrm{d}s}{v(s - s_+) - K(s) + K(s_+)}, \tag{14}$$

where ξ_* is the coordinate location of the arbitrarily selected saturation s_* ($s_- < s_* < s_+$). The inverse of the function $\xi(s)$ is called the basic solution and will be designated as $s_0(\xi)$. A typical plot of this solution is presented in Figure 1. By the nature of the solution and the included functions ($K(s)$ and $P(s)$) the saturation decreases monotonically from s_+ at $+\infty$ to s_- at $-\infty$.

The stability analysis is based on a small perturbation applied to the basic solution $s_o(\xi)$. The perturbed saturation field is represented as

$$s(x, y, z, t) = s_o(\xi) + \varepsilon e^{i\omega_x x + i\omega_y y + kt} s_1(\xi) + O\left(\varepsilon^2\right), \tag{15}$$

where the ω_x and the ω_y are characteristic wave numbers in the x and y directions, respectively, the k is the amplification factor (or growth factor), the function $s_1(\xi)$ describes the variation of the bounded perturbation in the ξ coordinate and vanishes at $\pm\infty$, and ε scales the magnitude of the perturbation.

The perturbed solution is obtained by substituting expression (15) into equation (4) and dropping terms of order ε^2. Accounting for the equation for the basic solution and collecting like terms we arrive at a locally

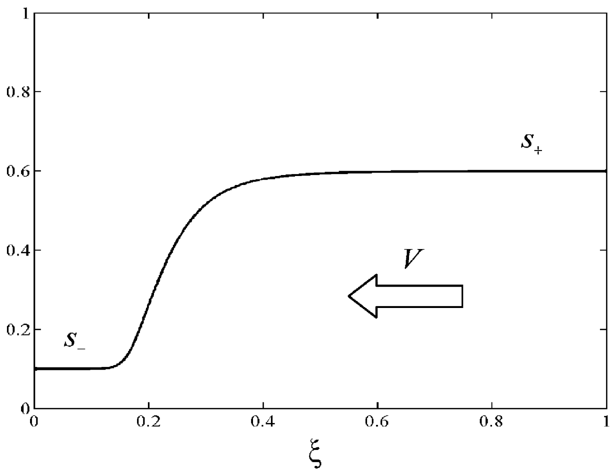

Figure 1. A typical plot of saturation s versus dimensionless variable ξ as a result of the solution of the traveling wave form of the RE. This solution comprises the basic solution s_o.

linearized perturbation equation in the form of a spectral problem for determining nontrivial s_1 and $k = k(\omega)$ for arbitrary ω, that is

$$-\frac{d^2}{d\xi^2}(D(s_o)s_1) + \frac{d}{d\xi}\left((V - K'(s_o))s_1\right) + \omega^2 D(s_o)s_1 = -ks_1, \quad -\infty < \xi < \infty. \tag{16}$$

An equation of similar form to equation (16) was also derived by Du *et al.* (2001).

Now the problem is the analysis of the spectrum of the problem (16). If the equation admits a solution (s_1, k) with $k > 0$ then we have instability of the RE. If all solutions have $k < 0$ then the flow governed by the RE is stable. Analytical investigation of the spectral problem is difficult in the form of equation (16) because the equation is not self-adjoint. To make the analytical study tractable we perform a transformation using new variables ζ and θ to replace ξ and s_1 respectively,

$$\zeta = \int \frac{d\xi}{\sqrt{D(s_o)}}, \quad \theta = \frac{D^{1/4}(s_o)}{\sqrt{s_o'}} s_1, \tag{17}$$

which leads to

$$-\frac{d^2\theta}{d\zeta^2} + \left(\omega^2 D + F\right)\theta = -k\theta, \quad -\infty < \zeta < \infty, \tag{18}$$

where

$$F=\frac{1}{B}\frac{\mathrm{d}^2 B}{\mathrm{d}\zeta^2},\quad B=D^{1/4}\sqrt{s'_{\mathrm{o}}}.$$

Equation (18) is self-adjoint and therefore has been made tractable to theoretical analysis.

In mathematical physics equation (18) is known as the Schrödinger equation, and for different forms of the potential $(\omega^2 D+F)$ the spectral problem for the Schrödinger equation has been studied (Carmona and Lacroix, 1999), and therefore known techniques can be used to investigate the problem presented by equation (18). Such an analysis was performed in Egorov *et al.* (2003) in which it was shown that the spectrum of the problem is negative (i.e., $k<0$) for all non-zero frequencies ω of the perturbation.

So we can now state that the RE is unconditionally stable to infinitesimal perturbation. But it is legitimate to ask whether the occurrence of finite perturbations to the basic flow would be stable. This query has been addressed by Otto (1996, 1997) and by Egorov *et al.* (2003). It was shown by Otto that the type of equation given by the RE is unconditionally stable for perturbations of finite magnitude in the case of homogeneous porous media. Otto's work was extended by Egorov *et al.* to show that the same conclusion is found for the case of heterogeneous media. While the linear stability analysis outlined in the foregoing description points toward unconditionally stability of the RE it does not prove the stability of the RE for all conditions. But the nonlinear stability analyses of Otto and Egorov *et al.* provides strong proof that the RE is unconditionally stable for all conditions. This also means that upscaling of the RE over a heterogeneous domain will lead to a governing equation that possesses the property of unconditional stability.

4. Stability Analyses of Selected Nonequilibrium Models

In this section we will consider the two types of nonequilibrium models that were outlined in Section 2, that is the NERE and the RNERE. The NERE will be described under the heading of the general nonequilibrium model, while the RNERE will be described under the heading of the relaxation nonequilibrium model.

4.1. GENERAL NONEQUILIBRIUM MODEL

The general nonequilibrium model was presented in Section 2 by the coupling of equation (1) and relation (6) and referred to as the NERE. Due to the non-specific form of relation (6) it is not possible to derive an explicit equation for analysis, but as shown by Egorov *et al.* (2003) it is possible to derive a useful stability criterion for the NERE.

A linear stability analysis is performed on the NERE using the same procedure we used for the stability analysis of the RE. First we define a basic solution based on the traveling wave form of the NERE. The traveling wave form of equation (1) for that model is independent of the form of the rheological relation. That traveling wave equation is given by

$$V\frac{\mathrm{d}s}{\mathrm{d}\xi}-\frac{\mathrm{d}}{\mathrm{d}\xi}\left(K(s)\frac{\mathrm{d}p}{\mathrm{d}\xi}\right)-\frac{\mathrm{d}K(s)}{\mathrm{d}\xi}=0. \tag{19}$$

After integrating once and applying the boundary conditions we have the following result,

$$\frac{\mathrm{d}p}{\mathrm{d}\xi}=\frac{V(s-s_+)+K(s_+)-K(s)}{K(s)}. \tag{20}$$

The transformation to the traveling wave variable for relation (6) gives

$$F\left(s, p, V\frac{\mathrm{d}s}{\mathrm{d}\xi}, V\frac{\mathrm{d}p}{\mathrm{d}\xi}, \ldots\right)=0. \tag{21}$$

Let us suppose that the solution to the traveling wave equation (20) and relation (21) exists and are represented by $s_0(\xi)$ and $p_0(\xi)$, respectively. The exact form of these basic solutions will depend on the form of the rheological relation (6), but it is not necessary to specify the form of that relation to perform the following stability analysis.

The next step in the linear stability analysis is to superimpose three-dimensional perturbations in saturation and pressure onto the basic solution in the form

$$s(x,y,z,t)=s_{\mathrm{o}}(\xi)+\varepsilon e^{i\omega_x x+i\omega_y y+kt}s_1(\xi)+O\left(\varepsilon^2\right), \tag{22}$$

$$p(x,y,z,t)=p_{\mathrm{o}}(\xi)+\varepsilon e^{i\omega_x x+i\omega_y y+kt}p_1(\xi)+O\left(\varepsilon^2\right). \tag{23}$$

These perturbation expressions are substituted into equation (1) and relation (6), and terms of order ε^2 are dropped to yield a system of locally linearized perturbation equations in the form of a spectral problem for determining nontrivial p_1 and s_1, corresponding to spectral parameter k for arbitrary frequencies ω. This spectral problem is expressed by

$$\frac{\mathrm{d}A}{\mathrm{d}\xi}+\omega^2K(s_0)p_1=-ks_1, \tag{24}$$

$$\Phi\left(s_1, p_1, \frac{\mathrm{d}s_1}{\mathrm{d}\xi}, \frac{\mathrm{d}p_1}{\mathrm{d}\xi}\ldots; s_0, p_0, \frac{\mathrm{d}s_0}{\mathrm{d}\xi}, \frac{\mathrm{d}p_0}{\mathrm{d}\xi}, \ldots; k\right)=0, \tag{25}$$

where A is the flux perturbation given by

$$A = -K(s_0)\frac{\mathrm{d}p_1}{\mathrm{d}\xi} - K'(s_0)\left(1 + \frac{\mathrm{d}p_0}{\mathrm{d}\xi}\right)s_1 + Vs_1. \tag{26}$$

Integration of equation (24) with the boundary condition such that A vanishes as $\xi \to \pm\infty$, leads to the integrals

$$\omega^2 \int_{-\infty}^{+\infty} K(s_0)p_1 \mathrm{d}\xi = -k \int_{-\infty}^{+\infty} s_1 \mathrm{d}\xi. \tag{27}$$

It is not possible to evaluate the signs of the integrals in equation (27) and thereby be able to find the sign of $k = k(\omega)$ without knowing the specific forms for s_0, s_1 and p_1. However, it is possible to perform an asymptotic analysis to derive an asymptotic solution for the eigenvalue k_0 at low frequency($\omega \ll 1$). This analysis begins by establishing the fact that the eigenfunction for s_1 and p_1 are equal to $\mathrm{d}s_0/\mathrm{d}\xi$ and $\mathrm{d}p_0/\mathrm{d}\xi$ when $\omega = 0$ as shown in Egorov *et al.* (2003). At low frequency the eigenvalue k_0 and the eigenfunctions s_1 and p_1 can be expanded in powers of ω^2 as

$$k_0 = 0 + b\omega^2 + \cdots,$$
$$s_1 = \mathrm{d}s_0/\mathrm{d}\xi + s_*\omega^2 + \cdots,$$
$$p_1 = \mathrm{d}p_0/\mathrm{d}\xi + p_*\omega^2 + \cdots$$

Substituting these expressions into equation (27) and dropping terms of order ω^4 leads to

$$b = -\frac{C}{s_+ - s_-}$$

with

$$C = \int_{-\infty}^{+\infty} K(s_0)\frac{\mathrm{d}p_0}{\mathrm{d}\xi} d\xi. \tag{28}$$

Therefore we have

$$k_0 = -\frac{C}{s_+ - s_-}\omega^2 + O(\omega^4). \tag{29}$$

Since ω^2 and $(s_+ - s_-)$ are inherently positive, the condition given by equation (29) means that flows will be unstable ($k_0 > 0$) when $C < 0$. Examining the expression for C in equation (28), the value of C will be negative when the pressure field is sufficiently non-monotonic. This result about the pressure gradient being opposed to the flow for gravity-driven unstable flows was also found by Raats (1973), Philip (1975a) and Parlange and Hill (1976).

The low frequency criterion established here will be used in later sections to evaluate the stability of the RNERE models presented in those sections. But here we should end with a note about the use of the low frequency criterion as a tool to evaluate the stability of the RE model. It was established in Section 3 that for infiltrating flows the pressure and saturation profiles in the RE model are monotonic, meaning that the pressure gradient $\mathrm{d}p_0/\mathrm{d}\xi$ is positive for all cases of the RE model. Using this result in equation (28) leads to $C>0$, and from expression (29) the value of $k_0<0$ for all small ω, meaning that infiltrating flows governed by the RE will be stable.

4.2. RELAXATION NONEQUILBRIUM MODEL

The relaxation non-equilibrium model is a special case of the generalized nonequilibrium model where the dynamic pressure is given by a first order kinetic rheological relation as in relation (7). For this model we have examined two conditions, one in which the initial saturation is above the residual, and the other where the initial saturation is less than the residual. These distinct cases are both important because most models of unsaturated flow have involved saturation conditions above residual, while in many realistic field conditions, and also in many laboratory experiment conditions the saturations within the flow domain can be below residual. Each of these cases will be examined in the following subsections.

4.2.1. *RNERE Model for Initial Moisture Greater than Residual*

The RNERE model is given by the combination of equations (1) and relation (7). The traveling wave form of those equations are given by the coupled equations

$$\frac{\mathrm{d}s}{\mathrm{d}\xi}=\frac{p-P(s)}{V\tau\,(p,s)}, \tag{30}$$

$$\frac{\mathrm{d}p}{\mathrm{d}\xi}=\frac{V(s-s_+)+K(s_+)-K(s)}{K(s)} \tag{31}$$

subject to the initial conditions $s(-\infty)=s_-$ and $p(-\infty)=P(s_-)$. Equation (31) was obtained after once integrating with respect to ξ and applying the boundary condition $s=s_+$ at $\xi=\infty$.

We now investigate the situation where τ is factorized into a constant τ_o, a function of pressure $\tau_\mathrm{p}(p)$ and a function of saturation $\tau_\mathrm{S}(s)$. This factorization is expressed by

$$\tau(s,p)=\tau_0\tau_\mathrm{p}(p)\tau_\mathrm{S}(s). \tag{32}$$

A number of functions could be used to express the pressure and the saturation dependencies. We have used the following functions:

$$\tau_S(s) = \frac{dP(s)}{ds}, \tag{33}$$

$$\tau_S(s) = s^{\gamma}(1-s)^{\delta}, \tag{34}$$

$$\tau_p(p) = (p_* - p)^{\eta}, \quad \eta > 0. \tag{35}$$

The other parameters that need to be specified are those defining the capillary pressure – saturation relation, and the hydraulic conductivity – saturation relation. The more common types of forms used in modeling unsaturated flows are those referred to as the van Genuchten relations and the Brooks–Corey relations. Both of these types of relations were used in the present study. The van Genuchten relations (van Genuchten, 1980) are given by

$$P(s) = -(s^{-1/nm} - 1)^{1/n}, \tag{36}$$

$$K(s) = \sqrt{s}\left[1 - \left(1 - s^{1/m}\right)^m\right]^2, \tag{37}$$

where n and m are porous media dependent parameters. The relation for the hydraulic conductivity is for the special case of a Mualem–Burdine type of pore-scale model where $m = 1 - 1/n$.

The relations for $P(s)$ and $K(s)$ for the Brooks–Corey formulation (Brooks and Corey, 1964) are given by

$$P(s) = -s^{-\beta}, \quad 0 < \beta < 1, \tag{38}$$

$$K(s) = s^{\alpha}, \quad \alpha > 2. \tag{39}$$

For these models hysteresis in the $P(s)$ function was represented by the Mualem (1974) independent domain model.

4.2.1.1. Basic Solution. In this section we will present numerical solutions of equations (30) and (31) with the associated initial condition. A similar analysis was presented by Cuesta *et al.* (2000) wherein they analyzed the existence, uniqueness and monotonicity of the solution to Equation (8) instead of the system of equations (1) and (7). In the following we will show results from our own calculations about monotonicity of the solution of this system of equations, and where it is pertinent we will relate our results to those of Cuesta *et al.*

Solutions (that is basic solutions) to Equations (30) and (31) were performed numerically using the relaxation function expressed by relation (32) with relations (33) and (35) in particular. A sample set of solutions are illustrated in Figure 2, where all parameters are kept constant except for the value of τ_0. The invariant parameters are: $s_+ = 0.6$, $s_- = 0.1$, $n = 10$,

$\alpha = 2.5$, and $\eta = 0$. The value set for η makes the relaxation coefficient independent of pressure for these simulations. The results for six values of τ_0 are presented in the plot. It is seen that as the value of τ_0 increases the solution becomes more non-monotonic. For the case with $\tau_0 = 0$ the solution is the same as the solution to the RE, and the profile is seen to be monotonic.

The magnitude of the relaxation coefficient necessary to produce non-monotonicity in the basic solution is estimated from the parameter $\tau_F(s_+)$, given by,

$$\tau_F = \tau_F(s_+) = \frac{\left(s_+ P'(s_+)\right)^2}{4\left(s_+ K'(s_+) - K(s_+)\right)}. \tag{40}$$

Equation (40) is derived from analysis of the traveling wave equations (30) and (31) with the underlying assumption that $s_+ \gg s_-$. For the parameters used in producing Figure 2, equation (40) gives $\tau_F(s_+) = 0.036$. Therefore, when $\tau(s_+) \geqslant 0.036$ the traveling wave solution is non-monotonic. For the cases shown in Figure 2, this occurs for the values of τ_0 exceeding about 0.08.

It is observed that the tails of the non-monotonic profiles shown in Figure 2 are oscillatory. This feature can be understood upon viewing the

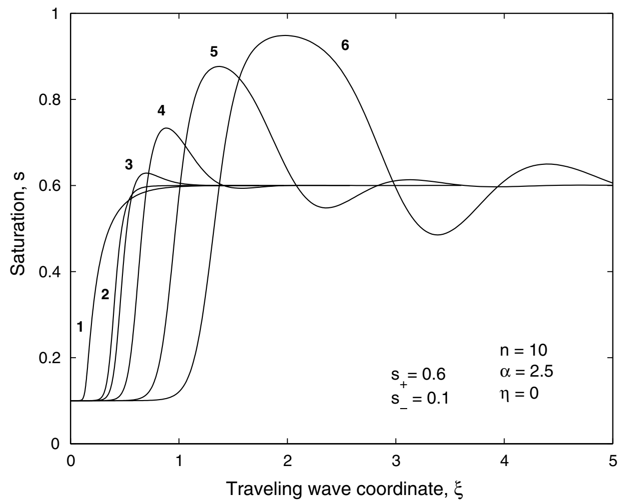

Figure 2. Plots of saturation versus traveling wave variable for various values of τ_0. The curve labels 1 to 6 correspond to the following values of $\tau_0 = 0$, 0.07, 0.1, 0.2, 0.5 and 1.0. The relaxation function $\tau(s, p)$ is given by relation (32) in conjunction with (33) and (35). The critical value of τ_F for non-monotonicity is 0.036. The first two curves are monotonic and $\tau(s_+, p_+) > \tau_F$, while curves 3–6 are non-monotonic and $\tau(s_+, p_+) > \tau_F$. The larger the value of τ, the more non-monotonic the saturation profile.

phase plane shown in Figure 3(a), which is derived from the same solution for $\tau_0 = 0.5$ shown in Figure 2. There we see that the trace starting at s_- ends at a focus point around s_+. In contrast, as shown in Figure 3(b) for the monotonic solution (derived with $\tau_0 = 0.07$) the end point at s_+ is nodal and therefore the tail is non-oscillatory. Although the result is not shown here, we found the tail of a non-monotonic solution to be non-oscillatory (ends at a nodal point at s_+) when the equilibrium capillary pressure – saturation relation $P(s)$ is hysteretic.

For the model just presented we used relation (33) which yields a saturation dependence to the relaxation coefficient similar in behavior to that derived by Panfilov (1998) in his analysis for upscaling dynamic capillary pressure for two-phase flows. This relation shows (see Figure 4) that the saturation dependent part of the coefficient is unbounded at the extreme ends of the effective saturation range. In using this model we found that as $s_- \to 0$, the pressure at the wetting front becomes unbounded and physically unrealistic. A sample result of this is shown in Figure 5(a). The parameters used to derive this were the same as those used to derive Figure 2, with $\tau_0 = 0.5$. It is observed that as s_- progressively decreases, the water pressure at the wetting front increases to the point where it becomes positive, which is a physically unrealistic result. Even further reduction in s_- leads to pressure at the front approaching infinity.

A solution we discovered to resolve this problem of unbounded pressure was to apply a non-unity pressure factorization into the relaxation coefficient, such as the factorization given by relation (35). With this factorization, as $s_- \to 0$ the pressure at the wetting front is limited to p_*. A sample result of this solution is shown in Figure 5(b), wherein the parameters are

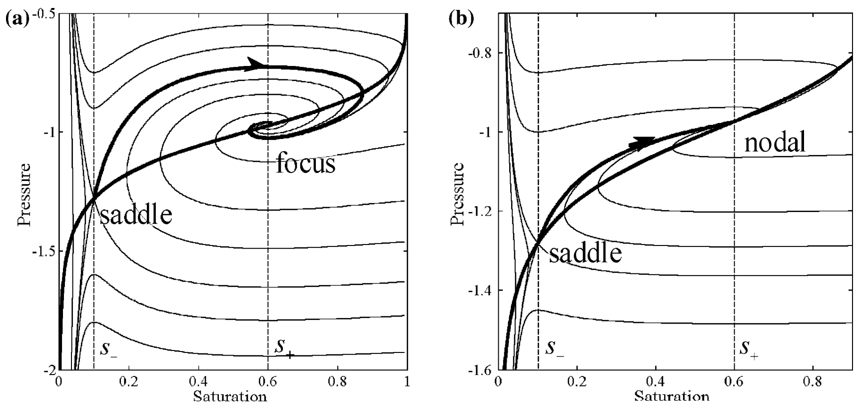

Figure 3. A typical phase plane plot for the basic solution to the RNERE equations for two cases of τ: (a). Where the τ is sufficiently large ($\tau \geqslant \tau_F$) to lead to a non-monotonic saturation profile, and (b). where the τ is small enough ($\tau \ll \tau_F$)to lead to a monotonic saturation profile.

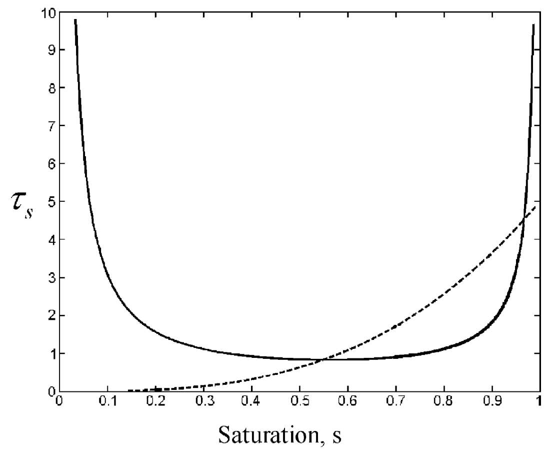

Figure 4. Alternative forms of the saturation component of the relaxation coefficient. These are based on Equations (33) (solid line) and (34) (dash line).

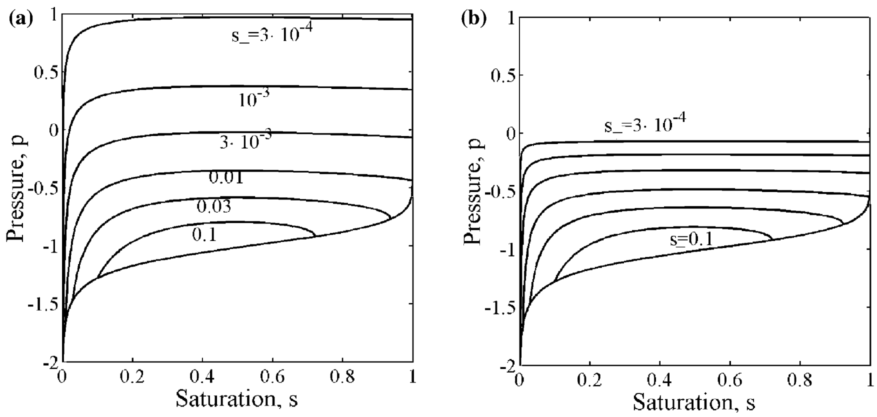

Figure 5. The effect of a pressure limit function used in the relaxation coefficient function. As the initial saturation decreases, the pressure at the front increases. In (a) the pressure limitation is not imposed and as $s_- \to 0$, the pressure at the front increases without bound. In (b) the limitation on pressure is imposed and is in the form of a water entry pressure p_* and therefore the pressure at the front is bounded from above.

all the same as for the solution shown in Figure 5a, but in this case the pressure factorization is applied. For this case the parameter values in the pressure function were set to $\eta = 1.0$ and $p_* = -0.1$.

An approach different from this was presented by Cuesta *et al.* (2000). In their analysis the hydraulic functions were taken from the Brooks–Corey functions. For the relaxation coefficient they used the formula $\tau = \tau_0 s^\gamma$ (same as relation (34) but with $\delta = 0$). A qualitative description of this function is illustrated in Figure 4 with $\gamma > 0$, where it is seen that the relaxation

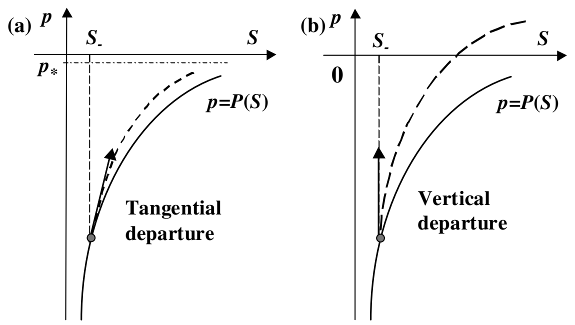

Figure 6. Phase plane diagrams showing the effect of porous media hydraulic and non-equilibrium characteristics on the shape of the phase plane trace. The dividing point between the two behaviors is the parameter $\gamma = (\alpha - 2 - 2\beta)$. For (a) the $\gamma > (\alpha - 2 - 2\beta)$, and the solution to the traveling wave equation is bounded from above. For (b) the $\gamma < (\alpha - 2 - 2\beta)$ and the traveling wave solution is not bounded, and therefore the solution does not exist.

coefficient approaches zero as the saturation approaches zero while it is finite and non-zero at full saturation.

Cuesta *et al.* (2000) stated that the solution to the traveling wave form of the RNERE exists and is unique for all intial conditions when $s_- > 0$. However, for the condition where $s_- \to 0$, they found the same result as we did where the pressure at the front became unbounded. Rather than use a pressure factorization as we did, they instead defined the range of parameters that would allow the solution pressure to be bounded as $s_- \to 0$. Their analysis showed that for the solution to be bounded the parameter γ needs to be constrained by the inequality $\gamma > (\alpha - 2 - 2\beta)$.

A qualitative result showing the effect of setting γ according to this criterion is illustrated in Figure 6 where the phase plane for saturation versus. pressure is plotted. Shown on each plot are the equilibrium pressure curve and the trace set by the evolution of saturation in the traveling wave solution. For the case shown in Figure 6(a) the value of $\gamma > (\alpha - 2 - 2\beta)$. For this case the trace makes a tangential departure from the equilibrium curve, and at the end the trace reaches a pressure that is bounded from above. In contrast, for the case shown in Figure 6(b), the value of $\gamma < (\alpha - 2 - 2\beta)$, and for this situation the trace makes a vertical departure from the phase plane, effectively causing the trace to reach pressures that are not bounded from above.

4.2.1.2. Stability Analysis for the RNERE. The linear stability analysis for the RNERE is performed similarly to that for the NERE (see equations (24) and (25)). We need only to specify the equation due to the relaxation law. The resulting perturbed equations are given by

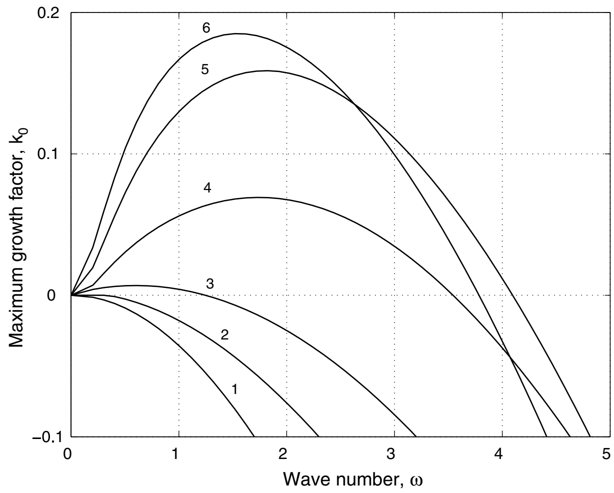

Figure 7. Plots of the critical eigenvalue as a function of wave number of disturbance for various values of τ_0. The curve labels 1–6 correspond to the following values of $\tau_0 = 0$, 0.07, 0.1, 0.2, 0.5 and 1.0.

$$\frac{\mathrm{d}A}{\mathrm{d}\xi} + \omega^2 K(s_0) p_1 = -k s_1, \tag{41}$$

$$V\tau_0 \frac{\mathrm{d}s_1}{\mathrm{d}\xi} + \left(P'(s_0) + V\frac{\partial \tau(s_0, p_0)}{\partial s}\frac{\mathrm{d}s_0}{d\xi}\right) s_1 + \left(V\frac{\partial \tau(s_0, p_0)}{\partial p}\frac{\mathrm{d}s_0}{\mathrm{d}\xi} - 1\right) p_1 = -k\tau_0 s_1 \tag{42}$$

with the same definition for A given by equation (26).

Equations (41) and (42) are in the form of a spectral problem for which we are interested in the sign of the spectrum especially for the sign of the critical eigenvalue k_0 if it exists. The equations are not readily amenable to analytical solution, so a numerical solution for the eigenvalue problem will be presented.

Results of the numerical solution of the eigenvalue problem given by equations (41) and (42) for the critical eigenvalue $k_0(\omega)$ are presented in Figure 7 for various values of the parameter τ_0. The other parameters needed for the solution are the same as those used in developing Figure 2. The result for $\tau_0 = 0$ (curve 1) is essentially the same result that would be obtained for solving the RE eigenvalue problem given by equation (18) for equivalent sets of porous media parameters. From Figure 7 it is observed that the critical eigenvalue for the solution with $\tau_0 = 0$ (RE solution) is negative for all perturbation frequencies, and therefore the RE is unconditionally stable, and this agrees with the conclusion derived in Section 3 by analytical means. The critical eigenvalue is also negative for all frequencies for $\tau_0 = 0.07$. However, for $\tau_0 > 0.07$ the saturation profile is sufficiently non-monotonic (see curves 3–6 in Figure 2) for the critical eigenvalues to be positive over a range of frequencies. For this set of parameters then we can establish the critical value of τ_0 for instability to be slightly less than 0.1. Also, we can say that somewhere within the range of $0.08 < \tau_0 < 0.10$ the critical eigenvalues will be negative although the saturation profiles within that range are somewhat non-monotonic. These results on the conditional stability of the RNERE have shown that the advancing flow can be unstable if the parameters fall within a specified range.

The low frequency criterion derived in Section 4.1 also applies to the results obtained here for the RNERE model. Equation (29) indicates that if the value of C is negative then the flow will be unstable. As shown earlier in this section, the pressure profiles generated by the basic solution of the RNERE model can be non-monotonic if the value of the relaxation coefficient is large enough. However, it was just shown that non-monotonicity by itself is not a sufficient condition to guarantee instability. Instead, the degree of non-monotonicity has to be large enough to lead to instability.

As a reminder we should note that the results presented up to this point have all been for the condition where the initial saturation is at or above the residual saturation. Therefore, one might argue that our results are contradictory to experimental evidence that overwhelmingly has shown that flows generally become unstable where the initial saturation is below the residual. This argument then motivates us to investigate the case where $S_{\mathrm{init}} < S_{\mathrm{r}}$. This is done in the next section.

4.2.2. *RNERE Model for Initial Moisture Less than Residual*

Most models of unsaturated flow are concerned with flows that occur at saturations above the residual. For the case where the initial saturation is less than the residual, an extended model is required. We will now present analyses for an extended model for unsaturated flow. Both the basic solution and a stability analysis for the basic solution will be presented.

4.2.2.1 Basic Solution for the Extended Model. The governing equations are changed slightly using saturation S as the primary variable, as opposed to effective saturation s as before. The traveling wave form of the RNERE therefore becomes (analogous to equations (30) and (31))

$$\frac{\mathrm{d}S}{\mathrm{d}\xi} = \frac{p - P(S)}{V\tau(S)}, \tag{43}$$

$$\frac{\mathrm{d}p}{\mathrm{d}\xi} = \frac{V(S - S_+) + K(S_+) - K(S)}{K(S)}. \tag{44}$$

The usual pressure-saturation and conductivity-saturation relations apply for the saturation range from residual to full saturation. To apply equations

(43) and (44) over the full range of saturation from $S=0$ to $S=1$ we need an extended model for pressure-saturation and conductivity-saturation. For this we use the approach of Rossi and Nimmo (1994) who extended the modified Brooks–Corey model for the range $0 \leqslant S \leqslant S_j$, except that we use the conventional Brooks–Corey function for the range $S_j \leqslant S \leqslant 1$. The parameter S_j is the value of saturation joining the two ranges of saturation. The pressure-saturation model now becomes

$$P(S) = -p_0 \exp(-aS), \quad 0 \leqslant S \leqslant S_j,$$
$$P(S) = -\left(\frac{S-S_r}{1-S_r}\right)^{-\beta}, \quad S_j \leqslant S \leqslant 1. \tag{45}$$

The conductivity-saturation relation is given by

$$K(S) = \sqrt{S}\,[I(S)/I(1)]^2, \tag{46}$$

where

$$I(S) = 1 - \frac{1}{ap_0} e^{aS}, \quad 0 < S < S_j, \tag{47}$$

$$I(S) = 1 - \frac{1}{ap_0} e^{aS_j} + \frac{1-S_r}{\beta+1}\left[\left(\frac{S_j-S_r}{1-S_r}\right)^{\beta+1} - \left(\frac{S-S_r}{1-S_r}\right)^{\beta+1}\right], \quad S_j < S \leqslant 1. \tag{48}$$

The computed parameter a and S_j provide first-order continuity for these functions. The S_j is set at a saturation slightly above S_r.

For the relaxation coefficient we used relation (34) with $\delta = 0$. Asymptotic analysis showed that for bounded solutions as $S_{\text{init}} \to 0$ we need $\gamma > 0.5$.

Parameter values for the model were chosen to fit the experimental data of Bauters *et al.* (2000), who performed experiments to evaluate the effect of initial saturation on flow stability. They examined initial water contents ranging from air-dry conditions to residual water content. For the analysis to follow we examined a subset of their experiments, using initial water contents θ_{init} :0.001, 0.01, 0.02, 0.03, 0.04 and 0.047. The residual water content for their porous media was 0.047 and saturated water content was 0.348. Parameter values obtained from the published moisture retention data were $S_r = 0.135$ and $\beta = 0.18$, while for the conductivity function we used $p_0 = 10^5$ m and $a = 1.5$. We also calibrated the relaxation coefficient relation using the published water content and pressure profiles for the experimental run for $\theta_{\text{init}} = 0.001$, and obtained $\tau_0 = 1.5$ and $\gamma = 1.5$.

The saturation profiles resulting from the solution to equations (43) and (44) with the specified parameters are shown in Figure 8 for the various values of S_{init} corresponding to the various initial water contents. The profiles for the very dry initial conditions are clearly non-monotonic, while

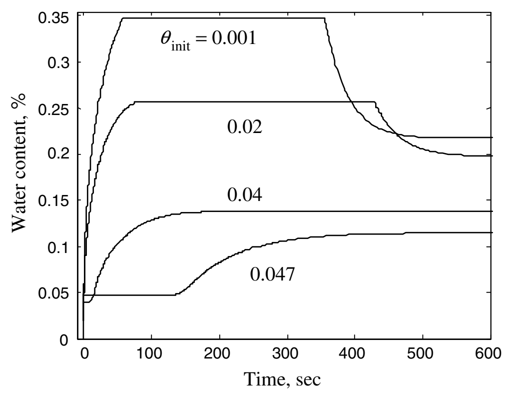

Figure 8. Water content as a function of dimensional time at any particular point within the flow domain. The cases $\theta_{\text{init}} = 0.01$ and 0.03 represented in Table I are not shown.

the profiles for the higher initial saturations are essentially monotonic. The characteristics of these profiles with respect to flow stability will be discussed in the next section.

4.2.2.2. Stability Analysis for the Extended Model. The analysis of flow stability for the extended RNERE model follows the same procedures as for the RNERE model outlined in Section 4.2.1. The resulting spectral problem is essentially the same as that shown by equations (41) and (42). The main difference between the current model and the previous model is in the parameters of the system due to the extension to dry conditions. As before, the complexity of the resulting perturbation equation makes it necessary to solve the eigenvalue problem by numerical means.

When we attempted the numerical evaluation of the spectral problem for the extended RNERE we found the numerical procedures used previously to be inadequate to get accurate results. The reason for the numerical difficulty is the extremely steep wetting front that develops for the basic solution in the case of the dry initial condition (see Figure 8). Therefore, to derive some useful results the direct evaluation of the spectral problem was abandoned for the time being and the low-frequency criterion analysis derived by Egorov *et al.* (2003) and outlined in Section 4.1 was applied. Revisiting the direct spectral problem will have to await further investigation into more accurate means to solve the steep front problem.

The low-frequency criterion for flow stability was given by equations (28) and (29). These equations state that when the pressure profile is sufficiently non-monotonic the value of C will be negative, and this will then lead to a positive value of k_0, indicating the flow will be unstable. So the determination of the stability of flows generated from dry initial conditions is to simply evaluate expression (28) with the $K(s_0)\mathrm{d}p_0/\mathrm{d}\xi$ derived from the

Table I. Finger widths as a function of initial water content observed in the experiments of Bauters *et al.* (2000), and corresponding values of C evaluated by Equation (28)

θ_{init}	0.001	0.01	0.02	0.03	0.04	0.047
Finger (cm)	2.5	1.25	3.0	7.5	11.0	30.0
C	−2.46	−2.85	−0.96	−0.087	−0.093	0.009

traveling wave solution for a specific set of porous media parameters, and if the value of C is negative to then conclude that the flow will be unstable.

The value of C evaluated with equation (28) for the various initial water contents is presented in Table I. Finger widths reported by Bauters *et al.* (2000) for the corresponding cases are also listed. The experimental chamber had a width of 30 cm. It is observed from the table that as the initial water content approached the residual of 0.047 the finger width increased to the size of the experimental chamber.

From the values presented in the table it appears that the only case of stable flow ($C > 0$) occurs for $\theta_{\text{init}} = 0.047$. All the other cases have negative values of C, indicating instability of flow. The finger widths observed by Bauters *et al.* (2000) are in agreement with this result. The largest finger width was observed for $\theta_{\text{init}} = 0.047$, with the finger width being at least equal to the width of the chamber. The next largest finger width was 11.0 cm for the case with $\theta_{\text{init}} = 0.04$. While the plot in Figure 8 for $\theta_{\text{init}} = 0.04$ does not appear to be non-monotonic, it was sufficiently non-monotonic so that the value of C was negative in the evaluation of equation (28). For the other two cases shown in Figure 8, $\theta_{\text{init}} = 0.001$ and $\theta_{\text{init}} = 0.02$, the saturation profiles are clearly non-monotonic, and this is manifested in the values of C presented in Table I.

5. Summary and Conclusion

We have presented several alternative forms of the equations for flow in unsaturated porous media. All of the various forms contain two coupled equations, the mass balance equation derived from a combination of conservation of mass and a linear flux law, and a relationship for the pressure that appears in the mass balance equation. The differences between the different forms of equations are contained completely in the definition of the pressure function. For the conventional equation for unsaturated flow, given by the RE, the pressure function is given by the equilibrium capillary pressure – saturation relationship. A more general equation system is derived using a generalized non-equilibrium relationship of the pressure function, and this is called the NERE. A specific form of the non-equilibrium relationship is given by a relaxation function expressed by a first-order rate process. The equation system using this relaxation function is referred to as the RNERE.

The traveling wave solution was studied for each of these models and stability analysis of these traveling wave solutions was performed. The characteristics of the traveling wave solutions for the RE and the RNERE were analyzed in detail, and expressed in terms of the monotonicity or non-monotonicity of the traveling wave saturation and pressure profiles. These solutions were derived for the standard case where the initial saturation is above residual saturation. The RNERE was also extended to the case where the initial saturation is less than the residual, since this corresponds better with conventional laboratory experiments on unstable flows.

For the linear stability analysis the solution to the system of equations in the traveling wave variable yielded a basic solution that was then perturbed by infinitesimal fluctuations. Stability of the perturbed flow was then analyzed by the method of spectral analysis. The stability of the NERE was analyzed at low-frequency only because of the general form of the non-equilibrium pressure function, and the resulting criterion is called the LFC. The stability analysis for the RNERE for initially dry conditions was also limited to the LFC because of the numerical difficulty to accurately solve the perturbation equation with extremely sharp fronts.

From the analyses presented here we can conclude the following.

(1) The RE is unconditionally stable to any perturbation, whether infinitesimal or finite in magnitude, in homogeneous or heterogeneous porous media. The traveling wave saturation and pressure profiles for the RE are monotonic for standard type boundary conditions.
(2) The analysis of the stability of the NERE model using the LFC shows that infiltrating flows governed by the NERE can become unstable for conditions where the flow profile is sufficiently non-monotonic.
(3) The saturation and pressure profiles for the RNERE model were found to be non-monotonic for a sufficient large value of the relaxation coefficient parameter τ_0. The larger this parameter the larger is the degree of non-monotonicity of the profiles. Assessments of stability over a wide range of perturbation frequencies were completed showing that flows are stable even for slight non-monotonicity, but transition to unstable as the degree of non-monotonicity increases.
(4) For initially dry conditions, the LFC assessment of the RNERE indicated unstable flow for initial conditions from absolutely dry up to near residual saturation. With initial saturation equal to the residual, the LFC indicated that the flow may be stable. These stability assessments were in good agreement with the stability experiments of Bauters *et al.* (2000).

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