Dynamic capillary pressure, hysteresis and gravity-driven fingering in porous media

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Abstract. Experimental data collected from the unstable, or fingered, flow of water through soils have shown that the traditional porous media equation is unable to explain the characteristic structure of the moisture distribution within these fingers. One and two-dimensional numerical solutions are presented for an alternative non-equilibrium porous medium equation as proposed by [1] which incorporates a dynamic hysteretic capillary pressure model. Computed profiles capture both the non-monotonic property of finger evolution as well as the limited lateral growth of the instabilities.

1. Introduction

The unsaturated flow of water in soil occurring through unstable wetting fronts has been documented widely both in the field and the laboratory over the past three decades (for example see [2] – [13]). Wetting front instability leads to the development of unstable or fingered flow profiles which significantly increase the transport velocity of dissolved pollutants to groundwater through the unsaturated zone. Critical practical applications for studying fingered profiles centre on quantifying the vulnerability of aquifers to contamination, determining recharge rates for aquifers, managing waste disposal sites, and in agriculture where there is particular interest in the movement of pesticides and fertilizers which rely on residence time in the upper soil profile for their degradation. Groundwater is a very important component of water resources, and issues of groundwater quality and pollution become significant and controversial particularly where there is a diverse range of interest groups. To be able to make effective and realistic predictions concerning groundwater quality requires a thorough understanding of the physics of the transport mechanisms through the unsaturated zone and their corresponding mathematical representation. In a related problem, it is also known that fingering plays a significant role in the heterogeneous distribution of moisture and nutrients in arid environments, leading to the scattered growth of deep rooted species and therefore desertification ([14]).

There have been many experimental papers (see above) which have led to a very good understanding of the physics of finger development. The question as to whether the porous medium equation (in particular Richards’ equation) can actually reproduce various known behaviour in finger growth and evolution has recently received a lot of attention ([15] – [22]). A key characteristic feature of fingers is that the capillary pressure distribution is non-monotonic, and there is a reversal in the pressure gradient immediately behind the advancing finger tip. Secondly, once formed, fingers tend to propagate into the soil at a constant velocity while maintaining their shape. Usually, two-dimensional fingers have been created experimentally through (i) introducing water via a continuous constant point
source in a dry soil [13], and (ii) applying water uniformly at a constant rate at the top of a dry two-
layered soil profile of fine (top layer) over coarse sand, [3], [6]. Stability analysis of Richards’
equation by [18], [19], [23] clearly shows that for flows under the above conditions, solutions must be
monotonic and is in contrast to the characteristic non-monotonic saturation profile found in
experimental fingers. Numerical solutions of Richards’ equation under constant initial and boundary
conditions by [15] strongly support the results of stability analysis.

The authors of [15] believe that Richards’ equation “does not contain the critical physics required
to model gravity-driven fingers”, which has led these authors to postulate a modified Richards
equation [16] that takes into account non-equilibrium or dynamic processes for describing the fingers. As noted by [24], evidence of dynamic behaviour in the capillary pressure – water content relationship
can be found in past experiments by [25], [26] and [27]. They have proposed using the dynamic
capillary pressure relationship of [1] in combination with Richards’ equation to explain these
experiments. Within the multiphase flow literature non-equilibrium models have also been required to
explain experimental data on the spontaneous countercurrent imbibition of oil and water ([28], [29],
[30]). However the non-equilibrium component here is introduced through a dynamic saturation
relation rather than through the capillary pressure as used by [24].

Taking the non-equilibrium model of [1], a stability analysis by [18] and [20] demonstrated the
existence of non-monotonic solutions. While both [20] and [31] showed that one-dimensional
travelling wave solutions of the Hassanizadeh and Grey model have the required non-monotonicity
structure to model finger evolution, their solutions did not include hysteresis. Since the slope of the
capillary pressure – saturation relation changes dramatically at any reversal point, the behaviour of the
travelling wave solution is expected to differ significantly from this point, in comparison to a non-
hysteretic solution. Apart from the effect hysteresis has on the shape of the saturation profile after
pressure reversal, it is postulated by [8] that hysteresis provides the physical mechanism by which the
lateral spread of two-dimensional fingers are constrained, and therefore would be the mechanism that
ensures the stability of the finger itself.

In this paper the non-equilibrium model of [1] is considered. Following [20] we first develop a
one-dimensional travelling wave solution and analyse the stability of its critical points with the effects
of hysteresis included. While a phase plane analysis shows that the stability of the critical points in
the dynamic model is independent of hysteresis effects, the type of critical point and the phase plane
trajectory followed are not. Second, both a one and two-dimensional numerical solutions for the non-
equilibrium model with hysteresis are also developed. Validations of both the one and two –
dimensional numerical solutions are confirmed through a comparison with the travelling wave solution
and by using two different numerical schemes. As yet the Hassanizadeh and Gray model has not been
tested for its capacity to model two-dimensional finger evolution. Thus in the final section of this
paper we produce some preliminary results on producing numerical fingers using their model. The
only other numerical solutions to be found in the literature which have developed finger type profiles
are for the non-equilibrium model of [16] which contains quite a simple linear interpolation hysteresis
model.

2. Theory
In one vertical spatial dimension Richards’ equation is given by

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \frac{\partial p}{\partial z} \right] - \frac{\partial K(\theta)}{\partial z},$$  \hspace{1cm} (1)$$

where $\theta = (\Theta - \Theta_r)/(\Theta_{sat} - \Theta_r)$ is the effective water content ($0 \leq \theta \leq 1$), $\Theta_{sat}$ = the saturated water
content, $\Theta_r$ = residual water content, $p$ (cm) is the water pressure, $K$ (cm hr$^{-1}$) is the hydraulic
conductivity, \( T = t / (\Theta_{sat} - \Theta) \) where \( t \) is time and \( z \) is distance measured positive downwards with gravity \( g \). The actual water content \( \Theta(z,t) \) is defined on the REV (representative elementary volume) scale, [32], as the volume of water per REV and is therefore dimensionless. The flux of water in the \( z \) direction is given by \( K(1 - \partial p / \partial z) \) where the 1 is the scaled gravity effect. Richards’ equation is given by (1) with \( p = \psi(\theta) \), where \( \psi(\theta) \) (\( < 0, \text{cm} \)) is the capillary pressure – water saturation relationship, and is based on the assumption of local equilibrium. Thus the conductivity and water pressure can be expressed solely as functions of the local water content \( \theta(z,t) \), and this model is generally applicable for uniform stable flow through the soil.

While conditions at or close to equilibrium exist between the different pores in a soil during uniform flow, this is generally not the case during preferential or more rapidly time varying flow. It is considered that a non-equilibrium balance or behaviour is the most important feature of preferential flow. Preferential flow is defined essentially as a flow regime whereby infiltrating water does not have sufficient time to equilibrate with the slowly moving resident water in the bulk of the soil matrix. Examples of preferential flow are (i) fingered profiles in completely homogeneous soils, and (ii) dual porosity or dual permeability soils; these media consist of two interacting regions, one associated with the inter-aggregate macropore or fracture system, and one consisting of intra-aggregate or micropores [33]. The simplest non-equilibrium model is to take a kinetic description for the movement of the water pressure to equilibrium. Thus the equilibrium pressure relationship \( p = \psi(\theta) \), is now replaced with the additional differential equation ([1], [20], [24]),

\[
\frac{\partial p}{\partial T} = \psi(\theta) + \tau(p,\theta) \frac{\partial \theta}{\partial T},
\]

where \( \tau \) is a relaxation function that is a measure of the equilibration time (which is allowed to depend on the prevailing local pressure and water content). The full non-equilibrium flow model, in dimensional form, is then given by coupling (2) with (1).

It was noted on page 383 of [31] that experiments by [27] showed \( \tau \to 0 \) as \( \theta \to 0 \), and they proposed the following simple power law form for \( \tau \) as

\[
\tau = \epsilon \theta^\gamma,
\]

where \( \gamma \) and \( \epsilon \) are positive constants. This model suggests that equilibrium conditions for \( p \) as a function of \( \theta \) always hold in the dry state. An alternative possible form is ([20])

\[
\tau = \epsilon \theta^\gamma (1 - \theta)^\beta,
\]

which also requires that equilibrium of pressure with the water content holds in the saturated state.

3. Alternative one-dimensional non-equilibrium models

While the Hassanizadeh and Gray non-equilibrium model is defined by (1) and (2), there are several other dynamic models available in the literature. The model of Barenblatt and co-workers ([28] – [30]) is given by

\[
\frac{\partial \theta}{\partial T} = \frac{\partial}{\partial z} \left[ K(\sigma) \frac{\partial \psi(\sigma)}{\partial z} - K(\sigma) \right],
\]

\[
\sigma = \theta + \tau(\theta) \frac{\partial \theta}{\partial T},
\]
where $\sigma$ is the effective water content and $\tau_0$ is the Barenblatt relaxation function. The main difference with the Hassanizadeh and Gray model is that in (5) and (6), the dynamic effect is also included in the hydraulic conductivity function. To first order though, both models are related through (7)

$$\tau(\theta) = \left| \frac{d\psi}{d\theta} \right| \tau_0(\theta), \quad (7)$$

Additionally it is worth noting that while $\tau$ has units of LT, $\tau_0$ has units of time only.

In the dynamic model of [16], an extended Richards’ equation is proposed as

$$\frac{\partial \theta}{\partial T} = \frac{\partial}{\partial z} \left[ K(\theta) \frac{\partial \psi}{\partial z} - K(\theta) \frac{\partial \theta}{\partial T} \right] + R(\theta), \quad (8)$$

where the functional form of $R(\theta)$ in (8) is chosen to yield the desired non-monotonic behaviour in the solution. Three different forms for $R$ are suggested, being

$$R_{\text{diff}}(\theta) = \frac{\partial}{\partial z} \left[ F(\theta) \frac{\partial \theta}{\partial z} \right], \quad (9)$$

$$R_{\text{hyper}}(\theta) = -\frac{\partial}{\partial T} \left[ G(\theta) \frac{\partial \theta}{\partial T} \right], \quad (10)$$

$$R_{\text{mixed}}(\theta) = \frac{\partial}{\partial z} \left[ L(\theta) \frac{\partial}{\partial z} \left( \frac{\partial \theta}{\partial T} \right) \right], \quad (11)$$

and are referred to as the hyperdiffusive, hyperbolic and mixed forms respectively with the functions $F(\theta) < 0$, $G(\theta) > 0$ and $L(\theta)$ being new constitutive properties to be determined. It is only for the mixed form of $R(\theta)$ can (8) be written in an equivalent form to the Hassanizadeh and Gray model. This occurs in the special case where $L(\theta) = \tau K(\theta)$ and $\tau$ being constant.

4. Travelling wave solutions and non-monotonic profiles

Experimental data ([6] – [8], [10]) show very clearly that when the fingered profiles form, they travel downwards at a fairly constant velocity. This suggests that we should look for travelling wave solutions of (1) and (2) of the form $\theta(\xi)$ where $\xi = vT - z$. We take the following boundary conditions ($\theta_s < \theta_i$)

$$z \to \infty, \quad \xi \to \infty, \quad \theta = \theta_s$$

$$z \to -\infty, \quad \xi \to -\infty, \quad \theta = \theta_i$$

(12)

where $\theta_i$ is the initial water content ahead of the wave, and $\theta_s$ is the upstream water content once the wave has passed. Then (1) and (2) using $\theta(\xi, t) = \theta(vT - z) = \theta(\xi)$, and similarly $p(\theta(\xi)) = p(\xi)$, $\psi(\theta(\xi)) = \psi(\xi)$, reduce to the autonomous system

$$\frac{d\theta}{d\xi} = \frac{p - \psi}{v \tau(\theta, p)} = X(\theta, p),$$

$$\frac{dp}{d\xi} = \frac{K_s - K + v(\theta - \theta_s)}{K} = Y(\theta, p). \quad (13)$$

To obtain the first equation in (13) we use (2) directly, while the second equation is found from (1) after integration and using the first condition in (12). The wave speed is then determined by applying the second condition in (12) and assuming that $dp/d\xi = d\theta/d\xi = 0$ as $|\xi| \to \infty$ by
\[ v = \frac{K_s - K_o}{\theta_s - \theta_o}, \quad (14) \]

where \( K_s = K(\theta_s) \) and \( K_o = K(\theta_o) \).

We consider (as usual) only monotonic \( K(\theta) \) in \( \theta \) for \( 0 < \theta < 1 \), and note that the system (13) has only the two critical points, c.p., \((\theta_s, \psi_s), (\theta_o, \psi_o)\) (we assume \( \tau(\theta,p) \geq 0 \) in our region of interest).

Then the corresponding linearised system is

\[
\begin{bmatrix}
X_\theta & X_p \\
Y_\theta & Y_p
\end{bmatrix} =
\begin{bmatrix}
\frac{\psi - p}{v \tau} - \frac{\psi'}{v \tau} & \frac{\psi - p}{v \tau^2} + \frac{1}{v \tau} \\
\frac{K - K_o - v(\theta - \theta_o)}{K^2} & K' + \frac{v - K'}{K} \\
\end{bmatrix} \cdot \quad (15)
\]

where \( K' = dK / d\theta \), \( \psi' = d\psi / d\theta \) and (15) is evaluated at each critical point in turn. Noting that this occurs for \( \psi = p \) and \( K - K_s - v(\theta - \theta_s) = 0 \), then at the downstream critical point, \( \theta = \theta_o \), the eigenvalues of (15) are given from (\( \tau(\theta_o) = \tau_o \))

\[
\lambda = -\frac{\psi_o}{2v \tau_o} \pm \frac{\sqrt{\left(\frac{\psi_o}{\tau_o}\right)^2 + 4(v - K_o)}}{v \tau_o K_o}. \quad (16)
\]

For functions where \( K(\theta), K'(\theta), K''(\theta) > 0 \), in other words \( K \) is convex in \( \theta \) as well as monotonic and positive, we have \( K'' < v \) and \((\theta_o, \psi_o)\) is a saddle point. For the upstream critical point, \( \theta = \theta_s \), the eigenvalues of (15) are given from (\( \tau(\theta_s) = \tau_s \))

\[
\lambda = -\frac{\psi_s}{2v \tau_s} \pm \frac{\sqrt{\left(\frac{\psi_s}{\tau_s}\right)^2 - 4(K_s' - v)}}{v \tau_s K_s}. \quad (17)
\]

Since \( K'(\theta) > v \) and \( -\frac{\psi_o}{v \tau_o} < 0 \), the critical point \((\theta_s, \psi_s)\) is stable, and we have

- (a) \( \frac{(\psi_o')^2}{v^2 \tau_o^2} > \frac{4(K_s' - v)}{v \tau_o K_s} \) (stable node)
- (b) \( \frac{(\psi_o')^2}{v^2 \tau_o^2} = \frac{4(K_s' - v)}{v \tau_o K_s} \) (stable improper node)
- (c) \( \frac{(\psi_o')^2}{v^2 \tau_o^2} < \frac{4(K_s' - v)}{v \tau_o K_s} \) (stable spiral)

It is clear that hysteresis only effects the type of stable point in (a) – (c), it does not affect its actual stability, since \( \theta = \theta_s \) is a stable critical point whether or not hysteresis is actually present. Note the surprisingly simple form of these results occurring from the potentially more complicated third order partial differential equation that arises for \( \theta \) when (2) is substituted into (1). This is because first, we can integrate the basic equation for travelling waves to get the second order system of differential equations (13), and second, the monotonicity of the conductivity function \( K(\theta) \) has significant simplifying consequences. It is also noteworthy that \( \tau > 0 \) does not have any impact on the stability of the system (13), but only on the actual trajectory followed within the phase plane.

5. Hysteresis model and hydraulic functions
For the mathematical description of hysteresis, we take the model of [35] as extended by [36]. This takes the van Genuchten equation [37] for the main drying curve, \( \theta_d \).
\[ \theta_{d0} = \left[ \frac{1}{1 + (-\alpha \psi)^n} \right]^{1/n}, \]  

with \( n > 0 \) and the main wetting curve, \( \theta_{w0} \), then given by

\[ \theta_{w0} = \alpha \psi + \left[ 1 + (-\alpha \psi)^n \right]^{1/n}. \]

Subsequent scanning wetting, \( \theta_{wr} \), and drying, \( \theta_{dr} \), curves of order \( r \) are given by

\[ \theta_{w,r} = \theta_{w,0} + (\psi - \psi_{d,r-1})C(\psi_{w,r}) + \sum_{k=1}^{r-1} (\psi_{d,k} - \psi_{d,k-1})C(\psi_{w,k}), \]  

and

\[ \theta_{d,r} = \theta_{w,0} + (\psi - \psi_{d,r})C(\psi) + \sum_{k=1}^{r} (\psi_{d,k} - \psi_{d,k-1})C(\psi_{a,k}), \]

where \( C(\psi) = d\theta_{w,0}/d\psi \). In (20) and (21), \( \psi_{d,r} \) and \( \psi_{w,r} \) denote the values of \( \psi \) for the drying and wetting reversal points on the \( r \)th scanning curve respectively. Finally for the hydraulic conductivity we take ([38])

\[ K(\theta) = K_{sat} \sqrt{\theta} \left[ 1 - (1 - \theta_{w,0}^{-1})^{1-1/n} \right]^{n/2}, \]

where \( K_{sat} \) is the saturated conductivity. These forms of wetting and drying curves and conductivity function have been shown in the soil physics literature to model a wide range of soil types from sands to clays [39]. Figure 1 shows a typical hysteretic \( \psi(\theta) \) relation calculated from (18) - (21). For the relaxation function (4) will be used.

![Figure 1](image)

**Figure 1** \( \psi(\theta) \) hysteresis curves from the Parlange model for \( \alpha = 5 \) and \( n = 2 \).

### 6. Numerical solutions

#### 6.1 One-dimensional case

Define the dimensionless (starred quantities) variables, parameter and functions as

\[ \frac{z^*}{z} = \frac{\xi^*}{\xi} = \frac{p^*}{p} = \frac{\psi^*}{\psi} = \alpha, \quad r^* = \alpha K_{sat} T = \frac{\alpha K_{sat} t}{\Theta_{sat} - \Theta}, \]

and
\[ \frac{\varepsilon'}{\varepsilon} = \frac{\tau'(\theta)}{\tau(\theta)} = \alpha^2 K_{sat}, \quad \frac{\nu'}{\nu} = \frac{K'(\theta)}{K(\theta)} = \frac{1}{K_{sat}}. \]  

(24)

From now on we drop the stars and all variables are implicitly dimensionless, and consider solutions of (1) and (2) subject to the following initial and boundary conditions

\[
\begin{align*}
  z = 0, \quad & K - K \frac{dp}{dz} = q_s, \\
  z \to \infty, \quad & \theta \to \theta_o, \quad \psi \to \psi(\theta_o), \quad p \to \psi(\theta_o), \\
  t = 0, \quad & \theta = \theta_o, \quad \psi = \psi(\theta_o), \quad p = \psi(\theta_o),
\end{align*}
\]

(25)

where \( q_s \) is the constant surface flux and \( \theta_o \) is the uniform initial moisture content. Note that for the initial condition and the boundary condition at infinity, \( p = \psi \) since \( \partial \theta / \partial t = 0 \).

![Figure 2 Travelling wave profile with and without hysteresis](image)

To integrate (13) subject to (12) with hysteresis, the fourth order Runge-Kutta method is used. The resulting travelling wave solution can then be used as a check on the asymptotic large time numerical solution of (1) and (2) subject to (25). To confirm the reliability and accuracy of our numerical solutions prior to the formation of this asymptotic solution we have used two different methods, the method of lines and a standard finite difference discretization method (from now on referred to as the matrix method). Details of both of these methods are given in Appendices A and B respectively. For oscillatory or non-monotonic solutions, the phase plane analysis in section 4 showed that \( \tau_o \) must be greater than \( \tau_o^n \) where \( \tau_o^n = K_o(\psi_o')^2 / [4\nu(K_o' - \nu)] \), thus we take \( \varepsilon = a\tau_o^n \) with \( a > 1/[\theta_o'(1-\theta_o')^2] \) to ensure oscillatory solutions. A typical soil parameter value of \( n = 2 \) is also used throughout all the computations. While the method of lines is a quick and efficient scheme to program, a serious difficulty arises whenever \( \tau \to 0 \) with \( p \to \psi \), as in (3) with \( \theta \to 0 \) and (4) with \( \theta \to 0 \) or \( \theta \to 1 \), resulting in a numerically indeterminate equation for (A.7). This problem however does not arise with the scheme of (B.8) and (B.9) which simply reduces to a finite difference scheme for solving Richards’ equation as \( \tau \to 0 \).
Figure 2 shows the computed solutions from (13) with and without hysteresis included in the $\psi(\theta)$ relation. Additional parameter values used are $\theta_1 = 0.6$, $\theta_o = 0.4$ and $a = 200$. It is clearly seen that hysteresis has a huge damping effect on the oscillations. The reason for this is that at the point of reversal in either a hysteretic wetting or drying cycle, $\psi$ will either significantly increase or decrease respectively, while there is very little change to the water content $\theta$. In the absence of hysteresis though, significant changes in both $\psi$ and $\theta$ occur at the reversal point, hence the magnitude and number of oscillations increase. While there are still oscillations with hysteresis, far more realistic profiles are now obtained. Typical finger experiments tend to only detect the “first finger pulse” and not see any subsequent smaller oscillations. However [8] do detect some of these small oscillations in their figures (4) – (6), though they make no comment as to whether they believe these oscillations to be real, or are an artifact of the measurement process. As far as we are aware there have also been no comments made on these oscillations in any subsequent paper in the literature.

![Figure 3 Comparing solutions by the method of lines with the matrix method and with the travelling wave profile from (13) with hysteresis included.](image)

In figure 3 results from the method of lines ((A.6) and (A.7)) and the matrix method ((B.8) and (B.9)) with hysteresis are presented for the dimensionless times of 15, 60 and 240 along with the travelling wave solution from (13). The parameter values of figure 2 are used along with a surface flux of $q_s = K(\theta)$. Note that the travelling wave solution (invariant with respect to translations) has been deliberately offset slightly at $t = 240$ to show that the two numerical solutions evolve to the correct long time profile. At all three times, the numerical solutions give profiles which are indistinguishable from each other. Consequently we believe that both schemes have provided an accurate and reliable numerical solution to the non-equilibrium model of (1) and (2). Two interesting features to be observed in Figure 3 are (i) that the surface water content reaches a maximum which is
significantly greater than $\theta_s$ and (ii) there is a rapid decrease in $\theta$ from $\theta(0, t \to \infty)$ to $\theta_s$ over a small interval. Neither type of behaviour arises in solutions of Richards’ equation where for the same initial and boundary conditions $\theta(0, t)$ increases monotonically to $\theta_s$ as $t \to \infty$ and $\theta(z, t)$ is a monotonically decreasing profile. It is not just the presence of the dynamic capillary pressure which is responsible for the behaviour of $\theta$ near the surface boundary, but its combination with a hysteresis model. After the surface water content has increased monotonically from its initial value of $\theta_o$ to its maximum, it then dries along a scanning curve to its asymptotic steady state value, and as such, it must then be different to $\theta_s$. In the dynamic model of (8) and (9) of [17], numerical results presented in their figure 4 also show a rapid change in $\theta$ from $\theta(0, t \to \infty)$ to $\theta_s$ over a small spatial interval, however they find the opposite behaviour to that shown in Figure 3 here, i.e. $\theta$ increasing rapidly to $\theta_s$.

6.2 Two-dimensional profiles

The equivalent of (B.1) for two-dimensional flow is described by

$$
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ K(\theta) \frac{\partial \psi}{\partial z} - K(\theta) \right] + \frac{\partial}{\partial x} \left[ K(\theta) \frac{\partial \psi}{\partial x} + K(\theta) \frac{\partial \theta}{\partial t} \right] + \frac{\partial}{\partial x} \left( K(\theta) \frac{\partial \theta}{\partial t} \right).
$$

(26)

(Note that the dimensionless $x$, like $z$, is scaled by $\alpha$ as in (23)). Due to the symmetry in water content with respect to the centre axis of a finger we seek solutions of (26) subject to the following initial and boundary conditions

$$
\begin{align*}
&z = 0, \\
&\quad K - K \frac{\partial}{\partial z} \left( \psi + \tau \frac{\partial \theta}{\partial t} \right) = q_s, \quad 0 \leq x \leq x_w \\
&\quad K - K \frac{\partial}{\partial z} \left( \psi + \tau \frac{\partial \theta}{\partial t} \right) = 0, \quad x > x_w \\
&z \to \infty, \quad \theta \to \theta_o, \quad \psi \to \psi(\theta_o), \quad p \to \psi(\theta_o) \\
&x = 0, \quad \frac{\partial}{\partial x} \left( \psi + \tau \frac{\partial \theta}{\partial t} \right) = 0 \\
&x \to \infty, \quad \theta \to \theta_o, \quad \psi \to \psi(\theta_o), \quad p \to \psi(\theta_o) \\
&t = 0, \quad \theta = \theta_o, \quad \psi = \psi(\theta_o), \quad p = \psi(\theta_o)
\end{align*}
$$

(27)

where $x_w$ is approximately the half width of the finger.

For the parameter values $x_w = 0.1, \theta_o = 0.6, \theta_s = 0.3, q_s = K(\theta_o)$ and $a = 200$, a two-dimensional simulation of a finger is given in figure 4. The non-monotonic profile and rapid propagation in the $z$ direction is clearly evident in comparison to the limited lateral growth. The rate and the extent of the lateral growth is more clearly visualized in figure 5 where the evolution of the cross sectional water content is shown at $z = 2.3$. As explained by [8], hysteresis is responsible for controlling the finger’s sideways growth. As the finger moves through the soil, the saturation in the central core of the finger quickly increases along a wetting curve to reach a maximum before decreasing along a drying curve to its steady state value, as seen by the profiles at times 53.4 and 66.75 in figure 5. Denote this value as $\theta = \theta_{core}, \psi = \psi_{core}$. During this process, figure 5 shows that the sides of the finger are moving along a wetting curve. Thus by $t = 66.75$, the side and the core of the finger are respectively wetting and drying on different branches of $\psi(\theta)$. As $\psi \to \psi_{core}$, along the side of the finger $\theta \to \theta_{side}$ which because of hysteresis we have $\theta_{side} \neq \theta_{core}$ but $\psi_{side} = \psi_{core}$. Thus it is possible to achieve a steady state
condition where between the side and the core of the finger \( \frac{\partial \theta}{\partial x} \neq 0 \) but \( \frac{\partial \psi}{\partial x} = \frac{\partial p}{\partial x} = 0 \) and therefore the later growth of the finger ceases.

**Figure 4** A simulation of an evolving finger type profile at \( t = 66.75 \)

**Figure 5** Cross-sectional moisture content at \( z = 2.3 \) at various times.

### 7. Summary

One and two-dimensional numerical solutions to the Hassanizadeh and Gray dynamic capillary pressure model for the non-equilibrium hysteretic unsaturated flows of water through porous media are provided. We apply this model to simulate the propagation of unstable fingers which have been found to routinely occur in experiments on flow through layered soils. Two different numerical
solution methods are presented, the method of lines and a standard finite difference scheme. Both schemes produce solutions which are in agreement at all times as well as evolving onto the correct asymptotic travelling wave profile for large times. Our numerical simulations of finger profiles reproduce the non-monotonic saturation distribution as well as their restricted lateral growth observed in experiments. The focus of this paper has been on investigating whether or not two-dimensional numerical solutions of the Hassanizideh and Gray model can simulate finger properties. Future research directions are now centred on testing our numerical code against accurate and detailed experimental measurements of both finger velocity and width for a wide variety of soils.

8. Appendix A
To integrate using the method of lines we write (1) and (2) in the form of

\[
\frac{p - \psi}{\tau(\theta)} = \frac{\partial}{\partial z}\left(K(\psi)\frac{\partial p}{\partial z}\right) - \frac{\partial K}{\partial z},
\]

(A.1)

and

\[
\frac{\partial \theta}{\partial t} = \frac{p - \psi}{\tau(\theta)}.
\]

(A.2)

Discretize the spatial terms in (A.1) as

\[
\frac{\partial K}{\partial z} = \frac{1}{\Delta z}\left(K_{i+\frac{1}{2}} - K_{i-\frac{1}{2}}\right), \quad \left(K(\psi)\frac{\partial p}{\partial z}\right)_{i} = K_{i+\frac{1}{2}}(p_{i} - p_{i+1})/\Delta z,
\]

(A.3)

and

\[
\frac{\partial}{\partial z}\left(K(\psi)\frac{\partial p}{\partial z}\right)_{i} = \frac{1}{\Delta z}\left[K(\psi)\frac{\partial p}{\partial z}\right]_{i+1} - K(\psi)\frac{\partial p}{\partial z}\right]_{i} = \frac{1}{\Delta z^2}\left[K_{i+\frac{1}{2}}(p_{i+1} - p_{i}) - K_{i-\frac{1}{2}}(p_{i} - p_{i-1})\right],
\]

(A.4)

with

\[
K_{i+\frac{1}{2}} = \frac{1}{2}(K_{i+1} + K_{i}),
\]

(A.5)

where \( z = i\Delta z, i = 0, 1, 2 \ldots \) Substituting for (A.3) and (A.4) allows (A.1) and (A.2) to be written as

\[
\tau_{i}K_{i+\frac{1}{2}}p_{i+1} - \Delta z^2 + \tau_{i}\left(K_{i+\frac{1}{2}} + K_{i-\frac{1}{2}}\right)p_{i,j} + \tau_{i}K_{i+\frac{1}{2}}p_{i+1} = \Delta z\left(K_{i+\frac{1}{2}} - K_{i-\frac{1}{2}}\right)\tau_{i} - \Delta z^2\psi_{i},
\]

(A.6)

and

\[
\frac{\partial \theta}{\partial t} = \frac{p_{i} - \psi_{i}}{\tau_{i}}.
\]

(A.7)

After applying the boundary and initial conditions from (25), (A.6) can be written as tri-diagonal linear system for \( p_{i} \) with its solution then allowing (A.7) to be integrated directly with an appropriate ordinary differential equation integrator.

9. Appendix B
To obtain a standard finite differencing procedure, first substitute for \( p \) from (2) directly into (1) to give
\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( K \frac{\partial \psi}{\partial z} \right) - \frac{\partial K}{\partial z} \left( \frac{\partial \theta}{\partial t} \right),
\]  
(B.1)

The time derivative is approximated as
\[
\frac{\partial \theta}{\partial t} = \frac{\theta_{i+1}^k - \theta_i^k}{\Delta t},
\]  
(B.2)

where \( t = k \Delta t, k = 0, 1, 2, \ldots \). The first and second terms on the right hand side are still discretized as in (A.3) and (A.4). Applying this to the third term results in
\[
\frac{\partial}{\partial z} \left( \frac{\tau \frac{\partial \theta}{\partial t}}{\Delta t} \right) = \frac{1}{\Delta z^2} \left\{ K \left[ \left( \frac{\tau}{\Delta t} \right)_{i+1}^k \right] \left( \theta_{i+1}^k - \theta_i^k \right) - \tau \left( \frac{\partial \theta}{\partial t} \right)_{i+1}^k \right\} - \frac{1}{\Delta z^2} \left\{ K \left[ \left( \frac{\tau}{\Delta t} \right)_{i-1}^k \right] \left( \theta_{i-1}^k - \theta_i^k \right) \right\},
\]  
(B.3)

Substituting (B.2) into (B.3) gives
\[
\frac{\partial}{\partial z} \left( K \frac{\partial \theta}{\partial t} \right) = \frac{1}{\Delta z^2} \left[ \tau \left( \theta_{i+1}^k - \theta_i^k \right) - \tau \left( \theta_{i-1}^k - \theta_i^k \right) \right]
\]  
(B.4)

By combining (A.3), (A.4), (B.2) and (B.4), then (B.1) can be written as
\[
A_i^k \theta_{i+1}^{k+1} + B_i^k \theta_i^{k+1} + C_i^k \theta_{i-1}^{k+1} = A_i^k \theta_{i+1}^k + B_i^k \theta_i^k + C_i^k \theta_{i-1}^k + F_i^k,
\]  
(B.5)

where
\[
A_i = \frac{-1}{\Delta z^2} \left[ K_{i-1/2}^k \tau_{i-1/2}^k \right], \quad B_i = 1 + \frac{\tau_{i-1/2}^k}{\Delta z^2} \left( K_{i-1/2}^k + K_{i+1/2}^k \right), \quad C_i = \frac{-1}{\Delta z^2} \left[ K_{i+1/2}^k \tau_{i+1/2}^k \right],
\]  
(B.6)

\[
F_i = \frac{\Delta t}{\Delta z^2} \left[ K_{i-1/2}^k (\psi_{i+1} - \psi_i) - K_{i+1/2}^k (\psi_i - \psi_{i-1}) \right] - \frac{\Delta t}{\Delta z} \left( K_{i+1/2}^k - K_{i-1/2}^k \right).
\]

For this scheme the surface flux boundary condition in (25) must be applied in the form
\[
q_s = K - K \frac{\partial}{\partial z} \left( \psi + \tau \frac{\partial \theta}{\partial t} \right)
\]  
(B.7)

With (B.7), (B.5) becomes a tri-diagonal linear system for \( \theta_i \). If we had choose the coefficients \( A_s, B_s, C_s \) and \( F_s \) to be evaluated at time line \( k+1 \) instead of \( k \), then (B.5) would have been an implicit scheme rather than its current explicit form. This was a deliberate choice as once hysteresis is included, iteration is then required to obtain \( \psi(\theta) \) at every grid point. The additional iterations required on each time line for an implicit scheme, would then make the computation time overwhelmingly impractical.
9.1 Two-dimensional scheme.
The equivalent explicit scheme for the two-dimensional system of (26) is given by
\[
A_{ij}^k \theta_{i+1,j}^{k+1} + B_{ij}^k \theta_{i,j}^{k+1} + C_{ij}^k \theta_{i-1,j}^{k+1} + D_{ij}^k \theta_{i,j+1}^{k+1} + E_{ij}^k \theta_{i,j-1}^{k+1} = A_{ij}^k \theta_{i+1,j}^k + B_{ij}^k \theta_{i,j}^k + C_{ij}^k \theta_{i-1,j}^k + D_{ij}^k \theta_{i,j+1}^k + E_{ij}^k \theta_{i,j-1}^k + F_{ij}^k + G_{ij}^k,
\]
where
\[
A_{ij}^k = \frac{-1}{\Delta x^2} K \left[ \frac{1}{i+\frac{1}{2}} \right], \quad B_{ij}^k = 1 + \frac{1}{\Delta x^2} \left( K \left[ \frac{1}{i+\frac{1}{2}} + K \left[ \frac{1}{i+\frac{1}{2}} \right] \right] \frac{1}{\Delta \tau} \left( K \left[ \frac{1}{i+\frac{1}{2}} + K \left[ \frac{1}{i+\frac{1}{2}} \right] \right] \right) \right),
\]
\[
C_{ij}^k = \frac{-1}{\Delta x^2} K \left[ \frac{1}{i-\frac{1}{2}} \right], \quad D_{ij}^k = \frac{1}{\Delta x^2} K \left[ \frac{1}{i-\frac{1}{2}} \right], \quad E_{ij}^k = \frac{-1}{\Delta x^2} K \left[ \frac{1}{i-\frac{1}{2}} \right],
\]
\[
F_{ij}^k = \frac{\Delta \tau}{\Delta x^2} \left[ K \left[ \frac{1}{i+\frac{1}{2}} (\psi_{i+1,j} - \psi_{i,j}) \right] - K \left[ \frac{1}{i-\frac{1}{2}} (\psi_{i,j} - \psi_{i-1,j}) \right] \right] - \frac{\Delta \tau}{\Delta \tau} \left( K \left[ \frac{1}{i+\frac{1}{2}} - K \left[ \frac{1}{i-\frac{1}{2}} \right] \right] \right),
\]
\[
G_{ij}^k = \frac{\Delta \tau}{\Delta x^2} \left[ K \left[ \frac{1}{i+\frac{1}{2}} (\psi_{i-1,j} - \psi_{i,j}) \right] - K \left[ \frac{1}{i-\frac{1}{2}} (\psi_{i,j} - \psi_{i,j-1}) \right] \right],
\]
with \( x = j \Delta x, j = 0, 1, 2, \ldots \).

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