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The FEST model – a test bed for hysteresis in hydrology and soil physics

J P O’Kane

Department of Civil & Environmental Engineering, University College, Cork, Ireland
Boole Centre for Research in Informatics, University College, Cork, Ireland
Environmental Research Institute, University College, Cork, Ireland

E-mail: jpokane@ucc.ie

Abstract. The purpose of the paper is to develop two new models that capture much of the physics of flow through a slab of vegetated unsaturated soil. The first is a partial differential equation; the second is an ordinary differential equation derived from a simplified case. Both models are intended to serve as the initial test-bed for studying rate-independent soil-water hysteresis using the new concepts and tools.

1. Introduction

Rate-dependent hysteresis has been observed in hydrology for a long time, for example, in the looped-rating curve, and in similar plots of state and rate variables from systems of linear and non-linear differential equations that model hydrological processes. These rate-dependent hysteretic loops do not show *affine similarity with respect to time*, i.e. when the time argument of an input function is stretched, or speeded up, the corresponding output function is *not* stretched in the same way. For example, the attenuation of a sinusoidal input to a linear system depends on its frequency. Stretching the frequency changes the attenuation. Hence, any looped plot is rate dependent. In contrast to this, rate-independent hysteretic loops exhibit *affine similarity with respect to time*, i.e. when the time argument of an input function is stretched, the corresponding output function is stretched in the same way. No smooth differential, or integro-differential operator, has this property. Consequently, this kind of hysteresis cannot be represented by a Volterra series expansion.

Seventy-five years ago, Haines [10] observed the phenomenon of hysteresis in soil-water in soils that are not fully saturated *i.e.* when air is also present in the matrix of the porous soil. It is believed, without experimental verification, that the hysteresis of soil-water is rate-independent when considered on the time-scales of water flow.

New mathematical concepts and analytical and numerical tools for treating rate-independent hysteresis have recently been developed. Hysteresis is now recognized as the collective name for strongly nonlinear, rate-independent, phenomena. The modern mathematical concept of hysteresis was suggested by M. Krasnosel’skii and his co-workers [14]. See also [54, 1, 15].

The purpose of this paper is to develop two models that capture much of the physics of flow through a slab of vegetated unsaturated soil. The first is a partial differential equation; the second is an ordinary differential equation derived from a simplified case. Both models are

intended to serve as the initial test-bed for studying rate-independent soil-water hysteresis using the new concepts and tools.

In the first case, the non-linear equations and boundary conditions of the Philip-Richards model are derived for isothermal movement of water in both the liquid and vapour phase in a vertical column of soil. It encompasses the processes of infiltration, evaporation, redistribution, capillary rise and drainage at the pedon scale of one meter. The governing equation is a non-linear concentration-dependent diffusion equation. However, non-linearities also arise from two pairs of switches expressed in the boundary conditions: an outer pair always switching between wet and dry periods, and an inner pair switching intermittently from atmosphere-control to soil-control of the fluxes of water through the soil-atmosphere surface.

Particular attention is paid to units, since at least three different systems are in use in the literature, a source of confusion to the beginner. The preferred system of units may be called the strict *SI* system in contrast to the nominally simpler engineering system of mixed units.

2. Water movement in a soil column

2.1. Equations of motion and conservation of mass

The two equations that govern the vertical movement of water in an unsaturated rigid column of bare soil at the pedon scale are taken from soil-physics (See for example [9] or [5]). These are

- (1) a water balance, that states that water mass is conserved; and
- (2) a dynamic equation, with liquid and vapour water flux proportional to the gradient in soil-water potential.

If z is a position coordinate measured vertically downwards - the opposite direction to that used in many textbooks - from the soil surface, and t is time, we may write these equations as follows

$$\rho_w \frac{\partial \theta}{\partial t} = -\frac{\partial (f_l + f_v)}{\partial z}, \quad 0 \leq \theta \leq \theta_s < 1, \quad (1)$$

$$f_l = -k_l \frac{\partial \psi}{\partial z}, \quad (2)$$

$$f_v = -k_v \frac{\partial \psi}{\partial z}, \quad (3)$$

where ρ_w is the *density of water* (kg m^{-3}); θ is the *volumetric moisture content* (m^3 of soil water per m^3 of rigid soil/void matrix); θ_s is the *saturation* volumetric moisture content; f_l is the *flux density* of liquid water ($\text{kg m}^{-2} \text{s}^{-1}$) in the direction of positive z i.e. downwards, which is assumed to be proportional to the gradient in the *soil water potential* $\partial \psi / \partial z$ ([3]) - ψ is the total water potential and has three different sets units; f_v is the flux density of water vapour ($\text{kg m}^{-2} \text{s}^{-1}$), which is also assumed to be proportional to the gradient in the soil water potential $\partial \psi / \partial z$ [30]. The *liquid* and *vapour conductivities* k_l , and k_v , may be considered, in the first instance, to be functions of water content.

Some authors present the flux density, not as a mass flux, but as a volumetric flux of cubic meters of water per square meter of vertical column of soil per second ($\text{m}^3 \text{m}^{-2} \text{s}^{-1}$ or m s^{-1}) which has units of velocity.

2.2. Soil-water potential

Different authors define the *potential energy of soil water* at the pedon scale, in one of three equivalent ways [43] as

- (i) energy per unit mass, or
- (ii) energy per unit volume, or

(iii) energy per unit weight.

The difference between these three alternative sets of units may be seen most easily by considering the change in potential energy of a mass m of water - occupying a volume V at a density of $\rho_w = m/V$ - when it is moved from one elevation to another in the gravitational field close to the Earth's surface. The necessary force is $mg = \rho_w Vg$. The force is applied along any path connecting the initial and final vertical positions a distance z apart. We assume there is no conversion of energy to heat through friction. Consequently, the work done is dissipationless work against the force of gravity and is equal to $mgz = (\rho_w Vg)z$. The three alternative ways of representing the potential energy of this water as dissipationless work (a) per unit mass, (b) per unit volume, and (c) per unit weight, may be written correspondingly as follows:

$$\psi_{mass} = \frac{mgz}{\rho_w V} = \frac{\rho_w Vgz}{\rho_w V} = gz \quad (\text{J kg}^{-1}), \quad (4)$$

$$\psi_{volume} = \frac{mgz}{V} = \frac{\rho_w Vgz}{V} = \rho_w gz \quad (\text{J m}^{-3} \text{ or } \text{N m}^{-2}), \quad (5)$$

$$\psi_{weight} = \frac{mgz}{\rho_w Vg} = \frac{\rho_w Vgz}{\rho_w Vg} = z \quad (\text{m}). \quad (6)$$

Their ratios are

$$\psi_{mass} : \psi_{volume} : \psi_{weight} = g : \rho_w g : 1. \quad (7)$$

These may be used to convert from one form to the other [9].

There are three matching sets of units for each of the three quantities: flux density of soil-water, soil-water conductivity, and gradient in the soil-water potential. This arises from the generalised *Darcy equation* formed from equations (2) and (3)

$$\begin{aligned} f &= f_l + f_v \\ &= -(k_l + k_v) \frac{\partial \psi}{\partial z} \\ &= -k \frac{\partial \psi}{\partial z}. \end{aligned} \quad (8)$$

The three sets of units, and their underlying physical dimensions, must be self-consistent with respect to equation (8). Table 1 shows how the units of k are defined to ensure consistency.

The column headed "Mass" in the table shows

- (a) the water flux density measured as a mass flow rate per unit area perpendicular to the flow direction, and
- (b) the soil-water potential measured as energy per unit mass of water, both in strict *SI* units.

Consequently, the gradient in soil-water potential has units of Joules per kilogram per meter, which is equivalent to Newtons per kilogram of soil-water, which is also its acceleration, in accordance with the definitions of the Joule and the Newton. For consistency, k must have the units (kg s m^{-3}).

In the column headed "Volume", water flux density is measured as a volumetric flux per unit area and has units of velocity. From (5) the soil-water potential, measured as energy per unit volume, is equivalent to a pressure and is quoted in the literature in a variety of units, such as kilo-Pascals, bar or an equivalent column of mercury. The last two entries in the second column show the corresponding *SI* units for

- (a) the gradient in soil-water potential, and

Table 1. Consistent units of Hydraulic conductivity

Term\Basis	Mass	Volume	Mixed Volume & Weight
Water flux density (f)	$\text{kg m}^{-2} \text{s}^{-1}$	$\text{m}^3 \text{m}^{-2} \text{s}^{-1}$ or m s^{-1}	$\text{m}^3 \text{m}^{-2} \text{s}^{-1}$ or m s^{-1}
Soil-water potential (ψ)	J kg^{-1}	J m^{-3} or N m^{-2} or Pa	m
Gradient in potential ($\partial\psi/\partial z$)	$\text{J kg}^{-1} \text{m}^{-1}$ or N kg^{-1} or m s^{-2} or $\text{m}^3 \text{m}^{-2} \text{s}^{-2}$	Pa m^{-1} or $\text{kg m s}^{-2} \text{m}^{-3}$ or $\text{kg m}^{-2} \text{s}^{-2}$	m m^{-1} (dimensionless)
Hydraulic conductivity (k)	kg s m^{-3}	$\text{m}^3 \text{s kg}^{-1}$	m s^{-1}

(b) the hydraulic conductivity,

so that the whole column is self-consistent.

Finally, the last column shows a mixed system based on

(a) volume, rather than weight, for the water flux density, and

(b) energy per unit weight as the measure of soil-water potential in equation (6).

The potential energy per unit weight of soil-water is measured by the height of an equivalent column of water, or so-called *pressure head*. The gradient in potential energy has units of meter per meter. Consequently, for consistency, the hydraulic conductivity must be measured in the same units as the water flux density, namely, cubic meters of water per square meter per second, or a water velocity. This is the simplest system of all and may be called the engineering system of units.

2.3. Component soil-water potentials

The total potential ψ is assumed to be the sum of several *component potentials* measured with respect to a common *reference state*. The most important of these are the gravitational potential ψ_g and the matric potential ψ_m . Hence

$$\psi = \psi_m + \psi_g, \quad \psi \leq 0. \quad (9)$$

The *gravitational potential* is negative in equation (4) when the position coordinate is taken as positive downwards from the surface. Hence

$$\psi_g = -gz. \quad (10)$$

The equation corresponding to (9 and 10) in the engineering system of units is often presented as $\phi = h = p/\gamma + z$ i.e. “the potential ϕ will be equal to the *piezometric head* h i.e. the sum of the *pressure head* p/γ and the elevation z , where p is the pressure in the soil water, γ is the

weight density of the water, and z is the elevation *above* a fixed horizontal datum". In this case potential energy ϕ is represented as energy per unit weight with the weight density given by $\gamma = \rho_w g$. The corresponding gravitational potential is then z , not $-g \cdot z$, in accordance with the engineering system of units in (7) above. The sign is reversed whenever the vertical coordinate is taken as positive upwards, whereas it is positive downwards in this paper; this confusion is reflected in the eclectic literature on soil-water.

The matric potential of soil water ψ_m (J kg^{-1}) is also negative and is a function of water content. Thermo-mechanical work must be done in order to return the soil water to the reference state, by removing it from the soil, whether by suction, drainage or evaporation. In the engineering system of units "in order to avoid continual use of negative pressures, it is convenient and is customary in discussing unsaturated flow in porous media to use the negative of the pressure head and to describe this as soil suction (S_s)" i.e. $S_s = -p/\gamma$. The logarithm to the base 10 of S_s expressed as centimeters of water in tension is the pF scale of measurement, by analogy with the pH scale.

The relationship between water content and matric potential, the *soil-water characteristic* $\psi_m = \psi_m(\theta)$, is a constitutive property of the soil-air-water system and is determined by measurements on soil samples at the pedon scale. The inverse function $\theta = \theta(\psi_m)$ and its derivative, the *specific water capacity* $C(\theta) = d\theta/d\psi_m$, may be used to eliminate θ from equation (1a), from k_l , and k_v , yielding ψ_m as the dependent variable. θ may also be chosen as the dependent variable. When the soil is layered, θ_s and k_l are discontinuous functions of depth. Consequently, the choice of ψ_m as the dependent variable is more general than θ , since ψ_m may be a continuous function of z when θ is not.

2.4. The Philip-Richards equation

Combining equations (1—3, 8 and 9, 10) and eliminating the fluxes, we find the equation for the unknown matric potential ψ_m

$$\rho_w C \frac{\partial \psi_m}{\partial t} = - \frac{\partial}{\partial z} \left(k \frac{\partial \psi_m}{\partial z} - k g \right) \quad (11)$$

where $k = k_l + k_v$. When $k_v = 0$ this is known as Richards equation [42] of soil physics; the extension to include vapour transport is due to Philip [30]. This is a non-linear parabolic equation of the diffusion type with "concentration" dependent coefficients $C(\psi_m)$ and $k(\psi_m)$.

Extensions of this equation to include two or three space dimensions, the non-rigid matrices of soils, the presence of electrolytes and the effect of temperature gradients, and living plants are also possible. The above presentation is sufficient for this discussion.

2.5. Potential energy and the phase partitioning of water

The potential energy, ψ , of water in a state S is equal to the notional work that must be performed by a given process, in order to convert water from a reference state S_0 , to the state S . The reference state is free pure liquid water at $z = 0$ in isothermal equilibrium with its vapour at saturation in a standard atmosphere.

Liquid water in an unsaturated soil is not free, since it is bound to the soil matrix by capillary and adhesive forces. Furthermore, the concentration of water vapour in the soil-air, which is in equilibrium with liquid soil-water, has a value less than that in the reference atmosphere.

The work done, $\psi_h < 0$, in expanding isothermally the water vapour in the standard atmosphere in its reference state S_0 , to achieve a lower humidity is

$$\psi_h = \frac{RT}{M_w} \ln h, \quad 0 < h \leq 1, \quad (12)$$

assuming that atmospheric water vapour obeys the ideal gas and partial pressure laws. M_w is the molar mass of water (0.018 kg/mol), R the molar gas constant (8.314 J/mol K) and T the constant temperature in degrees Kelvin (293 K at 20 °C).

On the other hand, $\psi_m < 0$, is the work done in transferring isothermally the liquid water from the state S_0 into an inert rigid porous soil. We may equate ψ_h and ψ_m when the liquid and vapour phases of soil-water are in “thermodynamic” equilibrium. Substituting $\psi_m = \psi_h$ in equation (12) and inverting the logarithm we find the relative humidity of soil-air h as the so-called “thermodynamic function” of soil-water potential ψ_m at any z [8, 29, 43, 4]

$$h(z) = \exp \frac{M_w \psi_m(z)}{RT}. \quad (13)$$

instantaneously partitions $\theta(\psi_m)$ between the liquid and vapour phases, and allows us to use one, rather than two, state variables for soil-water content. The complication of hysteresis has been ignored in this brief survey.

In the language of the thermodynamics of Gibbs, ψ , is the partial specific free energy of the water in the soil-air-water system [8]. The work performed by the process in converting water from state S_0 to S must be reversible, independent of path, and depend solely on the initial and final states. Necessary conditions for this, are usually given as

- (a) the process is sufficiently slow to be represented as a succession of steady states,
- (b) friction is negligible, and
- (c) constant temperature [43].

Condition (a) contradicts equation (11), since this parabolic equation has the property that infinitesimal changes in ψ_m are propagated everywhere with infinite speed.

For a penetrating critique of the problematic foundations of classical thermo-dynamics and its development on a rigorous foundation, see Truesdell [50, 51] and Serrin [47].

Table 2 shows typical values of the matric potential and relative humidity of soil-air in the different sets of units

Table 2. Matric potential and relative humidity of soil-air

Conditions	Matric potential			Relative humidity of soil-air at 20°	
	J/kg	MPa	Bars	pF	Concentration
Close to saturation	-1	-10 ⁻³	-10 ⁻²	1.01	0.999993
Field capacity approx.	-10 ²	-10 ⁻¹	-1.0	3.01	0.999261
Permanent wilting point approx.	-10 ³	-10	-10 ²	5.01	0.928772
Air-dry	-10 ⁵	-10 ²	-10 ³	6.01	0.477632
Oven-dry	-10 ⁶	-10 ⁴	-10 ⁴	7.01	0.000618

The terms “field capacity” and “permanent wilting point” have a long history of use in agronomy, but they are not constitutive properties of soil. The potential of soil-water in air-dry samples varies with the relative humidity of the atmosphere, where the relative humidity of the atmosphere is calculated from equation (13).

2.6. Liquid and vapour conductivities

The conductivities for liquid and water vapour in soil at the pedon scale are k_l and k_v ($\text{kg m}^{-2} \text{s}^{-1}$). They depend on the properties of the soil matrix and on water content θ . The inverse function $\theta = \theta(\psi_m)$ of the soil-water characteristic may be used to express $k_l[\theta(\psi_m)]$ and $k_v[\theta(\psi_m)]$ as functions of ψ_m .

The liquid-water conductivity k_l is zero at zero water content, and is assumed to increase monotonically to a maximum at saturation. k_l is determined by measurement on soil samples at the pedon scale. In contrast to k_l , the vapour conductivity k_v is zero for both saturated and completely dry soil, and may rise to a maximum at a potential of roughly -10^4J kg^{-1} (equivalent to 100,000 cm of water, $pF = 5$, when potential is defined as energy per unit weight). In the early stages of drying, the relative humidity of soil air is one and k_v is negligible compared with k_l . However, when the water potential in the soil drops below -10^4J kg^{-1} , mass transfer takes place almost entirely in the vapour phase.

The flux density of water vapour, is given by the isothermal theory of vapour diffusion (Fick's law) in porous media [27, 30, 13, 5]

$$f_v = -D_v \frac{\partial c}{\partial z} \quad (14)$$

where c is the water vapour concentration in soil air (kg m^{-3}) and D_v the corresponding vapour diffusivity ($\text{m}^2 \text{s}^{-1}$). D_v is given by the expression

$$D_v = -\alpha D_0 [\theta_s - \theta(\psi_m)], \quad (15)$$

where D_0 is the binary diffusion coefficient of water vapour in still air, at the prescribed temperature; $[\theta_s - \theta(\psi_m)]$ is the air-filled porosity of tortuosity α , through which vapour diffusion can occur.

Accordingly, using the chain rule for the derivative $\partial c / \partial z$, the conductivity k_v is

$$k_v = -\alpha D_0 (\theta_s - \theta) c_{sat} \frac{dh}{d\psi_m} \quad (16)$$

where $h = c/c_{sat}$ is the relative humidity and c_{sat} is the value of c at saturation for the given temperature T . From expression (13) we can find $dh/d\psi_m$. Hence the vapour conductivity k_v can be expressed entirely in terms of ψ_m .

3. Boundary conditions at the pedon scale

3.1. Boundary conditions at the bottom of the soil column

The boundary condition at the bottom ($z = z_b$) of the column of unsaturated soil can be expressed in terms of the air-entry potential ψ_e ,

$$\psi = \psi_e \quad \text{at} \quad z = z_b, \quad (17)$$

$\psi_e < 0$ is the potential at which air first enters a saturated ($\theta = \theta_s$) sample of soil during drying, coinciding with the emptying of the largest pores in the soil matrix. This condition fixes the top of the saturated capillary fringe at a depth z_b below the surface. We will refer to z_b as the depth to the water table.

Water fluxes in either direction are possible across the lower boundary at z_b and represent capillary rise from or drainage to the saturated zone in the lower deposits of soil. A fixed value of z_b is adequate for simulating periods of infiltration or evaporation of a few days duration.

On longer time scales, z_b varies with time. z_b increases due to outflow of water to drains, and it decreases when rain-water infiltrates down to z_b . During prolonged periods of high evaporation z_b may also decrease.

We may derive a differential equation for $z_b(t)$ from a dynamic water balance on a column of saturated soil lying between z_b and z_d , the water level in the nearest surface drain.

The volume of water in a column of porosity ϕ_f per unit cross sectional area is $\phi_f(z_d - z_b)$. Assuming that the flow rate to (and from) the drain is proportional to the volume of water in the saturated column, we write the dynamic water balance

$$\rho_w \phi_f \frac{dz_b}{dt} = \kappa \rho_w \phi_f (z_d - z_b) - f_l(z_b) \quad (18)$$

as where $\kappa(s^{-1})$ is a fractional rate of adjustment in the relative water level $(z_d - z_b)$ due to drainage. $f_l(z_b)$ is the flux density of liquid water (1b) at z_b . We may ignore the vapour flux contribution in this case. Equation (18) is a first-order inhomogeneous ordinary differential equation for $z_b(t)$. It is also linear when the porosity ϕ_f is independent of depth. $f_l(z_b)$ couples equations (11) and (18).

Equation (11) must now be solved subject to a moving boundary condition (18). This is considerably more difficult than the fixed condition in (17). The parameter κ may be found using field measurements of $z_b(t)$ or simple models of saturated flow to drains. A more detailed treatment requires a two-dimensional theory of combined saturated and unsaturated flow.

3.2. Surface boundary condition for infiltration of rain

The boundary condition for infiltration of rain into soil is a prescribed flux at $z = 0$, equal to the rainfall rate $Q(\text{m}^3 \text{m}^{-2} \text{s}^{-1})$

$$f_l = -k_l \frac{\partial \psi}{\partial z} = \rho_w Q, \quad \theta < \theta_s, \quad \text{at } z = 0. \quad (19)$$

Vapour flux is not normally considered during infiltration.

As the solution of equations (11), (17) and (19) evolves in time, from a given initial condition $\theta(z, 0)$, $\theta(0, t)$ increases and may reach saturation. When saturation occurs at the ponding time t_p , the *first stage of infiltration* at the *atmosphere-controlled* rate is completed and the boundary condition *switches* to a prescribed concentration $\theta = \theta_s$

$$\theta(0, t_p) = \theta_s. \quad (20)$$

As the solution of equations (11), (17) and (20) evolves in time, the flux into the soil $f_l(0, t)$ decreases from its initial value of $\rho_w Q$. During the second stage of ponded infiltration, the surplus water accumulates on the surface of the ground and starts to flow horizontally.

In the first stage of infiltration, the flux into the soil is atmosphere-controlled. In the second stage, it is soil-controlled. Analytical solutions for both linear and nonlinear simplifications of the above equations are summarized in [16]. Approximate expressions for the “time to ponding” for soils that are initially dry, are given in [17]. Time to ponding may vary by several orders of magnitude depending on soil properties and rainfall. If the rainfall intensity is less than the liquid conductivity at saturation, the switch to the second stage (ponding) does not occur. We now consider the soil after rainfall has stopped. The patches of ponded water, if there are any, will gradually disappear due to infiltration and evaporation. The infiltrated water will also be redistributed within the soil due to matric forces and gravity.

3.3. Surface boundary conditions for isothermal evaporation

In order to simplify the presentation, we begin with a column of bare soil with an initial water content but no ponded water on the surface. The initial water content is the accumulated effect of past rainfall, evaporation and drainage, modified by spatially varying topography, atmospheric

and soil properties. The relative humidity of the air in the soil surface is 100% and evaporation begins at the potential rate E_p .

The boundary condition for evaporation at the surface is a flux E of water vapour from soil to atmosphere

$$f_l = -k_l \frac{\partial \psi}{\partial z} = 0 \quad \text{at } z = 0, \quad (21)$$

$$f_v = -k_v \frac{\partial \psi}{\partial z} = -\rho_w E \quad \text{at } z = 0. \quad (22)$$

The actual evaporation rate E ($\text{m}^3 \text{m}^{-2} \text{s}^{-1}$) may be defined as follows [2]:

$$E = H(w)[c_0 - c_a] \quad (23)$$

where $H(w)$ is a mass transfer coefficient that varies with wind speed w at a reference height above the ground. c_0 is the water vapour concentration in the air in the soil surface and c_a is the water vapour concentration at the reference height in the atmosphere. In order to combine this boundary condition with the Philip-Richards equation, we must relate c_0 to ψ_m at $z = 0$.

The simplest relationship between c_0 and $\psi_m(0)$ is obtained by assuming an isothermal soil-atmosphere continuum. Hence, we may define a potential or maximum evaporation rate E_p ($\text{m}^3 \text{m}^{-2} \text{s}^{-1}$) as the evaporation rate from a wet soil at the same uniform temperature as the atmosphere

$$E_p = H(w)[c_{sat} - c_a] \quad (24)$$

where c_{sat} is the saturation water vapour concentration in the soil surface at the given temperature.

Numerical experiments by van Bavel and Hillel [52], based on an albedo that varies with water content, show that potential evaporation is not a precise concept even under isothermal conditions. In general, evaporation depends on both the soil and the atmosphere. Nevertheless, it is a very useful first approximation.

Eliminating $H(w)$ from (23) and (24) we find [32]

$$E = E_p \left[\frac{h_0 - h_a}{1 - h_a} \right], \quad 1 \geq h_0 \geq h_a, \quad (25)$$

where $h_a = c_a/c_{sat}$ is the relative humidity of the atmosphere at the reference height; $h_0 = c_0/c_{sat}$ is the relative humidity of the air in the soil surface at $z = 0$, and is found by inserting $\psi_m(0)$ into (13).

During the isothermal drying of wet soils, the precise value of h_a is not important in equation (25) for small values of t , since $h_0 = 1$, $E/E_p = 1$, and E_p drives the model. Eventually h_0 may decrease from unity at a rate that depends on soil hydraulic properties, which control the upward supply of water. The evaporating surface, which is initially located in the soil surface at $z = 0$, starts to move downwards and transport of soil-water in the vapour phase appears. Eventually thermal gradients become important and must be considered.

Values of E_p may be estimated from Penman's equation [28] using standard meteorological data or from open water evaporation rates after correction by a pan factor. A diurnal cycle may be introduced into E_p in proportion to the elevation of the sun [52, 12].

Combining equations (22) and (25), we find a non-linear inhomogeneous boundary condition of the mixed type at $z = 0$

$$k_v \frac{\partial \psi_m}{\partial z} - \frac{\rho_w E_p}{1 - h_a} \exp \left[\frac{M_w \psi_m}{RT} \right] = k_v g - \frac{\rho_w E_p h_a}{1 - h_a} \quad (26)$$

for isothermal evaporation from wet bare soil at the scale of one meter.

At very low moisture content, thermal gradients cannot be neglected. An additional partial differential equation is required to model the flow of heat. The pair of partial differential equations for heat and moisture is coupled through the energy balance at the surface and also through their coefficients, in accordance with the theory of Philip and de Vries [31]. For numerical techniques for solving various forms of the above equations and their boundary conditions see [12, 53, 5, 25, 46].

3.4. Non-linear switching

The effect of the boundary condition (26) is to switch suddenly at some point in time from an evaporative flux controlled by the atmosphere to a flux controlled by the soil [33, 36, 38, 44, 13, 45]. The time of switching emerges from the combined solution of the Philip-Richards equation and the boundary condition (26). It is not prescribed in advance. This non-linear switching is mathematically similar to the switching during rain before and after ponding.

A simple two-stage approximation to (26) is sometimes used. In the first stage, a flux boundary condition equal to E_p is specified and lasts until the water content of the surface reaches a designated low value – the end of atmosphere control. A switch is then made to this low water content as the “concentration” boundary condition for the second stage – the start of soil control. The moisture profile at the end of the first stage provides the initial condition for the second stage. See [18] for approximate analytical solutions. Soil water responds to alternating wet and dry periods, each of which starts with a surface flux in or out of the bare soil that is set by atmospheric conditions. The moisture profile at the end of one period provides the initial condition for the next period. Within each period, a switch from atmosphere control to soil control may occur if the atmospheric conditions are strong enough and if they last for sufficient time. We refer to these times as the “time to ponding” in the case of infiltration of rain, and the “time to stage-two drying” in the case of evaporation. Consequently, there are two sets of switches in our computational clock: an outer pair always switching between wet and dry periods, and an inner pair switching intermittently from atmosphere control to soil control, see Figure 1. This strongly non-linear behaviour is modelled by switching to and from the appropriate boundary conditions given in the above discussion. Simultaneously, the bottom boundary condition continues to play its role in contributing to the dynamic redistribution of water within the unsaturated soil column[6].

The action of the two pairs of switches is expressed spatially as a set of dynamic patches covering the soil surface, with each patch in one of four possible states: surface water flux in or out, surface water flux controlled by the atmosphere or by the soil. These patches have a life cycle. They grow, coalesce, shrink and disappear. Their shape may be fractal and will reflect the structure of the atmospheric boundary layer, the detailed geometry of the ground surface, the properties of the soil underneath and the deeper drainage in the saturated zone. They await discovery in remotely sensed data.

The transpiration of plants can be included as a distributed sink-term in the water balance equation. Plants extract water from the three-dimensional space occupied by their roots. In contrast, surface evaporation passes through a thin two-dimensional vapour layer, or bottleneck, at the surface of the soil. The presence of macro-pores, arising from biological processes, and also cracks, allows some evaporation to occur from the three-dimensional volume of the soil. They also allow rapid infiltration to occur during rain. The above model must be modified when these factors are important. However, the modified model will retain the non-linear switches, which are seen most clearly in the case of bare homogeneous soil at the pedon scale. At larger scales, spatial averaging can be expected to attenuate their abrupt action.

For further detail, the reader is referred to the book by Slatyer [48], the papers by Philip

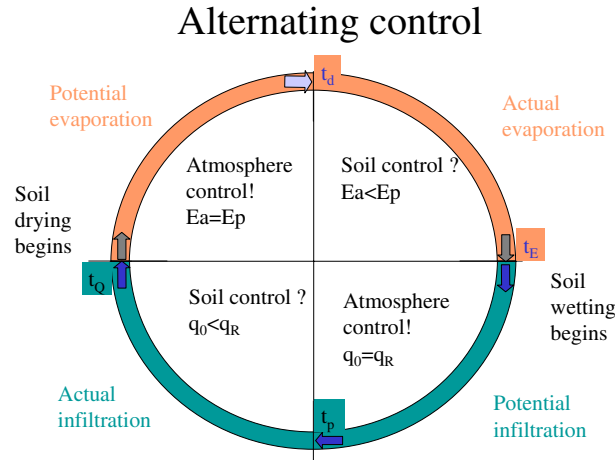


Figure 1. Computational clock with two pairs of switched boundary conditions. The outer pair shows fluxes at *potential* rates switching from red to green to red across a horizontal line and the inner pair shows fluxes at smaller *actual* rates switching across a vertical line through the clock. t_p is the time to ponding of water on the surface of the ground. t_Q is the time when rain stops. When ponding fails to occur $t_Q < t_p$. t_d is the time when phase 1 drying ends. t_E is the end of the dry period and the start of another rainy period. When phase 2 drying fails to occur $t_E < t_d$. The possible failure to switch to soil control is indicated by a question mark. The switching between wet and dry periods, initially always under atmosphere control, is indicated with an exclamation mark.

[35, 37] and more recent surveys of SVAT (Soil-vegetation-atmosphere) models at various scales.

3.5. The FEST model

The purpose of the FEST model is to provide a testbed for examining and demonstrating as clearly as possibly the effect of hysteresis on selected processes in a column of vegetated soil reacting to the atmosphere. A partial analysis of the full Philip-Richards equation begins by excluding all spatial variation requiring partial derivatives for the local description of water potential and the conservation of soil water.

The FEST model is a fully vegetated slab of soil and transpiring plants (FEST) with a water balance on the slab described by a first-order, ordinary differential equation. Transpiration is treated as capillary flow through a space-filling “wick” of roots extending from all points in the slab to a uniformly transpiring canopy above the surface of the slab. A preferential flow network due to decayed roots, animal burrows, and wormholes permits rainfall to infiltrate directly into the soil throughout the slab. A uniform matrix of soil surrounds the slab-filling wick and the preferential flow network. The soil matrix has (1) a standard soil-moisture characteristic, and (2) an unsaturated hydraulic conductivity function. All water flow into and out of the soil matrix, namely, transpiration, infiltration, drainage to and capillary rise from a water table below the slab, is driven by the appropriate difference in total potential energy multiplied by the unsaturated hydraulic conductivity K . This is a finite difference version of the generalised Buckingham/Darcy Law for unsaturated flow in porous media. These assumptions yield a non-linear, first-order ordinary differential equation.

Consequently, a uniform slab of vegetated soil of thickness L is considered with a position coordinate z pointing downwards into the soil. Its origin lies at the soil surface. Soil wetness is taken to be uniform throughout the slab with volumetric moisture content θ , measured as cubic meters of water per cubic meter of rigid soil matrix, satisfying the inequalities $0 \leq \theta \leq \theta_{sat} < 1$

where θ_{sat} is the saturation concentration of water. The scalar potential energy ψ of soil water is defined to be the sum of two partial potentials $\psi = \psi_g + \psi_m$. These are defined to be the thermo-mechanical work that must be performed on the soil-water to bring it to a common reference state. This work is done against (1) the field of gravity, yielding $\psi_g = -z$, and (2) all surface forces in the unsaturated soil, giving ψ_m , the matric potential. The reference state for the scalar potential is free water at the surface of the slab at $z=0$. Consequently, $\psi_g < 0$ and $\psi_m < 0$ in the case of both gravity and surface forces. The matric potential ψ_m is zero at saturation $\theta = \theta_{sat}$. The mixed system of units – the so-called engineering system – is used. Potential energy is expressed as energy per unit weight, which reduces to a “total head” with units of length. Volume replaces mass.

The water balance for the slab may be written as a first order ordinary differential equation with a prescribed initial condition

$$\begin{aligned} L \frac{d\theta}{dt} &= f(t), \\ \theta(0) &= \theta_0, \\ f(t) &= I(t) - E(t) - D(t), \end{aligned} \tag{27}$$

where I is the rate of infiltration of rain water, E the rate of transpiration from the soil slab, and D the rate of drainage below the soil slab. All rates are cubic meters of water per square meter of soil per unit time, in other words, a velocity. The vegetation excludes evaporation of water from the surface of the soil. Writing I , E , and D as functions of soil-water potential, which in turn is a function of soil-moisture, closes the water balance equation.

3.6. The rate of infiltration $I(t)$

The soil slab is assumed to contain a network of macro-pores, which bring rainfall into uniform contact with the micro-pores of the soil. The macro-pores are assumed to have a volume of zero in this simplified treatment. Ponding occurs when the soil cannot absorb, or imbibe, the available rain from the macro-pores. Accordingly, the rate of infiltration I per unit area as the lesser of two quantities at every point in time

$$I = \min \left(\frac{0 - \psi_m}{A}, Q \right) = \min \left(-\frac{\psi_m}{A}, Q \right).$$

When the first term is less than the rainfall rate Q , given as a volumetric rate per unit area, ponding of water on the surface of the slab is said to occur. The excess rain runs off immediately into a surface drain. The potential difference that drives the absorption, or imbibition, is assumed to be the difference between the potential at saturation, namely zero, in the macro-pores, and the potential in the soil proper $\psi_m < 0$. The parameter A is the associated adjustment time. This can be read as a negative feedback loop driving the moisture concentration to saturation and the associated matric potential to zero. The variation in the matric potential partitions the rainfall into infiltration I and surface runoff $(Q - I)$.

3.7. The rate of transpiration $E(t)$

The vegetation is assumed to have a uniform system of roots, which allows transpiration from all parts of the soil slab. We assume no evaporation from the surface of the soil. The rate of transpiration per unit area at all points in time is taken to be

$$E = E_p \frac{h_0 - h_a}{1 - h_a}, \quad h_0 = \frac{c_0}{c_{sat}}, \quad h_a = \frac{c_a}{c_{sat}}, \quad 1 \geq h_0 \geq h_a, \tag{28}$$

where E_p is the potential or maximum rate of transpiration per unit area and is controlled by conditions in the atmosphere. h_a is the relative humidity of the atmosphere, and h_0 is the relative humidity of the vacuoles in the leaves through which the plants transpire. c_{sat} is the saturation concentration of water vapour in air at the common temperature of the soil, plants and atmosphere – the isothermal assumption. When h_0 is unity, transpiration is at the maximum rate. When h_0 is less than one, due to the suction of the plant water in iso-potential contact with soil water near the plant roots, transpiration up the plant xylem is less than the maximum rate. Transpiration ceases when $h_0 = h_a$. No resistance to flow up the xylem is assumed.

The plant humidity h_0 can be related to the total potential ψ_0 at the canopy height by means of the so-called thermodynamic equation of soil physics

$$h_0 = \exp \left[\frac{M_w \psi_0}{RT} \right] = \exp \left[\frac{M_w}{RT} (\psi_m + z_c) \right], \quad (29)$$

where the total potential has been written in terms of its partial potentials and z_c is the canopy height. R is the gas constant, T the absolute temperature and M_w the molecular weight of water. Substituting equation (29) in (28) gives the rate of transpiration as a function of the potential of the soil water. These can be interpreted as a negative feedback loop, where the potential of soil-water drops, until the humidity of the plant vacuoles becomes equal to the humidity of the atmosphere, and transpiration ceases.

3.8. The rate of drainage $D(t)$

The rate of drainage per unit area is assumed to be driven by the difference in total potential between the centre of the soil slab and its base. We assume saturation immediately below the slab and a matric potential of zero. Consequently,

$$D = \frac{(0 - \psi_m) + (-L - (-L/2))}{B} = \frac{-\psi_m - L/2}{B} \quad (30)$$

where B is a second adjustment time. This can be interpreted as a negative feedback loop with the local equilibrium of $\psi_m = -L/2$ and the matric forces in the soil hold a quantity of water against gravity.

3.9. Closing the model

The model is closed with the *soil-water characteristic* $\psi_m = \psi_m(\theta)$, which can be taken as the Brooks-Corey or Van Genuchten relationships without hysteresis. This is the place where hysteresis may be introduced using a Preisach model [41].

3.10. Interpreting the model

The FEST equation can be interpreted as a set of competing feedback loops. The following feedback diagrams, written in Forrester's picture language as used in the STELLA software system, display the loops associated with infiltration, transpiration, and drainage or capillary rise. The two loops shown at Figure 2 drive the infiltration dynamics. Theta is the volumetric moisture content and ψ_m is its capillary or matric potential, or soil suction. Theta is associated with a rectangular box because it is a state variable that is conserved. All other variables are either rates or parts of rate variables.

Figure 3 shows the feedback loops driving transpiration

Figure 4 shows the feedback loops driving drainage or capillary rise of water to and from a water table beneath the vegetated slab.

An examination of the open loop structure of the FEST non-linear ordinary differential equation demonstrates its long-term dynamic behaviour, including the possibility of bifurcation and chaos. A very interesting bifurcation that depends on the ratio of the inputs P/E has been found.

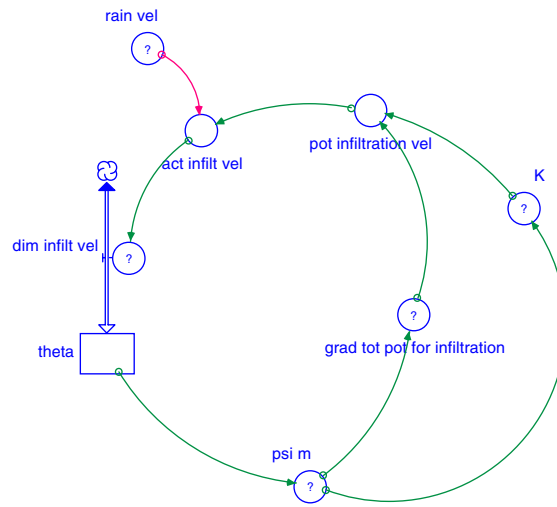


Figure 2. The feedback loops for infiltration

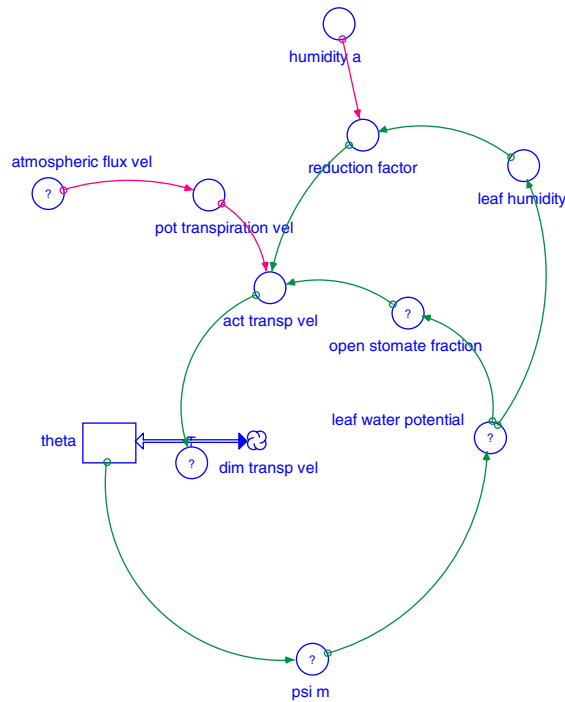


Figure 3. The feedback loops for transpiration.

4. Conclusions

The FEST model can be used to examine the effect of the hysteretic relationship between moisture content and its potential $\psi_{i,m}$. The difference between the cases with and without hysteresis, examined for a wide range of soil types and both deterministic and stochastic climates, will help to answer the question: *How important is hysteresis in soil physics and in terrestrial hydrology?*

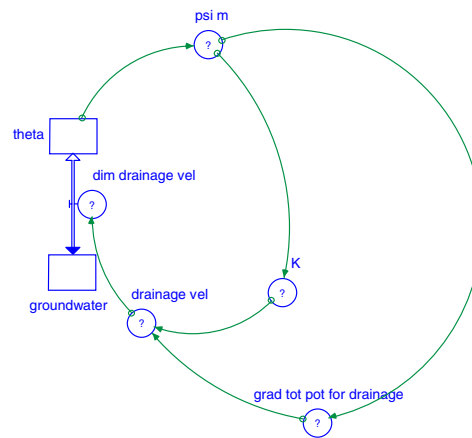


Figure 4. The feedback loops for drainage and capillary rise.

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