A conductivity relationship for steady-state unsaturated flow processes under optimal flow conditions

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Abstract

Optimality principles have been used for investigating physical processes in different areas. This work attempts to apply an optimal principle (that water flow resistance is minimized on global scale) to steady-state unsaturated flow processes. Based on the calculus of variations, we show that under optimal conditions, hydraulic conductivity for steady-state unsaturated flow is proportional to a power function of the magnitude of water flux. This relationship is consistent with an intuitive expectation that for an optimal water flow system, locations where relatively large water fluxes occur should correspond to relatively small resistance (or large conductance). Similar results were also obtained for hydraulic structures in river basins and tree leaves, as reported in other studies. Consistence of this theoretical result with observed fingering-flow behavior in unsaturated soils and an existing model is also demonstrated.

1.Introduction

Optimality principles refer to that state of a physical process is controlled by an optimal condition that is subject to physical and/or resource constrains. For example, Eagleson (2002) demonstrated that under natural conditions and in water-limited areas, vegetation tends to grow under maximum-productivity and unstressed conditions. He called function and forms of vegetation, following the optimality principle, results of “Darwinian expression”. After studying a variety of natural phenomena characterized by tree-like structures, Bejan (2000) proposed “constructal theory” that states that “for a finite-size open system to persist in time (to survive) it must evolve in such a way that it proves easier and easier access to the currents that flow through it”. While the definition of “easy access” is not always clear, Bejan (2000) demonstrated that tree-like structures are direct results of minimization of flow resistance across whole flow systems under consideration. Over the past 30 years, the maximum entropy production (MEP) principle has been successfully applied, in a heuristic sense, to the prediction of steady states of a wide range of systems (Niven, 2010; Kleidon, 2009). The MEP principle states that a flow system subject to various flows or gradients will tend towards a steady-state position of maximum thermodynamic entropy production (Niven, 2010). However, the theoretical connections between these optimality principles and the currently existing fundamental laws are not well established. The alternative point of view is that these principles are actually self-standing and do not follow from other known laws (Bejan, 2000).

The role of optimality principles in forming complex natural patterns has been recognized for many years in the surface hydrology community (Leopold and Langbein, 1962; Howard, 1990; Rodriguez-Iturbe et al, 1992; Rinaldo et al., 1992; Liu, 2010). For example, Leopold and Langbein (1962) proposed a maximum entropy principle for studying the formation of landscapes. Rodriguez-Iturbe et al (1992) postulated principles of optimality in energy expenditure at both local and global scales for channel networks. While previous studies mainly use spatially “discrete” approaches as a result of considering energy dissipation through channel networks only, Liu (2010) develop a group of (partial differential) governing equations for steady-state optimal landscapes (including both channel networks and associated hillslopes) using calculus of variations.

The importance of optimality principles has also been intuitively recognized in the vadose-zone hydrology community for a long time. For example, it seems to be well known that fingering flow is due to a fact that unsaturated water tends to form flow paths corresponding to the minimized flow resistances. However, rigorous applications of this optimality principle have not been fully explored. Fingering flow results in that liquid water propagates quickly to significant depths while bypassing large portions of the vadose zone, and solute travel times from the contamination source (located in soil surface or vadose zone) to groundwater are shorter than a prior expected. Because of the important effects of this flow process on groundwater contamination (an important issue for water resources management), preferential flow has been a major research area in the vadose zone hydrology community for a number of years and considered probably the most frustrating processes in terms of hampering accurate predictions of contaminant transport in the vadose zone (e.g., Glass et al., 1988; Flury et al., 1995; Liu et al., 2003; Simunek et al., 2003; Nimmo, 2010).

This note presents a conductivity relationship for unsaturated flow derived from a principle that energy dissipation rate (or flow resistance) is minimized for the entire flow system. Preliminary evaluation of this relationship is conducted by comparing it with relevant experimental observations and the currently existing models. The potential limitations and further improvements of this work are also briefly discussed.

2. Theory

As the first step, we consider a relatively simple, steady state unsaturated flow system associated with a homogeneous and isotropic porous medium. From the water mass (volume) conservation, the steady-state water flow equation is given by

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = 0 \qquad (1)$$

where x and y are two horizontal coordinate axes, z is the vertical axis, and q_x, q_y and q_z are water fluxes along x , y and z directions, respectively.

Accordingly, the energy expenditure rate for a unit control volume, ΔE, can be expressed as

$$\Delta E = \frac{\partial(q_x E)}{\partial x} + \frac{\partial(q_y E)}{\partial y} + \frac{\partial(q_z E)}{\partial z} \quad (2)$$

The above equation simply states that for a given unit volume, the energy expenditure rate at that location is equal to the energy carried by water flowing into the volume minus the energy carried by water flowing out of the volume. The *E* (a function of *x*, *y* and z) represents the total energy including both potential (corresponding to elevation *z*) and (capillary) pressure energy:

$$E = z + \frac{P}{\rho g} = z + h \quad (3)$$

where g is gravitational acceleration, P is capillary pressure, ρ is water density, and h is capillary pressure head. A combination of Equations (1) and (2) yields

$$\Delta E = q_x \frac{\partial E}{\partial x} + q_y \frac{\partial E}{\partial y} + q_z \frac{\partial E}{\partial z} \quad (4)$$

The water flux is generally given by Darcy's's equation

$$q_x = -K \frac{\partial E}{\partial x} \quad (5a)$$

$$q_y = -K \frac{\partial E}{\partial y} \quad (5b)$$

$$q_z = -K \frac{\partial E}{\partial z} \quad (5c)$$

where K is hydraulic conductivity and given by

$$K = K(h, S) \quad (5d)$$

$$S = \left(\frac{\partial E}{\partial x}\right)^2 + \left(\frac{\partial E}{\partial y}\right)^2 + \left(\frac{\partial E}{\partial z}\right)^2 \quad (5e)$$

In Equation (5d), hydraulic conductivity is assumed to be a function of both capillary pressure head (h) and the square of the energy gradient (S). Previous studies for optimal landscape (Liu, 2010) and hydraulic structure of water flow in tree leaves (Liu, unpublished manuscript) indicate that water-flow conductance is function of water flux in these systems. That is the motivation for assuming K to be function of water flux in Equation (5d). (Note that assuming K to be a function of water flux is equivalent to assuming it to be a function of energy gradient, because water flux, energy gradient and K are related through Darcy's law.) Function form of Equation (5d) is a subject of study in this work.

When we combine Equations (4) and (5), the global energy expenditure rate through domain Ω is given by

$$\iint_{\Omega} \Delta E dxdydz = \iint_{\Omega} (-KS) dxdydz \qquad (6)$$

The optimality principle in our problem is to minimize the absolute value of the above integral. To do so, we employ the calculus of variations that seeks optimal (stationary) solutions to a functional (a function of functions) by identifying unknown functions (Weinstock, 1974).

Based on Equations (1), (5) and (6), the Lagrange for the given problem is given by

$$L = -KS + \lambda_1[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}] + \lambda_2[S - \left(\frac{\partial E}{\partial x}\right)^2 - \left(\frac{\partial E}{\partial y}\right)^2 - \left(\frac{\partial E}{\partial z}\right)^2]$$

$$+ \lambda_3[q_x + K\frac{\partial E}{\partial x}] + \lambda_4[q_y + K\frac{\partial E}{\partial y}] + \lambda_5[q_z + K\frac{\partial E}{\partial z}] \qquad (7)$$

Note that the first term is from Equation (6) and other terms are constraints from Equations (1) and (5). Use of these constraint terms allows considering related functions to be independent when determining the optimal solution to Equation (6). The λ functions are Lagrange multipliers. A mathematically equivalent way to define L to avoid the use of some (or all) constraints is to directly insert Equations (1) and (5) into the first term of Equation (7) (Pike, 2001). In this case, the number of independent functions will be reduced. However, the use of Equation (7) is more straightforward and easier to handle for the given problem.

The following Euler-Lagrange equation is used to determine an unknown function w associated with L to minimize the integral defined in Equation (6) (Weinstock, 1974):

$$\frac{\partial L}{\partial w} - \frac{\partial}{\partial x}\left(\frac{\partial L}{\partial w_x}\right) - \frac{\partial}{\partial y}\left(\frac{\partial L}{\partial w_y}\right) - \frac{\partial}{\partial z}\left(\frac{\partial L}{\partial w_z}\right) = 0 \qquad (8)$$

where w_x, w_y and w_z are partial derivatives with respect to x, y and z, respectively. In this study, w corresponds to K, q_x, q_y, q_z, S and h (or E), respectively. (Also note that application of the Euler-Lagrange equation to Lagrange multipliers will recover Equations (1) and (5).)

Replacing w with q_x, q_y and q_z, respectively, in Equation (8) yields

$$\lambda_3 = \frac{\partial \lambda_1}{\partial x} \tag{9a}$$

$$\lambda_4 = \frac{\partial \lambda_1}{\partial y} \tag{9b}$$

$$\lambda_5 = \frac{\partial \lambda_1}{\partial z} \tag{9c}$$

Replacing w with S in Equation (8), we have

$$\lambda_2 = K + S\frac{\partial K}{\partial S} \tag{10}$$

Again, replacing w with h in Equation (8) and using Equation (1), we obtain

$$\frac{\partial K}{\partial h}\left[-S + \lambda_3\frac{\partial E}{\partial x} + \lambda_4\frac{\partial E}{\partial y} + \lambda_5\frac{\partial E}{\partial z}\right] + \frac{\partial[2\lambda_2\frac{\partial E}{\partial x}]}{\partial x} + \frac{\partial[2\lambda_2\frac{\partial E}{\partial y}]}{\partial y} + \frac{\partial[2\lambda_2\frac{\partial E}{\partial z}]}{\partial z} - \frac{\partial(\lambda_3 K)}{\partial x} - \frac{\partial(\lambda_4 K)}{\partial y} - \frac{\partial(\lambda_5 K)}{\partial z} = 0 \tag{11}$$

Replacing w with K in Equation (8) gives

$$S - \lambda_3\frac{\partial E}{\partial x} - \lambda_4\frac{\partial E}{\partial y} - \lambda_5\frac{\partial E}{\partial z} = 0 \tag{12}$$

Based on Equations (5e) and (9), solution to equation (12) can be given as

$$\lambda_1 = E \tag{13}$$

Then combining Equations (9), (10), (11) and (13) and using the continuity equation, we obtain the following equation

$$\frac{\partial(\frac{\partial K}{\partial(\log S)}\frac{\partial E}{\partial x})}{\partial x} + \frac{\partial(\frac{\partial K}{\partial(\log S)}\frac{\partial E}{\partial y})}{\partial y} + \frac{\partial(\frac{\partial K}{\partial(\log S)}\frac{\partial E}{\partial z})}{\partial z} = 0 \tag{14}$$

A comparison between the above equation with the continuity equation (Equations (1) and (5)) yields

$$\frac{\partial K}{\partial(\log S)} = AK \qquad (15)$$

where A is a constant.

To get practically useful results, we further consider K(h, S) to be further expressed by

$$K(h,S) = f(h)g(S) \qquad (16)$$

Substituting (16) into (15) results in

$$g(S) \propto S^{A} \qquad (17)$$

Based on Darcy's law, (17) can be rewritten as

$$g(S) \propto \left(\frac{|q|}{K}\right)^{A/2} \qquad (18)$$

where $|q|$ is the magnitude of water flux given by

$$|q| = \left[q_x^{\ 2} + q_y^{\ 2} + q_z^{\ 2}\right]^{1/2} \qquad (19)$$

Combining (18) and (16) gives our final conductivity relationship as follows

$$K = F(h)\left(\frac{|q|}{K_{sat}}\right)^{a} \qquad (20)$$

where a = A/(2+A). It is very interesting to note that although the mathematical derivation processes are considerably complex and involve solving a group of partial differential equations, the final result (Equation (20)) is amazingly simple.

3. Discussion

Under optimal flow conditions corresponding to the minimum energy dissipation rate (or flow resistance), the derived conductivity is a power function of water flux (Equation 20). This result physically makes sense. For the positive power values, the smallest flow resistance occurs within flow paths with the largest water flux. Intuitively, it is easy to understand that this conductivity distribution will result in total flow resistance globally. This finding is also consistent with our daily life experiences. For example, to maximize traffic transportation efficiency, our highways always have more lanes in locations with high traffic fluxes. Also note that conductivity-flux relationships with similar mathematical forms are derived under optimal flow conditions for tree leaves and surface water flow (Liu, unpublished manuscript; Liu, 2010). That explains why fingering flow patterns in unsaturated soils are similar to geometries of blades of tree leaves and drainage networks in river basins.

There may be different interpretations of Equation (20). One interpretation is that F(h) is the local-scale hydraulic conductivity within the fingering-flow zone and that the power function of flux in the equation represents the fraction of fingering flow zone in an area normal to water flux direction. This is justified because h is a local-scale variable. In this case, our result is supported by the analysis results of Wang et al. (1998). On the basis of a number of laboratory-experimental observations of vertical fingering flow in soils (reported in the literature), Wang et al. (1998) presented a relation between flow conditions and a parameter, F_a, defined as the ratio of horizontal cross-sectional area occupied by gravity fingers to the total cross-sectional areas:

$$F_a = \left(\frac{|q|}{K_{sat}} \right)^{0.5} \qquad (21)$$

Obviously, Equation (21) is identical to our theoretical result with a = 0.5. In other words, our theoretical result agrees with laboratory observations cited by Wang et al. (1998).

Our theoretical result is also consistent with the active region model (ARM) proposed by Liu et al. (2005) that is an extension of the active fracture model developed for modeling unsaturated water in fractured rock (Liu et al., 1998). Both the active fracture model and active region model have been evaluated with a variety of experimental data and remarkable agreements between the models and the data have been observed (Liu et al., 1998, 2003, 2005; Liu and Zhang, 2009; Sheng et al., 2009). The ARM assumes a flow domain to be divided into an active region (fingering flow zone) and an inactive region. Flow occurs only in the active region. The volumetric portion of the active region is given as

$$f = \theta^{\gamma} \qquad (22)$$

Where θ is the average effective water saturation across the whole flow domain (including both active and inactive regions), and γ is a constant factor between zero and one. Note that f is equivalent to F_a in Equation (21).

By definition, the average water saturation is related to the effective water saturation (θ_a) within the active region by

$$\theta = f\theta_a \qquad (23)$$

For gravity-dominated flow, the energy gradient equals one and the vertical water flux is the same as the hydraulic conductivity. Using the well-known Brooks-Corey relationship (1964) to describe hydraulic conductivity within the active region, we can write the total vertical water flux as

$$\frac{q}{K_{sat}} = \theta_a^{\beta} f \qquad (24)$$

where β is the Brooks-Corey factor. Combining Equations (22) to (24) yields

$$f = \left(\frac{|q|}{K_{sat}}\right)^{\frac{1}{1+\frac{\beta(1-\gamma)}{\gamma}}} \qquad (25)$$

Thus, Equation (25) derived from the ARM is equivalent to our conductivity relationship with

$$a = \frac{1}{1+\frac{\beta(1-\gamma)}{\gamma}} \qquad (26)$$

In the other worlds, we demonstrate the equivalence between our Equation (20) and the ARM for gravity-dominated unsaturated flow under the condition that the power function in Equation (20) is interpreted as a volumetric fraction of fingering flow zones within soils.

It is of interest to note that for typical values of β = 4 and γ = 0.7 (Brooks and Corey, 1964; Sheng et al., 2009), a = 0.4 is close to the value of 0.50 given in Equation (21). Whether or not a single value for parameter a is valid for different soils needs further research based on experimental observations. Nevertheless, single parameter (a) values seem to be able to describe water flow in tree leaves (a=1.0) and river basin (a = 2.2), respectively (Liu 2010; Liu, unpublished manuscript).

Finally, this work is the first step to incorporate the optimality principle into unsaturated flow. Consequently, some limitation of the current work still exists. For example, certain local-scale unsaturated-flow physics is not adequately incorporated yet. This physics requires that the upper limit of K in Equation (20) should be F(h), which, however, is not reflected in our theory except for gravity-dominated flow that automatically gives $\frac{|q|}{K_{sat}} \leq 1$. This can be approximately accounted for in practice by limiting the K value calculated from Equation (20) to the corresponding F(h) value. Nevertheless, the major focus of this note is to highlight the potential for developing new unsaturated water flow theories based on the optimal principle. This principle may hold the key to resolving a number of problems associated with emerging patterns in unsaturated soils.

4. Concluding remarks

Based on the calculus of variations, this work shows that under optimal conditions, hydraulic conductivity for steady-state unsaturated flow is proportional to a power function of the magnitude of water flux. It is consistent with an intuitive expectation that for an optimal water flow system, locations where relatively large water fluxes occur should correspond to relatively small resistance (or large conductance). Similar results were also obtained for hydraulic structures in river basins and tree leaves. Consistence between this theoretical result with observed fingering-flow behavior in unsaturated soils and the active region model is also demonstrated.

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