Upscaling of Richards equation for soil moisture dynamics to be utilized in mesoscale atmospheric models

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Abstract Water content and fluxes at the ground surface serve as lower boundary conditions to atmospheric mesoscale models (AMMs). Existing models for water movement (Richards equation) are however not suitable at the grid scale of AMMs and alternative techniques have to be utilized for determining the water content and fluxes at 10-60 km scale. It is found that perturbation techniques may be applied for spatial averaging of the point scale Richards equation for small variance in soil types. A simple rectangular profiles model is suggested for large variation in ground surface properties. Comparisons are made by spatial horizontal averaging of 3-d form of Richards point equation over a heterogeneous land surface.

INTRODUCTION

The processes coupling the soil surface and the atmosphere require special attention for climate modeling. Soil surface characteristics such as moisture availability, albedo, humidity and wind speed are some of the factors which are incorporated through boundary conditions in AMMs. At the large grid scales typically used in such models, spatial variability of soil surface parameters governing moisture availability becomes very significant. Water movement in the soil is frequently described by Richards equation. The validity of this equation at the laboratory scale has been established. This does not guarantee its applicability to averaged behavior over grid size of AMMs. Consequently, important questions arise: Can a spatially averaged form of Richards equation be used for such large numerical discretization blocks? If so, are there "effective properties" which represent the average behavior over such large areas/volumes? If not, what alternative techniques need to be evaluated for predicting average moisture dynamics? The answer to these questions will directly address the issue of upscaling of Richards equation for predicting average moisture dynamics at a scale appropriate for grid blocks in AMMs.

Richards equation at the laboratory or column scale is a nonlinear partial differential equation (PDE) and is based on Darcy’s law. The system state variable (water content) is related to soil properties (unsaturated hydraulic conductivity and soil suction pressure) in a complicated manner. Therefore simple geometric or arithmetic averages to describe the effective properties at a large scale fail to predict correct results. Stochastic approaches have been used to address this problem where local soil hydraulic properties are viewed as a realization of a three dimensional random field. Yeh et al. [1985a,b,c] utilized this approach to develop effective properties for steady
unsaturated flows. Mantoglou and Gelhar [1987a,b,c] extended this study to the time varying case. These studies emphasized the development of analytical expressions for effective properties which necessitated simplifying assumptions like stationarity, infinite flow domains and small fluctuation in soil properties. Mantoglou (1992) addressed the question of effective properties when dealing with finite domains and nonstationarity in parameters. All these studies were based on perturbation expansion of the nonlinear Richard’s equation.

This study addresses the issue of spatial averaging of moisture dynamics at the soil surface. It is shown that perturbation methods are applicable only for small fluctuations in soil parameters. Using this technique the resulting nonlinear PDE which describes average flow behavior over large spatial scales is more complicated than the original Richard’s equation. For large variances, a rectangular profiles model [Dagan and Bresler, 1983] is proposed to describe the local scale moisture dynamics. This equation, though approximate, can be easily upscaled to large spatial areas and yields good results when large variations exist in the soil properties. The parameterization of the hydraulic properties is after Brooks and Corey [1964]. This parameterization was adapted by Noilhan and Plankton [1989] for land surface processes in meteorological models. The saturated hydraulic conductivity of the soil is taken as a stochastic field with specified mean and covariance structure. It has been established in previous studies (Russo and Bresler, 1981a,b; Dagan and Bresler, 1983) that this quantity exhibits the maximum degree of spatial variability in many field soils.

MATHEMATICAL FORMULATION

The continuity equation (ensuring mass conservation) in the absence of sources and sinks is written as

\[
\frac{\partial \theta}{\partial t} + \nabla \cdot q = 0
\]  

(1)

where \( q \) is the volumetric soil-water content (\( \text{cm}^3/\text{cm}^3 \)) and \( q \) is the Darcian flux vector (\( \text{cm/hr} \)). Darcy’s law for isotropic porous media may be expressed as (Gardner, 1958; Philip, 1969)

\[
q = -K \left( \frac{\partial (\Psi - z)}{\partial z} + \frac{\partial \Psi}{\partial x} i + \frac{\partial \Psi}{\partial y} j \right)
\]  

(2)

where \( \Psi \) is the soil capillary pressure head (cm) and \( K \) is the unsaturated soil hydraulic conductivity (\( \text{cm/hr} \)). The total hydraulic head is taken as the algebraic sum of capillary pressure head \( \Psi \) and the elevation head \( z \). Potential gradients due to temperature, osmosis, salt concentrations, etc., are neglected. For convenience of notation, the matric flux potential is defined as (Gardner, 1958; Warrick, 1974),

\[
\Phi(\Psi) = \int_{-\infty}^{\Psi} K(h) dh
\]  

(3)
Combining (1), (2) and (3), the three-dimensional Richards equation in terms of matric flux potential becomes

\[
\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( \frac{\partial \Phi}{\partial z} K_s \right) + \frac{\partial}{\partial x} \left( \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial \Phi}{\partial y} \right)
\]

(4)

This equation is complicated because of the nonlinear water retention and hydraulic conductivity relationships. A physically consistent parameterization (Brooks and Corey, 1964) is quite popular in the soil physics literature (Dagan and Bresler, 1983; Noilhan and Plankton, 1989) and is adopted in this study. In terms of soil saturation \( s = (\theta - \theta_r)/(\theta_s - \theta_r) \), the hydraulic properties are defined as

\[
K_r(s) = s^\eta
\]

(5a)

\[
\Phi_f(s) = \frac{\Psi_w}{1 - s} s^{\frac{\eta}{\lambda}}
\]

(5b)

where equation (5b) is obtained by combining expression (3) with Brooks-Corey moisture characteristic. In equation (5a), the hydraulic conductivity is expressed as the product of the saturated hydraulic conductivity \( K_s(x) \) and the relative hydraulic conductivity \( K_r(s) \) and the flux potential is similarly the product of \( K_r(s) \) and the relative flux potential \( \Phi_f(s) \). The saturated hydraulic conductivity \( K_s(x) \) is taken as a random function of location \( x \).

**Spatial horizontally averaged Richards' equation**

The spatial horizontally averaged Richards equation (SHARE) is obtained by performing areal integration over both sides of equation (4)

\[
\frac{\partial}{\partial t} \left( \frac{1}{A} \iint_A \Phi_f \, dx \right) = \frac{\partial}{\partial z} \left[ \frac{1}{A} \iint_A \left( \frac{\partial \Phi}{\partial z} - K_s \right) \, dx \right] + \frac{1}{A} \iint_A \left( \frac{\partial^2 \Phi}{\partial x^2} + \frac{\partial^2 \Phi}{\partial y^2} \right) \, dx
\]

(6)

It may be noted that the first integral on the right hand side of equation (6) is the area averaged flux value at \( z \) direction. The last area integral can be expressed as a closed line integral of the flux around the boundary of the area \( A \) by using the divergence theorem and is zero because of no flux condition at the sides of the flow domain. The mean areal saturation and flux are defined through the following expressions

\[
<s>(z,t) = \frac{1}{A} \iint_A s(z,t; x) \, dx
\]

(7a)

\[
<q_z>(z,t) = <K> \cdot \frac{\partial <\Phi>}{\partial z}
\]

(7b)

\[
<K>(z,t) = \frac{1}{A} \iint_A K(z,t; x) \, dx
\]

(7c)
\[
<\phi>(z,t) = \frac{1}{A} \int_A \Phi(z,t;\xi) d\xi
\]

in which \(\xi\) is the horizontal coordinate and \(A\) indicates the horizontal averaging area. The principal variable of interest has been chosen as \(<s>\). Expanding \(K\) in Taylor series about \(<s>\), neglecting higher order terms and taking expectations yield

\[
\langle K \rangle = \langle K_s \rangle K_r \langle \langle s \rangle \rangle + K'_r \langle \langle s \rangle \rangle \text{Cov}[s,K_s]
\]

in which

\[
\text{Cov}[s,K_s] = \text{Cov}[s(x),K_s(x)] = \frac{1}{A} \int_A [s(x)-<s>][K_s(x)-<K_s>] d\xi
\]

is the cross-covariance function. The equation for \(\text{Cov}[s,K_s]\) is obtained in a similar manner and after simplification the following system of equations is obtained

\[
(\beta_s-\theta_r) \frac{\partial <s>}{\partial t} = -\frac{\partial \langle q_z \rangle}{\partial z}
\]

(9a)

\[
(\beta_s-\theta_r) \frac{\partial \text{Cov}[s,K_s]}{\partial t} = -\frac{\partial}{\partial z} \text{Cov}[q_z,K_s]
\]

(9b)

\[
\langle q_z \rangle = -\langle K_s \rangle \left[ \frac{\partial \Phi_T(\langle s \rangle)}{\partial z} - K_r(\langle s \rangle) \right]
\]

\[-\frac{\partial}{\partial z} \left[ \Phi_T(\langle s \rangle) \text{Cov}[s,K_s] \right] + K'_r(\langle s \rangle) \text{Cov}[s,K_s]
\]

(9c)

\[
\text{Cov}[q_z,K_s] = \text{Var}(K_s) \left( \frac{\partial \Phi_T(\langle s \rangle)}{\partial z} - K_r(\langle s \rangle) \right)
\]

\[+\langle K_s \rangle (1+\rho_k^2) \left( \frac{\partial}{\partial z} \left[ \Phi_T(\langle s \rangle) \text{Cov}[s,K_s] \right] - K'_r(\langle s \rangle) \text{Cov}[s,K_s] \right)
\]

(9d)

in which \(\rho_k\), the coefficient of variation of \(K_s\), is defined as

\[
\rho_k = \sqrt{\frac{\langle K_s(x) - <K_s> \rangle^2}{<K_s>^2}}
\]

Therefore the system state variables in the perturbated SHAREs are \(<s>\), the mean saturation, and \(\text{Cov}[s,K_s]\), the cross-covariance of \(s(x)\) and \(K_s(x)\). Numerical solutions of the perturbated SHAREs can now be obtained for given boundary and initial conditions. When the surface soil-water content is held constant (as in surface saturation conditions) then \(s(0,t;\xi) = s_c\) and for the constant surface soil-water flux boundary condition \(q_z(0,t;\xi) = q_c\), until the surface reaches saturation.

**Rectangular profile model**

Under the rectangular profiles assumption, the following holds
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\[ s(t,z;K_s) = \begin{cases} s_t & \text{for } z < L(t;K_s) \\ s_i & \text{for } z > L(t;K_s) \end{cases} \]  

(10)

where \( s_t \) is the saturation of the top soil, \( s_i \) is the initial saturation of the soil profile and \( L(t;K_s) \) is the approximate front location of the rectangular profile. Using saturation as the principle state variable, integration of Darcy’s law from the top soil to the infiltration front \( L_f \) produces the integrated Darcy’s law

\[ \int_0^{L_f} q_x(z,t) dz = K_s \int_0^{L_f} K_f(L_f,t) dz + K_s \{ \Phi_f[s(0,t)] - \Phi_f[s(L_f,t)] \} \]

(11)

Integrating the continuity equation from the soil surface to wetting front yields

\[ q_x(0,t) = K_s \Phi_f(L_f,t) - \frac{\partial}{\partial t} \{ s(0,t) - s(L_f,t) \} \]

(12)

In the rectangular profile approximate model, the integrated Darcy’s law and the integrated continuity equation are the two basic equations from which local approximate solutions of \( s \) can be obtained. When the soil surface is held at constant saturation i.e. \( s_t = s_0 \), the only unknown variable of the rectangular profile is the approximate front location \( L(t;K_s) \). Defining the following expressions

\[ K_{sz} = \frac{z - \alpha \ln(1 + z/\alpha)}{\mu t} \]  

(13a)

\[ \alpha = \frac{\Phi_f(s_t) - \Phi_f(s_i)}{K_f(s_t) - K_f(s_i)} \]  

(13b)

\[ \mu = \frac{K_f(s_t) - K_f(s_i)}{(\theta_S - \theta_f)(s_t - s_i)} \]  

(13c)

The analytical expression for the spatial horizontally averaged soil-water content is

\[ \langle s \rangle(z,t) = \frac{1}{A} \int s(t,z;K_S(x)) dx = s_t P(z,t) + s_i [1 - P(z,t)] \]

(14)

in which

\[ P(z,t) = \frac{1}{A} \int_0^{K_{sz}} dK_S = \text{Pr} \{ 0 < K_S(x) < K_{sz} \} = \int_A f_{K_S}(K_S) dK_S. \]

Function \( f_{K_S}(K_S) \) is the probability density function or the frequency distribution function of \( K_S \) over the area \( A \). \( A_i \) is the horizontal area in which the soil is still at initial state and has a \( K_S(x) \) value such that \( 0 < K_S(x) < K_{sz} \). When the distribution of \( K_S \) is lognormal, the mean time-space varying areal saturation is

\[ \langle s \rangle(z,t) = s_t + \frac{s_t - s_i}{2} \text{erfc} \left( \frac{1}{2} \ln \left[ \frac{z - \alpha \ln(1 + z/\alpha)}{\mu t K_s^*} \right] - m_y \right) \]

(15)

in which \( K_s^*, m_y \) and \( s_y \) are the known parameters of the distribution of \( K_s \). The
analysis for \( <s> \) under the boundary condition of constant flux at soil surface proceeds in the similar fashion. The details have been omitted for brevity.

A 3-d centered implicit finite difference model is developed to simulate field-scale unsaturated flow field in order to check the results from the spatial horizontally averaged solutions obtained by perturbation method and rectangular profile method. The 3-d Richard’s equation is discretized using the Crank-Nicholson difference scheme in time and center difference scheme in space. The resulting nonlinear system of equations is solved by the generalized Newton-Raphson iterative method. The resulting coefficient matrix for the simultaneous equations in each iteration is tridiagonalized to ensure that the efficient Thomas algorithm could be used. An adaptive grid scheme is also used to reduce the computer storage and computer time requirement. In the 3-d model, the \( K_s \) is represented as a horizontal 2-d random field. All \( K_s \) values in the vertical direction remain unchanged. This 2-d random \( K_s \) field is generated with correlation lengths of 4 units in x-direction and 8 units in y-direction. The mean soil-water content at each depth in the soil is obtained by averaging all areal saturation values at that depth.

**DISCUSSION OF RESULTS**

The performance of the SHARE model and the rectangular profiles model is evaluated by comparison with the results from 3-d simulations. The results obtained by using the one dimensional Richards equation with a weighted average \( K_s \) are also included. The parameter values used for the simulations are: \( q_s = 0.37, q_r = 0.01, \eta = 2.59 \) and \( \lambda = 0.36 \). The soil is uniformly dry \((s(z,t;x) = 0)\) at beginning of all the simulations considered in this paper. Figure 1 shows the mean saturation \((<s>)\) after 7 hours as a function of depth in the soil \((z)\) when the soil surface is hold at

![Fig. 1 Comparison of areal mean saturation <s> profiles under surface saturation condition with small and larger coefficient of variation of K_s fields computed by four different methods.](image)
Fig. 2 Comparison of areal mean saturation \(< s >\) profiles under constant surface flux condition with small and larger coefficient of variation of \(K_s\) fields computed by four different methods.

saturation. The results in Fig. 1a were obtained for a \(K_s\) field with a small variance \((\rho_k = 0.68, K_s^* = 0.5, m = -0.01, s = 0.5)\). The SHARE model performs well under this small variance for shallow depths. Because of the truncation of higher order moments, it does not capture the tail of the mean behavior exhibited by 3-d simulations. The rectangular profiles model is able to simulate the tail behavior at deeper depths, but it overestimates the mean water content. This is because the water flux at the soil surface is overestimated by this approximate model. The results in Fig. 1b were obtained for a \(K_s\) field with a larger variance \((\rho_k = 1.52, K_s^* = 0.5, m = -0.1, s = 1)\). In this case, the rectangular model is able to match the mean water content behavior of the 3-d simulations at all depths. Again, the SHARE model is unable to replicate the tail behavior at large depths. Similarly, Figure 2 shows the mean saturation \(< s >\) after 7 hours as a function of depth in the soil \((z)\) when a constant flux of \(q_0 = 0.1 \text{ cm/hr}\) is applied at the soil surface. The parameters in Figures 2a and 2b are the same as in Figures 1a and 1b respectively. Because of the larger variance of \(K_s\) in Fig. 2b, the rectangular profile model performs relatively better than it does in Fig. 2a.

It appears that the rectangular profiles model is a better choice when the soil exhibits large spatial variability because the model errors are insignificant in comparison to errors introduced by soil heterogeneity. This simplified model yields analytical solutions and can be upscaled to large spatial blocks. On the other hand, the SHARE model requires expensive numerical solutions. In both Figures 1 and 2, the numerical solutions of the 1-D Richards equation with areally averaged \(K_s\) yield discouraging results and leave unresolved the issue of utilizing such an approach for field-scale soils.

In order to be able to treat arbitrary weather sequences, we plan to extend this study to include space-time varying flux at the soil surface and consider the effects of temporal scales also on the mean behavior of the moisture dynamics. Data from a
watershed in California will be used for evaluating the performance of this model when linked to an AMM.

REFERENCES


