Effective hydraulic parameters for steady state vertical flow in heterogeneous soils

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[1] In hydroclimate and land-atmospheric interaction models, effective hydraulic properties are needed at large grid scales. In this study, the effective soil hydraulic parameters of the areally heterogeneous soil formation are derived by conceptualizing the heterogeneous soil formation as an equivalent homogeneous medium and assuming that the equivalent homogeneous soil will approximately discharge the same total amount of flux and produce same average pressure head profile in the formation. As compared to previous effective hydraulic property studies, a specific feature of this study is that the derived effective hydraulic parameters are mean-gradient-dependent (i.e., vary across depth). Although areal soil heterogeneity was formulated as parallel homogeneous stream tubes in this study, our results appear to be consistent with the previous findings of mean-gradient unsaturated hydraulic conductivity [*Yeh et al.*, 1985a, 1985b]. Three widely used hydraulic conductivity models were employed in this study, i.e., the Gardner model, the Brooks and Corey model, and the van Genuchten model. We examined the impact of parameter correlation, boundary condition (surface pressure head), and elevation above the water table on the effective saturated hydraulic conductivity and shape parameter. The correlation between the saturated hydraulic conductivity K_s and the shape parameter α increases the effective saturated hydraulic conductivity, while it does not affect the effective α. The effective α is usually smaller than the mean value of α, while the effective K_s can be smaller or larger than the mean value depending on no correlation or full correlation between K_s and α fields, respectively. An important observation of this study is that Gardner and van Genuchten functions resulted in effective parameters, whereas it is difficult to define effective parameters for the Brooks Corey model since this model uses a piecewise-continuous profile for hydraulic conductivity. *INDEX TERMS:* 1875 Hydrology: Unsaturated zone; 1836 Hydrology: Hydrologic budget (1655); 1869 Hydrology: Stochastic processes; 1833 Hydrology: Hydroclimatology; 1829 Hydrology: Groundwater hydrology; *KEYWORDS:* effective hydraulic parameters, heterogeneous soil formation, Gardner's model, Brooks and Corey model, van Genuchten model

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1. Introduction

[2] Simulations of unsaturated flow and solute transport in soil typically use closed-form functional relationships to represent water-retention characteristics and unsaturated hydraulic conductivities. The Gardner and Russo exponential model [*Gardner*, 1958; *Russo*, 1988], the Brooks and Corey piecewise-continuous model [*Brooks and Corey*, 1964], and the van Genuchten model [*van Genuchten*, 1980] represent some of the most widely used and practical hydraulic property models. Basically, based on a point-scale hydrologic process, these parameter models are valid at the point or local scale. When these models are used in larger-scale (plot, field, watershed, or regional) processes, major questions remain about how to average the spatially variable hydraulic properties over a heterogeneous soil volume [e.g., *Yeh et al.*, 1985a, 1985b, 1985c; *Russo*, 1992; *Desbarats*, 1998; *Govindaraju et al.*, 2001] and what averages of hydraulic property shape parameters to use for these models [e.g., *Yeh*, 1989; *Green et al.*, 1996]. During the past 2 decades, many research efforts have been dedicated to this issue, and the problem is usually analyzed using stochastic models [e.g., *Montoglou and Gelhar*, 1987a, 1987b, 1987c; *Ünlü et al.*, 1990a; *Ferrante and Yeh*, 1999].

[3] *Smith and Diekkruger* [1996] studied one-dimensional vertical flows through spatially heterogeneous soils. They assumed that there was no cross correlation between the soil characteristic parameters. *Green et al.* [1996] investigated methods for determining the upscaled water-retention characteristics of stratified soil formations using the van Genuchten model for soil hydraulic properties. While they compared the linear volume average (LVA) and the direct parameter average for an upscaled water retention curve of periodically layered soils, their approach remains to be justified under flow conditions. *Chen et al.* [1994a, 1994b] developed the spatially averaged Richards equation for the mean water saturation in each horizontal soil layer and the cross covariance of

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the saturated hydraulic conductivity and the water saturation in each soil layer in a heterogeneous field. Their approach, however, is restricted to the uncertainty from spatial variability in the saturated hydraulic conductivity. *Govindaraju et al.* [2001] studied field-scale infiltration over soils. They only considered the spatial variability of saturated hydraulic conductivity, which is represented by a homogeneous correlated lognormal random field. *Kim et al.* [1997] investigated the significance of soil hydraulic heterogeneity on the water budget of the unsaturated zone using the Brooks and Corey model, based on a framework of approximate analytical solutions. In their work, the geometrical scaling theory was assumed appropriate and the air entry value ($1/\alpha_{BC}$) was assumed to be deterministic.

[4] While stochastic analysis of flow through fully three-dimensional heterogeneous media [e.g., *Yeh et al.*, 1985a, 1985b, 1985c] is most appropriate, one-dimensional models has been used as approximations for various simplified problems under investigation (e.g., shallow subsurface dominated by vertical flows). For one-dimensional analyses, two physical scenarios need to be distinguished: (1) vertical layering (heterogeneity), where variations in soil properties are in the vertical directions only [e.g., *Yeh*, 1989], and (2) vertically homogeneous soil columns with variations of the soil properties in the horizontal plane only [e.g., *Rubin and Or*, 1993]. Our study focuses on the latter case, where the variability is in the horizontal plane. The domain is assumed to be composed of homogeneous soil columns without mutual interaction to simplify the analysis while keeping the focus on some of the main process of many practical field applications. For example, in meso-/regional-scale soil-vegetation-atmosphere transfer (SVAT) schemes used in hydroclimatic models, pixel dimensions may range from several hundred square meters to several hundred square kilometers, while the vertical scale of subsurface processes near the land-atmosphere boundary (the top few meters) is considerably small. In such a large horizontal scale, the areal heterogeneity of hydraulic properties dominates. Therefore it is reasonable to consider only the areal heterogeneity of soil. On the other hand, the parallel column approach will not apply to scenarios where the vadose zone is very deep and vertical heterogeneity dominates or the topography of the region varies considerably and thus mutual interactions between soil columns might be significant. Pixel-scale soil hydraulic parameters and their accuracy are critical for the success of hydroclimatic and soil hydrologic models. Our study tries to answer a major question: What will be the effective/average hydraulic properties for the entire pixel (or footprint of a remote sensor) for a typical soil textural combination in a real field condition, if the soil hydraulic properties can be estimated for each individual texture?

[5] Typically, the p-order power average or p-norm has been used in determining the parameters for the upscaled hydraulic conductivity function [e.g., *Green et al.*, 1996; *Korvin*, 1982]. It is, however, often difficult to determine p-value, which can range from $-\infty$ to $+\infty$. Furthermore, most previous studies of similar context usually either assumed that the driving force of heterogeneity was solely from saturated hydraulic conductivity or the parameters considered were statistically independent. In the study of *Yeh et al.* [1985a, 1985b, 1985c], the perturbation equation of the steady stochastic flow in unsaturated media was solved by spectral representation techniques, while *Zhang et al.* [1998] developed first-order stochastic models in second-order stationary media with both the Brooks-Corey and the Gardner-Russo constitutive relationships. While the mathematical approaches of *Yeh et al.* [1985a, 1985b, 1985c] and *Zhang et al.* [1998] were quite generic, they typically worked well in the deep and unbounded vadose zone where gravity-dominated infiltration is the main process and the mean hydraulic gradient is approximately constant. In this study, we consider the influence of parameter correlation on upscaled effective parameters without using a specific averaging scheme for the hydraulic parameters. The results apply equally well to both infiltration and evaporation scenarios in the shallow vadose zone bounded by atmospheric boundary. Specifically, we analyze the effective soil hydraulic parameters of the heterogeneous soil formation by conceptualizing the areally heterogeneous soil formation as an equivalent homogeneous medium and assuming that the equivalent homogeneous soil will approximately discharge ensemble-mean flux and produce ensemble-mean pressure head profile in the heterogeneous formation for the steady state flows. Three widely used hydraulic conductivity models were employed in the study, i.e., the Gardner model, the Brooks and Corey model, and the van Genuchten model. We examined the impact of parameter correlation, boundary condition (surface pressure head), and elevation above the water table on effective saturated hydraulic conductivity and shape parameter α. In this study, spatial correlation structure for each parameter field was assumed absent.

2. Hydraulic Property Models

[6] Soil hydraulic behavior is characterized by the soil water retention curve, which defines the water content (θ) as a function of the capillary pressure head (ψ), and the hydraulic conductivity function, which establishes relationship between the hydraulic conductivity (K) and water content or capillary pressure head. Simulations of unsaturated flow and solute transport typically use closed-form functions to represent water-retention characteristics and unsaturated hydraulic conductivities. It is assumed that the constitutive relationships apply at every point in the soil and the soil hydraulic property areal variation between sampling points can be described by the spatial variations of the parameters in the hydraulic characteristic functions [e.g., *Russo and Bouton*, 1992]. Some of the commonly used functional relationships include the Gardner-Russo model [*Gardner*, 1958; *Russo*, 1988], the Brooks-Corey model [*Brooks and Corey*, 1964], and the van Genuchten model [*van Genuchten*, 1980]. A brief review of these models is given below. Interested readers are referred to *Leij et al.* [1997] for more comprehensive review and discussion on various closed-form expressions of hydraulic properties, including the models given below.

2.1. The Gardner-Russo Model

[7] The unsaturated hydraulic conductivity (K)-capillary pressure head (ψ) and the reduced water content (S_e)-

capillary pressure (ψ) are assumed to be represented by the Gardner model [*Gardner*, 1958; *Russo*, 1988]

$$K = K_s e^{-\alpha_G \psi} \tag{1a}$$

$$S_e(\psi) = \left[e^{-0.5\alpha_G\psi}(1 + 0.5\alpha_G\psi)\right]^{2/(\ell+2)} \tag{1b}$$

where K_s is the saturated hydraulic conductivity, α_G is known as the pore-size distribution parameter, ℓ is a parameter that accounts for the dependence of the tortuosity and the correlation factors on the water content estimated, to be about 0.5 as an average for many soils [*Mualem*, 1976], $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ is the effective, dimensionless reduced water content, θ is the total volumetric water content, and θ_s and θ_r are the saturated and residual (irreducible) water contents, respectively. For notational convenience, ψ for the remainder of this paper is taken positive for unsaturated soils (i.e., it denotes suction).

2.2. The Brooks-Corey Model

[8] *Brooks and Corey* [1964] established the relationship between K and ψ using the following empirical equations from analysis of a large database:

$$S_e(\psi) = (\alpha_{BC}\psi)^{-\lambda} \qquad \text{if } \alpha_{BC}\psi > 1 \tag{2a}$$

$$S_e(\psi) = 1 \qquad \text{if } \alpha_{BC}\psi \le 1 \tag{2b}$$

$$K(\psi) = K_s(\alpha_{BC}\psi)^{-\beta} \qquad \text{if } \alpha_{BC}\psi > 1 \tag{2c}$$

$$K(\psi) = K_s \qquad \text{if } \alpha_{BC}\psi \le 1 \tag{2d}$$

where $\beta = \lambda(\ell + 2) + 2$. The λ is a parameter used by Brooks and Corey to define the relationship between water content and ψ (retention function) affecting the slope of the retention function.

[9] This model has been used successfully to describe retention data for relatively homogeneous and isotropic samples. The model may not describe the data well near saturation where the saturation is fixed and a discontinuity occurs at $\psi = 1/\alpha_{BC}$.

2.3. The van Genuchten Model

[10] *Van Genuchten* [1980] identified an S-shaped function that fits measured water-retention characteristics of many types of soil very well. The function was also combined with Mualem's hydraulic conductivity function [*Mualem*, 1976] to predict unsaturated hydraulic conductivity. Subsequently, the van Genuchten function has become one of the most widely used curves for characterizing soil hydraulic properties. The van Genuchten equation of soil water retention curve can be expressed as follows:

$$S_e(\psi) = \frac{1}{\left[1 + (\alpha_{vG}\psi)^n\right]^m} \tag{3}$$

where α_{vG}, n, and m are parameters that determine the shape of the soil water retention curve. Assuming $m = 1 - 1/n$, *van Genuchten* [1980] combined above the soil water retention function with the theoretical pore-size distribution model of *Mualem* [1976] and obtained the following relationships for the hydraulic conductivity in terms of the reduced water content or the capillary pressure head:

$$K(S_e) = K_s S_e^{\ell}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{4}$$

$$K(\psi) = \frac{K_s\{1 - (\alpha_{vG}\psi)^{mn}[1 + (\alpha_{vG}\psi)^n]^{-m}\}^2}{[1 + (\alpha_{vG}\psi)^n]^{m\ell}} \tag{5}$$

[11] There are then four parameters for the Gardner-Russo model to describe the soil hydraulic characteristics of each sample: K_s, α_G, θ_s, and θ_r; five parameters for the Brooks-Corey model: K_s, α_{BC}, λ, θ_s, and θ_r; and five parameters for the van Genuchten model: K_s, α_{vG}, n, θ_s, and θ_r. A study by *Hills et al.* [1992] showed that the water-retention characteristics could be adequately modeled using either a variable parameter α_{vG} with a constant van Genuchten parameter n, or a variable n with a constant α_{vG}, with better results when α_{vG} was variable. Because the van Genuchten n is closely related to the Brooks-Corey λ, we shall treat the Brooks-Corey λ as a deterministic constant in our subsequent analysis to reduce the number of parameters needed to describe the spatial distribution of the hydraulic properties. In the light of their results, we will consider only the spatial variability introduced by the spatial variation of the parameter K_s and α for both the Gardner-Russo and the Brooks-Corey models. In this study, we adopt a typical value of $\lambda = 0.4$, $\overline{K_s} = 1.0 \times 10^{-5}$ (cm/s), $CV(K_s) = 0.4$, and $\overline{\alpha} = 0.0225$(1/cm), $CV(\alpha) = 0.4$ [e.g., *Ünlü et al.*, 1990b]. Other values can also be used [e.g., *Philip*, 1969; *Braester*, 1973; *El-Kadi*, 1992; *Fayer and Gee*, 1992; *Rawls et al.*, 1992; *Mohanty et al.*, 1994].

[12] There are many studies about the correlation between characteristic parameters for the hydraulic properties of soil in the literature [e.g., *Yeh et al.*, 1985a, 1985b, 1985c; *Montoglou and Gelhar*, 1987a, 1987b, 1987c; *Russo and Bouton*, 1992]. Some of their results show no consensus about parameter correlation. For example, after analyzing soil samples gathered on the Krummbach and Eisenbach catchments in northern Germany and from a field experiment near Las Cruces, New Mexico, *Smith and Diekkruger* [1996] concluded that no significant correlation was observed among any of the characteristic parameters and suggested that most random variation in soil characteristic parameters could be treated as independent. However, in another study, *Wang and Narasimhan* [1992] indicated that K_s was proportional to α^2. In this research, we will study both correlated and independent cases and the significance of their correlation on the ensemble behavior of soil dynamic characteristic of unsaturated flow.

3. Steady State Vertical Flow

[13] General equations relating pressure head and elevation above the water table for steady state vertical flows can

be expressed as [e.g., *Zaslavsky*, 1964; *Warrick and Yeh*, 1990]

$$z = \int_0^{\psi} \frac{K(\psi)d\psi}{K(\psi) + q} \tag{6}$$

where z is the vertical distance above the water table with the water table location being at $z = 0$, and q is the steady state evaporation (positive) or infiltration (negative) rate. Its dimensionless form can be expressed as

$$\alpha z = \int_0^{\alpha\psi} \frac{K_r(x)dx}{K_r(x) + q'} \tag{7}$$

where the dimensionless hydraulic conductivity $K_r = K/K_s$, the dimensionless pressure head $x = \alpha\psi$, and the dimensionless flux rate $q' = q/K_s$. When the pressure head at the surface, ψ_L, is known, the dimensionless state steady flux q/K_s can be found out from the following equation:

$$\alpha L = \int_0^{\alpha\psi_L} \frac{K_r(x)dx}{K_r(x) + q'} \tag{8}$$

where L is the elevation of the ground surface above the water table. From equation (8), it can be seen that the dimensionless steady state flux rate q' itself is not related to the saturated hydraulic conductivity K_s. In other words, the flux rate q is a linear function of K_s. In turn, we can infer from equation (7) that the capillary pressure head ψ is not related to the saturated hydraulic conductivity K_s if the dimensionless flux q' is specified.

[14] When the Gardner hydraulic conductivity model is used, the capillary pressure profile (ψ) and the dimensionless flux rate ($q' = q/K_s$) can be analytically expressed as

$$\psi = \ln\left(\frac{e^{\alpha_G L} - 1}{e^{-\alpha_G z} + e^{-\alpha_G \psi_L} - e^{-\alpha_G L} - e^{-\alpha_G (z+\psi_L)}}\right)^{1/\alpha_G} - L \tag{9}$$

$$q' = \frac{1 - e^{-\alpha_G(\psi_L - L)}}{e^{\alpha_G L} - 1} \tag{10}$$

[15] For the Brooks-Corey model, analytical solutions are also possible, but the evaporation and infiltration cases need to be analyzed separately. The capillary pressure head (ψ) can be related to the elevation above the water table (z) as the following series relationship for steady state evaporation [*Warrick*, 1988]:

$$\alpha_{BC} z = \frac{1}{\beta}(q')^{-1/\beta} \times B_U\left(\frac{1}{\beta}, 1 - \frac{1}{\beta}\right) - \frac{\beta q'}{(1+\beta)(1+q')^2} \times {}_2F_1\left(1, 2; 2 + \frac{1}{\beta}; \frac{q'}{1+q'}\right) \tag{11}$$

where B_u is the incomplete Beta function with $u = q'\alpha_{BC}^{\beta}\psi^{\beta}/(1 + q'\alpha_{BC}^{\beta}\psi^{\beta})$ and ${}_2F_1$ is the Gaussian hypergeometric function. The relationship between the dimensionless evaporation rate q' and the surface pressure head ψ_L can be established iteratively by the following equation:

$$\alpha_{BC} L = \frac{1}{\beta}(q')^{-1/\beta} \times B_{u_L}\left(\frac{1}{\beta}, 1 - \frac{1}{\beta}\right) - \frac{\beta q'}{(1+\beta)(1+q')^2} \times {}_2F_1\left(1, 2; 2 + \frac{1}{\beta}; \frac{q'}{1+q'}\right) \tag{12}$$

where $u_L = q'\alpha_{BC}^{\beta}\psi_L^{\beta}/(1 + q'\alpha_{BC}^{\beta}\psi_L^{\beta})$, while for steady state infiltration, the relationship can be established as follows [*Zhu and Mohanty*, 2002] with $p' = -q'$:

$$\alpha_{BC} z = \alpha_{BC}\psi \times {}_2F_1\left(\frac{1}{\beta}, 1; 1 + \frac{1}{\beta}; p'\alpha_{BC}^{\beta}\psi^{\beta}\right) + \frac{\beta p'}{(1-p')(1+\beta)} \times {}_2F_1\left(1, \frac{1}{\beta}; 2 + \frac{1}{\beta}; p'\right) \tag{13}$$

The relationship between the dimensionless infiltration rate p' and the surface pressure head ψ_L can be established iteratively by the following equation:

$$\alpha_{BC} L = \alpha_{BC}\psi \times {}_2F_1\left(\frac{1}{\beta}, 1; 1 + \frac{1}{\beta}; p'\alpha_{BC}^{\beta}\psi_L^{\beta}\right) + \frac{\beta p'}{(1-p')(1+\beta)} \times {}_2F_1\left(1, \frac{1}{\beta}; 2 + \frac{1}{\beta}; p'\right) \tag{14}$$

[16] These analytical solutions will be required to calculate the derivative terms in deriving effective parameters in the next section. For the van Genuchten model, the integrations in equations (7) and (8) were carried out numerically.

4. Effective Hydraulic Parameters

[17] The effective soil hydraulic parameters of the heterogeneous soil formation are derived by conceptualizing the soil formation as an equivalent homogeneous medium. It is assumed that the equivalent homogeneous soil will approximately discharge the same ensemble-mean flux [e.g., *Milly and Eagleson*, 1987; *Kim et al.*, 1997] and produce the same ensemble-mean pressure head profile in the formation. Since ψ is only related to α based on the previous discussions for the three functions, approximating ψ by the first two terms of a Taylor expansion around the mean parameter $\overline{\alpha}$ and taking the expected value of the resulting equation lead to

$$\overline{\psi(\alpha)} = \psi(\overline{\alpha}) + \frac{1}{2}\frac{\partial^2\psi}{\partial\alpha^2}(\overline{\alpha})\sigma_\alpha^2 \tag{15}$$

Since q is a linear function of K_s, a similar operation in terms of q leads to

$$\overline{q(K_s, \alpha)} = \overline{K_s} q'(\overline{\alpha}) + \frac{\overline{K_s}}{2}\frac{\partial^2 q'}{\partial\alpha^2}(\overline{\alpha})\sigma_\alpha^2 + \frac{\partial q'}{\partial\alpha}(\overline{\alpha})\rho\sigma_{K_s}\sigma_\alpha \tag{16}$$

In equations (15) and (16), σ_{K_s} and σ_α are the standard deviations of K_s and α, respectively, and ρ is the correlation coefficient of K_s and α, defined as

$$\rho = \frac{\mathrm{cov}(K_s, \alpha)}{\sigma_{K_s}\sigma_\alpha} = \frac{\overline{(K_s - \overline{K_s})(\alpha - \overline{\alpha})}}{\sigma_{K_s}\sigma_\alpha}.$$

Approximation of $\psi(\alpha)$ and $q(K_s, \alpha)$ to the first order of a Taylor expansion around the mean parameters yields

$$\psi(\alpha_{\text{eff}}) = \psi(\overline{\alpha}) + \frac{\partial\psi}{\partial\alpha}(\overline{\alpha})(\alpha_{\text{eff}} - \overline{\alpha}) \tag{17}$$

$$q\left(K_{s\text{eff}}, \alpha_{eff}\right) = \overline{K_s}q'(\overline{\alpha}) + q'(\overline{\alpha})\left(K_{s\text{eff}} - \overline{K_s}\right) + \overline{K_s}\frac{\partial q'}{\partial\alpha}(\overline{\alpha})(\alpha_{\text{eff}} - \overline{\alpha}) \tag{18}$$

In using equations (17) and (18), we made two assumptions. First, it is a Taylor series expansion with higher-order terms truncated. Second, the derivative terms in the expansions are also evaluated approximately assuming that the derivative terms in the hypothetic layered formation are closed to those in the homogeneous formation. Both approximations require the variance of the random parameters to be small. Following *Milly and Eagleson* [1987] and *Kim et al.* [1997], we set $\psi(\alpha_{\text{eff}}) = \overline{\psi(\alpha)}$ and $q(K_{s\text{eff}}, \alpha_{eff}) = \overline{q(K_s, \alpha)}$ and use equations (15) through (18), which yield,

$$\alpha_{eff} = \overline{\alpha} + \frac{1}{2}\left(\frac{\partial^2\psi}{\partial\alpha^2}(\overline{\alpha}) \Big/ \frac{\partial\psi}{\partial\alpha}(\overline{\alpha})\right)\sigma_\alpha^2 \tag{19}$$

$$K_{s\text{eff}} = \overline{K_s} + \frac{\overline{K_s}}{2q'(\overline{\alpha})}\left\{\frac{\partial^2 q'}{\partial\alpha^2}(\overline{\alpha}) - \left[\frac{\partial q'}{\partial\alpha}(\overline{\alpha}) / \frac{\partial\psi}{\partial\alpha}(\overline{\alpha})\right] \times \frac{\partial^2\psi}{\partial\alpha}(\overline{\alpha})\right\}\sigma_\alpha^2 + \left[\frac{\partial q'}{\partial\alpha}(\overline{\alpha}) \Big/ q'(\overline{\alpha})\right]\rho\sigma_{K_s}\sigma_\alpha \tag{20}$$

[18] Since predicting the ensemble-mean flux rate is usually a main concern in most practical soil-vegetation-atmospheric transfer (SVAT) models, we can use an alternative and simpler approach to derive effective hydraulic parameters by assuming that the equivalent homogeneous medium will discharge the same amount of flux as the heterogeneous one. Because of the nature of areally heterogeneous vertical flow, in this study we consider the arithmetic average (mean) for the saturated hydraulic conductivity as an appropriate effective parameter, i. e., $K_{s\text{eff}} = \overline{K_s}$, and determine the other effective parameter, α_{eff}, by only matching the flux rate q. In this way, by equaling $q(\overline{K_s}, \alpha_{\text{eff}})$ to $\overline{q(\overline{K_s}, \alpha)}$ we have the following simple expression for effective parameter α_{eff}:

$$a_{\text{eff}} = \overline{\alpha} + \frac{1}{2}\left[\frac{\partial^2 q'}{\partial\alpha^2}(\overline{\alpha}) \Big/ \frac{\partial q'}{\partial\alpha}(\overline{\alpha})\right]\sigma_\alpha^2 \tag{21}$$

[19] In this sense, the equivalent homogeneous formation so defined would only deliver approximately ensemble-mean flux, while there would be no guarantee in term of ensemble-average pressure profiles in the formation.

5. Higher-Order Approximation and Comparison With Monte Carlo Simulations and Previous Studies

[20] Using a procedure similar to the first-order approximation but truncating the Taylor expansion around the mean parameters to the second order yields (note $\psi = \psi(\alpha)$ and $q = K_s q'(\alpha)$)

$$\psi(\alpha_{\text{eff}}) = \psi(\overline{\alpha}) + \frac{d\psi}{d\alpha}(\overline{\alpha})(\alpha_{\text{eff}} - \overline{\alpha}) + \frac{1}{2}\frac{d^2\psi}{d\alpha^2}(\overline{\alpha})(\alpha_{\text{eff}} - \overline{\alpha})^2 \tag{22}$$

$$q(K_{s\text{eff}}, \alpha_{\text{eff}}) = \overline{K_s}q'(\overline{\alpha}) + q'(\overline{\alpha})\left(K_{s\text{eff}} - \overline{K_s}\right) + \overline{K_s}\frac{dq'}{d\alpha}(\overline{\alpha})(\alpha_{\text{eff}} - \overline{\alpha}) + \frac{K_s}{2}\frac{d^2q'}{d\alpha^2}(\alpha_{\text{eff}} - \overline{\alpha})^2 + \frac{dq'}{d\alpha}\left(K_{s\text{eff}} - \overline{K_s}\right)(\alpha_{\text{eff}} - \overline{\alpha}) \tag{23}$$

[21] Setting $\psi(\alpha_{\text{eff}}) = \overline{\psi(\alpha)}$ and $q(K_{s\text{eff}}, \alpha_{eff}) = \overline{q(K_s, \alpha)}$ leads to

$$\alpha_{eff} = \overline{\alpha} - \left\{\frac{d\psi}{d\alpha} + \left[\left(\frac{d\psi}{d\alpha}\right)^2 + \left(\frac{d^2\psi}{d\alpha^2}\right)^2\sigma_\alpha^2\right]^{1/2}\right\} \Big/ \frac{d^2\psi}{d\alpha^2} \quad \text{if } \frac{d\psi}{d\alpha} < 0. \tag{24}$$

$$\alpha_{\text{eff}} = \overline{\alpha} - \left\{\frac{d\psi}{d\alpha} - \left[\left(\frac{d\psi}{d\alpha}\right)^2 + \left(\frac{d^2\psi}{d\alpha^2}\right)^2\sigma_\alpha^2\right]^{1/2}\right\} \Big/ \frac{d^2\psi}{d\alpha^2} \quad \text{if } \frac{d\psi}{d\alpha} > 0. \tag{25}$$

$$K_{s\text{eff}} = \overline{K_s} + \frac{\frac{\overline{K_s}}{2}\frac{d^2q'}{d\alpha^2}\left[\sigma_\alpha^2 - (\alpha_{\text{eff}} - \overline{\alpha})^2\right] + \frac{dq'}{d\alpha}\rho\sigma_{K_s}\sigma_\alpha - \overline{K_s}\frac{dq'}{d\alpha}(\alpha_{\text{eff}} - \overline{\alpha})}{q' + \frac{dq'}{d\alpha}(\alpha_{\text{eff}} - \overline{\alpha})} \tag{26}$$

[22] We have also conducted Monte Carlo simulations of 10,000 realizations and compared the results with the results of both first- and second-order approximations in order to verify our findings. Both K_s and α are assumed to obey the lognormal distribution. The cross-correlated random fields of the parameters K_s and α were generated using the spectral method proposed by *Robin et al.* [1993]. Random fields were produced with the power spectral density function, which was based on exponentially decaying covariance functions. The coherency spectrum, given by equation (27), is an indicator of parameter correlation,

$$R(\mathbf{f}) = \frac{\phi_{12}(\mathbf{f})}{\left[\phi_{11}(\mathbf{f})\phi_{22}(\mathbf{f})\right]^{1/2}} \tag{27}$$

where $\phi_{11}(\mathbf{f})$, $\phi_{22}(\mathbf{f})$ are the power spectra of random fields $\log(K_s)$ and $\log(\alpha)$, respectively, and $\phi_{12}(\mathbf{f})$ is the cross spectrum between $\log(K_s)$ and $\log(\alpha)$. Having $|R|^2 = 1$ indicates perfect linear correlation between the random fields. The random fields are assumed to be isotropic,

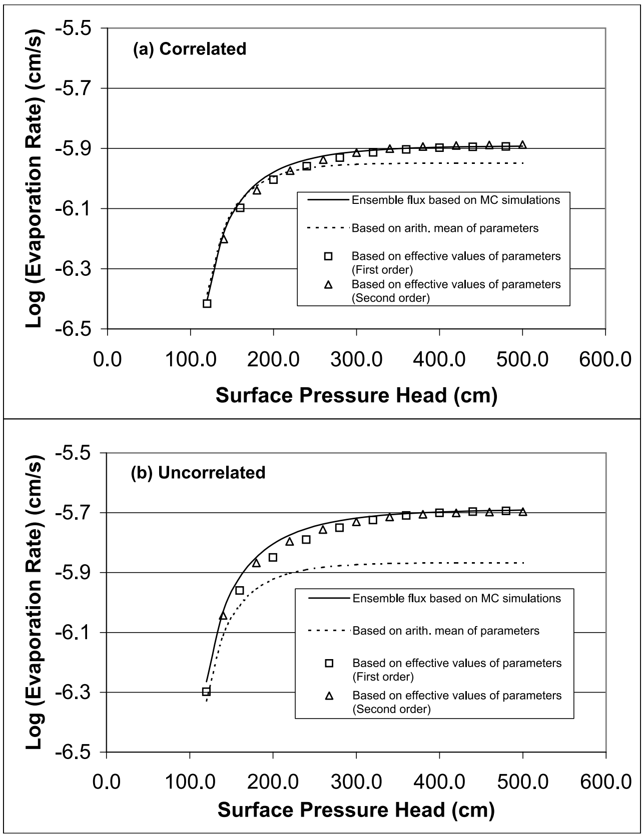

Figure 1. Comparison of evaporation rate versus surface pressure head: (a) correlated, and (b) uncorrelated.

with the domain length being equal to 10 correlation lengths, which in turn corresponds to 50 grid lengths. Random fields of 10,000 (100 × 100) values were generated for log(K_s) and log(α) field. After generating the random fields K_s and α, the pressure profile and the flux are calculated using the analytical solutions (9) and (10). Then the statistics of the dependent variables q and ψ can be computed over the entire domain. Figures 1 and 2 show the results of evaporation rate versus surface pressure head and pressure profiles versus elevation above the water table, respectively. We have only shown the results for evaporation using the Gardner model. The results for the other two models (i.e., Brooks and Corey and van Genuchten) demonstrate a similar trend. For comparison, we have also plotted the results based on arithmetic means of the hydraulic parameters (i.e., K_s and α). The solid lines represent the ensemble mean based on Monte Carlo simulations with the random fields of K_s and α generated by the direct Fourier method developed by *Robin et al.* [1993]. The squares and triangles represent the results based on the effective parameters of first- and second-order approximation calculated from equations (19) and (20) or (24) and (25), respectively. Since the effective parameters are mean-gradient-dependent (i.e., they vary across depth), these results are calculated as if the soil formation were layered with hydraulic parameters varying with depth. The improvement of using effective parameters, which are related to the boundary pressure condition and the vertical location, over using constant arithmetic means for the hydraulic parameters is apparent from these figures. However, the efficacy of the effective parameters in simulating the transition of evaporation rate curve from rapid change to approaching an asymptotic value needs to be improved further. The results demonstrated that both the first-order and the second-order approximations predict the ensemble evaporation rates and pressure profiles reasonably well with the results based on the second-order approximation performing slightly better. In light of these comparisons, we use the results from the first-order approximation for the discussion below.

[23] Next we will compare some of the results in this study (denoted by ZM) with those of *Yeh et al.* [1985b], *Yeh* [1989] (denoted by Y), and *Rubin and Or* [1993] (denoted by RO). For the sake of brevity, we compare some results for the scenario where only the parameter α is a heterogeneous field. This is partly because we deal with K_s while *Yeh et al.* [1985b] and *Rubin and Or* [1993] dealt with lnK_s. For infiltration, both the mean pressure head and the head variance approach an asymptotic value at a location far away from the water table, which represents a stationary limit for the pressure head profile. At the water table both of these values are zero. We shall compare these asymptotic values to show how our results are different from the results of *Rubin and Or* [1993], *Yeh et al.* [1985b], and *Yeh* [1989]. We want to emphasize that the comparison was made on a simple scenario (i.e., a special case for each of the three

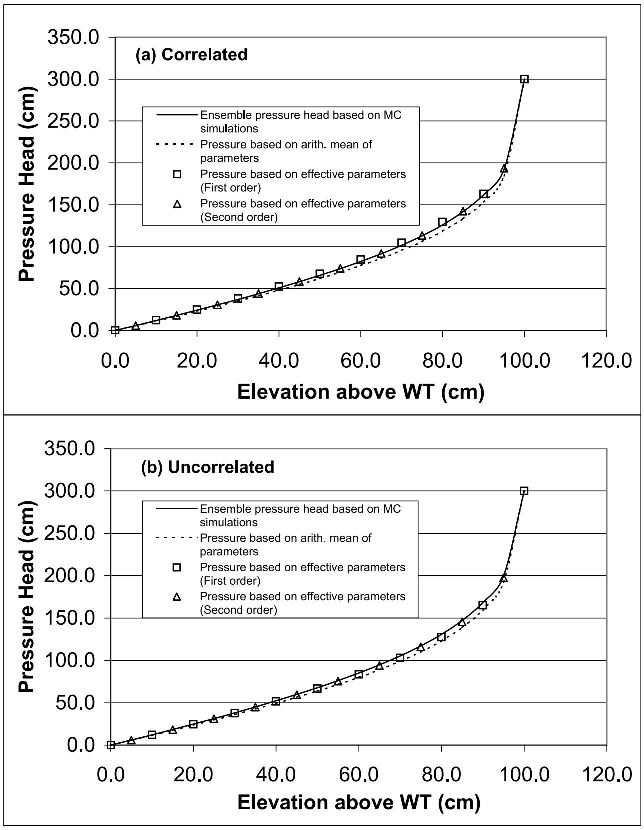

Figure 2. Comparison of pressure profiles versus elevation above the water table: (a) correlated, and (b) uncorrelated.

approaches, *Yeh* [1989], *Rubin and Or* [1993], and this study). In our study, the horizontal stationarity is implicitly assumed, meaning that the mean and variance are constant in the horizontal directions. Vertically, the hydraulic parameters were assumed homogeneous. *Yeh* [1989] assumes vertical variability of hydraulic parameters and unit mean gradient; his model can be compared with our study by taking very large values of the vertical integral scales of the random hydraulic parameters. The work of *Rubin and Or* [1993] also considered the effect of root water uptake, which is taken to be zero when comparing with our study.

[24] For this special case, the vertical pressure profile by using the Gardner hydraulic function can be easily expressed as

$$\psi(z) = -\ln[e^{-\alpha z} - q'(1 - e^{-\alpha z})]/\alpha \quad (28)$$

It can be seen that ψ and σ_ψ^2 approach an asymptotic limit as z (the distance from the water table) increases. At a location far away from the water table (i.e., unit gradient),

$$\psi = -\ln(-q')/\alpha \quad (29)$$

[25] For a lognormally distributed variable α, its probability distribution function is

$$f(\alpha) = \begin{cases} \frac{1}{\sqrt{2\pi}\xi} \exp\left[-\frac{(\ln\alpha - \mu)^2}{2\xi^2}\right] & \alpha > 0 \\ 0 & \alpha \le 0 \end{cases} \quad (30)$$

with the parameters μ and ξ being determined from the mean of α, $\overline{\alpha}$, and the coefficient of variations of α, c_α, as follows:

$$\xi = \sqrt{\ln(c_a^2 + 1)} \quad (31)$$

$$\mu = \ln\left(\frac{\overline{\alpha}}{\sqrt{c_\alpha^2 + 1}}\right) \quad (32)$$

Then the mean value and the variance of ψ at a location far away from the water table can be calculated as

$$\overline{\psi} = -\ln(q')\int_0^\infty \frac{f(\alpha)d\alpha}{\alpha} = -\frac{\ln(-q')}{\overline{\alpha}}\left(1 + c_\alpha^2\right) \quad (33)$$

$$\sigma_\psi^2 = \overline{\psi^2} - (\overline{\psi})^2 = \left[\frac{\ln(-q')}{\overline{\alpha}^2}\right]^2 \left(1 + c_\alpha^2\right)^2 c_\alpha^2 \quad (34)$$

The variance of pressure head from this study can be expressed as

$$\sigma_\psi^2 = \overline{[\psi(\alpha) - \psi(\alpha_{\mathrm{eff}})]^2} = \left(\frac{\partial\psi}{\partial\alpha}\right)^2 \overline{(\alpha - \alpha_{\mathrm{eff}})^2} \quad (35)$$

[26] Using the mean pressure head profile of equation (17) and the variance of (35) and evaluating at locations far away from the water table, we have

$$\overline{\psi}_{ZM} = \psi(\alpha_{\mathrm{eff}}) = -\frac{\ln(-q')}{\overline{\alpha}}\left(1 + c_\alpha^2\right) \quad (36)$$

$$\sigma_{\psi ZM}^2 = \left[\frac{\ln(-q')}{\overline{\alpha}}\right]^2 c_\alpha^2\left(1 + c_\alpha^2\right) \quad (37)$$

It can be seen that the results of this study predict exact mean pressure value (33) and underpredict the head variance (34) by a factor of $(1 + c_\alpha^2)$.

[27] The results of *Rubin and Or* [1993] for the mean and the variance of the pressure head are as (simplified from their equations (17) and (19) using our notations)

$$\overline{\psi}_{RO} = -\frac{\ln(-q')}{\overline{\alpha}} \quad (38)$$

$$\sigma_{\psi RO}^2 = \left[\frac{\ln(-q')}{\overline{\alpha}}\right]^2 c_\alpha^2 \quad (39)$$

The results of *Rubin and Or* [1993] suggested that the mean pressure head is the pressure head using the mean value of α.

[28] The head variance based on *Yeh et al.* [1985a, 1985b] can be expressed as

$$\sigma_{\psi Y}^2 = \overline{\psi}_Y^2 \sigma_\alpha^2 / \overline{\alpha}^2 \quad (40)$$

[29] The effective value for α from *Yeh* [1989] for this special case can be simplified by taking a very large value for the correlation scale in their results [e.g., *Yeh*, 1989, equation (16)],

$$\alpha_{\mathrm{eff(Y)}} = \overline{\alpha} - \frac{\sigma_\alpha^2}{\overline{\alpha}} = \overline{\alpha}\left(1 - c_\alpha^2\right) \quad (41)$$

[30] The mean pressure head and the variance can then be obtained by using $\alpha_{\mathrm{eff}(Y)}$ into pressure head and variance expressions,

$$\overline{\psi}_Y = -\frac{\ln(-q')}{\overline{\alpha}\left(1 - c_\alpha^2\right)} \quad (42)$$

$$\sigma_{\psi Y}^2 = \frac{[\ln(-q')]^2}{\overline{\alpha}^2} \frac{c_\alpha^2}{\left(1 - c_\alpha^2\right)^2} \quad (43)$$

[31] Figure 3 shows a comparison of mean and variance of pressure head for the three methods (ZM, RO, Y) using two selected values for c_α, 0.25 (Figure 3a) and 0.5 (Figure 3b), respectively. For a smaller coefficient of variation for α (c_α = 0.25), all three approaches predict

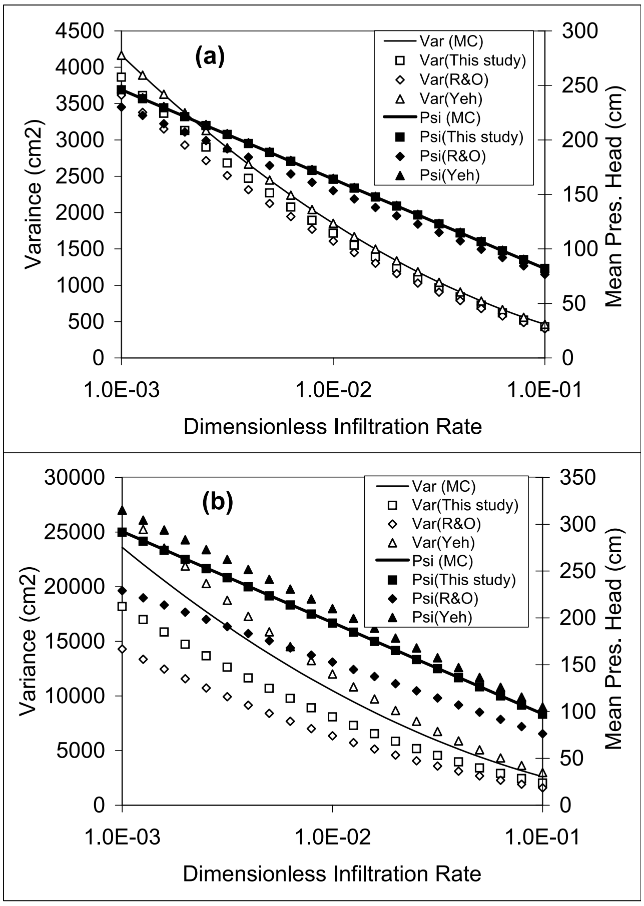

Figure 3. Comparison of mean pressure and variance between this study and those of *Yeh et al.* [1985b], *Yeh* [1989], and *Rubin and Or* [1993]: (a) $c_\alpha = 0.25$, and (b) $c_\alpha = 0.5$.

the mean and variance of the pressure reasonably well. The results of *Rubin and Or* [1993] underestimate both mean and variance of the pressure head, suggesting the arithmetic mean is too large as an effective parameter. The results based on *Yeh et al.* [1985b] and *Yeh* [1989] overestimate both mean and variance of the pressure head. However, the variance based on *Yeh* [1989] is closest to the theoretical results. It can be seen that the results of this study predict the mean pressure head exactly and underestimate the pressure variance.

[32] As a caveat, we want to point out that a general matching of mean pressure head and mean flux does not imply an equally good comparison of other details for a given scenario. The effective parameter idea developed in this study means to predict mean flux and pressure head in heterogeneous soils for steady state flows.

6. Results and Discussion

[33] Figure 4 shows effective saturated hydraulic conductivity K_{seff} as functions of surface pressure head and distance above water table when K_s and α are uncorrelated ($\rho = 0$) for all three hydraulic conductivity models considered with a water table depth of 100 cm. At the dividing line between the evaporation and infiltration when the surface pressure head is equal to the elevation of ground surface above the water table, a situation corresponding to static condition where no moisture flow is possible; the effective parameters are therefore not defined. However, the effective parameter patterns are continuous when going from evaporation to infiltration (i.e., the surface pressure head varying from very large values to zero). The continuity of effective parameters can be seen by observing how the patterns continue from the right edge of evaporation effective parameter contours to the left edge of the infiltration contours. Since water table is at 100 cm, the surface pressure head of 100 cm is the no-flow boundary which distinguishes between evaporation and infiltration. When the pressure head at the ground surface is smaller than the elevation, it depicts a situation of downward flow (infiltration), while the surface suction head larger than the elevation denotes upward flow (evaporation). It should be noted that the mean value of K_s used is $\overline{K_s} = 1.0 \times 10^{-5}$(cm/s). The other input values used for the analysis are $c_{Ks} = 0.4$, and $\overline{\alpha} = 0.0225$(1/cm), $c_\alpha = 0.4$. Therefore we can infer from Figure 4 that the effective saturated hydraulic conductivity is typically smaller than the mean value for the uncorrelated scenario. When the surface pressure head becomes large, the effective parameters approach an asymptotic value. In other words, the effective parameters typically vary only along the elevation when the suction head at the surface is large. The whole areally heterogeneous system would behave similar to a stratified medium with the effective parameters getting larger as it approaches the ground surface.

[34] It is interesting to note that the effective saturated hydraulic conductivity shows some unusual pattern as shown in Figure 4b. The way the Brooks and Corey model defines the water retention curve attributes to this unusual behavior. For the Brooks and Corey model, the hydraulic conductivity curve is piecewise-continuous and has a nonsmooth transition at pressure head $1/\alpha_{BC}$. Physically, it means that the definition of parameter α_{BC} is not continuous in terms of the pressure head regime. When the pressure head is smaller than the threshold value, the α_{BC} parameter is not defined. Mathematically, the slope (derivative) of the Brooks and Corey hydraulic conductivity curve at $1/\alpha_{BC}$ is not defined. Therefore we may expect some problems in the region where the pressure head is in the vicinity of $1/\alpha_{BC}$ in defining the effective parameters. Because in this study, a mean value of $\overline{\alpha} = 0.0225$(1/cm) has been used for α, which indicates a nonsmooth transition of hydraulic conductivity at a pressure head value of $1/\overline{\alpha} = 44$(cm). For the evaporation case, the pressure profile near the water table is almost equal to the elevation above the water table, as the hydraulic head is nearly zero. That explains the sudden changes experienced by the effective parameters in the vicinity of $z \approx 40$(cm) for the specific parameter input used in this study. For the infiltration case where both the pressure in the field and the elevation above the water table can fall in the vicinity of $1/\alpha_{BC}$, the effective parameters in the entire region are virtually undefined when the Brooks and Corey model is used. Therefore the results for the Brooks and Corey model are not shown for the infiltration zone, which is labeled "zone of model limitation" in the plot (Figure 4b).

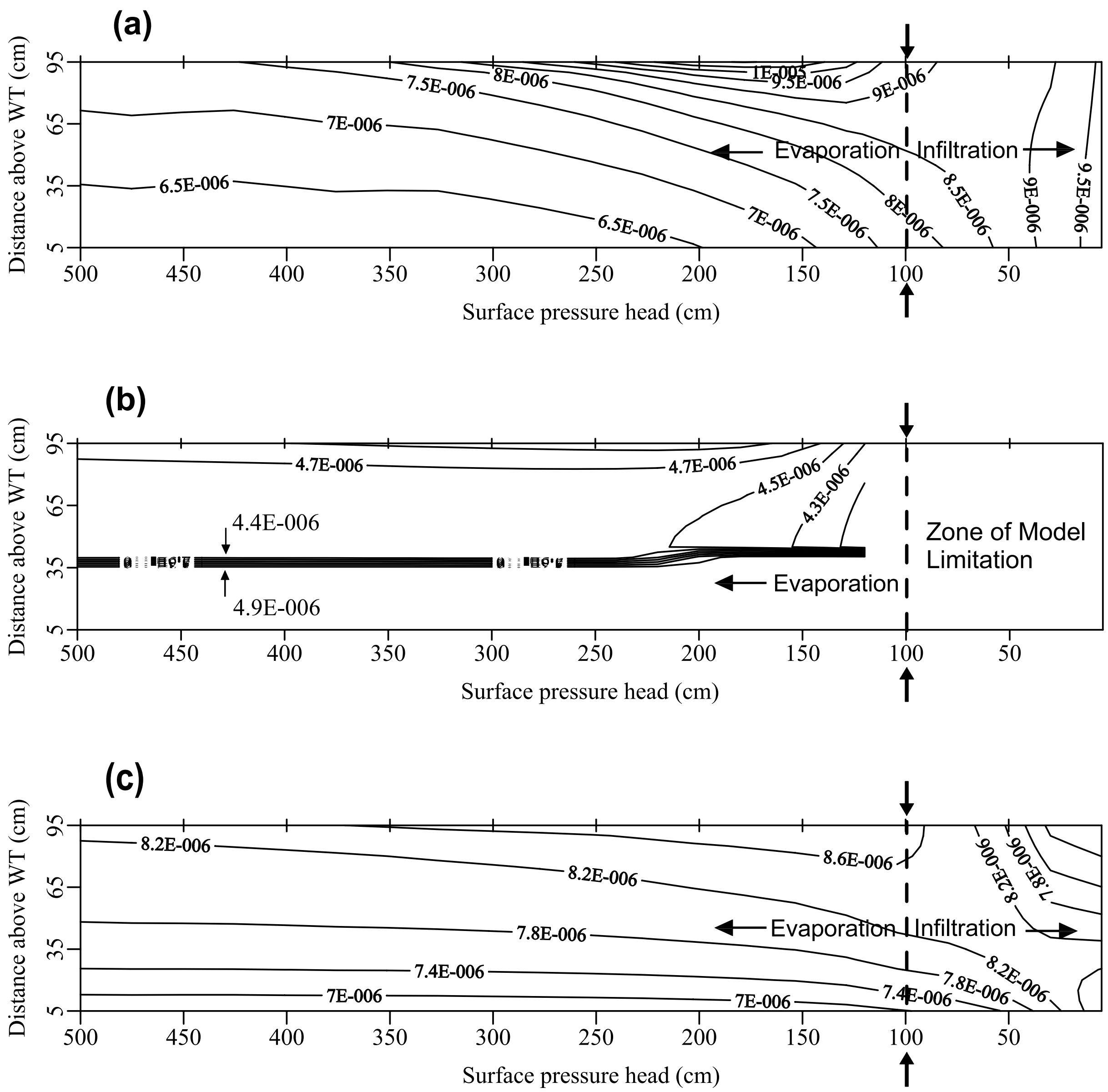

Figure 4. Effective saturated hydraulic conductivity K_{seff} as functions of surface pressure head and distance above water table when K_s and α are uncorrelated: (a) Gardner model, (b) Brooks and Corey model, and (c) van Genuchten model.

[35] Figure 5 shows effective saturated hydraulic conductivity K_{seff} as functions of surface pressure head and distance above water table when K_s and α are fully correlated ($\rho = 1$) for all three hydraulic conductivity models considered. The variation of effective saturated hydraulic conductivity follows the similar general pattern with the uncorrelated case, but the correlation between K_s and α increases the effective saturated hydraulic conductivity. Because of correlation with α, the effective saturated hydraulic conductivity is usually larger than the mean value of $\overline{K_s} = 1.0 \times 10^{-5}(\mathrm{cm/s})$ (cm/s), which can been seen in Figures 5a and 5c for the Gardner and van Genuchten functions, respectively.

[36] Figure 6 demonstrates effective α parameter (α_{eff}) as a function of surface pressure head and distance above water table for all three hydraulic conductivity models considered. Effective parameter α_{eff} is not affected by correlation between K_s and α, as shown in equation (19). Therefore the overall effect of parameter correlation makes the soil behave more like sand, i.e., a larger effective saturated hydraulic conductivity and an unaffected effective α. In general, notice that the effective α is usually smaller than the mean value of $\overline{\alpha} = 0.0225(1/\mathrm{cm})$. In other words, if α is assumed to be lognormally distributed, its geometric mean (smaller than the arithmetic mean) is probably a better indicator of effective value. From Figure 6, it can also be seen that the largest effective α values are observed near the ground surface and around the static condition. It is interesting to note that for infiltration scenario the effective α parameter shows approximately diagonal symmetry in the surface pressure head and elevation plots, especially for the Gardner-Russo model

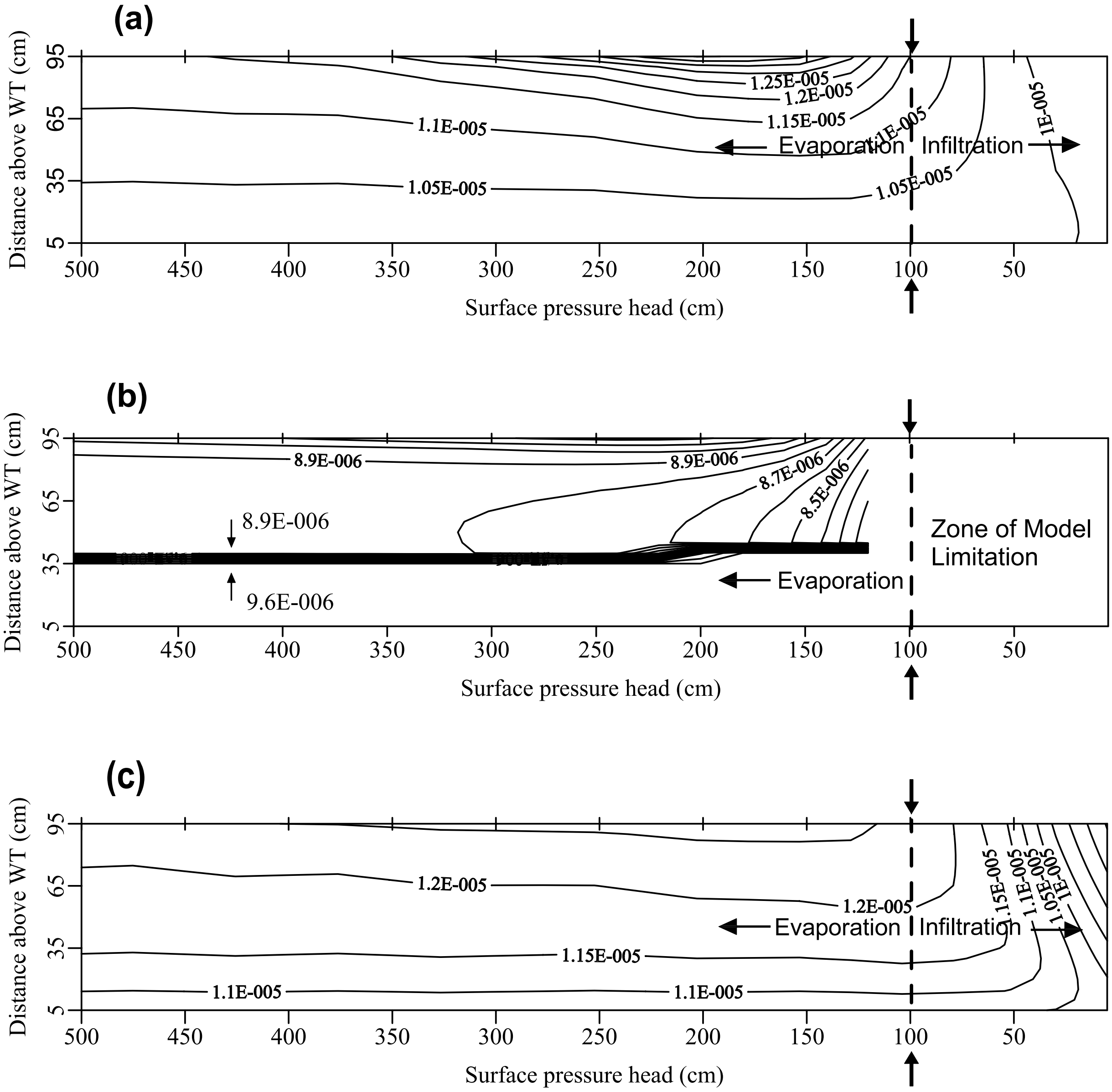

Figure 5. Effective saturated hydraulic conductivity $K_{s\mathrm{eff}}$ as functions of surface pressure head and distance above water table when K_s and α are fully correlated: (a) Gardner model, (b) Brooks and Corey model, and (c) van Genuchten model.

(Figure 6a). It means that the surface pressure head and the elevation would have similar effects on the effective α parameter.

[37] Figure 7 shows α_{eff} as a function of surface pressure head when $K_{s\mathrm{eff}}$ is assumed to take an average value of K_s, as determined from equation (21). The effective α decreases asymptotically as the flow scenario shifts from infiltration to evaporation, i.e., surface pressure head going from zero to infinity. Similar to the previous scenario of fitting both pressure head profile and flux rate, the effective α for the Gardner-Russo model is larger than for the other two models. In the event of only fitting flux rate, the effective α is a function of only surface pressure since the flux rate is uniform across the entire soil profile. The effective α is typically smaller than the mean value except for the Brooks and Corey model when the surface pressure head is near $1/\overline{\alpha}$ where the effective α approaches infinity.

[38] Our study suggested that we are still able to use the same form of hydraulic conductivity function for the local scale as well as for large-scale modeling, while using the effective parameters which are variable according to the boundary conditions and are also mean-gradient-dependent. The approach applies equally well to both infiltration and evaporation scenarios. With the mean-gradient-dependent effective parameters, the approach in this study allows the boundary conditions to be accounted for and it can be used to address the land surface and atmosphere interaction where the boundary between them must be considered.

7. Concluding Remarks

[39] The following main conclusions were drawn based on the results of our study.

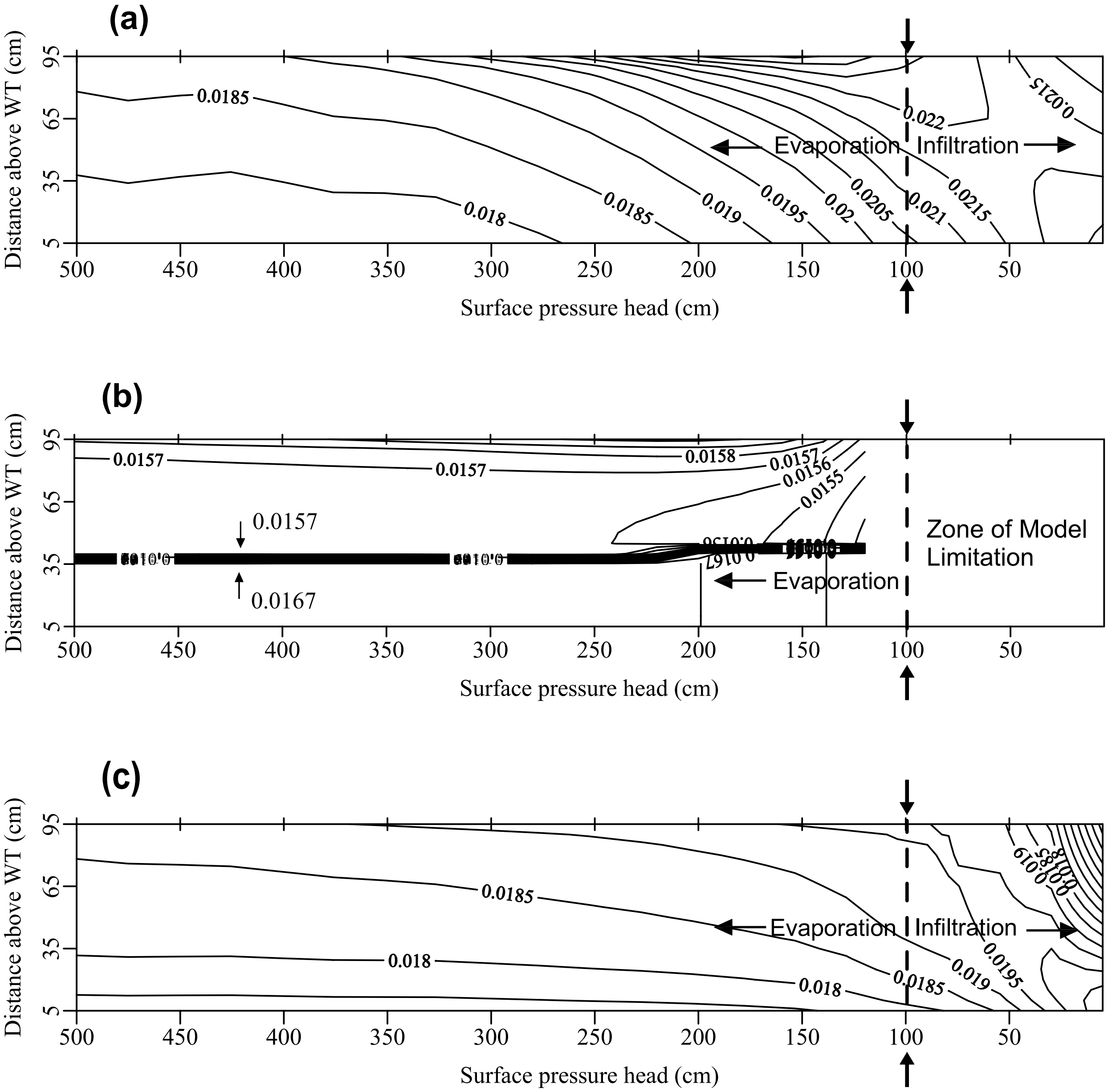

Figure 6. Effective α parameter α_{eff} as functions of surface pressure head and distance above water table: (a) Gardner model, (b) Brooks and Corey model, and (c) van Genuchten model.

[40] 1. The correlation between K_s and α increases the effective saturated hydraulic conductivity across the soil profile, while it does not affect the effective α. The effective α is usually smaller than the mean value of α, while the effective K_s can be either smaller or larger than the mean value for the uncorrelated case or fully correlated case, respectively.

[41] 2. For evaporation, the effective parameters typically vary along the distance above the water table while their variations due to the varying surface pressure head are less significant. The areally heterogeneous system would behave similar to a stratified medium with both effective parameters getting larger as it approaches the ground surface, especially at large surface pressure head. For infiltration, the surface pressure head and the elevation above the water table have similar effects on the effective α parameter.

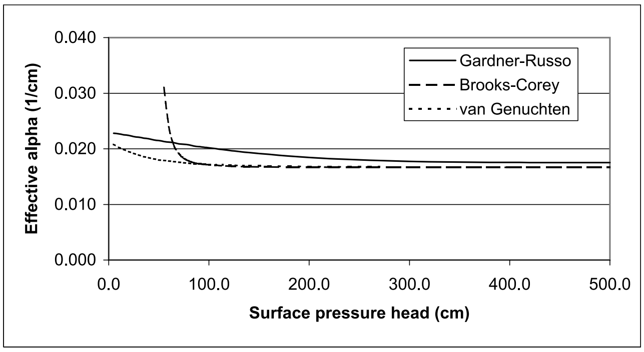

Figure 7. Effective α parameter α_{eff} as a function of surface pressure head when K_{eff} is assumed to take an average value of K_s.

[42] 3. It is difficult to define effective parameters for the Brooks Corey model since this model uses a piecewise-continuous profile for the hydraulic conductivity.

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