Soil Hydraulic Parameter Upscaling for Steady-State Flow with Root Water Uptake

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ABSTRACT

In this study we investigate effective soil hydraulic parameter averaging schemes for steady-state flow with plant root water uptake in heterogeneous soils. "Effective" soil hydraulic parameters of a heterogeneous soil formation are obtained by conceptualizing the soil as an equivalent homogeneous medium. The "effective" homogeneous medium is only required to discharge the same ensemble-mean flux across the soil surface. One-dimensional flow at the local scale has been used as an approximation for various simplified problems under investigation (e.g., a shallow subsurface dominated by vertical flows). The domain is assumed to be composed of homogeneous one-dimensional soil columns without mutual interactions. Using Gardner's unsaturated hydraulic conductivity model, we derive the effective value for the parameter α. While root water uptake influences the overall water budget, its impact on the effective hydraulic parameter averaging scheme was found to be secondary. Results show that the arithmetic mean of Gardner's α is usually too large to serve as an effective parameter. Deviations of the effective parameter from the arithmetic mean become larger as the surface suction increases; that is, the flow scenario switches from infiltration to evaporation. The results consistently show a smaller effective parameter for evaporation scenarios than for infiltration scenarios. The effective parameter α_{eff} decreases with an increase in the mean value of α. Spatial variability in α also decreases the effective value of α_{eff}. Alternative root water uptake distributions do not produce significant differences in both the water budget and the averaging scheme as long as total water loss to the plant roots remains the same.

UNSATURATED SUBSURFACE FLOW and solute transport are important components of studies of many large-scale hydrological and environmental processes, such as regional–global water balance, estimation of surface fluxes for soil–vegetation–atmospheric transfer (SVAT) algorithms, groundwater flow and contaminant transport models, and others. Simulations of unsaturated flow and solute transport in soil typically use closed-form functional relationships to represent soil hydraulic properties. The soil hydraulic properties have been studied extensively at the centimeter scale (measurement scale), but application to large heterogeneous areas remains an outstanding issue (e.g., Yeh et al., 1985a, 1985b, 1985c; Yeh, 1989; Russo, 1992; Green et al., 1996; Desbarats, 1998; Govindaraju et al., 2001; Zhu and Mohanty, 2002a, 2002b, 2003a, 2003b). Hydraulic property upscaling is a process that aggregates hydraulic properties defined at the measurement (support) scale into a coarser mesh with effective or average hydraulic properties that can be used in large-scale (e.g., basin-scale, watershed-scale, or regional-scale) hydrologic models.

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Dagan and Bresler (1983) and Bresler and Dagan (1983) developed models for water flow in the upper soil layer of spatially variable fields where spatial variability of the saturated hydraulic conductivity is assumed to take place in the horizontal plane. They found that effective properties may be meaningful only under very restricted and special conditions, such as steady gravitational flow where the effective saturated hydraulic conductivity varies between the geometric mean and the arithmetic mean. Kim and Stricker (1996) employed Monte Carlo simulation to investigate the independent and simultaneous effects of horizontal heterogeneity in soil hydraulic properties and rainfall intensity on various statistical properties of the components of the one-dimensional water budget for a large area up to 10^4 km^2. The effective hydraulic parameters were calculated by minimizing the squared differences of the capillary pressure profiles in the formation. Zhang et al. (1998) developed first-order stochastic models for stationary media using both the Brooks–Corey and the Gardner–Russo hydraulic property models. Kim et al. (1997) investigated the impact of heterogeneity of the soil hydraulic properties on the spatially averaged water budget of the unsaturated zone using a framework of analytical solutions (Kim et al., 1996). Their results indicate that the "effective" set of hydraulic parameters depends on the specific climate and the spatially uniform parameters, in addition to the obvious dependence on the mean, variance, and covariances of the spatially variable parameters.

Moisture flux across the land–atmosphere boundary (through infiltration, bare soil evaporation, and plant transpiration) is an important component of many large-scale hydrological processes. The hydraulic properties of the unsaturated zone usually exhibit high degrees of spatial variability over a range of scales because of the heterogeneous nature of soil formations. Because of the high nonlinear nature of unsaturated flow processes, the impact of soil heterogeneity on the average hydrological behavior is difficult to predict. Therefore the issue has received considerable attention in the recent past. In a series of previous studies related to this topic (Zhu and Mohanty, 2002a, 2002b, 2003a, 2003b), we investigated the use of effective hydraulic parameters for both steady-state and transient flow in bare heterogeneous soils. Zhu and Mohanty (2002a) investigated several hydraulic parameter averaging schemes and the ensemble hydraulic conductivity, in particular their appropriateness for predicting the ensemble behavior of the pressure head profile and the ensemble fluxes of heterogeneous formations for steady-state infiltration and evaporation. They used two hydraulic property models, the Gardner–Russo exponential model (Gardner, 1958) and the Brooks–Corey model (Brooks and Corey, 1964). Zhu

Abbreviations: SVAT, soil–vegetation–atmospheric transfer.

and Mohanty (2002b) provided practical guidelines on how commonly used averaging schemes (arithmetic, geometric, or harmonic) perform when compared with effective parameters for steady-state flow in bare heterogeneous soils using the widely used van Genuchten (1980) hydraulic property model. In the study by Zhu and Mohanty (2003a), the effective soil hydraulic parameters of a horizontally heterogeneous soil formation were derived by conceptualizing the heterogeneous formation as an equivalent homogeneous medium and assuming that the equivalent homogeneous soil will approximately discharge the same total amount of flux and produce the same average pressure head profile in the formation. A specific feature of the study by Zhu and Mohanty (2003a) is that the derived effective hydraulic parameters vary across the formation depth.

The objective of this study was to consider the effect of plant root water uptake on the averaging scheme for the hydraulic parameters for steady-state flow. As before, the effective parameter is obtained by conceptualizing the heterogeneous soil formation as an equivalent homogeneous medium that will discharge the same flux as the ensemble flux of the heterogeneous formation. The effective parameters so calculated are able to simulate the large-scale ensemble flux, which is an important quantity in modeling subsurface flow processes for land–atmosphere interactions. One-dimensional models have been used as approximations of various simplified problems under investigation (e.g., shallow subsurface dominated by vertical flows). For one-dimensional analyses, two physical scenarios need to be distinguished: (i) vertical layering (heterogeneity), where variations in soil properties are in the vertical directions only (e.g., Yeh, 1989), and (ii) vertically homogeneous soil columns with variations of the soil properties in the horizontal plane only (e.g., Dagan and Bresler, 1983; Bresler and Dagan, 1983; 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 one-dimensional soil columns, without mutual interaction, to simplify the analysis while keeping focus on some of the main process of many practical field applications. For example, in meso- or regional-scale 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 (top few meters) is considerably smaller. For such a large horizontal scale, the horizontal heterogeneity of hydraulic properties dominates. Therefore, it is reasonable to consider only horizontal soil heterogeneity. Using the simple Gardner hydraulic conductivity model (Gardner, 1958), we address the impact of horizontal hydraulic property heterogeneities and plant root characteristics on the effective hydraulic parameters during steady-state vertical flow in large heterogeneous fields.

FLUX EXCHANGE ACROSS SOIL SURFACE

In the vadose zone, the water conservation equation can be written as

$$\frac{dq(z)}{dz} = -G(z) \qquad [1]$$

and Darcy's Law as

$$q(z) = K(\psi)\left(\frac{d\psi}{dz} - 1\right) \qquad [2]$$

where q is the flux, z is the vertical coordinate (positive upwards, with $z = 0$ at the water table and $z = L$ at the soil surface, see Fig. 1), ψ denotes the suction head (a positive quantity), and q is the water flux (positive upwards). $G(z)$ is the water extraction term by plant roots expressed as volume of water per unit volume of soil per unit time, and $K(\psi)$ is the unsaturated hydraulic conductivity, which is modeled after Gardner (1958):

$$K(\psi) = K_s \exp(-\alpha\psi) \qquad [3]$$

where K_s is the saturated hydraulic conductivity of the soil, and α represents the rate of reduction in hydraulic conductivity with increasing suction head, ψ. K_s and α are assumed not to vary in the vertical direction, that is, not related to z.

The solution to Eq. [1] can be simplified significantly by defining the matric flux potential as follows (Rubin and Or, 1993; Warrick, 1974; Raats, 1974):

$$\phi = \int_{\psi}^{\infty} K(h)dh \qquad [4]$$

By using the matric flux potential and Gardner's (1958) hydraulic conductivity model, one can obtain the following equation:

$$\frac{d^2\phi}{dz^2} + \alpha\frac{d\phi}{dz} = G(z) \qquad [5]$$

The flux rate is given by

$$q(z) = -\frac{d\phi}{dz} - \alpha\phi \qquad [6]$$

Integrating Eq. [1] leads to

$$q(z) = q_0 - \int_0^z G(s)ds \qquad [7]$$

where q_0 is the flux rate at the water table (i.e., at $z = 0$), while the last term is the total flux rate lost to plant roots from $z = 0$ to $z = z$. The total flux rate lost via the entire root zone (transpiration) is then

$$A = \int_0^L G(z)dz \qquad [8]$$

The flux rate across the soil surface (i.e., water exchange between the subsurface and the atmosphere is then

$$q_L = q_0 - A \qquad [9]$$

Equation [6] can be solved for the matric flux potential to give

$$\phi = \left[\frac{K_s}{\alpha} - \int_0^z q(s)\exp(\alpha s)ds\right]\exp(-\alpha z) \qquad [10]$$

The suction head profile is then given by

$$\psi(z) = z - \frac{1}{\alpha}\ln\left[1 - \frac{\alpha}{K_s}\int_0^z q(s)\exp(\alpha s)ds\right] \qquad [11]$$

Substituting Eq. [7], [8], and [9] into Eq. [11] and rearranging, we can now relate the flux rate across the soil surface, q_L, to the suction head at the soil surface, ψ_L, as follows:

$$\frac{q_L}{K_s} = \frac{1 - \exp[\alpha(L - \psi_L] - \frac{\tau}{K_s}[1 - \exp(-1)][\exp(\alpha L) - 1] + \frac{\alpha}{K_s}\int_0^L\left[\int_0^z G(u)\mathrm{d}u\right]\exp(\alpha z)\mathrm{d}z}{\exp(\alpha L) - 1} \quad [12]$$

Two types of distributions for the water uptake term $G(z)$ are considered in this study. The first one is an exponential distribution along the plant root zone (e.g., Rubin and Or, 1993; Raats, 1974):

$$G(z) = \begin{cases} \dfrac{\tau \exp[-(L - z)/\delta]}{\delta} & z \geq L - \delta \\ 0 & z < L - \delta \end{cases} \quad [13]$$

The second form for $G(z)$ is a uniform distribution along the root zone (e.g., Warrick, 1974)

$$G(z) = \begin{cases} \dfrac{\tau(1 - e^{-1})}{\delta} & z \geq L - \delta \\ 0 & z < L - \delta \end{cases} \quad [14]$$

where τ is the transpiration rate, and δ the rooting depth. Note that both distributions will result in the same cumulative water uptake rate by the entire root zone; that is, $\tau[1 - \exp(-1)]$. Figure 1 illustrates root water uptake as a function of depth for the exponential and uniform distributions. The dimensionless root water uptake distribution G^* shown in the figure is given by GL/τ. The figure indicates that while the two root water uptake functions show different distributions vs. depth, the total water uptake per unit time is the same.

Substituting the two types of root water uptake terms Eq. [13] and [14] into [12] and rearranging, we can obtain the water flux rate across the soil surface in dimensionless form as follows:

$$q_L^* = \frac{1 - \exp[\alpha^*(1 - \psi_L^*)]}{\exp(\alpha^*) - 1 - C(\alpha^*, \delta^*)\tau^*} \quad [15]$$

where

$$q_L^* = q_L/K_s \quad [16a]$$
$$\tau^* = \tau/q_L \quad [16b]$$
$$\alpha^* = \alpha L \quad [16c]$$
$$\delta^* = \delta/L \quad [16d]$$
$$\psi_L^* = \psi_L/L \quad [16e]$$

The functional form for $C(\alpha^*,\delta^*)$ depends on the form of the invoked root water uptake terms. For the exponential root water uptake function, we have

$$C(\alpha^*, \delta^*) = \frac{\exp(\alpha^*)}{(\alpha^*\delta^* + 1)}\{\exp[-(\alpha^*\delta^* + 1)] - 1 + \exp(-\alpha^*)[1 - \exp(-1)](\alpha^*\delta^* + 1)\} \quad [17]$$

and for the uniform root water uptake,

$$C(\alpha^*, \delta^*) = \frac{\exp(\alpha^*)[1 - \exp(-1)]}{\alpha^*\delta^*}[\exp(-\alpha^*\delta^*) - 1 + \alpha^*\delta^* \exp(-\alpha^*)] \quad [18]$$

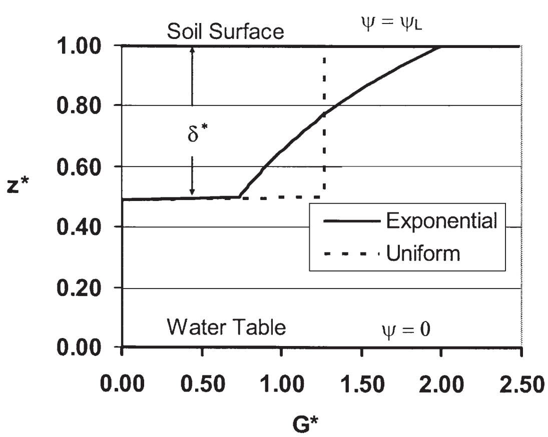

Fig. 1. Two different root water uptake distribution functions.

INFLUENCE OF INPUT PARAMETERS ON FLUX EXCHANGE

Before investigating the effects of parameter variability on the averaging scheme, it is useful first to discuss the influence of individual parameters on flux behavior.

Figure 2 illustrates the impact of the dimensionless root zone depth, δ^*, on the dimensionless flux, q_L^*, when $\tau^* = 1.0$, for low and high surface suction conditions. The surface suction conditions given in Fig. 2a and 2b represent a relatively wide range of values, from close to free drainage (a small value of 0.2 for ψ_L^*) to a very high suction ($\psi_L^* = 5.2$). The range of δ^* is also quite large, from a very shallow root zone close to the surface ($\delta^* = 0.1$) to a root zone extending almost to the water table ($\delta^* = 0.9$). Figure 2 shows that only for situations with small values of both the surface suction ψ_L^* and the Gardner parameter α^*, an increase in the soil root

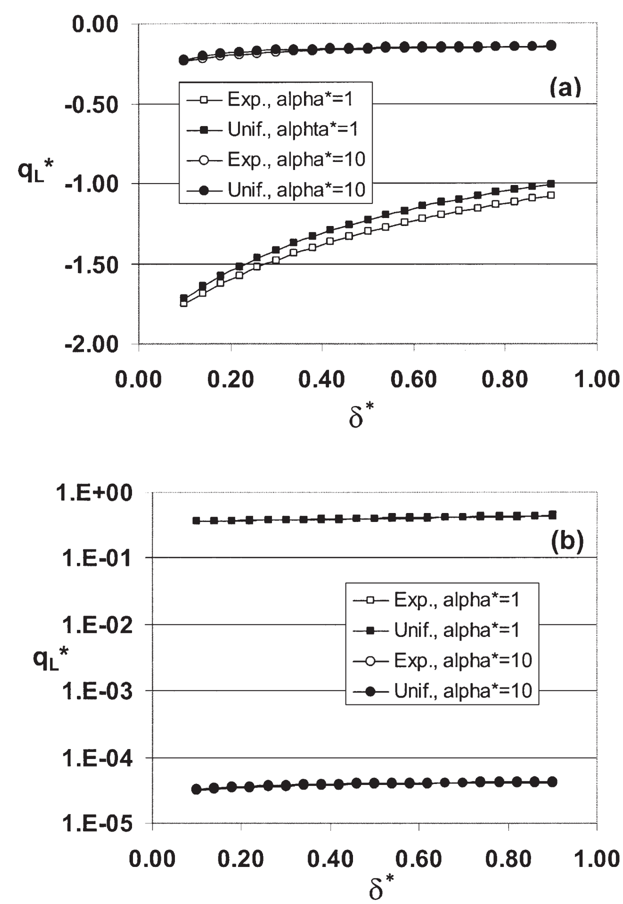

Fig. 2. Influence of dimensionless root zone depth, δ^*, on the dimensionless flux, q_L^*, when $\tau^* = 1.0$: (a) $\psi_L^* = 0.2$; (b) $\psi_L^* = 5.2$.

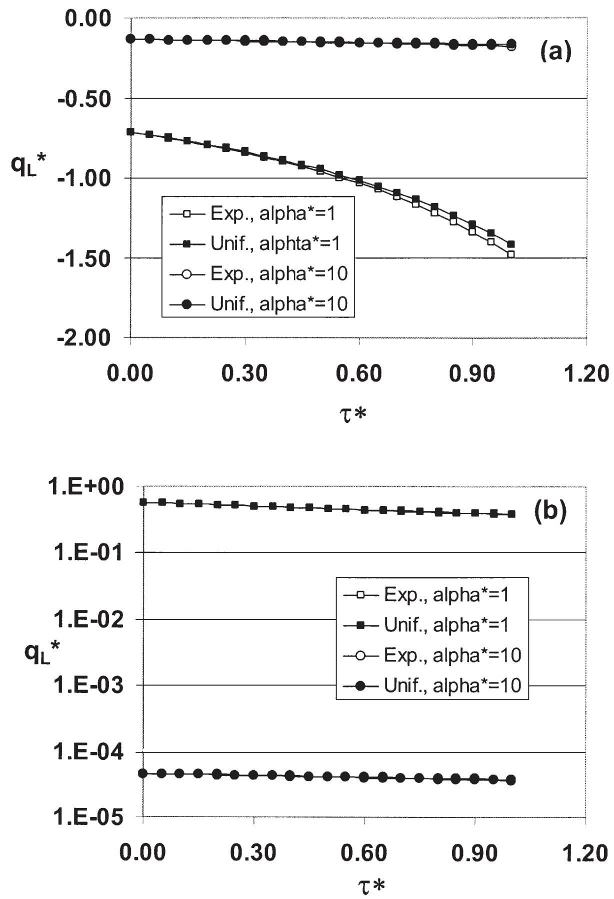

Fig. 3. Influence of dimensionless transpiration rate, τ^*, on the dimensionless flux, q_L^*, when $\delta^* = 0.3$: (a) $\psi_L^* = 0.2$; (b) $\psi_L^* = 5.2$.

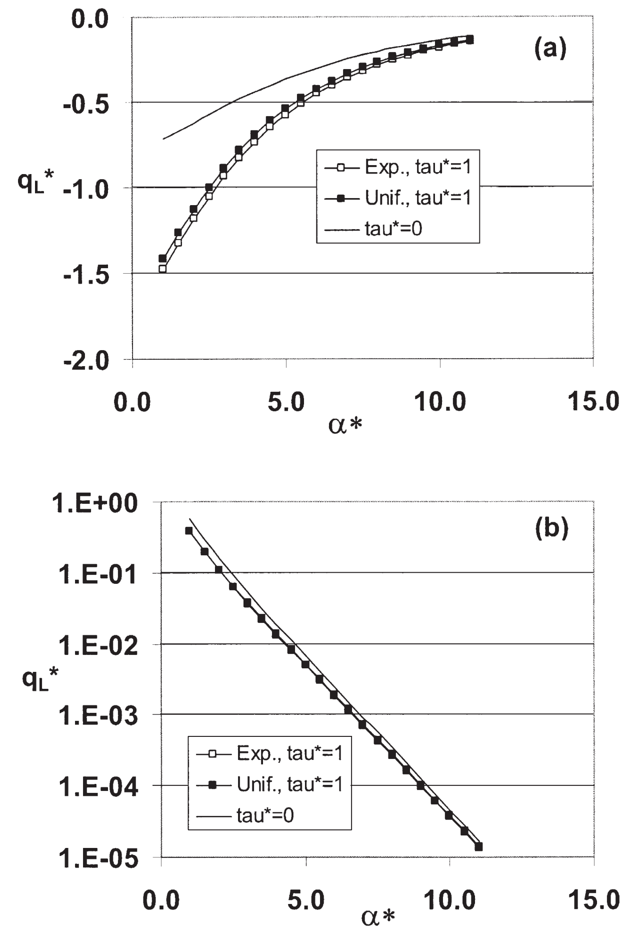

Fig. 4. Influence of α^* on the dimensionless flux, q_L^*, when $\delta^* = 0.3$: (a) $\psi_L^* = 0.2$; (b) $\psi_L^* = 5.2$.

zone depth will result in a lower (less negative) downward flux from the soil surface. Since the cumulative amount of water lost to plant transpiration is the same for all illustrated scenarios (it depends only on τ^*), the observed decrease in the downward flux across the soil surface indicates that steady-state groundwater recharge will be smaller because of the presence of a deeper root zone. For other scenarios the plant root zone depth has only minimal impact on the surface flux.

Figure 3 plots the dependence of the dimensionless surface flux, q_L^*, on the dimensionless transpiration rate, τ^*, when $\delta^* = 0.3$ for relatively low and high values of the surface suction head. The results are qualitatively the same as those in Fig. 2; that is, the transpiration rate is important only for conditions when both the surface suction and α^* are small. The observed increase in downward flux (more negative in value) across the soil surface is required to sustain the steady-state flux in response to increased transpiration (i.e., a higher value of τ^*).

Figure 4 shows the influence of α^* on the dimensionless flux, q_L^*, when $\delta^* = 0.3$ for relatively low and high values of the surface suction head. Results show a significant effect of α^* on the flux exchange between the subsurface and the atmosphere. An increase in α^* diminishes the surface flux significantly in both downward (i.e., less negative in values) and upward directions.

In summary, we note that the effects of τ^* and δ^* are important only when the flow scenario is near free drainage (i.e., relatively small ψ_L^*) and α^* is small. Therefore, α^* has the most significant impact on q_L^* for typical field conditions. In the following we treat flux heterogeneity by considering only spatial variability in the α^* field. In other words, the ensemble flux will be produced by an effective averaging scheme for the random α^* field. Figures 2, 3, and 4 show that in all cases the differences in results using the exponential and uniform root water uptake models are very small, indicating that the shape of root water uptake distribution does not make much difference as long as the total water loss to the plant roots remains the same. Therefore, we will only discuss results for the exponential root water uptake model; conclusions should apply equally to most of all other root water uptake models.

EFFECTIVE AVERAGING SCHEME FOR PARAMETER α^*

Since predicting the ensemble mean flux rate is usually a major focus of most practical SVAT studies, we can use a simple approach to derive effective hydraulic parameters by assuming that the equivalent homogeneous medium will discharge the same amount of moisture flux across the soil surface as the heterogeneous medium. Since the domain is assumed to be composed of homogeneous one-dimensional soil columns without mutual interactions, and flow is vertical in each column, we treat the arithmetic average (mean) for the saturated hydraulic conductivity as an appropriate effective parameter (e.g., Zhu and Mohanty, 2002b, 2003a) and determine the effective value for α^* by only matching fluxes across the soil surface.

For a lognormally distributed α^*, the probability distribution function is given by

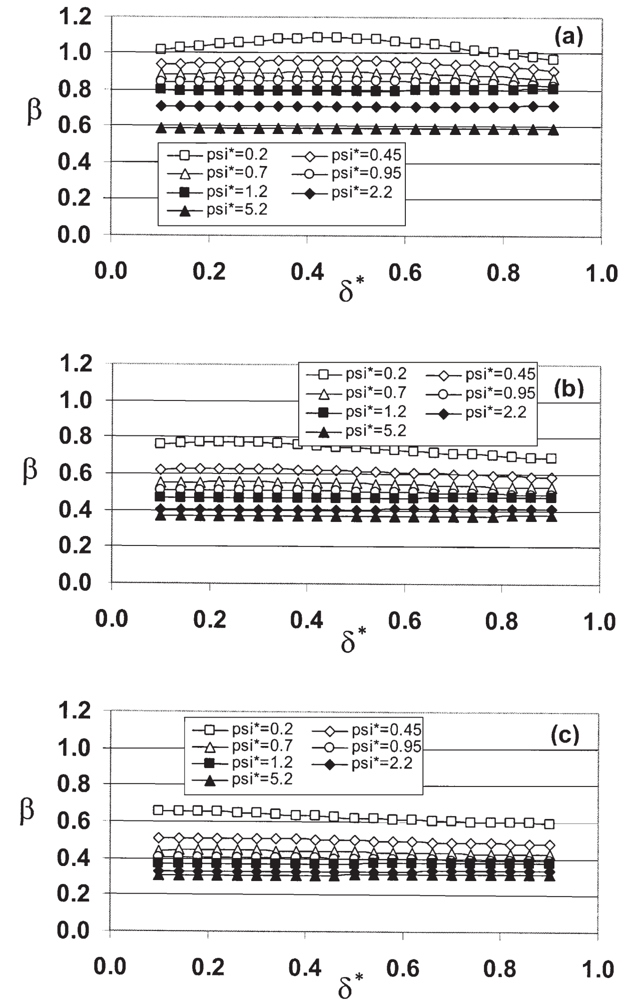

Fig. 5. Influence of dimensionless root zone depth δ^* on the effective coefficient for the α^* field when $\tau^* = 1.0$ and CV = 1.0: (a) $\overline{\alpha^*} = 1.0$, (b) $\overline{\alpha^*} = 6.0$, and (c) $\overline{\alpha^*} = 10.0$.

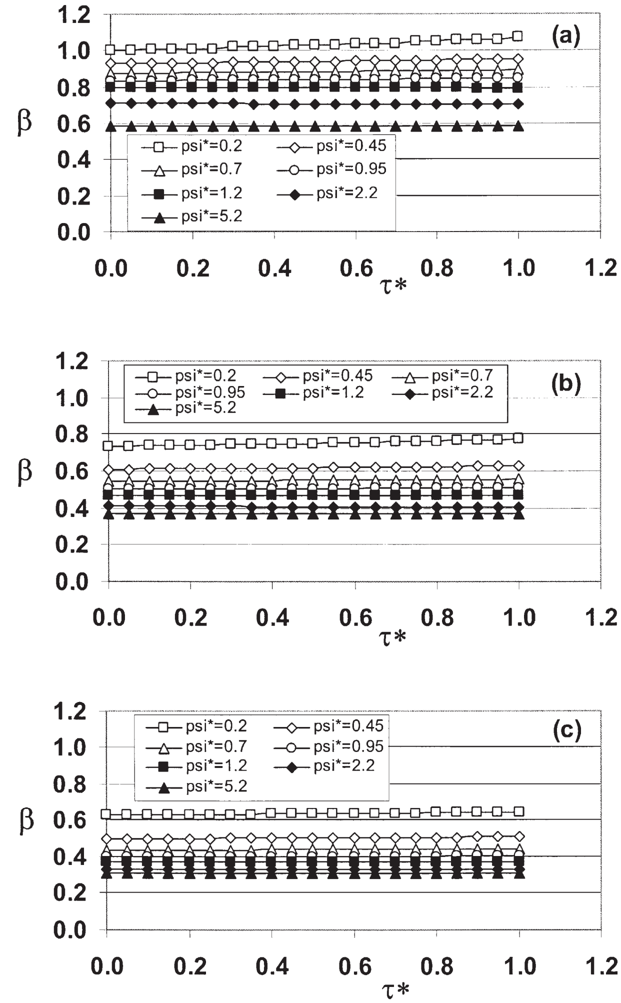

Fig. 6. Influence of dimensionless transpiration rate τ^* on the effective coefficient for the α^* field when $\delta^* = 0.3$ and CV = 1.0: (a) $\overline{\alpha^*} = 1.0$, (b) $\overline{\alpha^*} = 6.0$, and (c) $\overline{\alpha^*} = 10.0$.

$$f(\alpha^*) = \begin{cases} \dfrac{1}{\sqrt{2\pi}\sigma\alpha^*}\exp\left[-\dfrac{(\ln\alpha^* - \mu)}{2\sigma^2}\right] & \alpha^* > 0 \\ 0 & \alpha^* \leq 0 \end{cases} \qquad [19]$$

where the parameters μ and σ can be determined from the mean of α^*, (i.e., $\overline{\alpha^*}$), and the coefficient of variation of α^*, CV, as follows:

$$\mu = \ln\left[\frac{\overline{\alpha^*}}{\sqrt{CV^2 + 1}}\right] \qquad [20]$$

$$\sigma = \sqrt{\ln(CV^2 + 1)} \qquad [21]$$

Therefore, the ensemble dimensionless flux based on a log-normal distribution of α^* can be given by

$$\overline{q_L^*} = \int_0^\infty q_L^* f(\alpha^*)\mathrm{d}\alpha^* = \frac{1}{\sqrt{2\pi}\sigma}\int_0^\infty \frac{1 - \exp[\alpha^*(1 - \psi_L^*)]}{\alpha^*[\exp(\alpha^*) - 1 - C(\alpha^*,\delta^*)\tau^*]} \exp\left[\frac{(\ln\alpha^* - \mu)^2}{2\sigma^2}\right]\mathrm{d}\alpha^* \qquad [22]$$

The effective coefficient, β, for parameter α^* is determined from the following relationship

$$\frac{1 - \exp[\beta\overline{\alpha^*}(L - \psi_L)]}{\exp(\beta\overline{\alpha^*}L) - 1 - C(\beta\overline{\alpha^*}, \delta)\tau^*} = \overline{q_L^*} \qquad [23]$$

where the overbar denotes arithmetic mean (expectation). The left-hand side of Eq. [23] is $q_L^*(\beta\overline{\alpha^*})$. In other words, using the effective coefficient will produce the same ensemble flux exchange between the subsurface and the atmosphere. The coefficient β is therefore an indicator of how much the effective α^* deviates from the simple arithmetic mean, with $\beta = 1$ indicating that the arithmetic mean is the most appropriate for predicting the ensemble flux for the heterogeneous soils. We refer to β as the effective coefficient. Equation [23] was solved for β by using the golden section search (Press et al., 1992).

The influence of dimensionless root zone depth δ^* on the effective coefficient (β) for the random α^* field when $\tau^* = 1.0$ and CV = 1.0, is demonstrated in Fig. 5 for selected mean values of the α^* field. In the view of the fact that root zone depth is insignificant in relation to the surface flux in typical field conditions (see Fig. 2), the root zone depth has no significant influence on the α^* averaging scheme. The influence can be noticed when the surface suction is small (see open square curves for ψ_L^* in Fig. 5). The smaller the value of $\overline{\alpha^*}$, the more noticeable is the impact of the rooting depth, although the impact is relatively insignificant in all occurrences. While the

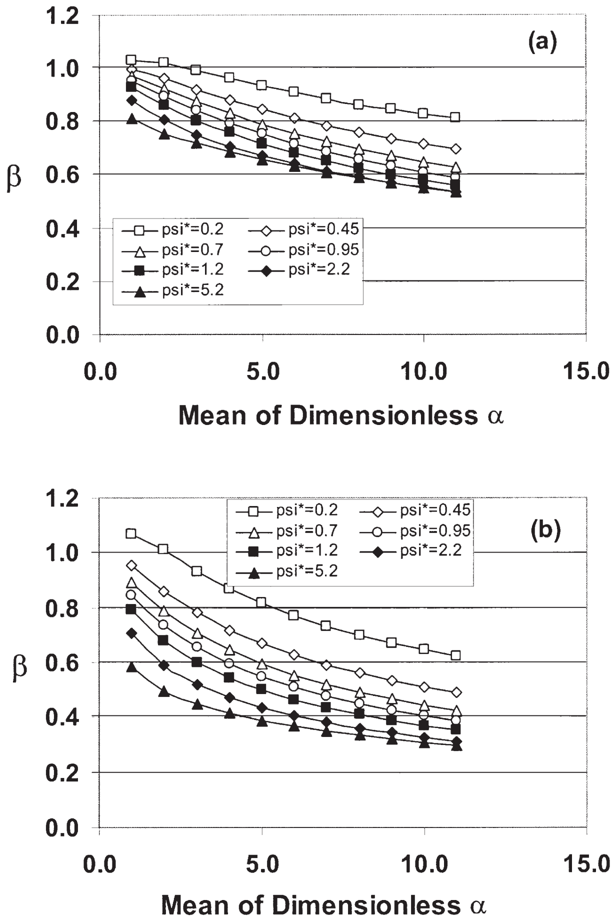

Fig. 7. Influence of $\overline{\alpha^*}$ on the effective coefficient for the α^* field when $\tau^* = 1.0$ and $\delta^* = 0.3$: (a) CV = 0.5 and (b) CV = 1.0.

impact of the plant root zone depth on the flux exchange between the subsurface and the atmosphere is not important, its influence on the effective parameter is even less significant.

Figure 6 shows the effect of the dimensionless transpiration rate τ^* on the effective coefficient (β) when $\delta^* = 0.3$ and CV = 1.0, for some selected mean values for the random α^* field. Results indicate that the transpiration rate has little impact on the averaging scheme. The effective coefficient β increases only slightly near the lower values of the surface suction.

Figure 7 shows the influence of $\overline{\alpha^*}$ on the effective coefficient β when $\tau^* = 1.0$ and $\delta^* = 0.3$, for two values of the coefficient of variation for the random α^* field. The effective coefficient β decreases as the mean of α^* increases. The effective coefficient β is typically smaller than 1.

The p-order power average (Korvin, 1982; Green et al., 1996; Gomez-Hernandez and Gorelick, 1989) or p-norm $\hat{\alpha}^*$ for a set of N α_i^* values is

$$\hat{\alpha}^*(p) = \left[(1/N)\sum_{i=1}^{N}\alpha_i^{*p}\right]^{1/p} \quad [24]$$

The arithmetic ($p = 1$), geometric ($p \rightarrow 0$), and harmonic ($p = -1$) means are all particular cases of the power average. For a lognormally distributed random variable, it can be shown that (Ababou and Wood, 1990)

$$\hat{\alpha}^*(p) = \overline{\alpha^*}\exp\left[\frac{(p-1)\sigma^2}{2}\right] \quad [25]$$

where σ^2 is the variance of $\ln\alpha^*$. Therefore, the power average for a lognormally distributed random variable increases with

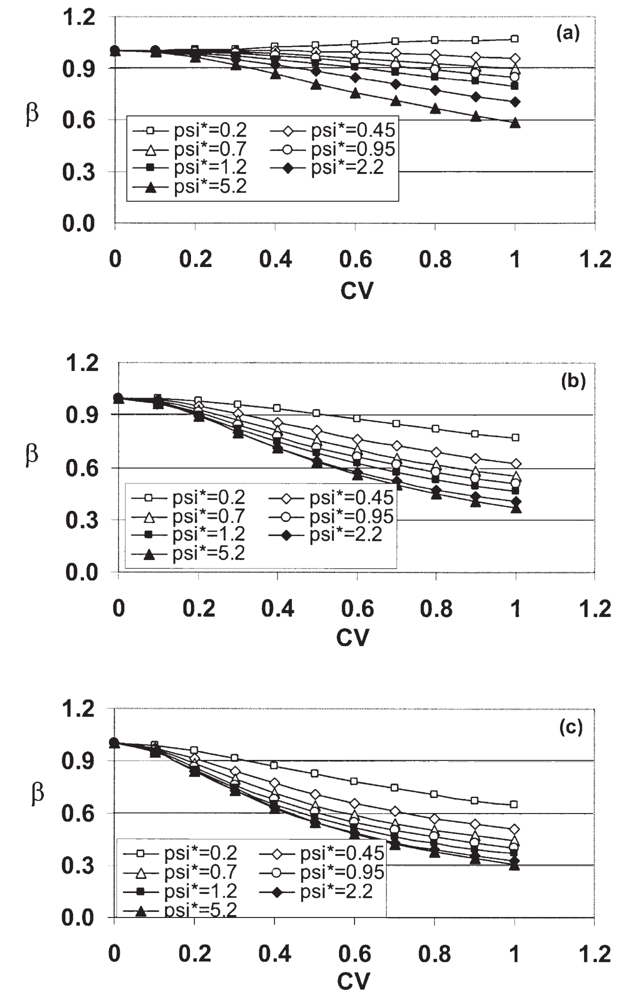

Fig. 8. Influence of coefficient of variation of the α^* field on the effective coefficient for the α^* field when $\tau^* = 1.0$ and $\delta^* = 0.3$: (a) $\overline{\alpha^*} = 1.0$, (b) $\overline{\alpha^*} = 6.0$, and (c) $\overline{\alpha^*} = 10.0$.

an increase in the power, p. Among the three commonly used averages, the arithmetic mean is the largest and the harmonic mean the smallest. Since the effective coefficient β is usually smaller than 1, this means that the arithmetic mean is too large to serve as a good effective parameter.

The importance of variability in α^* on the effective coefficient (β) is depicted in Fig. 8 when $\tau^* = 1.0$ and $\delta^* = 0.3$ for selected mean values of α^*. In general, spatial variability in α^* leads to a smaller effective coefficient β. The results indicate that the effective coefficient β deviates from the arithmetic mean as the CV increases. The deviation becomes larger as the surface suction increases, that is, as the flow scenario switches from infiltration to evaporation. The results show a consistently smaller effective coefficient for evaporation than for infiltration.

CONCLUSIONS

In this study we addressed the effects of horizontal hydraulic property heterogeneity and plant root characteristics on effective hydraulic parameters during steady-state vertical flow in large heterogeneous fields. Our main findings are as follows:

1. The influence of plant root water uptake on the averaging scheme of heterogeneous soil hydraulic

properties is secondary. Spatial variability in the nonlinear Gardner parameter α^* was found to dominate the averaging scheme.

2. Results show that the effective coefficient β of the α^* field is usually smaller than 1, indicating that the arithmetic mean is too large to serve as a good effective parameter.
3. Deviations of the effective coefficient β from 1 (i.e., from the arithmetic mean) become larger as the surface suction increases. Results indicate a smaller effective coefficient for evaporation than for infiltration.
4. The effective coefficient β decreases with an increase in the mean value of α^*. Spatial variability in α^* also leads to a lower effective coefficient β.

As a final caveat, predicting the ensemble flux on the basis of the upscaled hydraulic properties does not imply equally good predictions of other details of a given flow scenario.

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