Category: Subsurface Hydrology

Estimation of Internodal Permeabilities

for

Numerical Simulation of Unsaturated Flows

Josep Ma. Gastó and Jordi Grifoll

Departament d'Enginyeria Química, Escola Tècnica Superior d'Enginyeria Química
Universitat Rovira i Virgili, Catalunya, Spain.
E-mail jgrifoll@etse.urv.es

Yoram Cohen

Department of Chemical Engineering and Center for Environmental Risk Reduction
University of California, Los Angeles, Los Angeles, California 90095
E-Mail: yoram@ucla.edu

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Abstract

A scheme for the calculation of vertical interblock permeabilities for unsaturated flow in soil was developed and illustrated for one and two-dimensional unsaturated flows. In the proposed approach, interblock permeabilities were calculated from an average weight of contiguous grid point permeabilities. A large set of exact database weight values was fitted to a highly non-linear empirical-correlation equation as a function of the two contiguous block permeabilities, the dimensionless grid spacing and a soil dependent parameter. The present scheme was applied to the popular van Genuchten and, Brooks and Corey hydraulic functions for relative permeabilities ranging from 10-8 to 1, dimensionless grid spacing ranging from 0.01 to 1 and the soil parameter n of value between 1.05 and 5. The present approach is more accurate than other simple averaging schemes. At the same time, the computational effort for the present approach is comparable to that in which the arithmetic and geometric means are used, while enabling to estimate fluxes even with coarse grids.

GAP list

1875 Unsaturated zone
1866 Soil moisture
1894 Instruments and techniques

1. Introduction

The simulation of water flow in homogeneous unsaturated soil is typically accomplished by solving the unsaturated flow equation i.e., Richards' equation [*Richards,* 1931]. To solve the Richards' equation one requires a constitutive hydraulic function that describe the relationship among fluid capillary pressures, water content and relative permeabilities or conductivities. Two particularly popular forms of the hydraulic functions have been proposed by *van Genuchten* [1980] and by *Brooks and Corey* [1964] and these are designated hereinafter as VG and BC, respectively.

Numerical solutions of Richards' equation which are based on discritization of the flow domain require estimation of the relative permeability between adjacent control volumes. A popular procedure for estimating this interblock permeability is the arithmetic mean (AM) of the permeabilities of two neighboring cells [*Haverkamp and Vauclin*, 1979; *Celia et al.*, 1990; *Warrick*, 1991; *Zaidel and Russo*, 1992]. However, it is known that this procedure leads to an overestimation of the interblock permeability [*Zaidel and Russo*, 1992]. Another popular alternative scheme is the geometric mean (GM) that was shown to lead to better results relative to the AM approach under some conditions [*Schnabel and Richie*, 1984]. Other averaging schemes that have been proposed and tested in the literature, with less success than the preceding schemes, include the harmonic mean of conductivities, conductivity at the arithmetic or harmonic means of the capillary head, conductivity at the upstream node and numerical integration of conductivity [*Haverkamp and Vauclin*, 1979; *Srivastava and Guzman-Guzman*, 1995]. It has been suggested that, for a given soil, different averaging procedures should be used for the gravitational and capillary contributions to the flow and that each of these contributions in turn also depends on the internodal distance [*Baker*, 1995]. The above observation clarifies why different authors, when evaluating the internodal flow for different soil characteristics and grid spacing, have reached different conclusions regarding the most appropriate averaging scheme.

The piecewise Brooks-Corey Darcian mean approximation was introduced by *Baker et al.* [1999] as a way to calculate effective conductivities. Such an approximation was shown to be useful for simulating infiltration in a soil described by the Haverkamp's hydraulic function [*Haverkamp et al.,* 1977]; however, the implementation of the approach is complex and its performance for other soils has been not evaluated. In an earlier study, *Warrick* [1991] proposed a scheme whereby for a given pair of nodal capillary heads, the effective conductivity was calculated as a weighted average of the conductivities between adjacent nodes with weight values taken from previous exact calculations of the flux. In the numerical implementation of the approach, the weights were stored in the form of tables and interpolated when needed. This procedure led to excellent agreement with exact solutions of the Richards' equation but required the use of different tables for different soils and grid spacing (for a given soil). For a non-homogeneous grid simulation the procedure would require a separate table for each possible grid spacing.

The use of the integral average of the conductivity, with respect to the capillary head, between adjacent points to evaluate the effective conductivity is known as the Kirchhoff integral method and has received special attention. The Kirchhoff integral method provides an interblock conductivity that is exact for horizontal flow [*Schanbel and Richie*, 1984; *Warrick*, 1991], but does not consider the gravitational contribution to the integral for vertical fluxes. Nonetheless, the Kirchhoff integral method, in its original [*Srivastava and Guzman-Guzman*, 1994; *Miller et al.*, 1998] or modified [*Zaidel and Russo*, 1992; *Williams et al.*, 2000] forms, have been successfully applied to vertical fluxes. The use of the Kirchhoff integral form has two main disadvantages: (a) it is difficult to assess the error introduced by neglecting the gravitational term in the integral; and (b) it is not possible to express the transform analytically except for simple hydraulic functions. The later difficulty can be overcome using tables of suitable values and associated interpolation [*Ross*, 1992; *Grifoll and Cohen*, 1999]. It is worth noting that the Kirchhoff integral method has not been widely used for the solution of the Richards' equation mainly due to the complexity and computational effort involved.

In the present paper we present a simple procedure to calculate the weight values, as defined by *Warrick* [1991], for calculating interblock conductivities without the need of generating a table for each soil and grid spacing. Test cases are presented using the VG and BC hydraulic functions. The aim is to calculate accurate interblock conductivities, even with relative large internodal distances, and to provide an easy to implement numerical algorithm for such calculations.

2. Theory

2.1. Governing Equations

It is accepted that the flux or specific discharge, q, (m/s) for unsaturated soils, obeys the extension of Darcy´s law [*Hillel*, 1980], which, for one- dimensional (i.e. vertical) system, can be written as

$$q = -K_s\, k \left(\frac{\partial \psi}{\partial z} - 1 \right) \tag{1}$$

where K_s is hydraulic conductivity at saturation (m/s), k is the relative permeability, ψ is the water pressure head (m) and z (m) is vertical distance (positive downwards). The discritization of (1) between two adjacent vertical nodal points is typically written as

$$q_{eff} = -K_s\, k_{eff} \left(\frac{\Delta \psi}{\Delta z} - 1 \right) \tag{2}$$

where $\Delta\psi = \psi_L - \psi_U$ is the pressure head difference between two adjacent lower (*L*) and upper (*U*) nodes, $\Delta z = z_L - z_U$ is the internodal distance and q_{eff} and k_{eff} are the effective flux and effective relative permeability, respectively. It should be noted that the flux expression (2) is applicable for both steady and unsteady conditions and uniform or non-uniform control volumes (see Figure 1) An important requirement of the discritization methodology is that q_{eff}, calculated with (2) must be a representative value of the flux between cells *U* and *L*. Considering the continuous form of the Richards' equation in which the flux is given by (1), it is apparent that under unsteady state conditions q can vary along z, and this variation could be large when Δz, $\Delta\psi$ or both are large. Such flux variations cannot be handled by the discritized form of (1) as expressed in (2). Therefore, a unique flux value, between cells *U* and *L,* is assigned for both steady and unsteady conditions.

For a system described by a soil with a given hydraulic function, and given the values Δz, ψ_U and ψ_L, a coherent implicit definition of q_{eff} can be deduced from (1), as given by [*Warrick*, 1991]

$$\Delta z = \int_{\psi_U}^{\psi_L} \frac{d\,\psi}{1 - \dfrac{q(z)}{K_s\, k(\psi)}} = \int_{\psi_U}^{\psi_L} \frac{d\,\psi}{1 - \dfrac{q_{eff}}{K_s\, k(\psi)}} \tag{3}$$

Given the above implicit expression for q_{eff}, a consistent k_{eff} can be calculated with the aid of (2). As *Warrick* (1991) pointed out, k_{eff} must be bounded by $k_U = k(\psi_U)$ and $k_L = k(\psi_L)$. Therefore, for each case there is a weight w, $0 < w < 1$, such that

$$k_{eff} = w\,k_U + (1-w)\,k_L \tag{4}$$

If w is known, the calculation of q_{eff} is straightforward through (4) and (2). We note that the definition of w, as given in (4), differs from the definition given by *Warrick* (1991) who used a vertical coordinate defined as positive upwards with w multiplying k_L instead of k_U, as used in this work. The weight w defined in the present work is the complement (i.e., 1-w) to the one defined by *Warrick* (1991).

In order to integrate (3) one needs to specify the hydraulic function $k = k(\psi)$. For example, for the unsaturated zone the BC function can be written as

$$k = \left(\psi^*\right)^{1-3n} \tag{5}$$

where $\psi^* = \psi/\psi_{ref}$ is a dimensionless water pressure head and ψ_{ref} is the bubble head ψ_b (m), and $n = \lambda+1$, where λ is the pore size index as defined by *Brooks and Corey* (1964). The equivalent function for the VG hydraulic function is

$$k = \frac{\left\{1-\left[1-\dfrac{1}{1+\left(\psi^*\right)^n}\right]^m\right\}^2}{\left[1+\left(\psi^*\right)^n\right]^{m/2}} \tag{6}$$

where m = 1-1/n, and $\psi^* = \psi\,\alpha$, where α is a parameter of the VG equation (m^{-1}). It is interesting to note that in (5) and (6) the water pressure head is made dimensionless with respect a reference pressure head, ψ_{ref} (m), which is ψ_b for BC and 1/α for VG.

As defined by (2-4) and either (5) or (6), w depends on k_U, k_L, Δz, n and ψ_{ref}. However, a reduction of the number of independent variables can be achieved by considering a normalization procedure. First, we define the dimensionless variables $q^* = q/K_s$ and $z^* = z/\psi_{ref}$, and then transform (1) to

$$q^* = -k\left(\frac{\partial \psi^*}{\partial z^*} - 1\right) \quad (7)$$

which, when combined with (5) or (6), is independent of ψ_{ref}. Therefore, for a given type of hydraulic function [(5) or (6)] the weight w is only a function of k_U, k_L, Δz^* and n. We note that the approach presented above is applicable both to one-dimensional problems (Sections 3.1 and 3.2) and for the vertical component of multidimensional problems as illustrated in section 3.3. The specific correlations for the VG and BC functions are presented in the Section 2.2.

2.2 Hydraulic Function Correlation

Given a type of hydraulic function (VG or BC) and a set of ψ_U, ψ_L, Δz^* and n, (3) provides an implicit procedure for calculating q_{eff}^*. The weight w is then calculated from (2) and (4). In the present work, the integral in (3) was solved numerically with a globally adaptive scheme based on the Gauss-Kronrod rules [IMSL, 1997]. The value of q_{eff}^* was searched iteratively until the difference between the value of the integral in (3) and Δz was less than 10^{-4} %. As suggested by *Warrick* (1991), the transformation variable $u = \ln(-\psi^*)$ was used to alleviate integration accuracy problems. Using the above integration procedure, two databases, one for each type of hydraulic function, VG and BC, were created. Each database was designed to contain 13328 calculated w values for all combinations of the following values of the independent variables: k_U and $k_L = 10^{-i}$, $3\ 10^{-i}$ ($i = 1, 2,...,8$); $n = 1.05$, 1.5, 2, 2.5, 3, 4, 5 and $\Delta z^* = 0.01$, 0.1, 0.2, 0.4, 0.6, 0.8, 1. The database did not include the cases in which $k_U = k_L$ because in such a situation w cannot be calculated directly from (4). The VG database had only 13029 points since in 299 cases (all for $k_U \geq 0.1$ and $n = 1.05$) the iterative w calculation procedure did not converge. Non-convergence for the above cases was due to failure of the quadrature method for such highly non-linear $k(\psi)$ function. Clearly, the use of the weighting function for VG (as described below) for $n \sim 1.05$, $k_U \geq 0.1$ should be considered an extrapolation. We note, however, that the monotonic behavior of the function assures reasonable weight values for these latter conditions. For the BC hydraulic function only the region $\psi \leq \psi_b$ was included in the database. The case in which one internodal point is saturated ($\psi > \psi_b$) whereas the other contiguous point is not, is covered in the appendix. Finally, we note that when $k_U = k_L = 1$ it follows that $k_{eff} = 1$. We note that the range of n, $1.05 \leq n \leq 5$, considered in the present study, encompasses the range of values expected for natural soils. For VG, *Carsel and Parrish* (1988) reported average n values, for different types of soil, which ranged from 1.09 to 2.68. Similar range of n values was reported by *Rawls and Brakensiek* (1989) for the BC hydraulic functions.

The dependence of w on the variables k_U, k_L, n and Δz^* is highly nonlinear. The dependency of w with k_U and k_L was examined first, and after several trial and error searches, a general equation for w was deduced to be of the following form

$$w = \frac{1}{1 + \dfrac{a\ R}{1 + \beta_0\ R}} \tag{8.a}$$

$$R = \frac{k_U^b}{k_L^c} \tag{8.b}$$

for the condition whereby Δz^* and n where maintained as constants. For each pair of Δz^* and n, the parameters a, b, c and β_0 were searched by fitting (8.a) and (8.b) to the values of w from the database. The above parameters (a, b, c and β_0) displayed monotonic variations with Δz^* and n. The parameter β_0 was only slightly dependent on Δz^* and more sensitive to variations in n. For each n, the variation of a, b and c was also examined and several empirical equations were tested with respect to their ability to reproduce the functionality of the parameters respect Δz^*. The final set of equations, selected to describe the set of parameters in (8a) and (8b), are given below.

The parameter a is described by

$$a = \frac{1 - a_1\, \Delta z^*}{1 + a_2\, n^2\, \Delta z^*} \tag{9}$$

in which a_1 depends linearly on the decimal logarithm of n as given by

$$a_1 = a_{10} + a_{11} \log(n) \tag{10}$$

The powers b and c in (8.b) are linear functions of Δz^* given as

$$b = b_0 - b_1\, \Delta z^* \tag{11}$$

$$c = b_0 + c_0\, (n-1)\, \Delta z^* \tag{12}$$

Equations (11) and (12) share a similar intercept, dependent on the soil parameter n, through the relation for b_o

$$b_0 = \frac{b_{01}\, n}{b_{02}\, n - 1} \tag{13}$$

Finally, β_0 was found to be directly proportional to n according

$$\beta_0 = \beta\, n \tag{14}$$

Equations (8-14) include eight constants (a_{10}, a_{11}, a_2, β, b_{01}, b_{02}, b_1, c_0) which when properly chosen approximate the w weights stored in the database. These constants were determined by fitting the w values contained in the database using the Marquardt-Levenberg optimization algorithm [*Press et al.*, 1990] to minimize the sum of the squared differences between the observed and predicted values of the dependent variable (w). The optimization procedure was initiated with values of the parameters obtained during the sequential deduction of the form of the equations as described above, thereby, enabling smooth convergence to the final values. The parameter values that resulted from the optimization procedure for the BC and VG hydraulic functions are provided in Table 1 and the statistical parameters that qualify the goodness of the fit are given in Table 2. The average absolute errors for both correlations were less than 0.025 with standard deviations less than 0.041. The corresponding average relative error of the fit was 22% and the correlation coefficients for both cases were greater than 0.99, indicating a good correlation of w with the independent variables (k_U, k_L, n and Δz^*).

A comparison of the w values from the database and the fitted function is provided in Figures 2a and 2b that show the variation of the weights for the BC and VG hydraulic functions with k_U for different values of k_L, at fixed values of n = 2 and Δz^* = 0.20. For both the BC and VG hydraulic functions, the variation of w with k_U for a given k_L has a typical sigmoidal shape. For most conditions, higher weight values are obtained for the lowest conductivity, either k_U or k_L. This characteristic behavior is also shared with the geometric mean, which may explain why researchers have often found the geometric mean to be a preferred choice among the traditional means. It is emphasized that when the k_U and k_L are very dissimilar, the geometric mean yields too low k_{eff} and q_{eff} values, as revealed, for example, by the numerical experiments of *Schanbel and Richie* (1984).

An illustration of the type of errors expected from the use of the weighting average, with weights taken from the present correlation, and other averaging procedures is given in Table 4 for the fluxes calculated based on (2-4) for a typical sandy loam soil. The computed fluxes using AM averaging are greater than the *integral value* in all the cases presented except when ψ_U = -0.01 m and ψ_L = -0.1 m. On the other hand, GM averaging led to underprediction of the fluxes, except for (ψ_U, ψ_L)= (-0.1 m, -0.01 m) and (-1 m, -0.1 m). Finally, WM averaging resulted in either under- or over-predictions, but with greater accuracy than both the AM and GM averaging procedures, except for (ψ_U, ψ_L)= (-0.1 m, -0.01 m) where the GM coincides with the integral value and the weighted mean overpredict it by 17%. It is important to note that, for the conditions listed in Table 4, the arithmetic mean can lead to overprediction of the flux by a factor of nearly 9000, whereas the geometric mean can underpredict it by a factor of nearly 5000 times. In contrast, the WM averaging procedure results in a maximum overprediction factor of about 60 and a maximum underprediction factor of about 2.5 relative to the *integral* flux value.

3. Results and discussion

3.1 Test Cases and Numerical Approach

The effectiveness of the proposed hydraulic function correlations, for flux calculations in numerical simulations, was demonstrated with via four different test cases. The first test case is infiltration under fixed head gradient, performed to compare the classical means and the present approach of internodal averaging. The second test case is infiltration with fixed moisture content at the surface presented to check the performance of the present approach for different internodal distances and the type of hydraulic function. The third test case is a computationally intensive two-dimensional axisymmetric infiltration from a surface area source that further demonstrate the advantage of the present approach. Finally, infiltration into a layered soil is presented to illustrate the potential application of the proposed approach to non-homogeneous systems.

All the numerical simulations employed a Newton-Raphson iterative scheme. When using the weighted average, a series of test calculations demonstrated that the inclusion of the dependence of w on ψ, when calculating the Jacobian of the Newton-Raphson method, did not improve the convergence speed or the stability of the procedure. Therefore, the above approach was not utilized in the examples presented. The simulations were performed using the "mixed form" of Richards' equation (*Celia et al.*, 1990). The proposed weighting procedure described earlier is directly applicable to all discritized forms of the Richards' equation in which the pressure head gradient is used as the dependent variable when calculating the flux. This includes the standard "ψ-base" form and the "mixed" form of the Richards' equation. Numerical permeabilities, as estimated in this paper, provide accurate fluxes when using (2) and where the numerical approximation of the driving force is given in terms of $\Delta\psi/\Delta z$. Therefore, when using the "θ-base" form (*Celia et al.*, 1990) and other forms that are based on the transformation of the pressure head gradient [*Williams et al.*, 2000] as a driving force, the calculated fluxes would be less accurate.

3.2 Vertical flux under constant head gradient and different soils

The first test case of one-dimensional vertical infiltration under a constant head gradient illustrates the effect of different averaging procedures on the flux calculation between two internodal points. In this example, the flux was estimated between two grid points with $\Delta z^* = 0.5$, having dimensionless matric heads of $\psi_U^* = -1$ and $\psi_L^* = -2$ and soil properties described by the VG hydraulic function. The dimensionless flux between these points is given by

$$q^* = -k_{eff}\left(\frac{\psi_L^* - \psi_U^*}{\Delta z^*} - 1\right) \quad (15)$$

with k_{eff} calculated using the arithmetic mean (AM), the geometric mean (GM) or the present weighted mean (WM) calculation. The variation of the dimensionless flux, q^*, with respect to the parameter n in the VG function, for the above conditions, is shown in Figure 3 along with a fine grid (1000 grid points) steady state solution of the problem. The fine grid solution represents the grid-independent solution, which also does not does not depend on the averaging procedure for calculating k_{eff}. For values of n below 1.5 the predicted q^* values are very similar; however, as n increases differences among the different averaging procedures become more pronounced. For this test case, the geometric average led to the worst result, always underestimating the flux relative to the fine grid solution, while the arithmetic mean consistently resulted in overestimates of q^*. The weighted mean is indistinguishable from the fine grid solution for $n < 2.5$, but above this value, it slightly underpedicts the fine grid result. In all cases, the maximum discrepancy is at $n = 5$ where the GM approach underpredicts the fine grid solution by 91%, the AM overpredicts it by 45%, whereas the weighted average results in 7% underprediction.

3.3 Infiltration for an upper constant moisture condition

Infiltration into a Yolo light clay soil, with an upper constant moisture boundary condition, was selected for a time-dependent infiltration example. This same example was employed by *Warrick* (1991) to test his procedure. Soil parameters for this example are listed in Table 3 as given by *Warrick* (1991). Initial and surface boundary conditions were set as constant volumetric water content of $\theta = \theta_{\mathrm{ini}} = 0.235$ and $\theta = \theta_s = 0.495$, respectively. The lower boundary condition was taken as a unit gradient at a depth of 1 m. The simulation was performed with a fixed grid version of the numerical algorithm of *Grifoll and Cohen* (1999) using a time step of 1 s. Further reduction of the time step did not affect the results. The above simulation scheme assured that global mass balance errors were less than 0.05%.

The cumulative infiltration, CI (m) at any given time was calculated as

$$CI = \int_0^L \left(\theta - \theta_{ini}\right) dz \qquad (16)$$

where *L* (m) is the total length of the system considered. Equation (16) is appropriate when the flux at the bottom soil boundary is negligible, as was indeed the case for all of the simulations performed in this test case. An illustrative solution of this example was obtained for $\Delta z = 0.05$ m ($\Delta z^* = 0.10$) and $\Delta z = 0.10$ m ($\Delta z^* = 0.20$) with the cumulative infiltration results shown in Figures 4a and 4b. The cumulative infiltration was also calculated by the three-term quasi-analytical solution [*Philip*, 1969] with the coefficients provided by *Warrick et al.* (1985). The fine grid solution (Δz = 0.001 m), which coincided with the above quasi-analytical solution, was independent of the averaging procedure. The fine grid solution, for the volumetric water content profile, was compared to the solutions obtained for coarser grids and different averaging procedures. As seen in Figure 4, for grid spacing of both 0.05 m and the 0.10 m, use of the geometric mean resulted in fluxes and correspondingly cumulative infiltration values (CI) which, after 100 hours of infiltration, were too low by about 7.0% and 19.3%, respectively, thus resulting in shallow penetration into the soil. In contrast, use of the arithmetic mean resulted in excessively high relative permeabilities, and as a consequence higher cumulative infiltration (by 3.8% and 7.4% for grid spacing of 0.05 and 0.10m, respectively, after 100 hours of infiltration) and deeper penetration of water into the soil. The solution in which the weighted mean was used resulted, after 100 hours of infiltration, in a deviation of 1.0% and 3.6% below the fine grid solution for the grid spacing of 0.05 m and 0.10 m.

3.4 Infiltration from an area source

In order to illustrate the beneficial performance of the present weighted mean (WM) approach of estimating internodal fluxes for multi-dimensional simulations, two test cases are presented for infiltration from an area source (at the soil surface). The problem is formulated in a two-dimensional axisymmetric coordinate system with the mass conservation equation given as

$$\frac{\partial \theta}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}\left(r\, q_r\right) + \frac{\partial q_z}{\partial z} = 0 \qquad (17)$$

where q_r (m/s) and q_z (m/s) are the radial and vertical components of the flux, and r (m) is the radial coordinate. For the BC hydraulic function, the flux in the radial direction can be computed exactly by the Kirchhoff transformation

$$q_r = -K_s \frac{\phi_R - \phi_L}{r_R - r_L} \tag{18}$$

where R and L refer to right and left nodes and ϕ is the Kirchhof transform that for the BC [obtained from integration of (5)] as

$$\phi = \int_{-\infty}^{\psi} k \, d\psi \quad = \frac{k\,\psi}{2 - 3\,n} \tag{19}$$

The discritized form of (17) was solved using the alternating direction implicit (ADI) method (*Ferziger*, 1981). According to *Kirkland et al.* [1992] the ADI method for solving the two-dimensional Richards' equation worked well and was computationally more efficient relative to other methods considered in their study.

The soil domain, for the present 2D simulations, extended vertically from $z = 0$ (surface) to a depth $z = Z_T$ and radially from $r = 0$ (centerline) to $r = R_T$. The initial condition was set as constant water pressure inside the domain ($\psi_{initial}$). At the surface the vertical flux from the circular source area ($0 \le r \le r_{bc}$) was set as

$$q_z(r, 0) = q_0 \text{ for } 0 \le r \le r_{bc} \tag{20 a}$$

The flux boundary conditions for the remainder of the surface area and the lateral boundary are given as

$$q_z(r, 0) = 0 \text{ for } r_{bc} \le r \le R_T \tag{20 b}$$

$$q_r(R_T, z) = 0 \text{ for } 0 \le z \le Z_T \tag{20 c}$$

Finally, the gradient at the bottom boundary was specified as

$$\frac{\partial \psi}{\partial z}(r, Z_T) = 0 \text{ for } 0 \le r \le R_T \tag{20 d}$$

The first axisymmetric simulation test case was rapid infiltration into a loamy sand (test 2DA) with domain and simulation system parameters given in Table 5 and soil parameters given in Table 3. Simulations using the AM, GM and WM internodal averaging methods were performed with a fixed grid of Δz = 8 cm and Δr = 1 cm and time step Δt = 2 s. The contour profiles after 4 days of continuous infiltration are depicted in Fig. 5. Simulations with successively smaller grid size, Δz, demonstrated that at a grid spacing of Δz=0.02 m, the solution for the three different averaging methods was sufficiently accurate to be considered a fine grid solution (with maximum deviations <1% among the different averaging methods

All of the simulation results were obtained with a water mass balance error that was no greater than about 2x10^{-4} %. We note that for all the above simulations smaller time steps (i.e. Δt <2 s) did not improve the results depicted in Figure 5. The contours were very similar, except for the GM simulation for which the θ = 0.20 and 0.15 contours profiles appear flattened as a result of the excessive error introduced by the overprediction of the permeability by the GM method. For the above series of simulations, the computation time for the coarse z-grid was between 62 and 76 min, whereas it took 5 hours of computation for the fine grid (both simulations performed on a PC with a 866 MHz Pentium III Xeon processor).

The second axisymmetric test case was for a slow infiltration into a silty clay soil with the system domain and simulation parameters given in Table 5 and soil hydraulic parameters in Table 3. For this test case a fixed coarse grid was set as Δz = 0.30 m and Δr = 0.04 m with a time step of Δt = 500 s. The fine grid solution was obtained for a grid of $\Delta z = 0.04$ m ($\Delta r = 0.04$ m, $\Delta t = 500$ s). This is the larger Δz for which the discrepancies, in terms of the centerline-depth at which $\theta = 0.24$ at the end of the simulation, were less than 1% when using the AM, GM and WM internodal averages. Further time step reduction, for all simulations of the above test case, did not produce appreciable changes in the solution for the simulation of 1 year of infiltration. The volumetric water content contours, at the end of a 1 year of infiltration, are depicted in Figure 6 for the different averaging methods. While the contours appear to be qualitatively similar, severe deviations from the fine-grid solution are noticeable for the GM and WM and AM procedures for $\theta = 0.24$, which at r = 0 are ahead of the fine grid-solution contours (for $\theta = 0.24$) by 6.2%, 8.9% and 18.3%, respectively. We note that the one-year fine-grid simulation required about 23-28 minutes of computer time for the coarse grids. In contrast, 2 hours and 45 minutes were required to complete the computations for the fine grid solution.

The above two-dimensional infiltration examples illustrate that the present approach makes it feasible to use a coarse grid which results in significant computational time reduction. Moreover, it is noted that only the WM procedure provides the proper θ-contour profiles for both of the test cases considered above.

3.5 Infiltration into a layered soil

The proposed method of computing internodal conductivities can also be applied to layered soils as illustrated in this section for one-dimensional infiltration. The application of the algorithm involves the location of a grid nodal point at the boundary between layers, and the use of pressure as a continuum variable along the system [*Bear and Bachmat*, 1991]. The above strategy assures that all internodal fluxes are calculated within a homogeneous soil layer.

The layered soil structure selected for the present example follows *Hills et al.* [1989]. The soil domain consists of alternating layers of Berino loamy fine sand and Glendale clay loam, each 20 cm thick with a total soil depth of 1m. Both soil types were described by the VG hydraulic function with the parameters (Table 3) as reported by *Hills et al.* [1989]. The soil system was set with an initial uniform water pressure head of -100 m and a top boundary condition of constant water pressure head of ψ = -0.50 m. An illustrative results of the above test case, after a 2 day infiltration period, are shown in Figure 7 for a grid of spacing of Δz = 5 cm. and Δt = 1 s. Also shown in Figure 7 are a fine-grid solution (Δz = 0.005 m, Δt = 1 s) and the initial condition profile. We note that the simulation results (for all cases) were invariant to further decrease of the time step. Comparison of the volumetric water content profiles for the different solutions (Fig. 7) demonstrates that the WM procedure closely tracks the fine grid solution. The profile front, located at a depth of 0.725 m according to the fine grid solution, is overestimated by 3.45% (depth of 0.75 m). According to the fine grid solution the total volume that has entered the system is 0.1409 m^3/m^2, while the WM simulation results in a discrepancy of only 0.2%. The AM method overshoots the location of the front, setting it at 0.8 m with a corresponding 5.1% overestimate of the water volume that entered the system relative to the fine grid solution. The GM averaging method resulted in the greatest deviation with the water front predicted at a depth of about 0.5 m and a total infiltrated water volume 20.3% below that of the fine grid solution.

Conclusions

A new procedure for evaluating interblock permeabilities for vertical flow in unsaturated soil is proposed. The approach is based on estimating the weight of a weighting average of contiguous grid point permeabilities. From a large set of refined numerical solutions of the steady state vertical unsaturated flow, a correlation of the weights as a function of the encompassing relative permeabilities, the dimensionless internodal distance and a soil dependent parameter, was developed for soils described by the hydraulic functions proposed by van Genuchten [1980] and Brooks and Corey [1964]. The correlation can be easily implemented in a numerical code with a level of complexity comparable to the popular geometric and arithmetic means. The proposed method can save computational time in multidimensional simulations with a reasonable level of accuracy. The method is also applicable to layered soils with an accuracy that is highest for the weighted mean procedure of averaging of internodal permeabilities. The present results, consistent with previous studies, show that use of the arithmetic mean averaging procedure overestimates the relative permeabilities while the geometric mean procedure tends to underestimate the relative permeabilities. The present proposed weighted averaging scheme allowed the use of coarse grids while maintaining a reasonably high accuracy (relative to a fine grid solution) when predicting moisture profiles and cumulative infiltration.

Appendix: Weighting scheme for transition from saturated to unsaturated conditions.

The interblock relative conductivity can be easily calculated when two contiguous grid points are locally saturated, since it is unity in both points and consequently, the interblock value is also unity. A question arises when, locally, one grid point is saturated and its neighboring grid point is unsaturated. In such a circumstance, the averaging scheme as presented in equations (3, 4) is not applicable and alternate scheme is required as presented below.

We consider an upper grid point (*U*) situated at z_U and a contiguous lower grid point (*L*) at z_L. The point *U* is saturated with a head ψ_U, whereas *L* is unsaturated with a head ψ_L. The goal is to calculate an effective relative conductivity, k', such as

$$q^* = -k'\left(\frac{\psi_L - \psi_U}{z_L - z_U} - 1\right) \quad \text{(A1)}$$

Between z_L and z_U there must be a point, z_S, at the border between the saturated and the unsaturated zone. The water head at this point is $\psi_S = 0$ for the VG type of hydraulic function, whereas $\psi_S = \psi_b$ for the BC hydraulic function. Since the flux in the saturated and the unsaturated contiguous parts must be equal the following must hold

$$q^* = -k_S\left(\frac{\psi_S - \psi_U}{z_S - z_U} - 1\right) = -k_w\left(\frac{\psi_L - \psi_S}{z_L - z_S} - 1\right) \quad \text{(A2)}$$

where $k_S = 1$ is the relative conductivity at saturation and k_W is the relative conductivity, calculated with the weighting procedure described in this paper, for the zone between z_S to z_L. Combining (A1) and (A2) leads to

$$k' = \frac{k_W (z_L - z_U)}{(z_L - z_S) + k_W (z_S - z_U)} \tag{A3}$$

where z_S is the single unknown necessary for calculating k_W and k'. This z_S can be calculated exactly from (A2) using an iterative procedure. However, a reasonable approximation can be arrived at by considering that the water head varies linearly between z_U and z_L. This approximation is true for the saturated segment and hold reasonably well for the unsaturated segment because it should be near saturation. Therefore, we can write

$$z_L - z_S = (z_L - z_U) \frac{\psi_L - \psi_S}{\psi_L - \psi_U} \tag{A4}$$

and finally,

$$k' = \frac{k_w (\psi_L - \psi_U)}{(\psi_L - \psi_S) + k_w (\psi_S - \psi_U)} \tag{A5}$$

Evaluation of internodal conductivities calculations by (A5 was tested for a loamy sand with the parameters (Table 3) reported by *Rawls and Brakensiek* [1989]. Comparison of the differently computed effective conductivities for this soil, for a constant ψ_L = -1.0 m and ψ_U ranging from ψ_b = -0.0869 to 0.5 m, is provided in Fig. A.1. Classical average calculations of k are insensitive to variations of the upper water pressure head once saturation is reached, while the lower water pressure is maintained constant. Figure A.1 shows these constant k values calculated with AM and GM. In contrast, k_{eff} values calculated by quadrature of (3) show a monotonic increase as the upper pressure increases. This increase is closely followed by k' as computed from (A5).

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Figure Captions

Figure 1. Schematic representation of the flux between non-uniform cells.

Figure 2. Weights from the correlation and exact database values for n = 2 and $\Delta z^{*} = 0.20$. (a) Brooks and Corey and (b) van Genuchten type of hydraulic function.

Figure 3. Dimensionless fluxes, based on the different averaging procedures, between two nodal points with $\psi_U^{*} = -1$, $\psi_L^{*} = -2$, and $\Delta z^{*} = 0.5$ as a function of the parameter n of the van Genuchten equation.

Figure 4. Cumulative infiltration (a, b) and volumetric water content profile (c, d) after 100 h of infiltration into a soil with $n = 2$ and van Genuchten type of hydraulic function. Numerical solution with Δz = 0.05 m (a, c) and Δz = 0.10 m (b, d).

Figure 5. Contours of the volumetric water content after 4 days of infiltration from a surface circular area source of 0.055 m. Comparison of a fine grid solution and results based on the different averaging procedures with Δz = 0.08 m.

Figure 6. Contours of the volumetric water content after 365 days of infiltration from a surface circular area source of 0.220 m. Comparison of a fine grid solution and results based on the different averaging procedures with Δz = 0.30 m.

Figure 7. Volumetric water content profile in a layered soil. Comparison of a fine grid solution with results from the different averaging procedures with Δz = 5.0 cm after 2 days of infiltration under a constant surface water pressure head.

Figure A.1. Interblock permeabilities for a saturated upper node with different water pressures and constant water pressure at the lower node (calculations for a loamy sand).

List of Tables

Table 1. Constants for the correlation $w = w(k_U, k_L, n, \Delta z^*)$ for the hydraulic functions of Brooks and Corey (BC) and van Genuchten (VG).

	a_{10}	a_{11}	a_2	b_{01}	b_{02}	b_1	c_0	β
BC	0.208	0.634	0.191	0.690	2.294	0.049	0.020	0.0080
VG	0.465	0.052	0.112	0.551	1.939	0.057	0.0090	0.011

Table 2. Statistical parameters for the errors and correlation coefficient for the fitting of the weights (w) to the databases values for Brooks and Corey (BC) and van Genuchten (VG) hydraulic functions.

	BC	VG
Average absolute error	0.013	0.025
Average relative errors	22%	20%
Correlation coefficient	0.998	0.992

$error_i = \left|(w_i)_{database} - (w_i)_{correlation}\right|$, for i = 1,..,ndb; where ndb is the number of points in the database; $average\ absolute\ error = \sum_{i=1}^{ndb} error_i \Big/ ndb$;

$average\ relative\ error = \sum_{i=1}^{ndb}\left(error_i / (w_i)_{database}\right) \Big/ ndb\ x\,100$

Table 3. Parameters used for different soils.

	Functions	ψ_{ref} (m)	n	θ_s	θ_r	K_s (m/s)
Sandy loam *Carsel and Parrish* [1988]	VG	0.133	1.89	0.41	0.065	$1.23\ 10^{-5}$
Yolo light clay *Warrick* [1991]	VG	0.667	2	0.495	0.124	$1.23\ 10^{-7}$
Loamy sand *Rawls and Brakensiek* [1989]	BC	0.0869	1.474	0.401	0.035	$1.70\ 10^{-5}$
Silty caly *Rawls and Brakensiek* [1989]	BC	0.3419	1.127	0.423	0.056	$2.50\ 10^{-7}$
Berino loamy fine sand *Hills et al*. [1989]	VG	0.357	2.2390	0.3658	0.0286	$6.26\ 10^{-5}$
Glendale clay loam *Hills et al*. [1989]	VG	0.962	1.3954	0.4686	0.1060	$1.52\ 10^{-6}$

Table 4. Dimensionless fluxes for an average sandy loam soil and ratio between the flux calculated using different averaging procedures and the integral value[(a)].

ψ_L (m)	ψ_U (m) -0.01	-0.1	-1	-10	-100
			q^* **(integral)**		
-0.01	0.805	0.110	-2.20e-2	-2.22e-2	-2.22e-2
-0.1	0.817	0.120	-6.64e-3	-6.80e-3	-6.80e-3
-1	0.819	0.123	3.86e-5	-4.60e-5	-4.60e-5
-10	0.819	0.123	7.96e-5	2.38e-9	-3.59e-8
-100	0.819	0.123	7.97e-5	3.80e-8	1.14e-13
			q^* **(arithmetic mean)/** q^* **(integral)**		
-0.01	1.00	2.31	72.4	889.	9062.
-0.1	0.82	1.00	31.7	430.	4420.
-1	2.92	2.69	1.00	18.5	207.
-10	25.1	24.8	11.2	1.00	14.9
-100	246.	245.3	120.	14.2	1.00
			q^* **(geometric mean)/** q^* **(integral)**		
-0.01	1.00	1.55	1.00	9.67e-2	7.61e-3
-0.1	0.55	1.00	1.14	0.12	9.59e-3
-1	4.05e-2	9.65e-2	1.00	0.29	2.51e-2
-10	2.72e-3	6.96e-3	0.17	1.00	0.23
-100	2.07e-4	5.32e-4	1.46e-2	0.22	1.00
			q^* **(weighted mean)/** q^* **(integral)**		
-0.01	1.00	0.89	1.17	0.77	0.41
-0.1	1.12	1.00	1.11	0.79	0.43
-1	1.12	1.31	1.00	0.86	0.51
-10	5.77	5.77	3.29	1.00	1.17
-100	55.9	55.7	27.4	3.58	1.00

[(a)]VG parameters for an average sandy loam soil as reported by *Carsel and Parrish* [1988] and given in Table 3. The internodal distance considered is Δz = 0.20 m.

Table 5. System, boundary and initial conditions for the examples in cylindrical coordinates.

Test	r_{bc} **(m)**	R_T **(m)**	Z_T **(m)**	q_0 **(m/s)**	**soil**	$\psi_{initial}$ **(m)**	**simulation time (days)**
2DA	0.055	0.70	1.100	$1.389\ 10^{-5}$	Loamy sand	-20.	4
2DB	0.220	2.80	4.100	$8.333\ 10^{-8}$	Silty clay	-100.	365

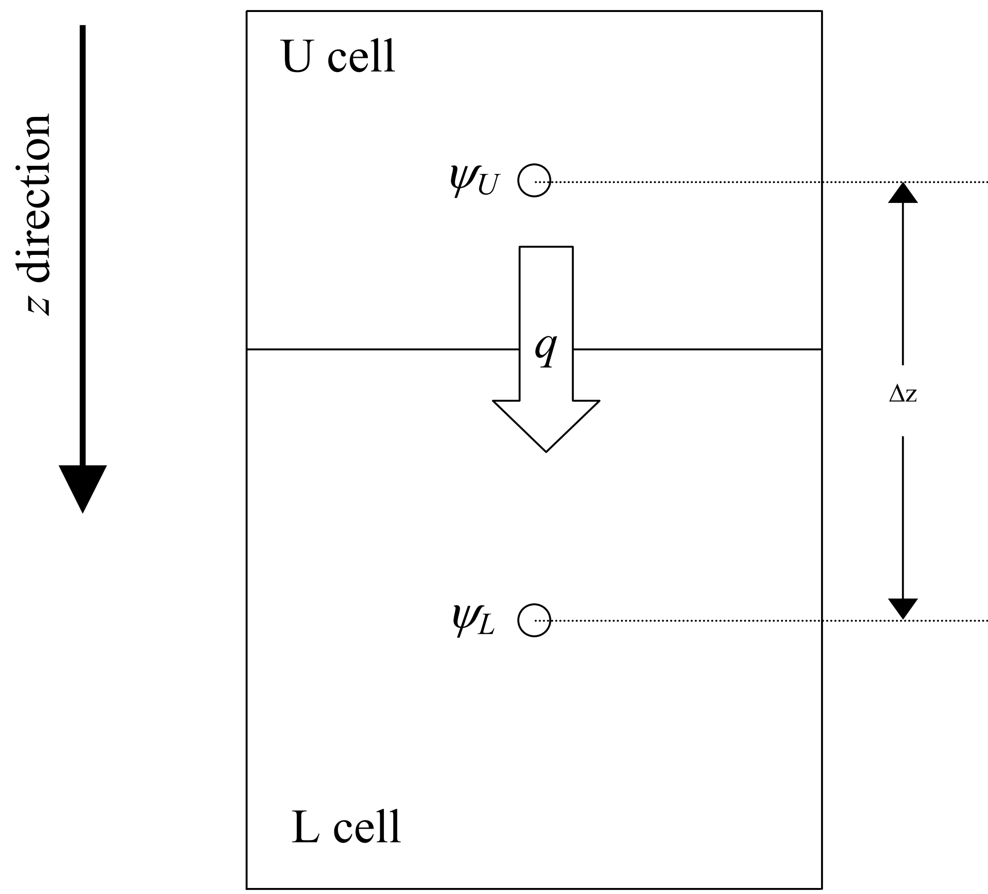


Figure 1

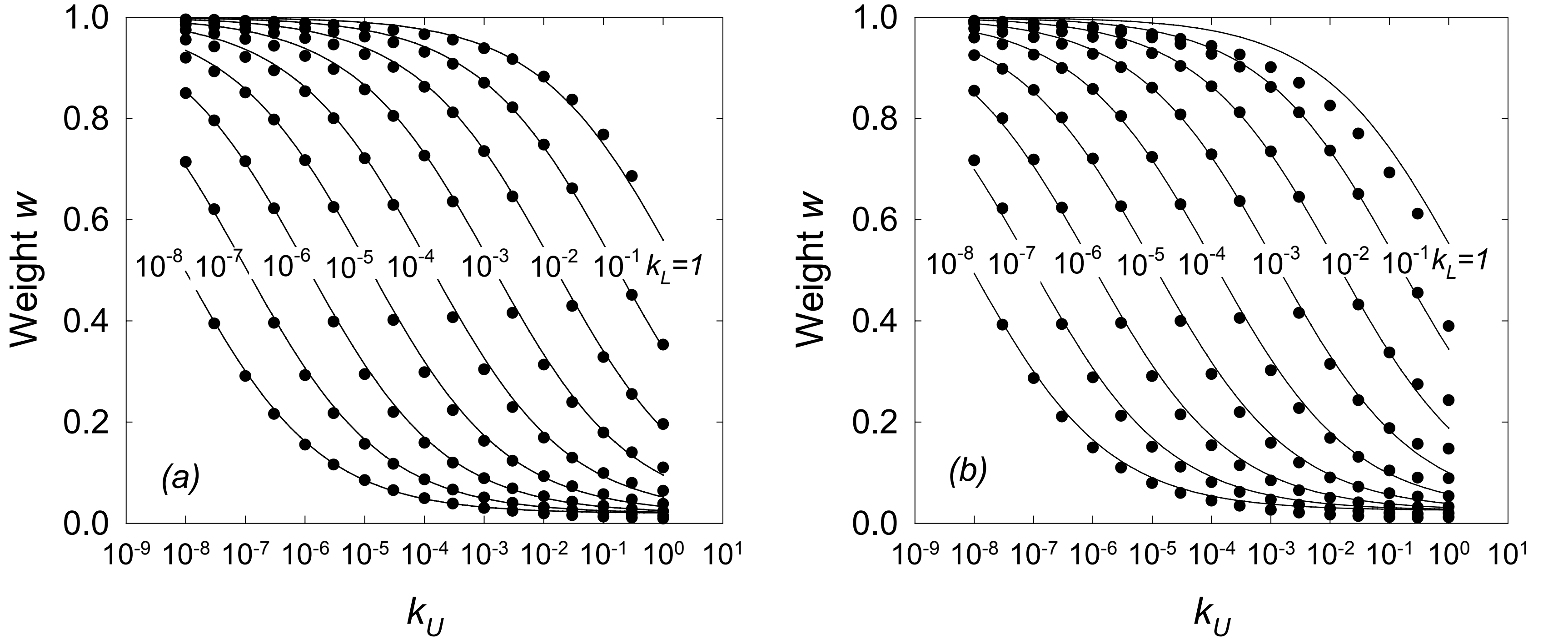

Weight w
1.0
0.8
0.6
0.4
0.2
0.0
10-8 10-7 10-6 10-5 10-4 10-3 10-2 10-1 kL=1
(a)
10-9 10-8 10-7 10-6 10-5 10-4 10-3 10-2 10-1 100 101
kU
(b)

Figure 2

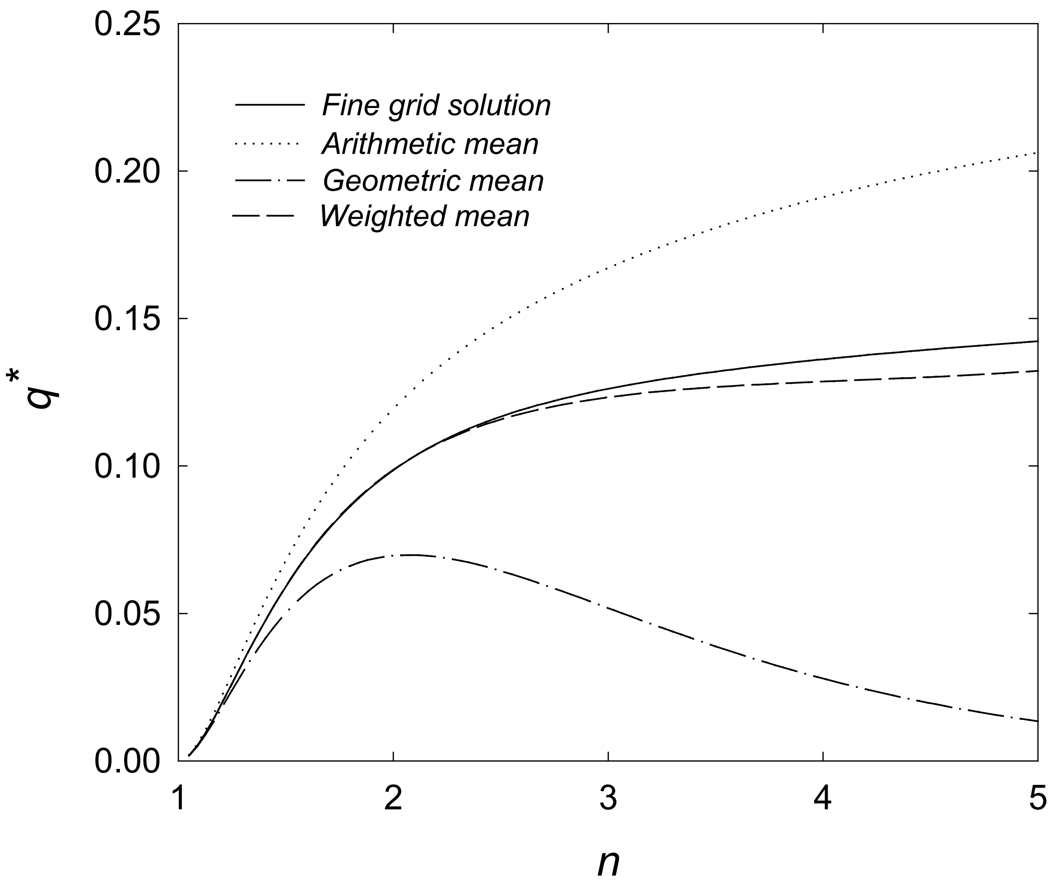
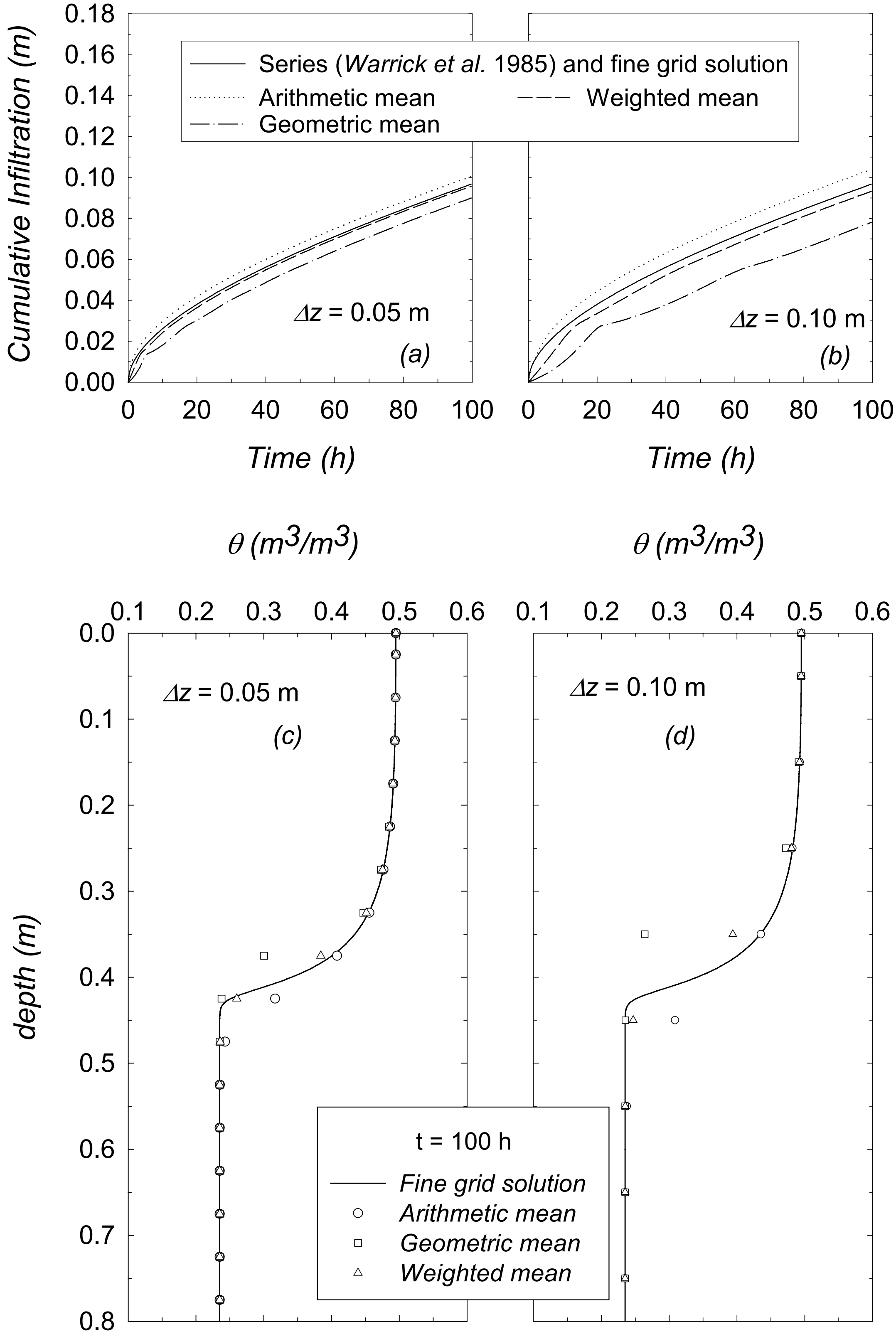

0.25
0.20
0.15
0.10
0.05
0.00
q*
Fine grid solution
Arithmetic mean
Geometric mean
Weighted mean
1
2
3
4
5
n

Figure 3



Cumulative Infiltration (m)
Series (Warrick et al. 1985) and fine grid solution
Arithmetic mean
Weighted mean
Geometric mean
Δz = 0.05 m
(a)
Δz = 0.10 m
(b)
Time (h)
Time (h)
θ (m3/m3)
θ (m3/m3)
Δz = 0.05 m
(c)
Δz = 0.10 m
(d)
depth (m)
t = 100 h
Fine grid solution
Arithmetic mean
Geometric mean
Weighted mean

Figure 4

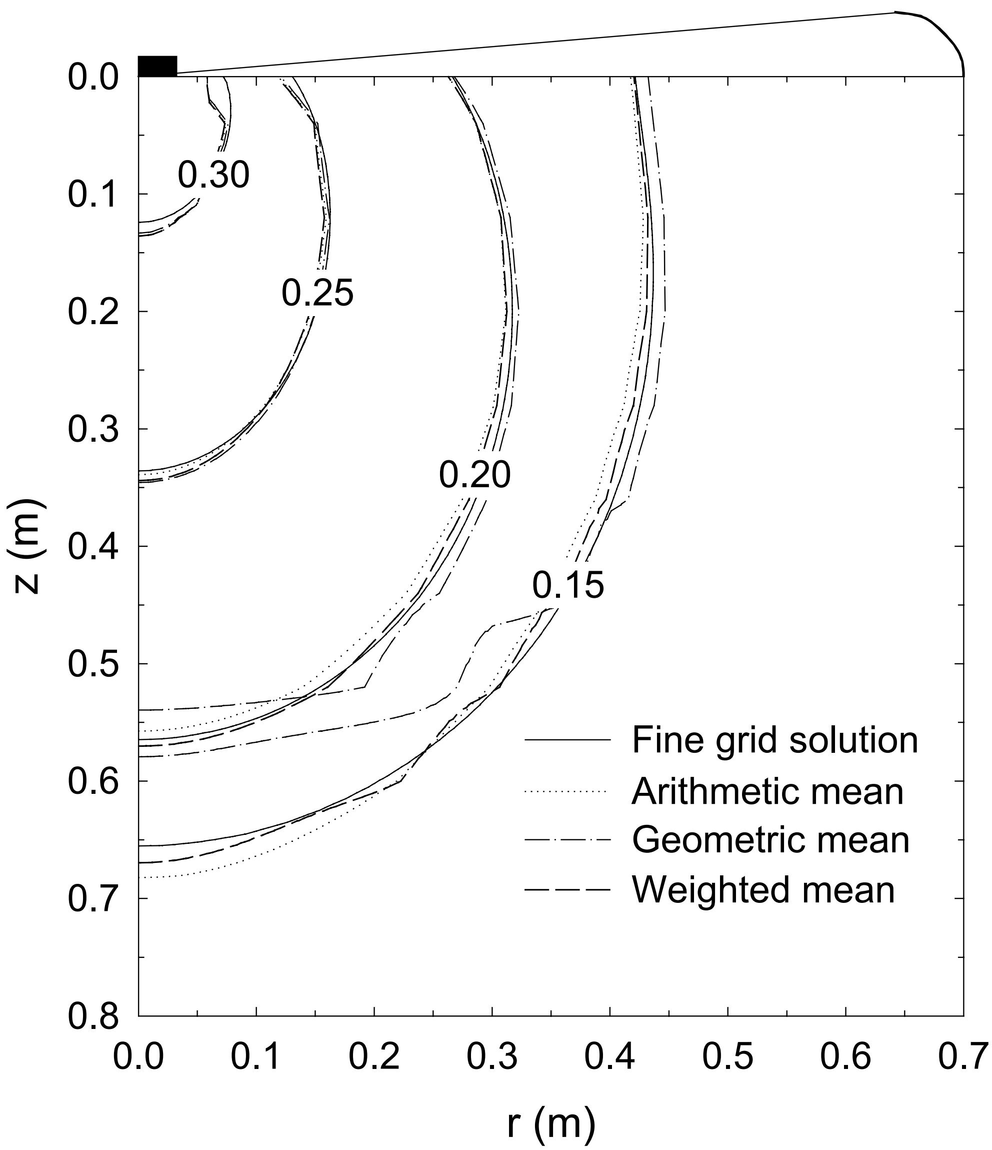
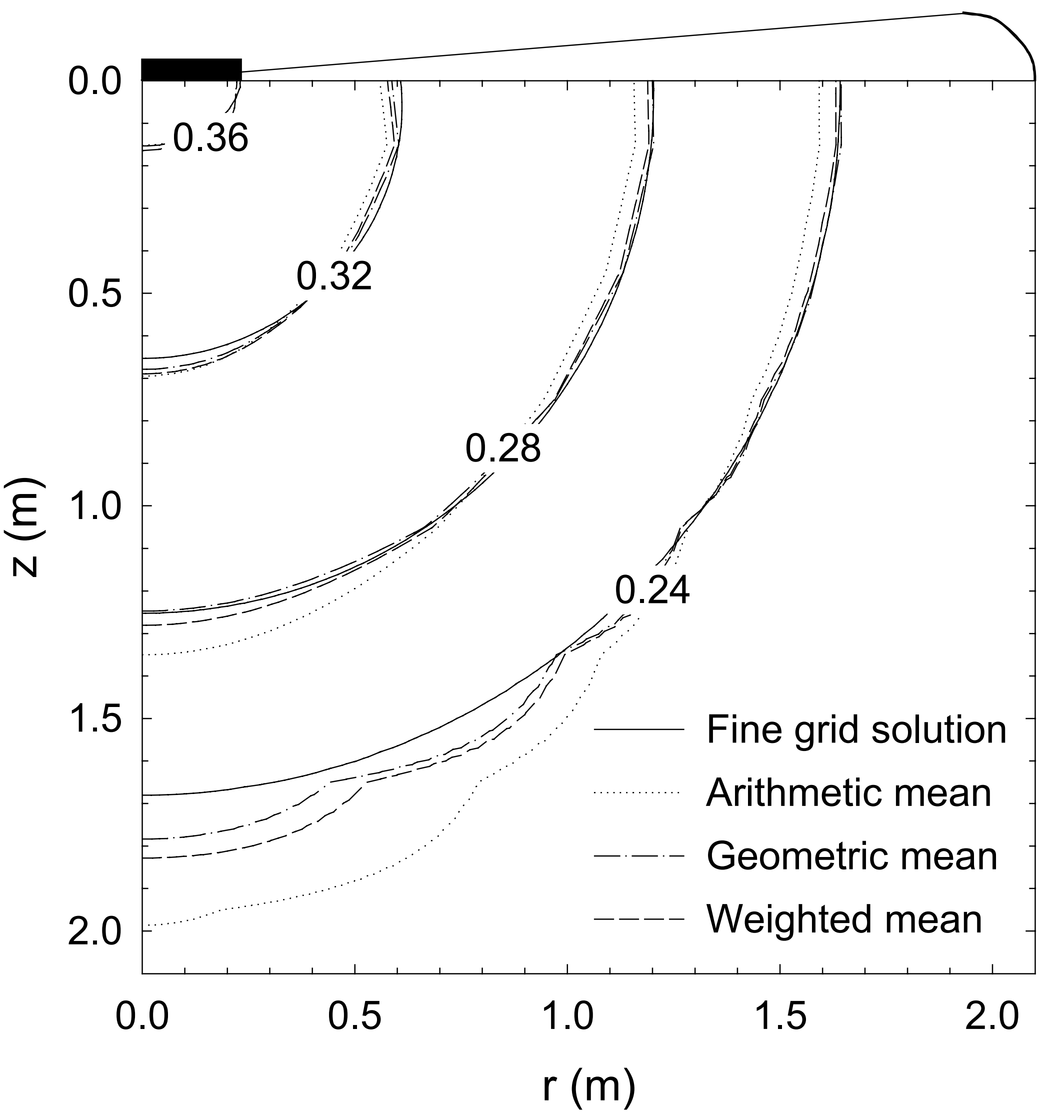
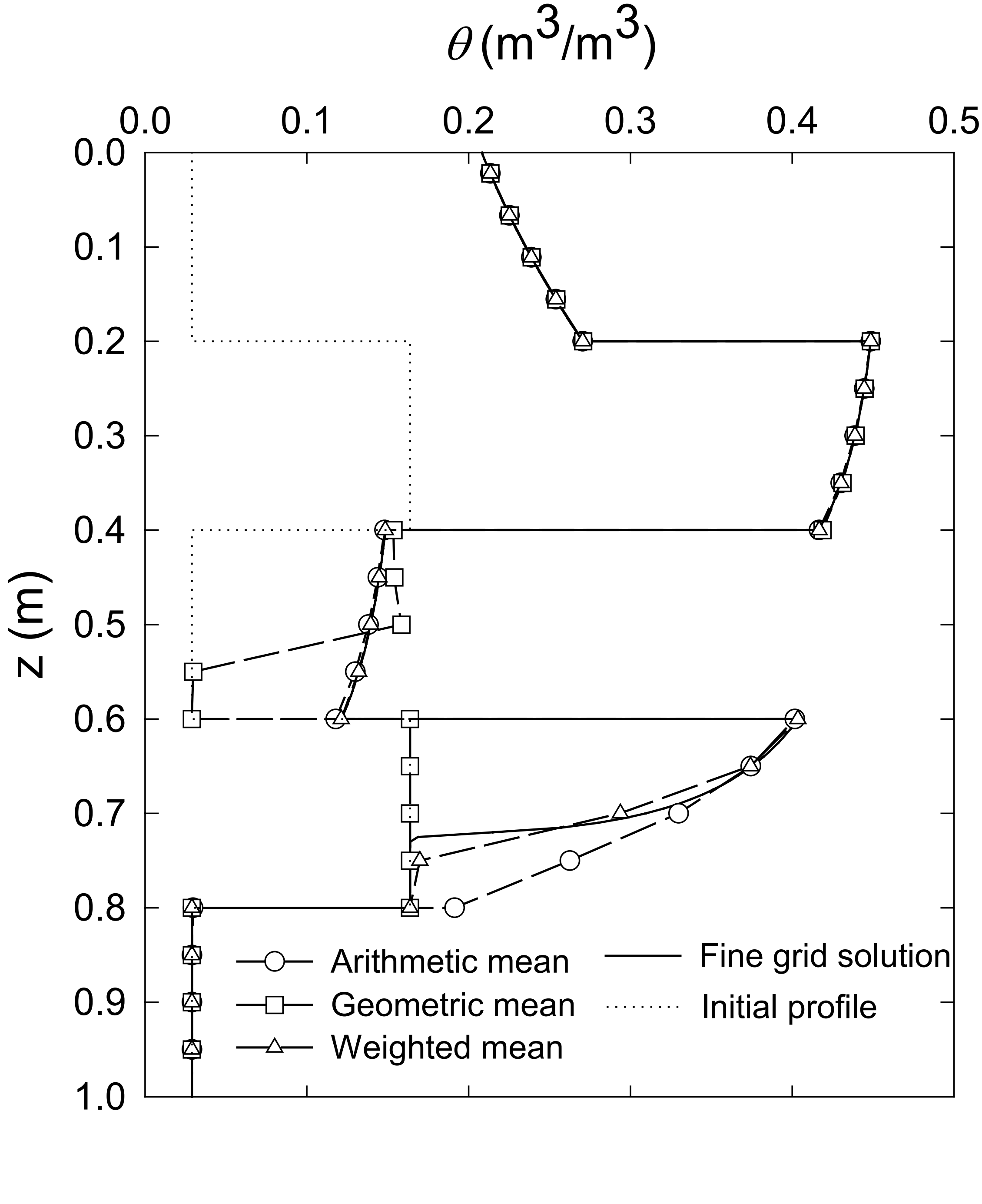

0.30
0.25
0.20
0.15
Fine grid solution
Arithmetic mean
Geometric mean
Weighted mean
z (m)
r (m)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8

Figure 5



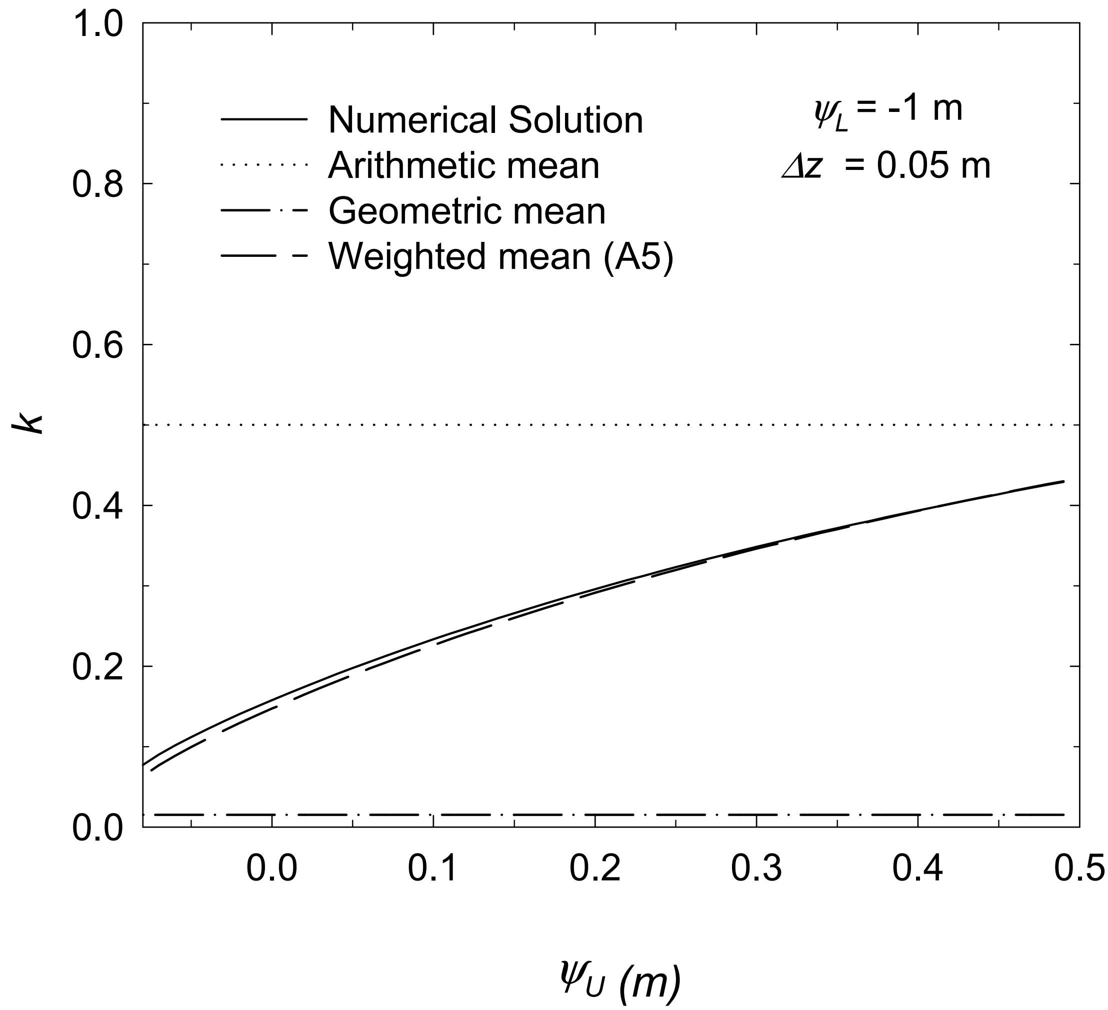
0.36
0.32
0.28
0.24
0.0
0.5
1.0
1.5
2.0
z (m)
0.0
0.5
1.0
1.5
2.0
r (m)
Fine grid solution
Arithmetic mean
Geometric mean
Weighted mean

Figure 6



θ (m3/m3)
0.0
0.1
0.2
0.3
0.4
0.5
z (m)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Arithmetic mean
Geometric mean
Weighted mean
Fine grid solution
Initial profile

Figure 7



1.0
0.8
0.6
0.4
0.2
0.0
k
Numerical Solution
Arithmetic mean
Geometric mean
Weighted mean (A5)
ψ_L = -1 m
Δz = 0.05 m
0.0
0.1
0.2
0.3
0.4
0.5
ψ_U (m)

Figure A1