Homogenization of Richards equation in permeability fields with different connectivities

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[1] Large-scale modeling of transient flow in the unsaturated zone is important for the estimation of the water budget and solute transport in the vadose zone. Upscaled flow models need to capture the impact of small-scale heterogeneities, which are not resolved by the model, on large-scale flow. We perform upscaling of the Richards equation in heterogeneous porous media with continuous distributions of the soil hydraulic parameters using homogenization theory and stochastic averaging techniques. We restrict the analysis to flow regimes in which the capillary-equilibrium assumption holds on the small scale. In order to account for effects of capillary entry pressure we apply the Brooks-Corey model for the soil retention and relative permeability curves and consider Leverett scaling for the coupling of intrinsic permeability and entry pressure. For this model we derive and analyze the ensemble-averaged parameter functions for the macroscopic flow equations. The effects of a definite entry pressure vanish with increasing variance of the log intrinsic permeability. We compare the statistically averaged parameter functions to numerically calculated effective functions for parameter fields with different connectivity properties. These results illustrate that soils with well-connected coarse materials differ in the relative permeability from those with well-connected fine materials or those without particular connectedness.

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1. Introduction

[2] A major problem of flow in natural porous media is the heterogeneity of the soil. Mostly, we are interested in the flow behavior on scales which are too large to resolve the details of soil-hydraulic parameter fields. Also, the exact distributions are generally not known. Thus we need equivalent flow models describing the flow on the large scale in an average sense. These so-called upscaled models are characterized by effective parameters or processes, which capture the influence of the small-scale heterogeneities on the larger scale. A common framework of upscaling is the stochastic one. Here the spatially variable parameters are interpreted as outcome of a random space process with known statistical properties, and the upscaled flow equations are derived by ensemble averaging the statistical (small-scale) flow equations. Typically, this is done by applying perturbation techniques, where terms of the flow equation are expanded to a certain order in the fluctuations of the parameter fields [see Zhang, 2002].

[3] In the unsaturated zone, not only the intrinsic permeability is an important spatially variable parameter, but also the capillary properties of the soil. These effects may counteract. Coarse materials show high permeability under

saturated conditions, but have a small entry pressure, and the total permeability drops off rapidly with decreasing saturation. By contrast, fine materials are low permeable under saturated condition, but remain rather wet at higher capillary pressures. As a result, materials with fine texture can have higher total permeabilities than those with coarse texture in regimes with high capillary pressure. As flow in the unsaturated zone is nonlinear, upscaling with statistical models is not straightforward, especially when transient flow processes are considered.

[4] Field-scale experiments on flow and transport in the unsaturated zone have shown, that these processes are very complex and are often prone to preferential flow and channeling [e.g., Roth *et al.*, 1991; Forrer *et al.*, 1999]. Deriving upscaled models, which capture these phenomena, is thus a challenging task. It requires good understanding how small-scale processes affect large-scale behavior, and appropriate models for the soil heterogeneity are needed, which reflect the properties influencing preferential flow.

[5] The steady state unsaturated flow equation, denoted Richards equation, has been analyzed in a stochastic framework by Yeh *et al.* [1985], Russo [1992], and Indelman *et al.* [1993], and the transient case has been analyzed by Mantoglou and Gelhar [1987] and Zhang [1999]. These authors derived ensemble moments of the soil parameters, such as the capillary pressure parameters and the permeability, as well as the statistical moments of the capillary

head and the flow velocities. Because of the nonlinearity of the flow equations, the results underly restrictions. A typical assumption is that the mean flow is exclusively driven by gravity, so that the mean capillary head is uniform. Another typical assumption is that the relationship between the capillary pressure and the saturation follows an exponential function [Gardner, 1958; Russo, 1988]. This model does not include entry pressure effects. Although entry pressure effects are less important for water in the unsaturated zone than for nonwetting fluids in multifluid flow, a model without entry pressure does not reflect the variability of saturation and thus relative permeability at low pressure values [cf. Zhang *et al.*, 1998]. The threshold behavior of the parameter functions in models which consider capillary entry pressure makes the averaging procedure more complex. Zhang *et al.* [1998] analyzed the Richards equation for the steady state using a Brooks-Corey model [Brooks and Corey, 1966], where effects of a definite entry pressure are accounted for. More recent studies also overcome the restriction of gravity-driven flow [see Zhang, 2002, chap. 5]. All of these studies, however, have used perturbation approximations in terms of the logarithm of the saturated permeability.

[6] Lewandowska and Laurent [2001] applied homogenization theory for media composed of several distinct materials to Richards equation for the strictly capillary-dominated flow regime, deriving exact upscaled flow parameters. Homogenization theory has the advantage that it yields upscaled equations, where effective parameters can be derived directly. The method introduces an expansion parameter, the ratio between two typical length scales. Since all terms in the flow equation are scaled with this parameter, results are restricted to certain flow regimes. The regimes are quantified by the scaling of the dimensionless characteristic flow parameters with this length scale ratio. Traditionally, homogenization theory is set up for deterministic fields with two (or more) distinct properties, where the interfaces between the two materials are clearly defined and the boundary conditions at these interfaces are considered in the upscaling procedure [cf. Hornung, 1997].

[7] In the statistical framework, the use of two-point covariances of the parameters requires a simple correlation structure, such as in multi-Gaussian fields. The parameter fields are therefore mostly assumed to be continuous and change smoothly. For these type of fields, homogenization theory can also be applied. Lunati *et al.* [2002] investigated macrodispersion for solute transport in continuously changing stochastic fields using homogenization theory. In this framework, two expansions are performed: the first in space, expanded about the ratio of the typical length scales, and the second in the parameter of interest (e.g., the conductivity), expanded about a mean parameter value. The latter expansion leads to ensemble-averaged parameters.

[8] In the present study, we apply homogenization theory to the Richards equation for continuously changing stochastic fields. With the homogenization approach, we derive the upscaled equation. The focus of the present study is on the effective retention curve and total permeability rather than on flow velocities. Therefore the application lies more in water budget related questions than on solute dispersion. The parameter fields are random and periodic [see Cirpka and Kitanidis, 2002]. We use the Brooks-Corey formulation to describe the relation between relative permeability and

pressure head and thus consider entry pressure effects. We assume that the entry pressure and the permeability are coupled according to Leverett [1941]. We restrict the analysis to the flow regime, which is dominated by capillary forces on the small scale, similar to Lewandowska and Laurent [2001]. Thus the results for the upscaled equations may not be as general as those obtained by general stochastic models. For this particular flow regime, the multiscale expansion performed in the homogenization approach leads to a saturation distribution, which can be considered static on the small scale. This allows to perform a perturbation expansion in terms of the logarithm of the total (unsaturated) rather than the saturated conductivity. Using this type of expansion, we calculate the statistically averaged parameter functions to second order. We show, that the results differ from the results of perturbation theory in terms of log saturated permeability. The differences are most pronounced at pressure values close to the geometric mean of the entry pressure.

[9] In stochastic theory, the heterogeneities of the soil are usually characterized by the mean, variance and integral scale of the parameters. Higher-order spatial properties such as the connectivity of certain parameter values are mostly neglected. However, it has been found in a number of field experiments on tracer transport, that statistic properties of second order are often not sufficient to characterize the soil in an appropriate manner [e.g., Desbarats and Srivastava, 1991; Labolle and Fogg, 2001]. Connectivity properties are especially important for nonlinear flow processes, where the flow can develop a channeling behavior. The importance of connectivity properties for the effective flow parameters has already been stressed by Gomez-Hernandez and Wen [1997] and Zinn and Harvey [2003] in single-phase flow. Here we analyze the impact of connectedness on unsaturated flow.

[10] In general, connectivity properties are difficult to quantify by statistical properties of the parameter field. Yet, percolation theory yields measures such as two-point cluster functions applied to a two-cut indicator field [e.g., Torquato *et al.*, 1988] which reflect the connectivity of certain parameter ranges. Such concepts have been applied to soil fields by Western *et al.* [2001]. Zinn and Harvey [2003] and Vogel [2002] introduced the absolute value transformation as an efficient method to generate fields with certain connectivity properties, providing the opportunity to investigate the impact of connectivity properties on effective flow behavior by Monte Carlo simulations. The result of the generator are fields with identical two-point correlation functions and probability distributions but differing in the parameter range forming continuous bands. We investigate such fields in order to discuss the influence of connectivity on the effective and ensemble-averaged relative permeability curves in unsaturated soils.

2. Homogenization of the Flow Equation in Capillary Equilibrium

2.1. Flow Equations

[11] We consider transient water flow in the unsaturated zone, described by Richards equation:

$$\Psi(h) \frac{\partial h}{\partial t} + \nabla \cdot \mathbf{u} = q \quad (1)$$

in which h [L] is the hydraulic head, having negative values in unsaturated systems, $\mathbf{u}$ [L/T] is the specific discharge of soil water, q [1/T] stands for volumetric sources and sinks and $\Psi(h) = d\Theta/dh$ [1/L] is the water retention function, where Θ (dimensionless) is the volumetric water content. The specific discharge follows Darcy's law:

$$\mathbf{u} = -\frac{K_0 k_r(h)g}{\nu}(\nabla h + \mathbf{e}_z) \quad (2)$$

in which K_0 [L²] is the intrinsic permeability, k_r (dimensionless) is the relative permeability, ν [L²/T] is the kinematic viscosity of water, g [L/T²] is the gravity constant, and $\mathbf{e}_z$ (dimensionless) denotes the vertical unit vector pointing upward. We assume the intrinsic permeability to fluctuate about a uniform mean permeability K_g [L²] by a lognormal scaling factor:

$$K_0(\mathbf{x}) = K_g \exp(f_k(\mathbf{x})) \quad (3)$$

in which f_k (dimensionless) is the logarithm of the permeability fluctuations. We could assume that the f_k field is a periodic, isotropic, multi-Gaussian random field characterized by second-order statistics. Applying the Brooks-Corey parameterization for the constitutive relationships $\Psi(h)$ and $k_r(h)$, the hydraulic head is in the order of the entry pressure head h_e which is also assumed to be spatially variable. At first, to be as general as possible, we do not assume particular correlations between the fields of entry pressure head $h_e(\mathbf{x})$ and log permeability fluctuations $f_k(\mathbf{x})$. Like the permeability, we expand the entry pressure head about its geometric mean, here denoted h_g [L], which is assumed uniform. The fluctuations of the entry pressure head are denoted by a lognormal scaling factor f_h (dimensionless), leading to:

$$h_e(\mathbf{x}) = h_g \exp(f_h(\mathbf{x})) \quad (4)$$

In a model lacking an entry pressure, we would expand about a different characteristic value of the hydraulic head.

[12] The Richards equation can be made dimensionless by introducing characteristic scales for all parameters and variables. The characteristic values for time and space are denoted T and L . We choose K_g as the characteristic value of permeability and h_g of the hydraulic head. We thus express the dimensional quantities by

$$h = h_g h^*, \quad \mathbf{x} = L \mathbf{x}^*, \quad t = T t^*, \quad \Psi = \frac{\Psi^*}{h_g} \quad (5)$$

in which symbols with stars are dimensionless. Note that by choosing the entry pressure head as scaling parameter, the relative permeability k_r becomes a function of the dimensionless pressure head h^* and the random variable f_h only. The typical timescale T is here chosen as a large-scale timescale:

$$T = \frac{\nu L^2}{h_g K_g g} \quad (6)$$

[13] A small-scale timescale is not taken into account. Substituting equation (2) into equation (1), and applying above mentioned scaling, the dimensionless Richards equation becomes:

$$\Psi^*(h^*) \frac{\partial h^*}{\partial t^*} + \nabla^* \cdot (\exp(f_k) k_r(h^*, f_h) (\nabla^* h^* + Bo \mathbf{e}_z)) = qT \quad (7)$$

in which ∇^* denotes the vector of derivatives with respect to the dimensionless coordinates $\mathbf{x}^*$, and the Bond number Bo is defined as

$$Bo = \frac{L}{h_g} \quad (8)$$

2.2. Homogenized Equations

[14] In homogenization theory, we consider two typical length scales of the system, a large and a small one [cf. *Hornung, 1997; Lewandowska and Laurent, 2001*]. We denote the characteristic length on the large-scale L [L] and that on the small-scale ℓ [L]. The ratio between these two scales is denoted ε (dimensionless):

$$\varepsilon = \frac{\ell}{L} \quad (9)$$

[15] In periodic domains, the large scale typically relates to the size of the domain, whereas the small scale relates to the size of the unit cell or to the size of the heterogeneity.

[16] Now, the functions $f(\mathbf{x})$ are expressed in terms of small-scale coordinates $\hat{\mathbf{Y}}$ and large-scale coordinates $\hat{\mathbf{X}}$. Like *van Duijn et al. [2002]* and *Lewandowska and Laurent [2001]*, we choose $\hat{\mathbf{X}}$ to be a continuous variable. Small-scale fluctuations of the functions are captured in the $\hat{\mathbf{Y}}$ dependence and large-scale fluctuations in the $\hat{\mathbf{X}}$ dependence. So far, that means only denoting variables $\mathbf{x}$ which are related to large-scale fluctuations as $\hat{\mathbf{X}}$ and those related to small scale fluctuations as $\hat{\mathbf{Y}}$.

[17] To make $\hat{\mathbf{X}}$ and $\hat{\mathbf{Y}}$ dimensionless, we now scale them with two different length scales, the large-scale length L and the small-scale length ℓ :

$$\hat{\mathbf{X}} = \hat{\mathbf{X}}^* L, \quad \hat{\mathbf{Y}} = \hat{\mathbf{Y}}^* \ell. \quad (10)$$

By making the variables dimensionless with the two different length scales we really separate the two variables. Now, the dimensionless nabla operator ∇^* has to be split into two dimensionless contributions [cf. *Hornung, 1997*]:

$$\nabla_{\mathbf{x}^*} = \nabla_{\hat{\mathbf{X}}^*} + \frac{1}{\varepsilon} \nabla_{\hat{\mathbf{Y}}^*} \quad (11)$$

in which $\nabla_{\hat{\mathbf{X}}^*}$ is the vector of derivatives with respect to the dimensionless large-scale coordinates $\hat{\mathbf{X}}^*$, whereas $\nabla_{\hat{\mathbf{Y}}^*}$ is that with respect to the small-scale ones $\hat{\mathbf{Y}}^*$. In the following, we will exclusively consider dimensionless variables, omitting the star in the notation.

[18] In the end, we average the fluctuations on the small scale out. In principle, this is not different from the usual stochastic approach, if we average over a sampling volume which is large enough to cover a representative sample of

the fluctuating parameter field. The average over the volume leads again to an upscaled continuous system on a larger scale [Dagan, 1989].

[19] We perform an expansion of the hydraulic head h in terms of ε

$$h(\hat{\mathbf{X}}, \hat{\mathbf{Y}}, t) = h^{(0)}(\hat{\mathbf{X}}, \hat{\mathbf{Y}}, t) + \varepsilon h^{(1)}(\hat{\mathbf{X}}, \hat{\mathbf{Y}}, t) + \varepsilon^2 h^{(2)}(\hat{\mathbf{X}}, \hat{\mathbf{Y}}, t) + \dots \quad (12)$$

[20] All functions of the hydraulic head, such as the retention curve $\Psi(h)$ and the relative permeability $k_r(h)$ can also be expanded by Taylor series about $h^{(0)}$. To keep the notations short, we will not formulate the expansions explicitly but use $\Psi(h) = \Psi^{(0)} + \varepsilon \Psi^{(1)} + \varepsilon^2 \Psi^{(2)} + \dots$ and $k_r(h) = k_r^{(0)} + \varepsilon k_r^{(1)} + \varepsilon^2 k_r^{(2)} + \dots$ with

$$\begin{aligned} \Psi^{(1)} &= \left. \frac{d\Psi}{dh} \right|_{h=h^{(0)}} h^{(1)} \\ \Psi^{(2)} &= \left. \frac{d\Psi}{dh} \right|_{h=h^{(0)}} h^{(2)} + \frac{1}{2} \left. \frac{d^2\Psi}{dh^2} \right|_{h=h^{(0)}} (h^{(1)})^2 \end{aligned} \quad (13)$$

and equivalent terms for k_r . To do so, all orders of the hydraulic head must be continuous. Also, the resulting flux must be continuous on all scales. Considering a periodic field, the fluctuations of h with the local coordinates $\hat{\mathbf{Y}}$ must be periodic.

[21] Substituting equation (11) and the expansions, equations (12) and (13), into the dimensionless Richards equation, equation (7), yields an expression containing all orders of ε . We assume now that the large and small scales are clearly separated, that is, ε is very small. Then, we may collect terms in equation (7) of equal order in ε leading to subequations for which we assume that they are met separately. That is, the original equation is split into a coupled system of equations for the different orders of h in ε . We will finally consider the limit $\varepsilon \rightarrow 0$. Therefore only the orders ε^m with $m \leq 0$ in equation (7) need to be considered [Hornung, 1997] (Appendix A).

[22] A prerequisite for collecting terms of equal order in ε is that the order of the Bond number Bo is known. We restrict our analysis to the case of Bo in the order ε^0 . As has been shown by others, and will be demonstrated in the following, this assumption leads to the capillary equilibrium condition [Pickup and Stephen, 2000]. A Bond number Bo in the order of ε^0 implies that the entry pressure head is in the same order as the large length scale. This choice is crucial, as a different order of Bo or other model parameters would lead to different upscaled equations [cf. Lewandowska et al., 2004].

[23] A second prerequisite for splitting equation (7) into separate equations of different orders in ε is that we restrict the functions k_r , Ψ and the parameters describing the spatial variability. The flow has to be in a regime, where these parameters do not contribute orders ε^m with m different from zero to equation (7). In such a case, the expansion in equation (13) would look different. In particular, under dry conditions, where the retention curve increases over orders of magnitude, this requirement may no longer be met. Also, the relative permeability has to be larger than ε , as otherwise the lowest order in the expansion of k_r would be of the order ε^1 . The following analysis holds therefore only if the saturation is not too small and its fluctuations are moderate.

[24] Under these conditions, the lowest-order equation obtained from equation (7) is of order ε^{-2} (see Appendix A):

$$\nabla_{\hat{\mathbf{Y}}} \cdot \left(\exp(f_k) k_r^{(0)}(f_h) \nabla_{\hat{\mathbf{Y}}} h^{(0)} \right) = 0 \quad (14)$$

This equation is solved by [see, e.g., van Duijn et al., 2002; Lewandowska and Laurent, 2001]:

$$h^{(0)} = h^{(0)}(\hat{\mathbf{X}}, t) \quad (15)$$

[25] Equation (15) states that the system on the small scale is in capillary equilibrium. On this scale the capillary forces are dominant (which is quantified by the Bond number) and lead to a very fast relaxation of head changes. From the standpoint of the large scale, the small-scale relaxation may be considered instantaneous. This concept is often applied when modeling two-phase flow and has also been compared to experiments [e.g., Desbarats, 1995; Braun et al., 2005]. A uniform distribution of the hydraulic head on the small scale does not imply other hydraulic quantities to be uniform because soil parameters still vary on that scale. However, the capillary equilibrium makes the relationship between small-scale hydraulic parameters and large-scale hydraulic head unique.

[26] Considering equation (15), the terms of order ε^{-1} in equation (7) become (see Appendix A):

$$\nabla_{\hat{\mathbf{Y}}} \cdot \left[\exp(f_k) k_r^{(0)}(f_h) \left(\nabla_{\hat{\mathbf{X}}} h^{(0)} + \nabla_{\hat{\mathbf{Y}}} h^{(1)} + Bo \mathbf{e}_z \right) \right] = 0 \quad (16)$$

[27] Finally, the equation of order ε^0 yields the homogenized large-scale flow equation. The upscaled equation is obtained by integrating the zeroth-order equation over the unit cell and dividing it by its volume Ω . As the fields are periodic, all terms in the equation of the type $\nabla_{\hat{\mathbf{Y}}} \cdot \mathbf{v}$ for any vector field $\mathbf{v}$ vanish upon integration. Considering equation (15), the small-scale averaged zeroth-order equation is (see Appendix A):

$$\begin{aligned} \frac{1}{\Omega} \int_{\Omega} \Psi^{(0)} \frac{\partial h^{(0)}}{\partial t} d\hat{\mathbf{Y}} + \frac{1}{\Omega} \nabla_{\hat{\mathbf{X}}} \cdot \int_{\Omega} \exp(f_k) k_r^{(0)}(f_h) \\ \cdot \left(\nabla_{\hat{\mathbf{X}}} h^{(0)} + \nabla_{\hat{\mathbf{Y}}} h^{(1)} + Bo \mathbf{e}_z \right) d\hat{\mathbf{Y}} = \frac{1}{\Omega} \int_{\Omega} q T d\hat{\mathbf{Y}} \end{aligned} \quad (17)$$

[28] In order to obtain the upscaled equation for $h^{(0)}$, we have to solve equation (16) (order $\varepsilon^{(-1)}$) for $h^{(1)}$ and substitute the solution into equation (17).

2.3. General Parameter Fields

[29] We express the first-order term $h^{(1)}$ of the head as a product of a vector of auxiliary variables χ , depending only on the small-scale coordinates $\hat{\mathbf{Y}}$ times the large-scale driving force $\mathbf{J}$ appearing in equation (16) [cf. Hornung, 1997]:

$$h^{(1)} = \chi(\hat{\mathbf{Y}}) \cdot \mathbf{J}(\hat{\mathbf{X}}, t) \quad (18)$$

with

$$\mathbf{J} = \nabla_{\hat{\mathbf{X}}} h^{(0)} + Bo \mathbf{e}_z \quad (19)$$

$\mathbf{J}$ does not depend on the small-scale coordinates $\hat{\mathbf{Y}}$. Now, equation (16) becomes:

$$\nabla_{\hat{\mathbf{Y}}} \cdot \left(\exp(f_k) k_r^{(0)}(f_h) (\mathbf{J} + \nabla_{\hat{\mathbf{Y}}}(\chi \cdot \mathbf{J})) \right) = 0 \quad (20)$$

χ as well as the resulting flux are periodic and continuous. Equation (20) has to be solved for the specific parameter field in the specific unit cell considered. With this approach we obtain for the zeroth-order equation (17) by inserting equations (18) and (19) into equation (17):

$$\Psi_a^{(0)} \frac{\partial h^{(0)}}{\partial t} + \nabla_{\hat{\mathbf{X}}} \cdot \left(\mathbf{K}_e \left(\nabla_{\hat{\mathbf{X}}} h^{(0)} + B o \mathbf{e}_z \right) \right) = q_a T \quad (21)$$

with the arithmetic means $\Psi_a^{(0)}$ and q_a :

$$\Psi_a^{(0)} = \frac{1}{\Omega} \int_{\Omega} \Psi^{(0)} d\hat{\mathbf{Y}} \quad (22)$$

$$q_a = \frac{1}{\Omega} \int_{\Omega} q d\hat{\mathbf{Y}} \quad (23)$$

and the effective dimensionless permeability tensor $\mathbf{K}_e$ (see Appendix B):

$$\mathbf{K}_e = \frac{1}{\Omega} \int_{\Omega} \exp(f_k) k_r^{(0)}(f_h) (\mathbf{I} + \nabla_{\hat{\mathbf{Y}}} \otimes \chi) d\hat{\mathbf{Y}} \quad (24)$$

in which $\otimes$ is the dyadic product operator. The same expression for the effective permeability, equation (24), has been obtained by *Lewandowska and Laurent* [2001] for noncontinuous fields.

[30] The pde for the auxiliary variable χ , equation (20), must be met for any driving-force vector $\mathbf{J}$. We can determine the components of the χ vector by subsequently choosing $\mathbf{J}$ as a unit vector in each principal direction. This leads to the following procedure to determine the functional relationship $\mathbf{K}_e(h^{(0)})$.

[31] 1. Choose a value for the mean hydraulic head $h^{(0)}$ within the unit cell.

[32] 2. Calculate the corresponding distribution of the permeability field $\exp(f_k) k_r^{(0)}(h^{(0)})$ throughout the unit cell.

[33] 3. Choose a unit hydraulic gradient in direction i and apply periodic boundary conditions for the steady state head equation within the unit cell. This results in the field of $\chi_i + \hat{Y}_i$.

[34] 4. Calculate the mean flux vector for $\chi_i + \hat{Y}_i$. This yields the i th column of the effective permeability tensor $\mathbf{K}_e$.

[35] 5. Repeat steps 3 and 4 with the other principal direction(s).

[36] For an arbitrary field, the computations in the outlined procedure have to be done numerically.

2.4. Ensemble Averaging

[37] Conceptually, we so far have analyzed single, spatially variable, periodic fields. In a stochastic framework, we consider these fields as outcome of a random process with known statistical parameters. For a sufficiently large unit cell, the ergodicity assumption holds and we may replace volume averages by ensemble averages. For a smaller unit

cell, the ensemble-averaged quantities are only the expected values of the volume-averaged one; the deviation of the volume average of an actual realization from the ensemble average could still be large.

[38] In the following, we assume the field of the log permeability fluctuations f_k to be multi-Gaussian and isotropic. We will calculate the ensemble-averaged effective parameter functions by a second-order approach. Without the nonlinear relative permeability $k_r^{(0)}$, the problem would be simplified to linear upscaling of saturated flow. In this particular case, the second-order effective permeability for an isotropic covariance function of f_k in a flow field of uniform mean flow is known to be the geometric mean of the permeability in two-dimensional systems, whereas three-dimensional systems require a correction term that is proportional to the variance σ_f^2 of log permeability fluctuations [King, 1987; Dagan, 1993].

[39] In unsaturated flow, however, we must account for the nonlinear relative permeability $k_r(h)$. The product $\exp(f_k) k_r^{(0)}$ is not multiGaussian, and thus the effective permeability may differ from the geometric mean. For stochastic averaging, it is more practical to consider equation (16) for the first-order head $h^{(1)}$ directly, rather than to introduce the auxiliary variable χ . Equation (16) has two spatial parameters varying on the small scale, the log permeability f_k and the log scaling factor of the entry pressure head f_h . We expand the relative permeability as

$$k_r^{(0)}(f_h, h^{(0)}) = k_r^{(0)}|_{f_h=0} + \frac{dk_r^{(0)}}{df_h}|_{f_h=0} f_h + \dots \quad (25)$$

[40] Substituting the perturbation expansion for the spatially variable parameters into the equation of order ε^{-1} , equation (16), yields:

$$\nabla_{\hat{\mathbf{Y}}} \cdot \left(k_r^{(0)}|_{f_h=0} P(\hat{\mathbf{X}}, \hat{\mathbf{Y}}) (\mathbf{J} + \nabla_{\hat{\mathbf{Y}}} h^{(1)}) \right) + k_r^{(0)}|_{f_h=0} \nabla_{\hat{\mathbf{Y}}}^2 h^{(1)} = 0 \quad (26)$$

in which P denotes the fluctuating terms:

$$P = \left(f_k + \frac{1}{2} f_k^2 + \dots \right) + \left(k_r^{(0)}|_{f_h=0} \right)^{-1} \left(\frac{dk_r^{(0)}}{df_h}|_{f_h=0} f_h + \dots \right) \cdot \left(1 + f_k + \frac{1}{2} f_k^2 + \dots \right) \quad (27)$$

Equation (26) can be transformed into the corresponding integral equation:

$$h^{(1)}(\hat{\mathbf{X}}, \hat{\mathbf{Y}}) = \int_{\Omega} G(\hat{\mathbf{Y}}, \hat{\mathbf{Y}}') \nabla_{\hat{\mathbf{Y}}'} \cdot \left(P(\hat{\mathbf{Y}}') (\mathbf{J} + \nabla_{\hat{\mathbf{Y}}'} h^{(1)}(\hat{\mathbf{X}}, \hat{\mathbf{Y}}')) \right) d\hat{\mathbf{Y}}' \quad (28)$$

which is recursive. G is the Green's function solving $\nabla_{\hat{\mathbf{Y}}}^2 G = \delta(\hat{\mathbf{Y}} - \hat{\mathbf{Y}}')$. In a two-dimensional, infinite domain it is given by $G = 1/(2\pi) \ln(|\hat{\mathbf{Y}} - \hat{\mathbf{Y}}'|)$. The periodicity may cause slight deviations.

[41] In the zeroth-order equation, equation (17), we now replace the spatial average by the ensemble average:

$$\langle \Psi^{(0)} \rangle \frac{\partial h^{(0)}}{\partial t} + \nabla_{\hat{\mathbf{X}}} \cdot \left(\langle \exp(f_k) k_r^{(0)}(f_h) \rangle (\nabla_{\hat{\mathbf{X}}} h^{(0)} + B o \mathbf{e}_z) \right) + \nabla_{\hat{\mathbf{X}}} \cdot \left(\langle \exp(f_k) k_r^{(0)}(f_h) \nabla_{\hat{\mathbf{Y}}} h^{(1)} \rangle \right) = q T \quad (29)$$

Figure 1. Effective dimensionless retention curve Ψh_g as function of $h^{(0)}/h_g$.

With this framework, the ensemble-averaged equation can be evaluated to a given order for given constitutive relationships.

3. Effective Constitutive Relations for the Brooks-Corey Model With Leverett Scaling

[42] In the following, we will discuss the averaged equation (29) in a two-dimensional medium for a Brooks-Corey model [Brooks and Corey, 1966]:

$$S(h) = \begin{cases} \left(\frac{h_e}{h}\right)^n & \text{if } |h| > |h_e| \\ 1 & \text{otherwise} \end{cases} \quad (30)$$

$$k_r(S) = \begin{cases} (S)^{2/n+3} = \left(\frac{h_e}{h}\right)^{2+3n} & \text{if } |h_e| \geq |h| \\ 1 & \text{otherwise} \end{cases} \quad (31)$$

with the entry pressure head h_e and the Brooks Corey parameter n . S is the water saturation. Here the residual saturation is assumed zero. The water retention curve is:

$$\Psi(h) = \phi \frac{dS}{dh} = \begin{cases} -\frac{n\phi}{h_e} \left(\frac{h_e}{h}\right)^{n+1} & \text{if } |h| > |h_e| \\ 0 & \text{otherwise} \end{cases} \quad (32)$$

h is negative under unsaturated conditions. ϕ is the porosity of the medium. We assume that the entry pressure is related to the permeability via Leverett scaling [Leverett, 1941]:

$$h_e \propto \frac{1}{\sqrt{K_0}} \quad (33)$$

[43] Under these conditions, the geometric mean of the entry pressure head h_g is the entry pressure head which corresponds to the geometric mean of the permeability, and the fluctuations are fully correlated:

$$f_h = -\frac{1}{2} f_k \quad (34)$$

$$\frac{h_e}{h_g} = \exp\left(-\frac{1}{2} f_k\right) \quad (35)$$

In the following, again, h and Ψ denote the dimensionless capillary pressure head and retention function, respectively.

3.1. Effective Retention Curve

[44] Accounting for equation (32), the retention curve field for a fixed pressure head (here $h^{(0)}$) is given by substituting the dimensionless pressure head h^* according to equation (5) and the random field according to equation (35) into the definition of equation (32):

$$\Psi(f_k, h^{(0)}) = \begin{cases} -n\phi \exp\left(\frac{n+1}{2} A - \frac{n}{2} f_k\right) & \text{if } f_k > A \\ 0 & \text{otherwise} \end{cases} \quad (36)$$

with $A = -2\ln(h^{(0)})$. The ensemble-averaged effective retention curve $\langle \Psi(h^{(0)}) \rangle$ can be computed by integrating the product of $\Psi(f_k, h^{(0)})$, given by equation (36), and the Gaussian probability density function $p(f_k)$ of f_k over all values of f_k :

$$\begin{aligned} \langle \Psi(h^{(0)}) \rangle &= \int_{-\infty}^{\infty} \Psi(f_k, h^{(0)}) p(f_k) df_k \\ &= \int_{-\infty}^{\infty} \Psi(f_k, h^{(0)}) \frac{1}{\sqrt{2\pi\sigma_{f_k}^2}} \exp\left(-\frac{f_k^2}{2\sigma_{f_k}^2}\right) df_k \\ &= \phi \frac{-n}{2} \exp\left(\frac{n+1}{2} A\right) \exp\left(\frac{n^2}{8} \sigma_{f_k}^2\right) \\ &\quad \cdot \left(1 - \operatorname{erf}\left(\frac{n\sigma_{f_k}^2}{2\sqrt{2}} + \frac{A}{\sigma_{f_k}^2 \sqrt{2}}\right)\right) \end{aligned} \quad (37)$$

[45] Ensemble-averaged retention curves $\langle \Psi(h^{(0)}) \rangle$ are plotted in Figure 1 for different values of log permeability variance $\sigma_{f_k}^2$. The curves get wider with increasing variance. Also, the effect of a definite entry pressure gets lost because the permeability K_0 is continuously distributed. Because of the Leverett scaling, also the entry pressure head h_e is a distributed quantity.

3.2. Statistical Properties of the Total Permeability Field

[46] In section 2.4, we have expanded the total permeability $K_{tot} = K_0 k_r$ about the zeroth-order term $K_g k_r^{(0)}|_{f_h=0, h^{(0)}}$. In the following, however, we will expand the total permeability about its geometric mean which differs from the homogeneous large-scale value used in section 2.4. This is a reasonable approach from a physical point of view. In order to do so, we determine the statistical and geostatistical properties of the total permeability. Subsequently, we will substitute the expansion about the geometric mean of the total permeability into equation (26).

[47] Applying the Brooks-Corey parameterization, the dimensionless total permeability is:

$$K_{tot} = K_0 k_r = \exp(f_k) S^{2/n+3} \quad (38)$$

Because of the Leverett scaling, only a single statistical parameter, namely f_k , remains and the total permeability is given by

$$K_{tot} = \begin{cases} \exp(f_k) & \text{if } f_k \leq A \\ \exp\left(\left(1 + \frac{3}{2}n\right)A - \frac{3}{2}nf_k\right) & \text{if } f_k > A \end{cases} \quad (39)$$

The expected value, or arithmetic mean of K_{tot} , denoted $\langle K_{tot} \rangle_a$, can be obtained by multiplying $K_{tot}(f_k)$ with the probability density function (pdf) of f_k and integrating over all possible values of f_k :

$$\begin{aligned} \langle K_{tot} \rangle_a &= \int_{-\infty}^{\infty} K_{tot}(f_k) \frac{1}{\sqrt{2\pi\sigma_{f_k}^2}} \exp\left(-\frac{f_k^2}{2\sigma_{f_k}^2}\right) df_k \\ &= \frac{1}{2} \left[\exp\left(\frac{\sigma_{f_k}^2}{2}\right) \left(1 + \operatorname{erf}\left(\frac{A - \sigma_{f_k}^2}{\sigma_{f_k}\sqrt{2}}\right)\right) \right. \\ &\quad + \exp\left(\left(1 + \frac{3}{2}n\right)A + \frac{9n^2\sigma_{f_k}^2}{8}\right) \\ &\quad \cdot \left. \left(1 - \operatorname{erf}\left(\frac{A + 3/2n\sigma_{f_k}^2}{\sigma_{f_k}\sqrt{2}}\right)\right) \right]. \end{aligned} \quad (40)$$

The geometric mean of the total permeability, denoted $\langle K_{tot} \rangle_g$, is the exponential of the expected value of the log total permeability, $\langle K_{tot} \rangle_g = \exp(\langle \ln(K_{tot}) \rangle)$. Thus we need to integrate over the probability density function of f_k times the log total permeability, leading to:

$$\begin{aligned} \langle K_{tot} \rangle_g &= \exp\left(\int_{-\infty}^{\infty} \frac{\ln(K_{tot}(f_k))}{\sqrt{2\pi\sigma_{f_k}^2}} \exp\left(-\frac{f_k^2}{2\sigma_{f_k}^2}\right) df_k\right) \\ &= \exp\left(\left(1 + \frac{3n}{2}\right)\left(\frac{A}{2} - \frac{\sigma_{f_k}}{\sqrt{2\pi}} \exp\left(-\frac{A^2}{2\sigma_{f_k}^2}\right)\right) \right. \\ &\quad \left. - \frac{A}{2} \operatorname{erf}\left(\frac{A}{\sigma_{f_k}\sqrt{2}}\right) - \frac{3|A|n}{4} \operatorname{erf}\left(\frac{|A|}{\sigma_{f_k}\sqrt{2}}\right)\right) \end{aligned} \quad (41)$$

The variance of the total permeability $\sigma_{K_{tot}}^2$ can be obtained with the same method:

$$\begin{aligned} \sigma_{K_{tot}}^2 &= -\langle K_{tot} \rangle_a^2 + \frac{1}{2} \left[\exp(2\sigma_{f_k}^2) \left(1 + \operatorname{erf}\left(\frac{A - \sigma_{f_k}^2}{\sigma_{f_k}\sqrt{2}}\right)\right) \right. \\ &\quad \left. + \exp\left(\left(2 + 3n\right)A + \frac{9n^2\sigma_{f_k}^2}{2}\right) \left(1 - \operatorname{erf}\left(\frac{A + 3n\sigma_{f_k}^2}{\sigma_{f_k}\sqrt{2}}\right)\right) \right] \end{aligned} \quad (42)$$

while the variance of the log total permeability is

$$\begin{aligned} \sigma_{\ln(K_{tot})}^2 &= \frac{1}{8} \left[4A^2 \left(1 + \frac{3}{2}n\right)^2 + 4\sigma_{f_k}^2 + 9n^2\sigma_{f_k}^2 \right. \\ &\quad - 8A \exp\left(-\frac{A^2}{2\sigma_{f_k}^2}\right) \sqrt{\frac{\sigma_{f_k}^2}{2\pi}} \left(1 + \frac{3}{2}n\right)^2 \\ &\quad - 3n \frac{\sqrt{A^2}}{A} \left(A^2(4 + 3n) + 3n\sigma_{f_k}^2\right) \operatorname{erf}\left(\frac{\sqrt{A^2}}{\sqrt{2\sigma_{f_k}^2}}\right) \\ &\quad \left. + 4\left(\sigma_{f_k}^2 - A^2\right) \operatorname{erf}\left(\frac{A}{\sqrt{2\sigma_{f_k}^2}}\right) \right] - \ln(\langle K_{tot} \rangle_g)^2 \end{aligned} \quad (43)$$

[48] The coefficients of variation of the effective total permeability, $\sigma_{K_{tot}}/\langle K_{tot} \rangle$ depend via $A = -2\ln(h^{(0)})$ strongly on the large-scale head $h^{(0)}$.

[49] The averaged total permeabilities according to equations (40) and (41) and the variances according to equations (42) and (43) do not show the effects of a definite entry pressure, since the latter has been averaged out. In this respect, both results differ from first-order results for the averaged log total permeability that have been obtained by Zhang *et al.* [1998]. Their first-order expression is identical to the zeroth-order expression, which is the total permeability of a homogeneous medium parameterized by the expected values of the independent, normally distributed parameters. In our notation the first-order total permeability of Zhang *et al.* [1998] for the capillary equilibrium case reads as

$$\langle K_{tot} \rangle_{ord.1} = \begin{cases} \exp\left(\frac{1}{h^{(0)}}\right)^{(2+3n)} & \text{if } h^{(0)} > 1 \\ 1 & \text{otherwise} \end{cases} \quad (44)$$

and the first-order variance of log permeability is:

$$\sigma_{\ln(K_{tot})}^2_{ord.1} = \sigma_{f_k}^2 \begin{cases} 1 - (2 + 3n) + \frac{1}{4}(2 + 3n)^2 & \text{if } h^{(0)} > 1 \\ 1 & \text{otherwise} \end{cases} \quad (45)$$

Figure 2 shows plots of the averaged total permeabilities according to equations (41) and (44) and the variances according to equations (43) and (45) for $\sigma_{f_k}^2 = 1.0$ and $\sigma_{f_k}^2 = 0.01$. The differences are pronounced most at pressure values in the range of the entry pressure h_g , where the geometric mean is much lower than the first-order mean. With decreasing variance $\sigma_{f_k}^2$ the averages converge to the same zeroth-order curve. The first-order approximation overpredicts the total permeability at low capillary pressure heads. The variance $\sigma_{\ln(K_{tot})}^2$ has a minimum at pressure heads below h_g , with a smaller value than the variance of the log intrinsic permeability $\sigma_{f_k}^2$. If the pressure head equals zero, the medium is water saturated and $\sigma_{\ln(K_{tot})}$ equals $\sigma_{f_k}^2$. As the pressure increases, the permeability of coarse material (high intrinsic permeability and low entry pressure) decreases. For small values of the pressure head $h^{(0)}$, the decrease of the total permeability with increasing head is still rather small, so that the total permeabilities within zones of high intrinsic permeability are in an intermediate range. With more values of the total permeability in the intermediate range, the variance of the log total permeability decreases with increasing pressure heads in the range of capillary pressures below the entry pressure. The latter effect is not captured by first-order theory. For high capillary pressures, the total permeabilities in the zones of high intrinsic permeability get very small, thus increasing the variance of log total permeability.

[50] The geometric mean $\langle K_{tot} \rangle_g$ according to equation (41) and variance $\sigma_{\ln(K_{tot})}^2$ according to equation (43) depend on the variance of log permeability $\sigma_{f_k}^2$ and the large-scale pressure in a complex way. Figure 3 shows a plot of the expected value $\langle K_{tot} \rangle_g$ as function of the variance of log permeability $\sigma_{f_k}^2$ for three different values of A ($A = 3$, $A = 0$ and $A = -3$). The first value corresponds to $h^{(0)} = 0.2$, the second one to

Figure 2. Mean $\langle K_{tot} \rangle$ of the total permeability and variance $\sigma_{\ln(K_{tot})}^2$ of the log total permeability normalized with σ_{fk}^2 . First-order mean and averages are according to equations (41) and (43)–(45).

$h^{(0)} = 1$, and the third one to $h^{(0)} = 5$. Figure 3 shows also the variances $\sigma_{\ln(K_{tot})}^2$ according to equation (43) as function of σ_{fk}^2 for the same values of A .

[51] If the nondimensionless entry pressure is high or low compared to h_g , the geometric mean of K_{tot} is almost constant, at least for the value range of σ_{fk}^2 considered here. If $h^{(0)}$ is very low, the medium is saturated and the intrinsic permeability determines K_{tot} . In this case, the geometric mean equals the geometric mean of the intrinsic permeability, independently of σ_{fk}^2 . This is consistent with the linear increase of the variance of $\ln(K_{tot})$ with a slope of 1 for $h^{(0)} = 0.2$. If $h^{(0)}$ is large compared to h_g there is hardly any water in the medium. The geometric mean of the total permeability is therefore very low, and the value does not depend on σ_{fk}^2 . Because of the low water content the variance $\sigma_{\ln(K_{tot})}^2$ is much larger than in the case of small pressure head $h^{(0)}$, and it increases also linearly with σ_{fk}^2 . In the case that the pressure head $h^{(0)}$ equals h_g , we are in an intermediate regime. At $\sigma_{fk}^2 = 0$, the pressure head equals the entry pressure in a homogeneous medium and the geometric mean of total permeability equals the geometric mean of the intrinsic one. As σ_{fk}^2 increases, more parts of the material have a lower entry pressure than h_g and thus have a water saturation $S < 1$. Their total permeability is smaller. Because

of the stepwise shape of the capillary pressure-saturation curve, the parts in the medium with higher entry pressure do not counterbalance this effect. As a result, the geometric mean $\langle K_{tot} \rangle_g$ decreases with σ_{fk}^2 . The variance $\sigma_{\ln(K_{tot})}^2$ also grows with σ_{fk}^2 but with a slope larger than unity, because the medium becomes less saturated with larger σ_{fk}^2 , leading to a higher variance than in the water-saturated case.

[52] In order to evaluate the ensemble averaged unsaturated flow equation, equation (29), the correlation structure of log total permeability is important. In this context, it is worth noting that the two-point autocovariance function cannot fully determine the statistics of the total permeability since the latter is, due to the nonlinear relative permeability, not a multi-Gaussian field. Nonetheless, we neglect higher moments in the present study. We denote the log intrinsic permeability at location $\mathbf{x}_1$ by f_1 and at location $\mathbf{x}_2$ by f_2 . The two-point autocovariance can then be computed by

$$\begin{aligned} & \langle \ln(K'_{tot}(\mathbf{x}_1)) \ln(K'_{tot}(\mathbf{x}_2)) \rangle - (\ln(\langle K_{tot} \rangle_g))^2 \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(\frac{\ln(K_{tot}(f_1)) \ln(K_{tot}(f_2))}{2\pi\sigma_{fk}^2 \sqrt{1-\rho^2}} \exp\left(-\frac{f_1^2 - 2f_1f_2\rho + f_2^2}{2\sigma_{fk}^2(1-\rho^2)}\right) \right) \\ & \quad \cdot df_1 df_2 - (\ln(\langle K_{tot} \rangle_g))^2 \end{aligned} \quad (46)$$

Figure 3. Expected value of total permeability $\langle K_{tot} \rangle_g / K_g$ and variance $\sigma_{\ln(K_{tot})}^2$ as function of the variance σ_{fk}^2 for different values of mean hydraulic head $h^{(0)}$.

Figure 4. Autocorrelation of the log of the total permeability, $\sigma_{f_k}^2 = 1.0$, $n = 2$, $\text{Corr}(\rho) = (\langle \ln(K_{tot}(f_1)) \ln(K_{tot}(f_2)) \rangle - (\ln(\langle K_{tot} \rangle_g))^2) / (\sigma_{\ln(K_{tot})}^2)$.

in which ρ is the correlation function of the log intrinsic permeability fluctuations, which may be parameterized by standard models such as the Gaussian and the exponential ones. To the best of our knowledge, the second integration of equation (46) cannot be performed in closed form. Instead, we apply numerical integration for the three examples discussed above ($A = -3$, $A = 0$ and $A = 3$) using the numerical integration tool of Mathematica [Wolfram, 1991].

[53] Figure 4 shows the correlation coefficient of the log total permeability as function of ρ for the given values of A and a variance of the intrinsic permeability of $\sigma_{f_k}^2 = 1.0$ and $n = 2$. For nondimensionless entry pressures $h^{(0)}$ much higher or lower than h_g , the correlation function is the same as the correlation function for f_k . If $h^{(0)}$ is in the range of h_g , the correlation function decreases faster than the correlation function of f_k . As high permeable zones are drained easier and thus have smaller total permeabilities, parts with high intrinsic permeability are flipped into the low end of the total permeability range, leading to a smaller correlation length of the field.

3.3. Effective Relative Permeability Curves in a Quasi-uniform Flow Field

[54] With the statistical properties calculated above, we can evaluate the effective total permeability by equation (29). As outlined above, we perform the expansion about $\langle K_{tot} \rangle_g$, computed by equation (41), with the expansion parameter $\sigma_{\ln(K_{tot})}^2$. The second term in equation (29) to the second order of this expansion reads:

$$\nabla_{\hat{\mathbf{x}}} \cdot \left(\langle K_{tot} \rangle_g \left(1 + \frac{1}{2} \sigma_{\ln(K_{tot})}^2 \right) \mathbf{J} \right)$$

[55] In order to calculate $h^{(1)}$ we have to solve the order ε^{-1} of the Richards equation, equation (26), which reads with the expansion in terms of $\sigma_{\ln(K_{tot})}^2$

$$\nabla_{\hat{\mathbf{y}}} \cdot \left(\left(\ln(K_{tot}) + \frac{1}{2} \ln(K_{tot})^2 + \dots \right) (\mathbf{J} + \nabla_{\hat{\mathbf{y}}} h^{(1)}) \right) + \nabla_{\hat{\mathbf{y}}}^2 h^{(1)} = 0 \quad (47)$$

The Green's function is:

$$G = \frac{1}{2\pi} \sum_{l=-\infty}^{+\infty} \sum_{j=-\infty}^{+\infty} \ln \left(\left| \hat{\mathbf{y}} + i\varepsilon^{-1} \mathbf{e}_1 + j\varepsilon^{-1} \mathbf{e}_2 - \hat{\mathbf{y}}' \right| \right) \approx \frac{1}{2\pi} \ln \left(\left| \hat{\mathbf{y}} - \hat{\mathbf{y}}' \right| \right) \quad (48)$$

in which the approximation denotes the two-dimensional solution for an infinite rather than a periodic domain. $\mathbf{e}_1$ and $\mathbf{e}_2$ are unit vectors in both spatial directions.

[56] With this expansion the third term in equation (29) can be determined to second order by

$$\begin{aligned} & \nabla_{\hat{\mathbf{x}}} \cdot \left(\langle \langle K_{tot} \rangle_g \exp(\ln(K_{tot})) \nabla_{\hat{\mathbf{y}}} h^{(1)} \rangle \right) \\ &= \frac{1}{2\pi} \nabla_{\hat{\mathbf{x}}} \cdot \left[\langle K_{tot} \rangle_g \int_{\Omega} \left(\nabla_{\hat{\mathbf{y}}}^2 \ln \left(\left| \hat{\mathbf{y}} - \hat{\mathbf{y}}' \right| \right) \right. \right. \\ & \quad \left. \left. \cdot \left(\ln(K'_{tot}(\hat{\mathbf{y}})) \ln(K'_{tot}(\hat{\mathbf{y}}')) \right) \mathbf{J} d\hat{\mathbf{y}}' \right) \right] \end{aligned} \quad (49)$$

This type of integral has been evaluated before by Dagan [1993] for single-phase flow in a macroscopically uniform flow field, using covariance functions with finite integral scale. In the multiscale framework, the constraint of a uniform flow field on the large scale is relaxed: Here large-scale trends may exist but must be negligible on the small scale. For isotropic media, the effective single-phase conductivity does not depend on the correlation scale of the medium. As the covariance of the total permeability decays at least as fast as the covariance of the log intrinsic permeability f_k , we assume that here the integral does not depend on the integral scale either and the covariance of $\ln(K_{tot})$ can be approximated as a Gaussian one. We furthermore assume, that the mean flow can be assumed uniform on the small scale. The result becomes thus:

$$\nabla_{\hat{\mathbf{x}}} \cdot \left(\langle \exp(f_k) k_r^{(0)} \nabla_{\hat{\mathbf{y}}} h^{(1)} \rangle \right) \approx -\frac{1}{2} \nabla_{\hat{\mathbf{x}}} \cdot \left(\langle K_{tot} \rangle_g \sigma_{\ln(K_{tot})}^2 \mathbf{J} \right) \quad (50)$$

Finally, the ensemble-averaged homogenized equation (29) is:

$$\langle \Psi^{(0)} \rangle \frac{\partial h^{(0)}}{\partial t} + \nabla_{\hat{\mathbf{x}}} \cdot \left(\langle K_{tot} \rangle_g \left(\nabla_{\hat{\mathbf{x}}} h^{(0)} + B o \mathbf{e}_z \right) \right) = qT \quad (51)$$

with the effective parameter functions $\langle \Psi^{(0)} \rangle$ and $\langle K_{tot} \rangle_g$.

[57] As the distribution of the total permeability is not multi-Gaussian, the next order with nonzero contribution to the effective parameters is the third one. It is quite expectable, that higher-order contributions are more important in unsaturated flow than in single-phase flow.

[58] Figure 5 shows an example for the effective curve $K_{tot}(h^{(0)})$ using the parameters $n = 2$, $\sigma_{f_k}^2 = 0.25$ and $\sigma_{f_k}^2 = 1.0$. The averaging of the entry pressure effect is clearly visible. In comparison to the homogeneous case, the effective total permeability $\langle K_{tot} \rangle_g$ is always smaller.

4. Effective Relative Permeability Curves for Differently Connected Fields

[59] Second-order ensemble averaging has been shown rather reliable in estimating the mean flow in saturated

Figure 5. $\langle K_{\text{total}} \rangle_g / K_g$ in relation to $h^{(0)} / h_g$ for different variances $\sigma_{f_k}^2$.

porous media. In unsaturated flow, however, the nonlinearity of relative permeability may restrict the parameter range in which the averaging procedure outlined above is appropriate. The total permeability field may exhibit distinct features that are not so pronounced in the intrinsic permeability field. When a water-saturated medium is drained, the zones of coarse material are the first to drain. In this process, the zones of highest permeability become the least permeable ones. Particularly, well-connected paths of either high or low total permeability may have a significant impact on the mean flow behavior. Well-connected zones of low conductivity may significantly reduce flow through the domain, whereas well-connected zones of high conductivity lead to channeling flow. Under such conditions, statistical approximations based on two-point correlations may become inappropriate, since this type of statistics does not cover connectivity properties.

[60] The connectivity of hydraulic conductivity and its effects on single-phase flow and solute transport have already been analyzed by *Gomez-Hernandez and Wen* [1997], *Zinn and Harvey* [2003], and *Vogel* [2002]. Here we consider unsaturated flow, where the connectivity of the total permeability does not only depend on the distribution of soil materials but also on the capillary pressure, and the effect may be even more pronounced.

[61] *Zinn and Harvey* [2003] presented the absolute value transformation as a method to transform fields with high connectivity of medium parameter values to fields with high connectivity of either low or high parameter values [see also *Vogel*, 2002]:

$$f_{\text{low}}(\mathbf{x}) = \sigma_f \operatorname{erf} \left(\frac{|f_{\text{nor}}(\mathbf{x})|}{\sqrt{2}} \right) - 1 \sqrt{2} \quad (52)$$

$$f_{\text{high}}(\mathbf{x}) = -\sigma_f \operatorname{erf} \left(\frac{|f_{\text{nor}}(\mathbf{x})|}{\sqrt{2}} \right) - 1 \sqrt{2} \quad (53)$$

in which $f_{\text{nor}}(\mathbf{x})$ is an autocorrelated field with zero mean and variance of unity, produced by a standard random field generator based on sequential Gaussian simulation, spectral methods, or the turning bands method [e.g., *Deutsch and*

Journal, 1992]. Typically, such fields show a high connectivity of intermediate values. Particularly when using autocovariance functions lacking small-scale variability, such as the Gaussian model, the generated fields exhibit separated blobs of high and low parameter values. By applying the absolute value transformation, all of these blobs get either high values only or low values only. The scaling with the error function and its inverse guarantees that the values of the transformed fields are again normally distributed. The resulting fields have either well-connected high values or well-connected low values. We use these type of fields to analyze the influence of connectivity properties on the effective parameter curves.

[62] The term connectivity is well defined for networks, whereas its applicability to continuous fields is somewhat ambiguous. Here we use the two-point cluster function of an two-cut indicator field as a way of quantifying connectivity properties [Torquato *et al.*, 1988; Western *et al.*, 2001]. The two-cut indicator field $I(\mathbf{x})$ is obtained from the log-intrinsic permeability field by applying an upper and a lower threshold value to the log permeability values and setting all values in between the two thresholds to one and all others to zero. The values of the thresholds are chosen by the user. We identify the clusters of regions with indicator value one and give each cluster an index. The field with the cluster numbers is denoted $CI(\mathbf{x})$. Finally, the two-point cluster function $C(h)$ is defined as the probability that two points with distance $|\mathbf{x} - \mathbf{x}'|$ belong to the same cluster [Torquato *et al.*, 1988]:

$$C(h) = \frac{\langle I(\mathbf{x})P(\mathbf{x}', \mathbf{x}) \rangle_{|\mathbf{x}-\mathbf{x}'|=h}}{\langle I(\mathbf{x}) \rangle} \quad (54)$$

with

$$P(\mathbf{x}', \mathbf{x}) = \begin{cases} 1 & \text{if } CI(\mathbf{x}) = CI(\mathbf{x}') \\ 0 & \text{otherwise} \end{cases} \quad (55)$$

Without the distinction of the different clusters, the two-point cluster function would be the correlation function of the indicator field.

[63] In order to analyze the influence of connected permeability zones on the effective parameter functions, we compare three test fields generated by the method of *Zinn and Harvey* [2003]. Starting point is a standard autocorrelated field with a Gaussian covariance function. From this, we generate fields with high connectivity of the high log intrinsic permeability values, denoted type 2, and those with high connectivity of low permeability values, denoted type 3. These fields are analyzed for their two-point autocovariance function by evaluating their power spectra. The fields of type 1 are generated with a standard spectral random field generator using the covariance function determined for the highly connected fields. That is, all three types have identical two-point correlation functions but have connected bands at different parameter values. All fields have a mean of $\langle f_k \rangle = 0$ and a variance of $\sigma_{f_k}^2 = 1.0$. Examples of all three types of fields (256×256 cells with a correlation length of 5 cells) are shown in Figure 6 together with three two-point cluster functions (54) for each field.

[64] The first cluster function, marked with a dashed line, is obtained for two-cut indicator fields with the thresholds

Figure 6. Test fields with different connectivity properties and corresponding two-point cluster functions.

$f_{\max} = \infty$ and $f_{\min} = 0.7$, thus indicating high permeabilities. The second cluster function, marked with a solid line, is obtained for two-cut indicator fields with the threshold values $f_{\max} = 0.7$ and $f_{\min} = -0.7$, indicating intermediate permeabilities, and the third cluster function, marked with dotted lines, is obtained from two-cut indicator fields with threshold values $f_{\max} = -0.7$ and $f_{\min} = -\infty$, indicating low permeabilities. The fields had the same properties as the example fields from Figure 6. The averaging, denoted as angular brackets in the definition of the two-point cluster function according to equation (54), was performed over an ensemble of 10000 fields for each of the three field types, where the location $\mathbf{x}$ was held constant in the middle of the field. As the fields are isotropic, the two-point cluster function is only a function of the distance h from $\mathbf{x}$; it is independent of the direction. It is therefore shown in Figure 6 only for the x direction. The ensemble-to-ensemble fluctuations of the two-point cluster functions, obtained from an average over a number of n and $n + 1$ realizations, was for all field types and threshold values lower than 0.001 for $n = 10000$. This was tested on an ensemble of 14000 realizations. An ensemble of 10000 fields was therefore considered to be sufficiently large. The two-point cluster functions reproduce the connectivity properties of the three types of fields rather well; each type has a slower decay for a single indicated permeability zone.

[65] Subsequently, we computed the effective parameter functions (effective retention curve according to equation (22) and effective total permeability according equation (24)) for all three types of fields. For the effective functions we used fields with the same parameters as the example fields of Figure 6; however, the fields were 512×512 cells large. An ensemble averaging was not necessary to calculate the effective parameter functions. The deviations between curves obtained from different fields were negligible.

[66] Using these three types of fields, we calculate the effective retention curve by calculating the arithmetic mean of the saturation fields for different values of $h^{(0)}$ and building the derivative with respect to the pressure head $h^{(0)}$ numerically. The retention curves for all types of fields are almost identical because they are the arithmetic means of the local values. Since the pdf of the f_k fields did not differ with connectivity type, identical retention curves are to be expected. The curves are not shown here.

[67] We evaluate the relative permeability curves by numerical simulation of the small-scale problem in a field for each type of fields, as outlined in section 2.3. We compare these curves to the geometric mean $\langle K_{\text{tot}} \rangle_g$ of the total permeability, evaluated by equation (41). The small-scale problem is solved by a cell-centered finite volume scheme applying periodic boundary conditions [see Cirpka and Kitanidis, 2002]. The resulting system of linear equations is solved by a conjugate gradient method with algebraic multigrid preconditioning [Ruge and Stüben, 1987]. Because of the periodic boundary conditions, the system of equations for the pressure is singular. However, the total permeability is calculated from the averaged flux and thus only from the pressure gradients. The singularity can therefore be overcome by fixing the pressure at one node to an arbitrary value, without changing the result for the effective total permeability. The resulting effective relative permeability curves are shown in Figure 7. In all three cases, the effective relative permeability curve evaluated numerically differ from the geometric mean. Considering relative errors (given by the dotted lines in the plots), however, large errors occurred only in the fields where either high or low permeabilities are well connected. In the first case, the stochastic theory overestimates the relative permeability, while in the second case it underestimates the relative permeability. This behavior is counterintuitive, but

Figure 7. Effective relative permeability curves for the test fields shown in Figure 6. Shown is a comparison between numerical upscaling and approximation by the geometric mean. Permeabilities were normalized by the effective saturated permeabilities. Deviations between the saturated permeabilities for the three fields were by a factor of 1.1.

can be explained by the statistical properties of the total permeability.

[68] For the field of type 3, the explanation is the most straightforward. The parameter distribution of the total

permeability is given by equation (39). The function monotonically increases with f_k for $f_k < A$, while it decreases for $f_k > A$, thus exhibiting a maximum at $f_k = A$.

[69] At capillary pressures where the maximum total permeability is in a well-connected regime (indicated by values of f_k yielding a slow decay of the two-point cluster function), the high total permeabilities (defined by the corresponding A) are well connected. This does not necessarily lead to channeling behavior. Channeling occurs only when, additionally to the connectedness of the high permeability zones, the variance of the total permeability field is high. In the three examples given above, this happens in the third case. Here low values of f_k are highly connected. At heads, where these values are similar to A , the high total permeability zones are well connected and the variance of the total permeability is high (see equation (42) and Figure 3). As stated above, the combined effects result in channeling. Obviously, channeling leads to a higher effective permeability than estimated by the geometric mean of the total permeability (see also the single-phase results of *Zinn and Harvey* [2003]). In the field of type 1, the well-connected values of f_k correspond to higher values of A , where the variance of the total permeability is smaller so that the channeling is less pronounced. In the field of type 2 we have the opposite effect to the third field. For the values of A corresponding to the values of $h^{(0)}$ shown here the low permeable parts are well connected. At the same time the variance of the total permeability is high. We thus get an antichanneling effect. The well-connected low permeable material blocks the flow, leading to a lower relative permeability than predicted by stochastic theory.

5. Discussion and Conclusions

[70] In this paper, we have analyzed the ensemble averaged Richards equation for periodic stochastic fields using homogenization theory. We restricted the analysis to the case, in which flow on the small scale is dominated by capillary forces. This restriction is severe, as it requires a scale separation factor ϵ that is much smaller than the ratio between typical capillary pressure head values and the large length scale of the flow process. Strictly speaking, the conditions for capillary-dominated flow can only be met when the large scale of the flow process is rather small, although significantly larger than the length scale of the heterogeneities, or when the entry pressure heads are very high. However, with the conditions for the validity of the results clearly defined, the presented methodology enables us to accurately investigate the averaged flow properties for the specified flow regime. We apply the Brooks-Corey model for the parameterization of unsaturated flow which accounts for capillary entry pressure effects. Because of the step-like shape of the entry pressure on the small scale, the ensemble-averaging procedure becomes difficult. In the capillary equilibrium flow regime, however, the effective parameter functions and ensemble-averaged flow parameters can be evaluated in terms of the logarithm of the total (unsaturated) permeability instead of the logarithm of the saturated one. The latter would be necessary in the general case, where no flow regime is specified.

[71] Our evaluation of the ensemble-averaged retention curves and total permeabilities shows that the sharp edges in the constitutive relations introduced by a definite entry

pressure are smoothed by the variability of the entry pressure. The degree of smoothing scales with the variance of the log intrinsic permeability and vanishes only at the limit of $\sigma_{f_k}^2 = 0$. Lacking a clear entry pressure, the ensemble-averaged constitutive relations resemble the general shape of the Mualem–van Genuchten parameterization [Mualem, 1976; van Genuchten, 1980]. These results are in contrast to the first-order approximation of Zhang *et al.* [1998] and illustrate that results of low-order perturbation can become questionable when the flow equations are highly nonlinear which, in our application, is the case for capillary pressures in the range of the entry pressure. In this range, the geometric mean of the total permeability is much smaller than the permeability predicted by first-order theory.

[72] In principle, homogenization theory is a volume-averaging technique. In the stochastic context, we have replaced the volume averages by ensemble averages, some of which we have solved in closed form. In general, with known fields, the volume average has to be computed numerically. We have compared the statistically averaged parameter functions to the effective ones, evaluated by numerical simulation, for fields with different connectivity properties. We compared fields where high permeable parts, low permeable parts and intermediate permeable parts are well connected. Although the patterns themselves look artificial, the effect of connectivity of the different parts could be illustrated with these fields. The examples illustrate, that the connectivity properties of the log intrinsic permeability field are important for the prediction of the upscaled effective parameter curves. Particularly under intermediate to dry conditions, high connectivity of fine materials lead to higher relative permeabilities than expected from stochastic theory. This is important in estimating soil hydraulic properties. As an example, soils classified as alfisols exhibit well-connected thin layers of clayey to silty materials encapsulating sand lenses. This type of soil will have a higher unsaturated conductivity under rather dry conditions than inceptisols with identical grain size distribution but different structure. The contrary effect is found for material with high connectivity of coarse material. Here statistical theory overpredicts the effective total permeability. These results illustrate that connectivity properties of the soil, in case they are available, should be considered in the upscaling of flow in the unsaturated zone.

Appendix A: Multiscale Expansion of Equation (7)

[73] Equation (7) is supposed to be dimensionless and the stars will be omitted. Inserting the expansions of equations (11), (12), and (13) into equation (7) yields

$$\begin{aligned} & \left(\Psi^{(0)} + \varepsilon \Psi^{(1)} + \dots \right) \frac{\partial}{\partial t} \left(h^{(0)} + \varepsilon h^{(1)} + \varepsilon^2 h^{(2)} + \dots \right) \\ & + \left(\nabla_{\hat{\mathbf{x}}} + \frac{1}{\varepsilon} \nabla_{\hat{\mathbf{y}}} \right) \cdot \left[\exp(f_k) \left(k_r^{(0)} + \varepsilon k_r^{(1)} + \varepsilon^2 k_r^{(2)} + \dots \right) \right. \\ & \left. \cdot \left(\left(\nabla_{\hat{\mathbf{x}}} + \frac{1}{\varepsilon} \nabla_{\hat{\mathbf{y}}} \right) \left(h^{(0)} + \varepsilon h^{(1)} + \varepsilon^2 h^{(2)} + \dots \right) + Bo \mathbf{e}_z \right) \right] = qT \end{aligned} \quad (\text{A1})$$

Assuming that scales are clearly separated implies that this equation has to be satisfied for each order of ε separately.

This yields a system of coupled equations for each order of ε . As we consider only the limit $\varepsilon \rightarrow 0$, all orders higher than ε^0 vanish. We therefore have to consider only the orders ε^{-2} , ε^{-1} and ε^0 in equation (A1). These equations read as

$$\varepsilon^{-2} : \nabla_{\hat{\mathbf{y}}} \cdot \left(\exp(f_k) k_r^{(0)} \nabla_{\hat{\mathbf{y}}} h^{(0)} \right) = 0 \quad (\text{A2})$$

$$\begin{aligned} \varepsilon^{-1} : & \nabla_{\hat{\mathbf{y}}} \cdot \left(\exp(f_k) k_r^{(0)} \left(\nabla_{\hat{\mathbf{x}}} h^{(0)} + Bo \mathbf{e}_z + \nabla_{\hat{\mathbf{y}}} h^{(1)} \right) \right) + \\ & \nabla_{\hat{\mathbf{x}}} \cdot \left(\exp(f_k) k_r^{(0)} \nabla_{\hat{\mathbf{y}}} h^{(0)} \right) + \\ & \nabla_{\hat{\mathbf{y}}} \cdot \left(\exp(f_k) k_r^{(1)} \nabla_{\hat{\mathbf{y}}} h^{(0)} \right) = 0 \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \varepsilon^0 : & \Psi^{(0)} \frac{\partial h^{(0)}}{\partial t} + \nabla_{\hat{\mathbf{x}}} \cdot \left(\exp(f_k) k_r^{(1)} \left(\nabla_{\hat{\mathbf{y}}} h^{(0)} \right) \right) + \\ & \nabla_{\hat{\mathbf{x}}} \cdot \left(\exp(f_k) k_r^{(0)} \left(\nabla_{\hat{\mathbf{x}}} h^{(0)} + Bo \mathbf{e}_z + \nabla_{\hat{\mathbf{y}}} h^{(1)} \right) \right) + \\ & \nabla_{\hat{\mathbf{y}}} \cdot \left(\exp(f_k) k_r^{(1)} \left(\nabla_{\hat{\mathbf{x}}} h^{(0)} + Bo \mathbf{e}_z + \nabla_{\hat{\mathbf{y}}} h^{(1)} \right) \right) + \\ & \nabla_{\hat{\mathbf{y}}} \cdot \left(\exp(f_k) k_r^{(0)} \left(\nabla_{\hat{\mathbf{x}}} h^{(1)} + \nabla_{\hat{\mathbf{y}}} h^{(2)} \right) \right) + \\ & \nabla_{\hat{\mathbf{y}}} \cdot \left(\exp(f_k) k_r^{(2)} \left(\nabla_{\hat{\mathbf{y}}} h^{(0)} \right) \right) = qT \end{aligned} \quad (\text{A4})$$

[74] If ε would be small but finite, the equations of order ε^1 , ε^2 , ... would yield the truncation error for the upscaled volume averaged equation (A4).

Appendix B: Derivation of the Effective Permeability in Equation (21)

[75] We obtain χ by solving equation (20) numerically (see the procedure explained in section 2.3). Once we have obtained χ , we can use equations (18) and (19) to write the second integral in equation (17) in the following way:

$$\begin{aligned} & \frac{1}{\Omega} \nabla_{\hat{\mathbf{x}}} \int_{\Omega} \exp(f_k) k_r^{(0)} \left(\mathbf{J} + \nabla_{\hat{\mathbf{y}}} h^{(1)} \right) d\hat{\mathbf{Y}} = \\ & \frac{1}{\Omega} \frac{\partial}{\partial \hat{X}_i} \int_{\Omega} \exp(f_k) k_r^{(0)} \left(J_i + \frac{\partial}{\partial \hat{Y}_i} h^{(1)} \right) d\hat{\mathbf{Y}} = \\ & \frac{1}{\Omega} \frac{\partial}{\partial \hat{X}_i} \int_{\Omega} \exp(f_k) k_r^{(0)} \left(\delta_{ij} J_j + \frac{\partial}{\partial \hat{Y}_i} \chi_j J_j \right) d\hat{\mathbf{Y}} = \\ & \frac{\partial}{\partial \hat{X}_i} \left(\frac{1}{\Omega} \int_{\Omega} \exp(f_k) k_r^{(0)} \left(\delta_{ij} + \frac{\partial}{\partial \hat{Y}_i} \chi_j \right) d\hat{\mathbf{Y}} \right) J_j = \\ & \frac{\partial}{\partial \hat{X}_i} K_{e,ij} J_j \end{aligned} \quad (\text{B1})$$

where the indices i and j stand for horizontal and vertical directions and we sum over all double indices in the equation. δ_{ij} is the Kronecker function, which equals zero if $i \neq j$ and equals one otherwise. K_{ij} is the tensor defined in equation (24).

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