UPSCALING FOR UNSATURATED FLOW INCLUDING CONNECTIVITY OF THE SOIL STRUCTURE

INSA NEUWEILER[1] AND MILOS VASIN[1]

[1]University of Stuttgart, Institute of Hydraulic Engineering, Pfaffenwaldring 61, 70659 Stuttgart, Germany

Abstract

In this contribution upscaling methods for flow in the unsaturated zone are discussed. The upscaled model is derived assuming capillary equilibrium conditions. The methods to calculate the effective retention function and the effective unsaturated permeability aim to reflect information about connected paths of the soil structure. This kind of information is usually not included in the characterization of heterogeneity, which is mostly based on second order stochastic properties. If parameter fields are non-Gaussian, this type of characterization might not capture the main features of the structure, but connectivity properties have a more important influence on the upscaled models.

1. INTRODUCTION

Modelling of water balances in the unsaturated zone on larger scales requires upscaling of the local flow equations. The heterogeneity of the soil structure is captured in the upscaled models by effective parameters or effective processes. As the soil structure is in general not known in detail, heterogeneity has to be characterized and quantified in a way, that it captures the main features of the structure.

Heterogeneity is often described in a stochastic framework (as explained e.g. in [Zhang, 2002] among many others). The parameters are modelled as correlated random fields. For practical reasons the fields are mostly characterized by their second order properties. An isotropic field is then described by its mean, variance and correlation length. If a field is Gaussian, it is completely described by these quantities. Natural soil is however in most cases not Gaussian. This has been illustrated e.g. by [Gomez-Hernandez and Wen, 1997], [Zinn and Harvey, 2003]. It has been suggested by [Knudby and Carrera, 2005] or [Vogel, 2002] that connected structures of the different material types are an important characteristic, that have a high importance for flow and transport characteristics on a large scale. It is therefore important to derive upscaled models which take these properties into account.

There are different approaches to quantify connectivity of certain parameters in a continuous field. They are based on indicator fields derived from the parameter fields. The information if there is a spanning cluster of material of a certain parameter range in the field can be derived by the two-point cluster density as defined by [Torquato, 2002]. The Euler characteristic (e.g. [Mecke and Wagner, 1991]), which is also calculated from indicator fields, has been used by [Vogel, 2002] as a criterion for connected structures.

[Hilfer, 1992] derived the probability distribution for a field, that a representative elementary volume (REV) with a given size has a spanning cluster to quantify connectivity properties.

For flow in the unsaturated zone these properties are important to characterize trapping effects or accessibility criteria, which have an influence on the upscaled retention curve. But it is also important information for the effective unsaturated permeability function. As second order stochastic methods do not quantify connected structures, this information is not contained in upscaled models derived with these methods. Some methods of effective medium theory (described e.g. in [Torquato, 2002]) can be used to incorporate connectivity, as they are based on a background - inclusion description of the parameter field. Percolation theory (e.g. [Hunt, 2005]) can also be useful to take information about connected structures into account.

In this contribution we will discuss simple upscaling methods for Richards equation, which reflect connected paths of the soil structure. The upscaled models will be derived assuming capillary equilibrium ([Pickup and Stephen, 2000]). The effective permeability curves will be derived using effective medium theory, similar to the methods discussed in [Neuweiler and Vogel, 2006], and with a percolation method similar to the method of [Hilfer, 1992]. Information about connected structures will also be included for the effective retention function.

2. UPSCALED RICHARDS EQUATION USING CAPILLARY EQUILIBRIUM

Flow in the unsaturated zone is described by Richards equation,

$$\frac{\partial \Theta(h)}{\partial t} - \vec{\nabla} \cdot K_0 k_r(h) \left(\vec{\nabla} h + \vec{e}_z \right) = 0, \tag{1}$$

which is a continuity equation for the water in the soil. $\Theta[-]$ is the water content, which is $\Theta = S n_f$, $S[-]$ being the water saturation and $n_f[-]$ the porosity. $h[L]$ is the hydraulic head of the water, which is negative under unsaturated conditions. It is assumed that the water saturation S and the hydraulic head h are uniquely related. $K_0[L/T]$ is the intrinsic permeability, or the permeability of the soil at saturated conditions. $k_r[-]$ is the relative permeability, which is assumed to be a unique function of the hydraulic head h. $\vec{e}_z$ is the unit vector in vertical direction.

2.1. **Heterogeneous model.** In heterogeneous media, the parameters and parameter functions of the soil depend explicitly on space. Heterogeneous parameters would be the parameters for the relation between S and h and for the relation between k_r and h, the porosity n_f and the intrinsic permeability K_0. We will assume here, that the porosity is constant and that the relative permeability and the saturation - hydraulic head relation have one common heterogeneous parameter, which corresponds to the entry pressure head of the material, h_e. All other parameters in these functions are assumed to be constant. We also assume that the entry pressure is correlated to the intrinsic permeability as in a Miller similar medium ([Sposito and Jury, 1990]). The intrinsic permeability is often written as

$$K_0(\vec{x}) = K_g \exp\left(f_k(\vec{x})\right), \tag{2}$$

where K_g is the geometric mean of the intrinsic permeability and f_k is the log permeability. For a Miller similar medium ([Sposito and Jury, 1990]) this yields

$$h_e(\vec{x}) \propto \frac{1}{\sqrt{K_0(\vec{x})}}, \rightarrow h_e(\vec{x}) = h_g \exp\left(-\frac{1}{2} f_k(\vec{x})\right), \tag{3}$$

where h_g is the entry pressure which corresponds to the geometric mean of the permeability. It is not necessarily the geometric mean of the entry pressure field. In this model there is only one heterogeneous parameter, which is the log intrinsic permeability f_k.

As an illustration a simple model for local parameter functions will be used. For the retention function a Brooks Corey model ([Brooks and Corey, 1966]) with a Brooks-Corey parameter $\lambda = 2$ is used. Taking the relation (3) into account, this yields

$$S(f_k, h) = \begin{cases} \frac{h_g^2}{h^2} \exp(-f_k) & \text{if } f_k > -2\ln\left(\frac{h}{h_g}\right) \\ 1 & \text{otherwise} \end{cases} \tag{4}$$

$$K_0 k_r(f_k, h) = \begin{cases} K_g \frac{h_g^8}{h^8} \exp(-3f_k) & \text{if } f_k > -2\ln\left(\frac{h}{h_g}\right) \\ K_g \exp(f_k) & \text{otherwise} \end{cases} \tag{5}$$

2.2. **Upscaled model with capillary equilibrium conditions.** The upscaled model describes the continuity of water on a large scale, where small scale heterogeneities are no longer resolved. The upscaled model has homogeneous, effective parameters. We will use here the upscaled model obtained assuming capillary equilibrium. Such models have been derived with homogenization theory by [Lewandowska and Laurent, 2001] among others. The method will not be explained here, but the assumptions and procedure will be outlined briefly.

Several assumptions have to hold for the applicability of homogenization theory. The medium has to be macroscopically homogeneous, and the length scale of the averaging volume (in the following called unit cell) has to be much smaller than the size of the medium. In homogenization theory this corresponds to the assumption of scale separation. The solution has to be locally stationary, that means, it is periodic or in average periodic over a unit cell. It is also assumed, that the flow processes on the large scale happen slowly, so that the effective parameters can be calculated from steady state conditions. The capillary equilibrium condition means that on the small scale capillary forces dominate, so that the hydraulic head can be assumed as locally constant (constant over the size of a unit cell). That means, on the small scale gravity forces have to be negligible compared to the capillary forces. If these conditions are fulfilled it has been shown ([Lewandowska and Laurent, 2001]), that the upscaled model has approximately the same form as the original Richards equation

$$\frac{\partial \Theta_{\text{eff}}(\langle h \rangle)}{\partial t} - \vec{\nabla} \cdot K_g k_{\text{eff}}(\langle h \rangle) \left(\vec{\nabla}\langle h \rangle + \vec{e}_z\right) = 0. \tag{6}$$

The angular brackets denote the hydraulic head which has been spatially averaged over a unit cell. There are effective relations between averaged saturation and averaged hydraulic head and between the averaged hydraulic and the unsaturated permeability.

To obtain the effective retention function several values for the averaged hydraulic head $\langle h \rangle$ are chosen. As the head is in capillary equilibrium locally constant, the local saturation distribution $S_{\langle h \rangle}(\vec{x})$ can be derived directly from the local parameter distribution. The saturation distribution is spatially averaged over a unit cell for a value of $\langle h \rangle$, yielding one point on the effective hydraulic head - saturation relation. By repeating this procedure for a set of values for the hydraulic head, the effective retention curve is obtained.

The effective permeability curve is also obtained by assuming one fixed value for the averaged hydraulic head $\langle h \rangle$. The local permeability field $K_{\text{tot}}(\vec{x}) = K_0(\vec{x}) k_{r\,\langle h \rangle}(\vec{x})$ can be calculated directly for this given value. The effective permeability value is obtained by assuming a unit pressure gradient in horizontal and in vertical direction over the unit cell, imposing periodic boundary conditions. From the averaged fluxes in horizontal and vertical direction the effective permeability for the given value of the hydraulic head $\langle h \rangle$ can be derived. By choosing again a set of values for the hydraulic head, the effective unsaturated permeability curve is obtained. This procedure is described in detail in [Lewandowska and Laurent, 2001].

The explicit parameter distribution of a medium is usually not known. This is not important for the effective retention curve, as the only information needed is the distribution of volume percentage the heterogeneous parameters (here only f_k), $\Phi(f_k)$. It allows for the calculation of the distribution of saturation values in a unit cell for a given hydraulic head. The saturation can then be averaged to obtain the averaged saturation distribution. The effective permeability has to be approximated for a given characterization of the field structure. The geometric mean of the local field or effective medium theory methods could be used to calculate the effective permeability from the local permeability distribution for a given hydraulic head $\langle h \rangle$.

3. CONNECTED FLOW PATHS

3.1. **Influence of connected structures on the upscaled model.** Usual upscaling methods do not take information of connected structures of material into account. The capillary equilibrium approach can lead to inconsistencies of the effective retention curve. They can be illustrated best by considering a cell of one material which is surrounded by a different material. For drainage at wet conditions (high hydraulic heads) a cell of coarse material is expected to drain with the capillary equilibrium approach, even if it is surrounded by fine material for which the entry pressure of air is not exceeded. In reality such parts of coarse material will remain wet. Also, for drainage at dry conditions (low hydraulic head) a cell of fine material is expected to drain if its entry pressure is exceeded, even if it is surrounded by coarse material that is very dry so that the permeability of these parts is extremely low. In reality such parts will drain extremely slowly so that they can be considered to remain wet at intermediate times.

The effective permeability curve will also be affected by the connectivity properties of the material. This would already be true for the effective intrinsic permeability. For unsaturated flow the effect will become more severe at certain ranges of the hydraulic head, where the variance of the unsaturated permeability becomes much larger than the variance of the intrinsic unsaturated permeability. A method that reflects connectivity properties, such as background-inclusion models or a percolation based model might yield better results than the methods which do not reflect connected structures, such as stochastic methods.

3.2. **Characterization of connected structures.** The important information for the upscaled models is, which material is connected throughout the medium and which material forms isolated structures. Three methods to quantify this criterion will here be shortly described.

3.2.1. *Two-point cluster density.* The two-point cluster density, as described by [Torquato, 2002], is a measure for connectivity of certain parameter ranges. It can be calculated for a two-cut indicator field, where the field is indicated with a one if the parameter f_k is inbetween two threshold values $f_{k\,1}$ and $f_{k\,2}$ and zero otherwise. The two-point cluster density is the probability, that two locations on the field, which are separated by a distance Δx, belong to the same cluster. If the two-point cluster density does decay over the length of a unit cell, the parameter range between the two thresholds can be considered as isolated, otherwise it is connected.

3.2.2. *Euler characteristic.* The Euler characteristic χ of a set has been used by [Vogel, 2002] to characterize connectivity of material properties. It can roughly be defined as the number of isolated objects N minus the number of holes C in 2d ($\chi = N - C$). In 3d it is the number of isolated objects N plus the number of enclosed cavities H minus the number of torus shaped holes C in 3d ($\chi = N + H - C$). A negative Euler characteristic describes a set of a connected structure with loops, while a positive Euler characteristic describes isolated objects. The Euler characteristic can thus be considered as a measure for connected structures.

The Euler characteristic can be derived from a one-cut indicator field of the parameter field, where the indicator value is increased continuously. If the Euler characteristic gets negative, the set with a parameter value below the threshold value becomes connected.

3.2.3. *Local percolation probability.* In the paper of [Hilfer, 1992] the local probability distribution is calculated. It is the probability that a sample of a field with the size of a unit cell has a connecting cluster. For a field with a parameter distribution this can be obtained from indicator fields, indicating e.g. the highly conductive parts. The local percolation probability is a useful measure if a medium can be considered as bi- or multivariate with a very poorly conductive part and the medium has an irregular structure.

4. INCLUDING INFORMATION ABOUT CONNECTED STRUCTURES INTO EFFECTIVE PARAMETER FUNCTIONS

With the characteristics described above, criteria for ranges of the parameter field f_k which are connected over a unit cell and for ranges which are isolated can be found. This information can then be included into the calculation of effective parameter functions.

In the following we will assume that there is one threshold value $f_{k,\,thr\,1}$ in the field, at which the low values of the parameter field become connected and below which they are unconnected. There is another threshold $f_{k,\,thr\,2}$, above which the high values of the field becomes disconnected. A field does not necessarily have to have this structure, however, the results can be extended to more complex structures. This will be illustrated with the heterogeneous model explained above, where the only heterogeneous parameter is the log intrinsic permeability.

4.1. **Retention function.** Using the capillary equilibrium approach, the effective retention function would just be the average over the local saturation distribution for a given averaged hydraulic head.

$$\Theta_{\mathrm{eff,\,cap.eq.}}(\langle h\rangle) = n_f \int S(f_k, \langle h\rangle)\Phi(f_k)df_k. \tag{7}$$

$\Phi(f_k)$ is the distribution of the parameter f_k.

If fine material is isolated and surrounded by coarse material, the effect of water trapping in fine material due to high permeability contrasts can be taken into account, by setting a contrast threshold for the permeability of fine inclusion material and connected coarse material, above the fine material is supposed to remain wet at the relevant time scales. In this model this is related to a critical parameter $f_{k\,crit}$. The trapping of water can then be taken into account by using the local relation

$$S(f_k, \langle h\rangle)_{\mathrm{tr}} = \begin{cases} \dfrac{h_g^2}{h^2}\exp(-f_k) & \text{if } f_k > \max\left(-2\ln\left(\dfrac{\langle h\rangle}{h_g}\right), f_{k\,crit}\right) \\ 1 & \text{otherwise} \end{cases} \tag{8}$$

instead of (4) to calculate the effective retention function (7).

The fact that coarse material which is surrounded by fine fully water saturated material cannot drain (as it is not accessible for air) can be taken into account using the threshold value $f_{k,\,thr\,2}$ above which the parameters form isolated structures. The effective retention function is then

$$\Theta_{\mathrm{eff,\,acc.}}(\langle h\rangle) = \begin{cases} \Theta_{\mathrm{eff,\,cap.eq.}} & \text{if } f_{k,\,thr\,2} > -2\ln\left(\dfrac{\langle h\rangle}{h_g}\right) \\ 1 & \text{otherwise} \end{cases} \tag{9}$$

An example of the three effective retention curves (capillary equilibrium only, capillary equilibrium with trapping due to large parameter contrasts and capillary equilibrium with accessibility criteria) is shown below. The f_k field is normally distributed with $\sigma_f^2 = 2$.

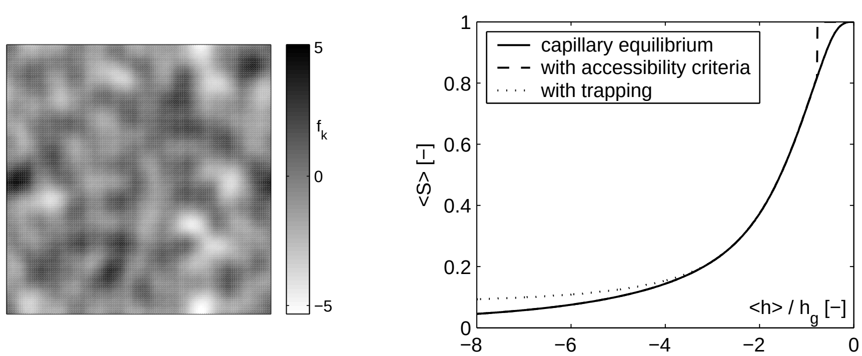

Figure 1: Test field (connected inbetween $f_k = -0.5$ and $f_k = 0.5$) and effective retention function according to (7), (9) with a ratio of the permeability of 100 as trapping criterion and according to (8).

4.2. **Unsaturated permeability.** If the medium is similar to a Gaussian field and has connected structures of material in the intermediate parameter range, while high and low values form isolated structures, the effective permeability function can be obtained using the geometric mean of the local parameter distribution $K_{\text{tot}} = K_0 k_r(\langle h \rangle, f_k)$.

If the medium has however connected structures in the high or low extremes of the parameter range, the effective permeability might be better derived with effective medium theory based on a background-inclusion model. Such models for the calculation of the effective permeability for unsaturated flow have been discussed by [Neuweiler and Vogel, 2006]. A simple model is the Maxwell approach (see e.g [Torquato, 2002]). If the parameters in a certain range between $f_{k,1}$ and $f_{k,2}$ are connected, a substitute permeability K_{conn} for this range can be assigned (e.g. the geometric mean of the values in this range). Applying the Maxwell approach, the effective permeability for a given value of $\langle h \rangle$ is defined by the equation

$$\frac{K_{\text{conn}} - K_{\text{eff}}(\langle h \rangle)}{K_{\text{conn}} + K_{\text{eff}}(\langle h \rangle)} = \int_{-\infty}^{f_{k,1}} \frac{K_{\text{conn}} - K_0(f_k) k_r(\langle h \rangle, f_k)}{K_{\text{conn}} + K_0(f_k) k_r(\langle h \rangle, f_k)} \Phi(f_k) df_k + \int_{f_{k,2}}^{\infty} \frac{K_{\text{conn}} - K_0(f_k) k_r(\langle h \rangle, f_k)}{K_{\text{conn}} + K_0(f_k) k_r(\langle h \rangle, f_k)} \Phi(f_k) df_k. \tag{10}$$

It should be mentioned, that this method might overpredict the background property, as it is derived for a model with spherical inclusions. An example for the effective permeability curves using the Maxwell approach for a test field is shown below. The field has connected parameters in the high range. The parameter distribution is here $\Phi(f_k) = \frac{1}{3}\delta(f_k + 1.75) + \frac{1}{3}\delta(f_k) + \frac{1}{3}\delta(f_k - 1.75)$. The curve is compared to the effective permeability obtained with the geometric mean of the local field (which would correspond to the effective permeability based on the second order properties of the field) and to the numerically calculated permeability curve. The Maxwell approach overemphasizes the background material, but gives better results than the geometric mean.

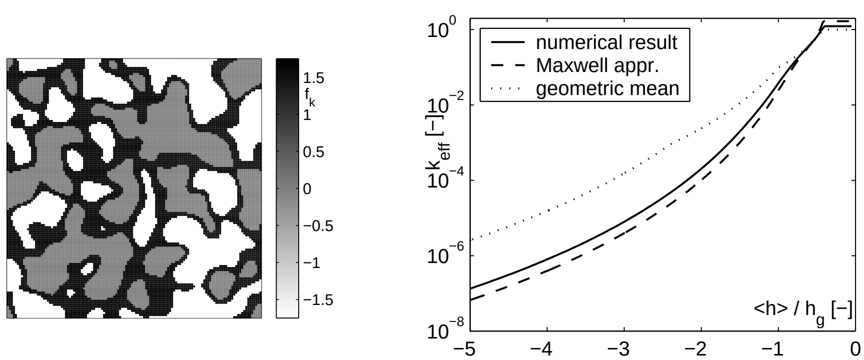

Figure 2: Test field (left) and effective unsaturated permeability curves (right).

If the parameter contrast in a medium is very high and the field does not have a regular structure (e.g. an uncorrelated field where the material with high permeability just exceeds the percolation threshold), percolation theory might be appropriate to model the effective permeability (e.g. [Hunt, 2005]). As an example an approach similar to that of [Hilfer, 1992] could be used. [Hilfer, 1992] used the self-consistent approach to describe the effective permeability in a pore scale model, where a certain part of the averaging cells have no connected path of pore space. He used then the percolation threshold obtained from percolation theory and the critical exponent from percolation theory to calculate the effective permeability instead the critical values obtained with the self-consistent approach. The model can also be used here, if the poorly conductive material is assigned to a constant low conductive permeability $K_{\text{lowcond.}}$. The highly conductive part covers a volume percentage of $\Phi_{\text{conn.}}$. Applying the method of [Hilfer, 1992] yields then the effective permeability

$$K_{\text{eff}}(\langle h\rangle) = K_{\text{lowcond.}} + (\Phi_{\text{conn.}} - \Phi_{\text{crit.}})^t \left[\int_{f_{thr}}^{\infty} \frac{\Phi(f_k)}{K_0(f_k)k_r(\langle h\rangle, f_k)} df_k\right]^{-1}. \qquad (11)$$

t is a critical exponent ($t = 1.3$ in 2d and $t = 2.0$ in 3d) and Φ_{crit} is the percolation threshold, depending on the coordination number of the grid.

An example for the effective permeability curves using the approach (11) for a test field is shown below. The field is uncorrelated and the material with the smallest value of f_k has a volume percentage of $\Phi_{\text{conn.}} = 0.66$. As the field has a square lattice, the percolation threshold is $\Phi_{\text{crit.}} = 0.59$. The parameter distribution is here $\Phi(f_k) = 0.66\,\delta(f_k + 1.4) + 0.17\,\delta(f_k - 1.3) + 0.17\,\delta(f_k - 2.0)$. At low pressures the material with $f_k = -1.4$ has a much higher conductivity than the other two materials. The curve is compared to the effective permeability obtained with the geometric mean of the local field (which would correspond to the effective permeability based on the second order properties of the field) and to the numerically calculated permeability curve.

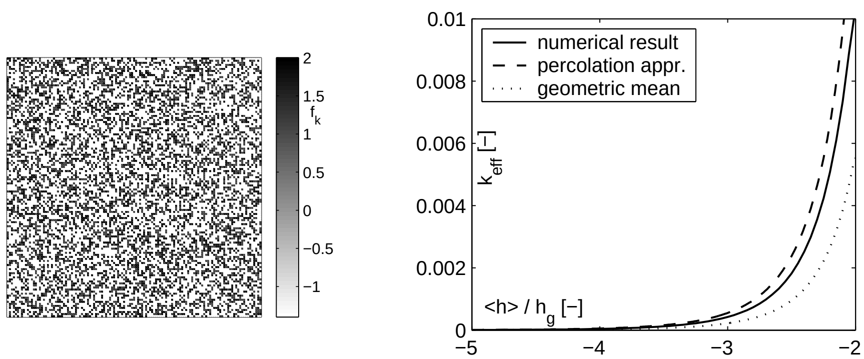

Figure 3: Test field (left) and effective unsaturated permeability curves (right).

5. CONCLUDING REMARKS

This contribution deals with upscaling of Richards equation for capillary equilibrium conditions. Methods to derive the effective retention curve and to derive the effective unsaturated permeability curve are discussed, where information about connected parts of the soil are taken into account.

Trapping of water is reflected in the effective retention curve. With the usual capillary equilibrium approach this is not taken into account. The effective unsaturated permeability function was calculated with an effective medium theory approach, which is based on a background - inclusion description of the medium. The connected parts of the material are assigned to the background material. A percolation theory approach was used to calculate the effective permeability function for an uncorrelated random field.

These methods include only information about the parameter distribution and some information about connected parameter values. This is still a quite simplified characterization. No information about the correlation structure of the medium or about the tortuosity of indicator fields is included. To improve the upscaled models, a more comprehensive description of heterogeneity are needed, which can still be obtained from local data.

References

Brooks and Corey, 1966. Brooks, R.H. and A.T. Corey (1966), Properties of Porous Media Affecting Fluid Flow, *Soil Sci. Soc. Am. J., 39 (2)*, 61-88.

Gomez-Hernandez and Wen, 1997. Gomez-Hernandez, J.J. and X.-H. Wen (1997), To be or not to be multi-Gaussian? A reflection on stochastic hydrogeology, *Adv. Water Resour., 21*, 47-61.

Hilfer, 1992. Hilfer, R. (1992), Local-porositz theory for flow in porous media, *Phys. Rev. B 45(13)*, 7115-7121.

Hunt, 2005. , Hunt, A. G. (2005), *Percolation theory for flow in porous media*, Springer, Berlin.

Knudby and Carrera, 2005. , Knudby, C. and J. Carrera (2005), On the relationship between indicators of geostatistical, flow and transport connectivity, *Adv. Water Resour., 28*, 405-421.

Lewandowska and Laurent, 2001. Lewandowska, J. and J.-P. Laurent (2001), Moisture transfer in an unsaturated heterogeneous porous medium, *Transport in Porous Media, 45*, 321-345.

Mecke and Wagner, 1991. , Mecke, K. and H. Wagner (1991), Euler characteristic and related measures for random geometric sets, *Journal of Statistical Physics 64*, 843-850.

Neuweiler and Vogel, 2006. , Neuweiler, I. and H.J. Vogel (2006), Upscaling of unsaturated flow considering connectivity, submitted to *Water Resour. Res.*.

Pickup and Stephen, 2000. Pickup G.E. and K. D. Stephen, An assessment of steady-state scale-up for small-scale geological models, *Petroleum Geoscience, 6*, 203-210, 2000.

Sposito and Jury, 1990. Sposito G. and W.A. Jury (1990), Miller similtude and generalized scaling analysis, in *Scaling in Soil Physics: Principles and Applications*, Eds.: D. Hillel and D.E. Elrick, SSSA Spec. Publ, 13-22.

Torquato, 2002. , Torquato, S. (2002), *Random Heterogeneous Materials*, Springer, New York.

Vogel, 2002. Vogel, H.-J. (2002), Topological characterization of porous media, In: Morphology of Condensed Matter - Physics and Geometry of Spatially Complex Systems, Mecke, K. and Stoyan, D. (eds), Lecture Notes in Physics, 600, 75-92.

Zhang, 2002. Zhang, D. (2002), *Stochastic Methods for Flow in Porous Media*, Academic Press, San Diego.

Zinn and Harvey, 2003. Zinn, B. and C.F. Harvey (2003), When good statistical models of aquifer heterogeneity go bad: A comparison of flow, dispersion and mass transfer in connected and multivariate Gaussian hydraulic conductivity fields, *Water Resour. Res. 39(3)* 1051, doi10.1029/2001WR001146.