# Hydraulic conductivity estimation for soils with heterogeneous pore structure

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# Hydraulic conductivity estimation for soils with heterogeneous pore structure

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**Abstract.** The hydraulic conductivity function, which is required to solve the Richards equation, is difficult to measure. Therefore prediction methods are frequently used where the shape of the conductivity function is estimated from the more easily measured water retention characteristic. Errors in conductivity estimations can arise either from an invalidity of the prediction model for a given soil, or from an incorrect description of the retention data. This second error source is particularly important for soils with heterogeneous pore systems that cannot be adequately described by the usually used retention functions. To describe the retention characteristics of such soils, a flexible $\theta(\psi)$ function was formed by superimposing unimodal retention curves of the van Genuchten (1980) type. By combining this retention model with the conductivity prediction model of Mualem (1976), conductivity estimations for soils with heterogeneous pore systems are obtained. Estimated conductivities by this model and the classical van Genuchten–Mualem method can differ by orders of magnitude. Thus reported disagreements between measured and estimated conductivities may in some cases be due to an inadequate description of the retention data rather than due to a failure of the prediction model.

## Introduction

The increasing concern with groundwater pollution and contamination of soils by hazardous substances has stimulated the development of numerous mathematical models of pollutant transport in soils. Today, the numerical simulation of water and pollutant transport in unsaturated soils has become a standard tool for assessing environmental pollution problems. Despite the existence and the use of simplistic models for management purposes [e.g., *Carsel et al.*, 1985; *Barraclough*, 1989] (see overviews by *Addiscott and Wagenet* [1985] and *Loague and Green* [1991]), as well as the recent intensive development of specific macropore models [e.g., *Jarvis et al.*, 1991; *Chen and Wagenet*, 1991; *Gerke and van Genuchten*, 1993], the most important approaches to modeling transient water and solute transport in the vadose zone are based on the Richards equation. To solve this equation, the knowledge of the effective soil hydraulic properties, namely, the soil moisture characteristic $\theta(\psi)$ and the $K(\theta)$ or $K(\psi)$ relationship over the whole range of moisture conditions is required. Here, $\theta$ (cubic centimeters per cubic centimeter) is the volumetric water content, $\psi$ (centimeters) is the matric pressure head, and $K$ (centimeters per day) is the hydraulic conductivity (a scalar property for the one-dimensional case). For use in models, the hydraulic properties are commonly expressed by analytical functions, often called parameteric models, as, for example, listed by *van Genuchten and Nielsen* [1985], *Bruce and Luxmoore* [1986], and *Mualem* [1986]. The parameters of these models can be obtained by fitting the functions to experimental water retention and conductivity data. Alternatively, they can be estimated from more easily measured soil properties [*Bloemen*, 1980; *Saxton et al.*, 1986; *Wösten and van Genuchten*, 1988; *Vereecken et al.*, 1989], or determined by parameter estimation techniques when the inverse problem is solved [*Zachmann et al.*, 1981, 1982; *Hornung*, 1983; *Kool et al.*, 1987; *Kool and Parker*, 1988].



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Of all hydraulic properties, the unsaturated hydraulic conductivity $K$ is most difficult to measure. Therefore the use of indirect methods where $K(\theta)$ is estimated from more easily measured soil properties has become more and more common [*van Genuchten and Leij*, 1992]. A potentially powerful class of methods results from pore-size distribution models, where the water retention curve of a porous medium is interpreted as statistical measure of its equivalent pore-size distribution [*Corey*, 1992]. In this approach, the conductivity is estimated by applying the concept of viscous fluid flow through capillaries and by using a conceptual model to describe the pore interaction and pore connectivity [*Mualem*, 1986]. Three basic groups of statistical prediction models may be distinguished: (1) the capillary-bundle model of *Purcell* [1949] with its subsequent tortuosity corrections by *Yuster* [1951], *Burdine* [1953], *Wyllie and Gardner* [1958], and *Alexander and Skaggs* [1986]; (2) the cut and random rejoin model of *Childs and Collis-George* [1950] with its subsequent modifications by *Marshall* [1958], *Millington and Quirk* [1961], *Campbell* [1974] and others; and, most recently, (3) the slab model of *Mualem* [1976]. *Mualem and Dagan* [1978] and *Mualem* [1986, 1992] provide comprehensive reviews for these groups of conductivity estimation models.

Closed-form expressions for the retention function and the conductivity function are often used in parameter estimation techniques where the inverse problem is solved [*Kool and Parker*, 1987a, b]. Applying a predictive model that couples the conductivity function with the retention function is then of particular advantage because it minimizes the number of parameters needed to express the hydraulic relationships. For the validity of this approach it is essential that the prechosen functional representation of both the retention curve and the conductivity curve as well as the model that couples the two functions are appropriate over the whole moisture range.

In principle, the statistical models can be used to estimate absolute conductivity values, but in practice they are used only to derive the shape of the conductivity function from the shape of the retention curve. To obtain absolute values, the estimated conductivity curve must be scaled with at least one measured conductivity, the "matching value" [*Nielsen et al.*, 1960]. Most frequently, the saturated conductivity is taken as matching value, although several authors [*van Genuchten and Nielsen*, 1985; *Mualem*, 1986; *Luckner et al.*, 1989; *Nielsen and Luckner*, 1992] have warned against this practice.

Errors of conductivity estimates may arise from two sources: (1) errors due to an inappropriate description of the soil moisture characteristic and (2) errors stemming from failure of the prediction model. Beginning with the work of *Nielsen et al.* [1960], numerous studies have compared estimated with measured conductivities and have discussed the validity of prediction methods from an empirical or semiempirical point of view [e.g., *Kablan et al.*, 1989; *Michiels et al.*, 1989; *Stephens*, 1992]. As a general result from these investigations, conductivity estimation methods appear to be relatively reliable for sandy soils with narrow particle size distributions, whereas for loamy and clayey soils they often fail. This failure is mostly attributed to incorrect values of the tortuosity coefficient (or pore-interaction factor) $\tau$ (dimensionless), which is an empirical parameter in the predicting equations (see (6) in the theory section). *Schuh and Cline* [1990] have shown that $\tau$ can vary over a wide range. In addition to these experimental investigations, theoretical discussions and reviews [*Brutsaert*, 1968; *Gardner*, 1974; *Mualem*, 1976; *Parkes and Waters*, 1980; *van Genuchten and Nielsen*, 1985; *Mualem*, 1986; *Alexander and Skaggs*, 1986] as well as mathematical sensitivity analyses [*Sakellariou-Makrantonaki et al.*, 1987; *Vogel and Cislerova*, 1988; *Sidiropoulos and Yannopoulos*, 1988] have been published. Despite the extensive treatment of the prediction problem and due to the lack of a reliable data base of measurements in undisturbed soils, the results appear ambiguous and inconclusive. A statement which was published a decade ago appears to be still valid: "The problem of which [conductivity] measurement method and which prediction method are most valid is undoubtedly one of the most vexing ones in contemporary soil physics" [*Ragab et al.*, 1981, p. 384].

When discussing validity problems, most investigators have concentrated on the failure of the predictive model, more or less disregarding the problem of interferences with the first error source. No investigation has been published so far on the systematic errors of conductivity estimation methods for soils with heterogeneous pore systems which arise from the use of nonoptimal water retention functions. The objective of this paper is to analyze conductivity estimations for such soils. After reviewing the characteristics of heterogeneous pore systems, conductivity estimates are obtained by combining a flexible retention function with *Mualem*'s [1976] model. The results of this method are compared with results obtained by classical unimodal models. The differences are analyzed and the general limitations of statistical conductivity estimation methods, particularly for soils with a nonnegligible fraction of large pores, are discussed.

## Theory

### Water Retention Curves and Equivalent Pore Size Distributions

The pore system of a rigid soil can be characterized by its equivalent pore-size distribution, which is commonly calculated from the specific moisture capacity $C^* = d\theta/d\psi$. According to Laplace's law, the matric pressure at which a water-filled pore starts to drain is inversely proportional to the equivalent radius $r$ of the pore necks. If $C^*$ as a measure of pore density is plotted versus $\psi$ on a linear scale, pores with large radii of different orders of magnitude are squeezed together, which masks the shape of the pore-size distribution at the hydrologically important range close to saturation. Since the matric pressure head varies over orders of magnitude, the retention characteristics are frequently plotted on a logarithmic pressure head scale, which is conveniently expressed in $pF$ units, defined for the unsaturated range by $pF \equiv \log_{10}(-\psi)$ [*Schofield*, 1935], where $\psi$ is expressed in centimeters. The $pF$ scale is equivalent to a logarithmic scale for the pore radius, and the derivative of the water content versus $pF$ therefore appropriate for visualizing the pore-size distribution over different orders of magnitude. The so-defined pore-size density is related to $C^*$ by

$$-\frac{d\theta(r)}{d\log_{10} r} = \frac{d\theta(pF)}{dpF} = \frac{d\theta(\psi)}{d\log_{10}|\psi|} = \frac{d\psi}{d\log_{10}|\psi|}\frac{d\theta(\psi)}{d\psi} = [\log_e(10)]|\psi|C^*. \qquad (1)$$

The pore-size distributions that are depicted in Figures 1–11 are calculated by (1). Accordingly, the shaded area between two $pF$ values indicates the fraction of pore space that drains when the pressure head is changed by one order of magnitude.

Numerous mathematical functions have been used in the literature to express $\theta(\psi)$ in analytical form [*Brooks and Corey*, 1964; *King*, 1965; *Brutsaert*, 1966; *Visser*, 1968; *Laliberte*, 1969; *Farrel and Larson*, 1972; *Rogowski*, 1972; *Su and Brooks*, 1975; *Haverkamp et al.*, 1977; *Gillham*, 1976; *Simmons et al.*, 1979; *D'Hollander*, 1979; *van Genuchten*, 1980]. Most popular among these functions are the equations of *Brooks and Corey* [1964] (here in a notation that is slightly modified from the original version):

$$\begin{aligned} S_e &= (\alpha|\psi|)^{-\lambda} \qquad & \alpha|\psi| > 1 \\ S_e &= 1 \qquad & \alpha|\psi| \le 1 \end{aligned} \qquad (2)$$

and, more recently, the equation of *van Genuchten* [1980]:

$$S_e = [1 + (\alpha|\psi|)^n]^{-m}, \qquad (3)$$

where $S_e$ is the effective saturation (dimensionless), defined by $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$, with $\theta_s$ and $\theta_r$ indicating the saturated and residual volumetric water contents, respectively, $\alpha > 0$ (centimeters) is a scaling factor that determines the position of the pore size maximum, and $\lambda$, $n$, and $m$ are dimensionless curve-shape parameters, subject to $\lambda > 0$, $m > 0$, and $n > 1$.

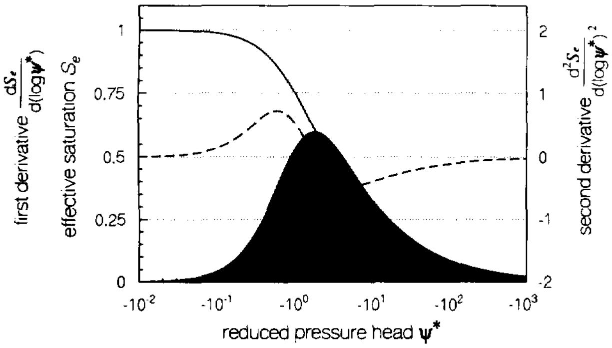


**Figure 1.** Retention curve (solid line), first derivative $dS_e/d \log \psi^*$ (shaded area), and second derivative $d^2S_e/d (\log \psi^*)^2$ (dashed line) of the van Genuchten function with $n = 1.5$ and $m = 1 - 1/n$. The reduced pressure head $\psi^*$ (dimensionless) is defined by $\psi/\alpha$. The shaded area represents the pore-size distribution. The position of maximum pore density is at $\psi^* = -(1/m)^{(1/n)}$.

Equation (2) and (3) can easily be combined with conductivity prediction models to obtain closed-form expressions for $K(\theta)$ and $K(\psi)$ [*Mualem*, 1992]. By this, both $\theta(\psi)$ and $K(\psi)$ are determined by the parameters of the retention curve plus one additional matching factor to scale the predicted hydraulic conductivity function. *Brooks and Corey* [1964] combined their function with the predictive model of *Burdine* [1953]; *Campbell* [1974] combined the same retention function with a simplified version of the *Childs and Collis-George* [1950] prediction model. The retention model of *van Genuchten* [1980] is most frequently coupled with the predictive model of *Mualem* [1976]. The resulting set of hydraulic functions has been thoroughly reviewed by *van Genuchten and Nielsen* [1985], *Luckner et al.* [1989], and *Nielsen and Luckner* [1992]. *Kool and Parker* [1987a] extended it to include hysteresis and air entrapment.

All the above-listed retention functions reflect unimodal and, if continuously differentiable, smooth normal to lognormal shaped pore-size distributions. This is illustrated by Figure 1, where the retention model of *van Genuchten* [1980] is depicted together with its underlying pore-size distribution (shaded area). As compared to the Brooks and Corey function, the van Genuchten function has the favorable property that its derivative $d\theta/dpF$ is continuous and becomes asymptotically zero toward the fine and large pores. The extension of the pore-size distribution toward the fine pores is determined by the product $mn$ (which for $\alpha\psi \gg 1$ is equivalent to $\lambda$ in the Brooks and Corey function), whereas the extension toward the large pores is determined by the ratio $m/n$. The larger this ratio is, the steeper is the decrease in pore density from its maximum toward the large pores. As will be shown later, the width of the pore-size distribution toward the large pores is of particular importance for estimating the conductivity function. Summarizing, the van Genuchten retention model in its general form (3) represents a continuous, smooth, unimodal, and bell-shaped pore-size distribution with the parameter $\alpha$ primarily determining the position of the pore density maximum and the parameters $m$ and $n$ determining the width toward the fine and large pore sizes. *Van Genuchten and Nielsen* [1985] compared various water retention models and concluded that (3) fits the water retention data of most soils almost perfectly.

However, to obtain the conductivity estimates as closed-form functions, the parameters of the van Genuchten equation must be subjected to the additional constraint $m + 1/n = i$, where $i$ is an integer value, for the van Genuchten–Mualem model generally taken as unity [*van Genuchten*, 1980]. This constraint eliminates some of the flexibility of the function, since a pore-size distribution that extends far toward fine pores is then always coupled with a relatively broad distribution towards the large pores, and vice versa. This is in fairly good accordance with experimental data for many soils. There are cases of fine-textured soils, however, where this constraint attributes a part of the pore space to unrealistically large pores.

There is some discussion whether the van Genuchten function is a physically realistic description of $\theta(\psi)$ over the whole moisture range when its parameter $n$ lies in the range $1 < n < 2$ [*Nielsen and Luckner*, 1992]. In this case, the second derivative, $d^2\theta/d\psi^2$, becomes infinite toward saturation, and the integral $\int_{\theta_s}^{\theta} \psi \, d\theta$ for $\lim_{\theta\to 0}$ is unbounded. This means that an infinite amount of work were necessary to extract all water from the soil [*Mualem*, 1978; *Sakellario-Makrantonaki et al.*, 1987]. According to our view, for practical purposes this does not restrict the usefulness of the van Genuchten function as an empirical model for the retention curve. Nevertheless, it appears important to realize that it expresses the retention characteristic as well as the derived property $C^*$ and the related conductivity estimation in a purely descriptive fashion. The coefficients should not be interpreted as parameters in a physical sense.

### Water Retention Characteristics of Soils With Heterogeneous Pore Systems

Undisturbed soils frequently have pore systems that are different from the unimodal, approximately normal distributed type which is represented by Figure 1. Consequently, attempts to fit their retention data with a simple sigmoidal curve lead to unsatisfying results. A scheme of typical fitting errors is depicted in Figure 2. It appears that such deviations are tacitly assumed to be within the confidence interval of the corresponding measured values. If they are not, such deviations would be relevant as will be shown later. This could be used to define the term "heterogeneous" with respect to hydrological properties. We can designate a pore system as heterogeneous if the pore-size distribution of a representative elementary area [*Bear and Bachmat*, 1991] cannot be correctly described by the van Genuchten function (or any other of the above mentioned unimodal retention functions).

Pore systems that are nonconform with a simple sigmoidal retention characteristic may be a result of specific particle-size distributions or be due to the formation of secondary pore systems by various soil genetic processes. Aggregation processes in loamy soils may lead to pore-size distributions that cause typical fitting problems in the midpore range, as illustrated in Figure 2 (bottom left) [e.g., *Sharma and Uehara*, 1968; *Smettem and Kirkby*, 1990]. Besides aggregation, biological soil-forming processes may lead to secondary pore systems in the large-pore range in soils of any texture (Figure 2 (top left)) [e.g., *Othmer et al.*, 1991; *De Jong et al.*, 1992]. Morainic soils and solifluction soils tend to have a significant fraction of pores over a wide range of tensions, which leads to fitting problems as illustrated in Figure 2 (top right) [e.g., *Parkes and Waters*, 1980; *Jacob-*

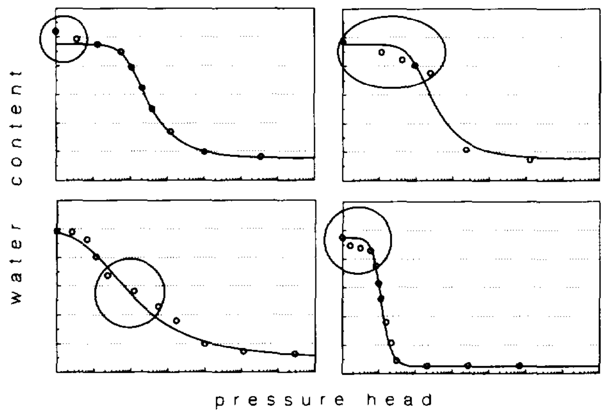


**Figure 2.** Schematic types of deviations between retention data of structured soils and fitted unimodal retention curves. The circles indicate typical trends, which help to identify structured pore systems even in cases where only few supporting data are available. (Top left) Increasing deviations between data and fitted curve when approaching saturation, observed in undisturbed soils of any texture [e.g., *Othmer et al.*, 1991; *De Jong et al.*, 1992]. (Top right) More or less straight retention characteristic in the wet range up to $pF3$–4, where the main pore system is located. Typical for morainic and solifluction soils [e.g., *Schjønning*, 1985; *Jacobsen*, 1989]. (Bottom left) Different slopes of fitted curve and data in the midpore range. Typical for aggregated loams [e.g., *Sharma and Uehara*, 1968; *Smettem and Kirkby*, 1990]. (Bottom right) Considerable change in water content very close to saturation, experimentally observed in unconsolidated sands (see, for example, *King* [1965] (liquid: soltrol C), *Ragab et al.* [1981], and *Stephens and Rehfeldt* [1985]).

*sen*, 1989; *Lafolie et al.*, 1989]. With unconsolidated sands, retention characteristics of the type in Figure 2 (bottom right) have been observed, even in cases where this cannot be due to boundary effects at the beginning of drainage [e.g., *King*, 1965; *Ragab et al.*, 1981; *Stephens and Rehfeldt*, 1985]. In natural soils, the schematic types of Figure 2 will always appear to some degree in combination (compare examples of *Boels et al.* [1978], *Currie and Rose* [1985], *Dixon* [1972], *Hantschel et al.* [1987], *Jeppson et al.* [1975], *Parker and van Genuchten* [1985], *Puckett et al.* [1985], and *Tsuji et al.* [1975]). Note that these heterogeneous pore systems can be found for field averages as well as for single soil samples [e.g., *Anderson and Cassel*, 1986].

### Multimodal Retention Function

To properly describe the retention characteristics of soils with heterogeneous pore systems, we introduce a multimodal retention function which is constructed by a linear superposition of subcurves of the van Genuchten type [*Durner*, 1991, 1992]:

$$S_e = \sum_{i=1}^{k} w_i \left[ \frac{1}{1 + (\alpha_i |\psi|)^{n_i}} \right]^{m_i}, \tag{4}$$

where $k$ is the number of "subsystems" that form the total pore-size distribution, and $w_i$ are weighting factors for the subcurves, subject to $0 < w_i < 1$ and $\sum w_i = 1$. As for the unimodal curve, the parameters of the subcurves ($\alpha_i$, $n_i$, $m_i$) are subject to the conditions $\alpha_i > 0$, $m_i > 0$, $n_i > 1$. We explicitly do not impose the additional constraint $m_i + 1/n_i = 1$. Figure 3 shows the superposition of two hypothetical pore-size distributions which define a bimodal pore system according to (4). The dark-shaded area can be interpreted as fine-textured pore system, with a maximum pore-size density around $pF4$ ($\triangleq r \approx 0.2$ μm), whereas the light-shaded area can be seen as a secondary pore system with its maximum density in the range of $r \approx 0.1$ mm.

The superposition of two unimodal pore systems has been previously used by *Peters and Klavetter* [1986] to describe the hydraulic properties of fractured rock. *Othmer et al.* [1991] and *Ross and Smettem* [1993] used this approach to describe the retention characteristics of soils with distinct secondary pore systems. *Pruess et al.* [1990] modeled the coupled transport of water, heat, and air in partially saturated porous rock by explicitly considering fracture effects. They compared the results with those obtained by treating the porous medium as a single continuum and derived simple criteria for the applicability of the effective continuum approximation. *Wang and Narasimhan* [1985, 1990] addressed the problem of finding effective parameter values and compared fractures in tuff with macropores in soil.

The multimodal retention model, (4), keeps the functional properties of the basic van Genuchten model, but is, due to the increased number of coefficients, able to account for the deviations discussed above. It is continuously differentiable, asymptotic to a zero slope towards the fine and large pores, and strongly monotonic over the whole moisture range. By keeping $k$ small, the function is well-behaved for interpolation purposes, reducing the noise in measured data while following the shape of the measured curve. *Hampton* [1990] showed that the use of unconstrained splines for describing

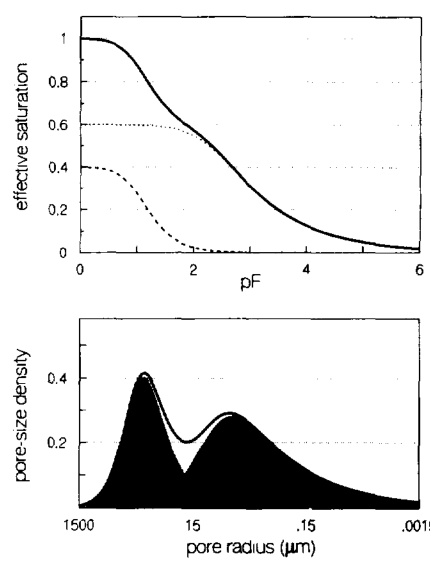


**Figure 3.** Construction of a multimodal retention function, (4). (Top) Bimodal retention curve (solid line), unimodal subcurve for the textural pore system (dotted line, $w_1 = 0.6$, $\alpha_1 = 0.005$ cm$^{-1}$, $n_1 = 1.4$, $m_1 = 1 - 1/n_1$), and unimodal subcurve for a secondary pore system (dashed line, $w_2 = 0.4$, $\alpha_2 = 0.1$ cm$^{-1}$, $n_2 = 2.2$, $m_2 = 1 - 1/n_2$). (Bottom) Pore-size distributions of bimodal function (solid line), of textural pore system (dark shaded), and of secondary pore system (light shaded).

retention data can lead to considerable problems in numerical simulations of water transport due to the rough shape of the water capacity function. In contrast to constrained spline interpolations, which appears to be the best alternative scheme, (4) requires less coefficients. Finally, its coefficients can, to a certain degree, be interpreted in the same manner as the basic van Genuchten coefficients, namely, $\psi_i = 1/\alpha_i$, indicating the positions of pore density maxima, and $n_i m_i$ and $n_i/m_i$, determining the width of the underlying pore-size distributions. However, if the pore system is not distinctly bimodal or multimodal, the coefficients of the multimodal retention function tend to be highly correlated. It is therefore important that they not be considered as "parameters" with a physical meaning; rather they must be seen as curve shape coefficients like those of any alternative interpolation function.

The multimodal retention function is fitted to data by minimizing the objective function $Z$:

$$Z(P) = \sum_{i=1}^{N} \omega_i \|\theta_i - \hat{\theta}(\psi_i, P)\|^{\mu}, \tag{5}$$

where $P = \{\theta_s, \theta_r, \alpha_i, n_i, m_i, w_i\}^T$ is the parameter vector, $N$ is the number of measured data, $\omega_i$ are the weights for the least squares minimization, $\mu$ determines the minimization norm, and $\theta_i$ and $\hat{\theta}(\psi_i, P)$ are the measured and calculated water contents at pressure $\psi_i$, respectively. If $\mu = 2$, (5) results in a weighted least squares scheme, which corresponds to a maximum likelihood fit under the assumption of independent and normally distributed data errors. If outliers are more frequent, $\mu$ can be set to unity. In this case, (5) minimizes the sum of absolute deviations between measured water contents and the retention curve. The fitting procedure we use is based on a multidimensional bracketing method. The numerical procedure is robust and unconditionally convergent, but computationally not very efficient. For each coefficient $p_i$, the following properties may be tailored for specific needs: (1) initial guess of $p_i$, (2) $p_i$ constant or optimized, and (3) allowed minimum and maximum value of $p_i$. The optimization is terminated when the improvement of the objective function or the changes of all parameter values are below their tolerance values between two iteration steps, ($\Delta Z < \varepsilon_Z$, $\Delta p_i < \varepsilon_{p_i}$), or when the maximum number of iterations is exceeded. (The program is available from the author on request.)

### Conductivity Estimation

The relative hydraulic conductivity function is computed by numerical evaluation of *Mualem*'s [1976] predictive model on base of the unimodal or multimodal representation of $\psi(S_e)$:

$$K = S_e^{\tau}\left[\frac{f(S_e)}{f(1)}\right]^2, \tag{6}$$

where $f$ is given by

$$f(S_e) = \int_0^{Se} \frac{1}{\psi(S_e')}\, dS_e'. \tag{7}$$

In (6), $S_e^{\tau}$ is an empirical correction function, which allows for a priori unknown effects of pore connectivity and tortuosity in Mualem's model. *Mualem* [1976] found an average value of $\tau = 0.5$ to be optimal for a set of 45 sample soils. The absolute conductivity $K_{\mathrm{abs}}(S_e)$ can be calculated by matching the predicted function $K(S_e)$ to a matching value $K_{\mathrm{ref}}$, measured at some reference saturation $S_{\mathrm{ref}}$, according to

$$K_{\mathrm{abs}}(S_e) = (S_e/S_{\mathrm{ref}})^{\tau} K_{\mathrm{ref}} K(S_e). \tag{8}$$

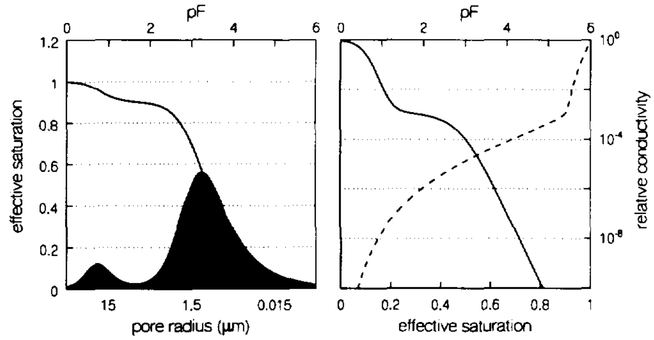


**Figure 4.** Conductivity estimation for a structured pore system. (Left) Bimodal retention curve (solid line) and underlying pore-size distribution (shaded area). (Right) Predicted relative conductivity functions $K(\psi)$ (from top left to bottom right, related to top axis) and $K(S_e)$ (from top right to bottom left, related to bottom axis). The coefficients are $w_1 = 0.1$, $\alpha_1 = 0.2\ \mathrm{cm}^{-1}$, $n_1 = 2.5$, $m_1 = 1 - 1/n_1$, $w_2 = 0.1$, $\alpha_2 = 0.001\ \mathrm{cm}^{-1}$, $n_2 = 2.2$, and $m_2 = 1 - 1/n_2$.

## Results and Discussion

### Conductivity Estimation for Heterogeneous Pore Systems

For the purpose of comparing conductivity estimates for bimodal and multimodal soils, we assume at this point that both the retention measurements of the example soils and the predictive model itself are free of error. Of course, these assumptions are not generally justified and have to be discussed later in their own right.

In Figure 4, the hydraulic properties of a hypothetical soil with a narrow textural pore-size distribution and distinct secondary pore system are shown. Two findings, which are of general nature, are clearly illustrated: (1) the shape of the retention curve is directly reflected in the shape of $K(\psi)$ and (2) the secondary pore system increases the conductivity by some orders of magnitude while taking only few percent of pore space. The particular shape of $K(\theta)$ cannot be reflected by unimodal models. The "similarity" between the shapes of $\theta(\psi)$ and $K(\psi)$ is physically meaningful: at pressure ranges where the specific water capacity is high, indicated by a steep slope of the retention function, the conductivity must drop steeply as well, since during a drainage process a large portion of the pore space empties in that range. A steep decrease of the conductivity close to saturation is typical for soils with a secondary pore system in the large-pore range. Composite conductivity functions with similar characteristics have been derived from explicit consideration of two porous systems, e.g., for fractured rock [*Wang and Narasimhan*, 1985; *Peters and Klavetter*, 1988] or for soils with macropores [*Othmer et al.*, 1991; *Chen and Wagenet*, 1991; *Chen et al.*, 1993].

If one attempts to describe a bimodal soil with simplified unimodal hydraulic functions, the error involved is much

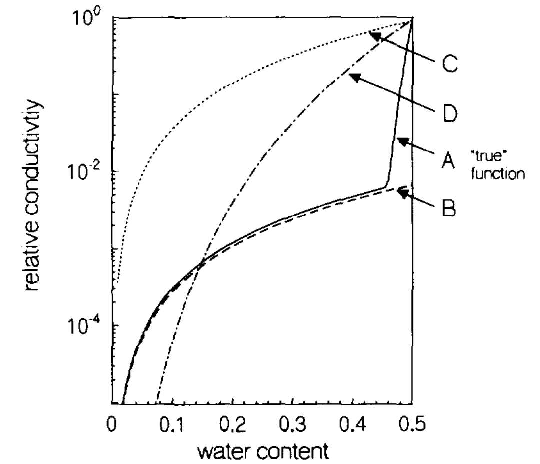


**Figure 5.** Schematic representation of the conductivity calibration problem for bimodal pore system. Line A, conductivity curve of a bimodal pore system; line B, unimodal predicted curve matched to unsaturated conductivity; line C, unimodal predicted curve matched to saturated conductivity; and line D, unimodal predicted curve with optimized pore interaction factor $\tau$.

larger for the conductivity estimations than for the retention function. Matching the unimodal conductivity function with the measured saturated conductivity value $K_s$, as is common practice, will lead to an overestimation of the unsaturated conductivity in the whole unsaturated moisture range (Figure 5, curve C). If, on the other hand, the unimodal predicted function is matched to an unsaturated conductivity value, the increase of hydraulic conductivity near saturation is not reflected, thus leading to a gross underestimation of the soil's conductivity near saturation (Figure 5, curve B). However, the use of this function in simulations of unsaturated water transport leads to a valid description of the hydraulic system as long as saturation is not approached [*Wang and Narashimhan*, 1985]. The double-porosity char-

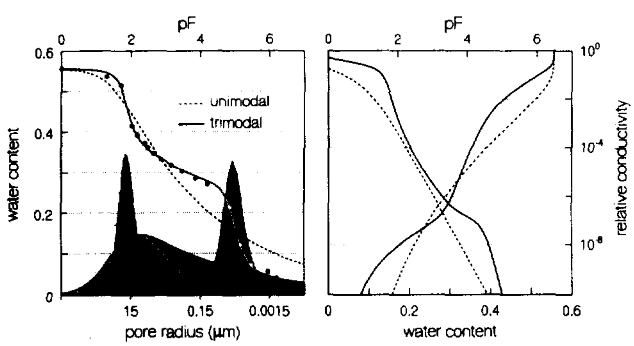


**Figure 6.** Hydraulic properties of Solar Village Clay [*Hampton*, 1989]. (Left) Measured retention data (solid circles), fitted bimodal (solid line), and unimodal (dashed line) retention curve, and corresponding bimodal (black shaded) and unimodal (light shaded) pore-size distributions. (Right) Predicted bimodal (solid lines) and unimodal (dashed lines) conductivity curves. The $K(\psi)$ curves, from top left to bottom right, are related to the top axis. The $K(\theta)$ curves, from top right to bottom left, are related to the bottom axis. The coefficients of the functions are listed in Table 1.

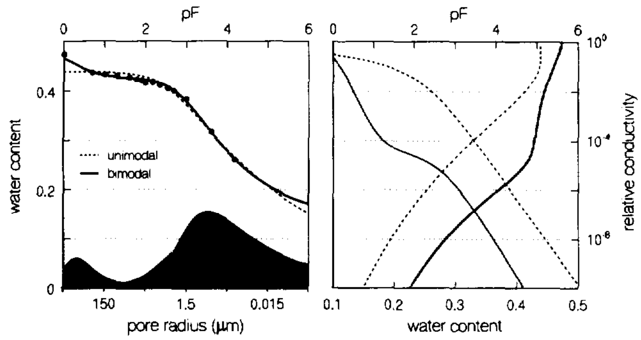


**Figure 7.** Hydraulic properties of Rideau Clay Loam [*De Jong et al.*, 1992]. See Figure 6 for explanations.

acteristic of the conductivity function cannot be reflected by the unimodal estimation, even if the tortuosity factor $\tau$ is manipulated (Figure 5, curve D).

In Figures 6, 7, and 8, measured retention data of three soils are depicted, representing structured pore systems which can be frequently found. The chosen examples are similar to the schematic soil types described in Figures 2 (bottom left), 2 (top left), and 2 (top right), respectively. In addition to the experimental data, Figures 6–8 show the least squares fitted unimodal and multimodal retention curves, the underlying pore-size distributions, and the estimated conductivity curves. Some physical properties of the soils and the coefficients of the fitted functions are listed in Table 1. Unlike the unimodal function, the multimodal function describes the measured data of each soil accurately, and it is obvious that in each case the two functions represent fundamentally different pore systems.

Figure 6 (left) depicts the hydraulic properties of a column packed with small clay aggregates [*Hampton*, 1989]. The pore-size distribution is distinctly bimodal, with a maximum pore density of the intra-aggregate pores at $r \simeq 0.01$ $\mu$m, and a secondary maximum for the interaggregate pores at $r \simeq 20$ $\mu$m. Whereas the primary pore system is determined by the particle-size distribution of that soil, the pore space between the aggregates depends only on the packing and is therefore essentially independent of the soil texture. Note that the existence and extent of secondary pore systems in undisturbed soils poses a limitation to the success potential of regression methods that seek to predict hydraulic relationships solely from particle-size distributions. Figure 7 (left) shows data of an undisturbed core of Rideau clay loam [*De*

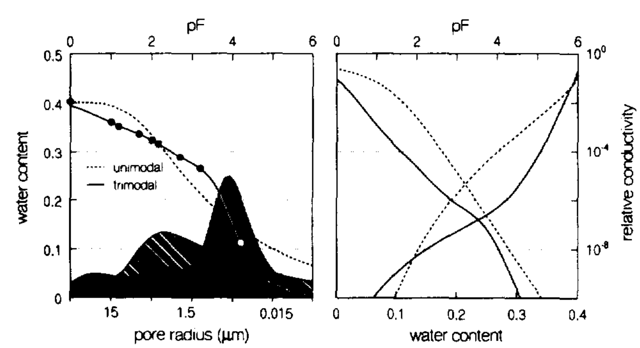


**Figure 8.** Hydraulic properties of Rønhave Sandy Loam [*Schjønning*, 1985]. See Figure 6 for explanations.

**Table 1.** Parameters of Example Soils

| Classification | Solar Village Clay* | Rideau Clay Loam† | Rønhave Sandy Loam‡ | Aggregated Loam§ | | |
|---|---|---|---|---|---|---|
| Texture | clay loam aggregates | heavy clay | coarse sandy loam | loam aggregates | | |
| Type | repacked | undisturbed | undisturbed | repacked | | |
| Density, g cm$^{-3}$ | 1.3 | | 1.55 | 0.98 | | |
| Porosity, % | 52.7 | | 41.3 | 0.63 | | |
| Sample volume, cm$^3$ | 12.3 | 345 | 100/250 | 750–1500 | | |
| log ($K_s$), m s$^{-1}$ | −5.7 | −4.6 | −5.3 | −4.4 | | |
| Unimodal van Genuchten | | | | | | |
| $\theta_s$, cm$^3$ cm$^{-3}$ | 0.556 | 0.439 | 0.403 | | | |
| $\theta_r$, cm$^3$ cm$^{-3}$ | 0.000 | 0.000 | 0.000 | | | |
| $\alpha$, cm$^{-1}$ | 0.0328 | 0.0027 | 0.0212 | | | |
| $n$ | 1.160 | 1.134 | 1.181 | | | |
| $m$ | 0.138 | 0.118 | 0.153 | | | |
| | Multimodal van Genuchten | | | | | |
| | Bimodal | Bimodal | Trimodal | Bimodal‖ | Bimodal¶ | Bimodal** |
| $\theta_s$, cm$^3$ cm$^{-3}$ | 0.556 | 0.473 | 0.403 | 0.633 | 0.633 | 0.633 |
| $\theta_r$, cm$^3$ cm$^{-3}$ | 0.044 | 0.132 | 0.000 | 0.160 | 0.160 | 0.154 |
| $w_1$ | 0.54 | 0.14 | 0.21 | 0.68 | 0.65 | 0.62 |
| $\alpha_1$, cm$^{-1}$ | 0.0252 | 0.6634 | 0.715 | 0.4422 | 0.3320 | 0.2799 |
| $n_1$ | 2.482 | 2.060 | 1.349 | 4.675 | 3.123 | 2.849 |
| $m_1$ | 0.243 | 0.515 | 0.210 | 0.304 | 0.680 | 1.000 |
| $w_2$ | 0.46 | 0.86 | 0.16 | 0.32 | 0.35 | 0.38 |
| $\alpha_2$, cm$^{-1}$ | 0.00006 | 0.0011 | 0.0093 | 0.0119 | 0.0112 | 0.0084 |
| $n_2$ | 2.272 | 1.286 | 1.550 | 3.471 | 2.527 | 1.741 |
| $m_2$ | 0.825 | 0.223 | 0.355 | 0.422 | 0.604 | 1.000 |
| $w_3$ | | | 0.62 | | | |
| $\alpha_3$, cm$^{-1}$ | | | 0.00017 | | | |
| $n_3$ | | | 1.818 | | | |
| $m_2$ | | | 0.450 | | | |

*Source: D. R. Hampton (personal communication, 1989).
†Source: *DeJong et al.* [1992].
‡Source: *Schjønning* [1985].
§Source: *Smettem and Kirby* [1990].
‖No constraint.
¶Here, $m_i = 1 - 1/n_i$.
**Here $m_i = 1$.

*Jong et al.*, 1992]. The pore-size distribution is again bimodal, but the secondary pore system is now less pronounced and shifted toward larger pore sizes, as compared to the previous example. For this soil we can deduce the existence, but not the actual shape of the secondary pore system, because the measurements are insufficient in the important range near saturation. For the purpose of analyzing bimodal conductivity estimations of such pore systems we assume here that the fitted bimodal function is a valid model of the soil's true retention properties even in the range where no data are available. As a third example, the retention properties of an undisturbed sample of Rønhave sandy loam [*Schjønning*, 1985] are depicted in Figure 8 (left). In a strict sense, this pore system is unimodal. Nevertheless, it cannot be adequately described by the classical sigmoidal retention curves. The continuous, almost linear decrease of the water content from $pF0$ to $pF3$ indicates a considerable pore density over a wide range of pore sizes, whereas the main pore system is located in the range of fine pores.

A comparison of the conductivity estimates from the uni- and the multimodal retention functions (Figures 6 (right) to 8 (right)) shows the following.

1. Conductivity estimates from uni- and multimodal descriptions of the retention curve can differ by orders of magnitude. These differences are visible in both the $K(\psi)$ and the $K(\theta)$ plane.

2. The largest differences occur in the wet moisture range, which is very important for solute transport processes.

3. The differences in the estimated $K(\psi)$ curves arise in most cases from different slopes near saturation. As the soil dries, the curves remain approximately parallel (Figure 7) or approach each other again (Figures 6 and 8), provided the same residual water content is approached by the retention functions.

Simplified sigmoidal retention functions cannot reflect the small but important changes in water content that take place in pore ranges distant from the main pore system. The limiting case for this inability is retention functions of the type of (2), where both water content and conductivity are constant between saturation and the air entry point. Functions of this type represent discontinuous pore-size distributions and are by definition not adequate for conductivity estimations in loamy and clayey soils.

Whether the conductivity estimation by a nonoptimal retention function will tend to lead to an overestimation or an underestimation can be simply evaluated by comparing the slope of the fitted retention curve with the slope of the measured data. If the fitted retention curve underestimates the true water release near saturation (as in Figures 2 (top left), 2 (top right), 2 (bottom right), 7 (left) and 8 (left)), the predicted change of $K(\psi)$ will as well be smaller than the true change. Consequently, if matched to $K_s$, the predicted curve results in an overestimation. In studies where conductivity predictions have been compared with measurements, this type of prediction error has, indeed, frequently been found [e.g., *Parkes and Waters*, 1980]. If, on the other hand, the fitted retention curve indicates a steeper slope than the measured water content data (as in the wet range of Figures 2 (bottom left) and 6 (left)), the predicted change of $K$ will be larger than the change that were predicted by a more accurate retention function. Accordingly, the two estimated $K(\psi)$ curves of the morainic soil (Figure 8) approach each other again at drier conditions, since the unimodal $\theta(\psi)$ curve has a steeper slope than the multimodal one at intermediate pore sizes.

Using conductivity estimations from multimodal retention curves as an investigation tool, some of the classical problems of the prediction methods will be discussed in the following sections, namely (1) the role of the parameter $\theta_r$, (2) the question whether the particular mathematical form of the retention function is of relevance, and (3) the sensitivity of conductivity predictions on the slope of the retention curve near saturation, which will be found to be most important.

**Role of $\theta_r$ and $\theta_s$**

Throughout the history of conductivity estimations, the search for a "correct" residual water content $\theta_r$ has been a continuous source of vexation. Statements on the role of $\theta_r$ for conductivity predictions range from "very important" [*Sidiropoulos and Yannopoulos*, 1988] to "unimportant" [*Vogel and Cislerova*, 1988]. Partly, this may be due to the fact that there is no agreement on the definition and, consequently, the correct determination of $\theta_r$ [*Sidiroupoulos and Yannopoulos*, 1988; *Luckner et al.*, 1989; *Nimmo*, 1991; *Nielsen and Luckner*, 1992]. *Mualem* [1976], who considered the correct value of the residual water content to be important for the prediction, devoted a considerable part of his classical paper to the determination of $\theta_r$. *Van Genuchten* [1980] proposed to set $\theta_r$ equal to a measured water content at a high suction. Recent reviews [*van Genuchten and Nielsen*, 1985; *Nielsen and Luckner*, 1992] recommend treating $\theta_r$ as a pure fitting parameter.

From (6) we can see that in principle the conductivity prediction in the wet range is not affected by the value of $\theta_r$, since the hydraulic conductivity of a soil is determined at any saturation by only a few percent of the largest water-filled pores. *Durner* [1992] confirmed this independency using water retention data of a loam from Roskilde, Denmark (similar to Figure 8). Contrary to a unimodal model, a change of $\theta_r$ from 0.0 to 0.19 had no influence on the conductivity prediction in the range of large pores, since it did not alter the shape of a fitted bimodal retention curve in that range. Any influence of $\theta_r$ in unimodal hydraulic models is therefore caused by interferences of the curve shape parameters. For the van Genuchten retention model, as an example, a decrease of the value of $\theta_r$ causes a shift of the parameter $n$ toward a smaller value. A similar effect is caused by an increase of the parameter $\theta_s$. Therefore if the interest lies purely in the wet moisture range, we can disregard data points in the dry range if this leads to a better description in the range of interest.

Effects of parameter correlations can be shown by data of *Kablan et al.* [1989], who compared conductivity measurements for a fine sand with conductivity estimates by the van Genuchten–Mualem model. In the fitting procedure for the retention curve, the parameter $\theta_s$ was set equal to the largest single measured water content. Since field data with a considerable scatter were used, this value was far higher than an optimally fitted value. As a consequence, the optimized values of $\theta_r$ and $n$ both became too small, and the predicted conductivity function correspondingly underestimated the decrease in conductivity at low saturation, thus leading to the conclusion that the predictive model worked well at high saturations, but failed at low saturations. The example exhibits a dilemma in fitting procedures for the retention curve. To get a best overall fit, all parameters should be simultaneously optimized [compare *Nielsen and Luckner*, 1992]. An independent determination, as is desirable for parameters of physical significance, e.g., in transport models, is here inappropriate. On the other hand, if an optimized value of $\theta_s$ is lower that actually observed values, information relevant for $K(\theta)$ at large pores may be masked by the overall fitting procedure [*Mualem*, 1992].

**Mathematical Formulation of the Retention Function**

As is expressed by (6), the conductivity prediction models estimate the relative conductivity function purely from the shape of the retention function. Thus we can postulate that the specific mathematical form of a retention model has no influence on the conductivity prediction as long as it provides a proper description of the measured data. We verify this by describing a strongly aggregated loam with a bimodal pore system (data by *Smettem and Kirkby* [1990]) using three different retention models, based on the bimodal form of (4): (1) the unconstrained model with varying $m_i$ and $n_i$, (2) the constrained model with $m_i = 1 - 1/n_i$, and (3) a simplified form with $m_i = 1$. For comparison, we also interpolate the retention data linearly, with extrapolations in the dry range to water content zero at $pF7$. To define the pore-size distribution toward the large pores, the measured value of $\theta$ at $pF0$ is taken as $\theta_s$. Figure 9 shows the retention characteristic, the underlying pore-size distribution, and the predicted $K(\psi)$ curve, as represented by this linear interpolation. The pore-size distribution has a very rugged shape and is noncontinuous. Such a description of the hydraulic properties would cause problems in numerical simulations [*Hampton*, 1990].

A comparison of all four retention models and the related estimated conductivity functions is shown in Figure 10. The agreement among the four models as well as the agreement between the estimated and measured conductivities is almost perfect (Figure 10 (right)). We conclude that any smooth function which describes the retention data accurately appears to be suitable in this case, regardless of its

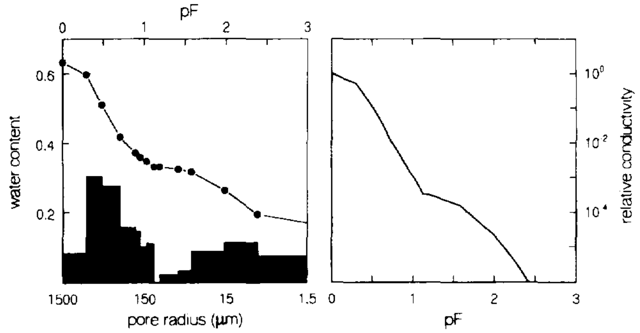


**Figure 9.** Hydraulic properties of Aggregated Loam [*Smettem and Kirkby*, 1990]. (Left) Experimental retention data (solid circles), linear interpolation (solid line), and pore-size distribution (shaded area), as represented by the linear interpolated retention curve. (Right) Estimated conductivity function.

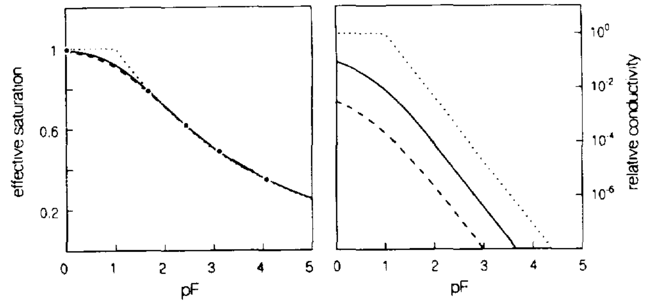


**Figure 11.** Dependence of conductivity estimations on the asymptotic slope of the retention curve near saturation. (Left) Retention curves: dotted line, Brooks and Corey function (2) ($\alpha^{-1}$ = 10 cm, $\lambda$ = 0.15); solid line, van Genuchten function (3), with constraint $m = 1 - 1/n$ ($\alpha^{-1}$ = 10.5 cm, $n$ = 1.15, $nm$ = 0.15); dashed line, van Genuchten function without constraint ($\alpha^{-1}$ = 10.5 cm, $n$ = 1.0, $nm$ = 0.15). (Right) Predicted conductivity curves.

mathematical type. As will be shown next, this is, however, only true as long as the functions do really correspond, and do not differ in their asymptotic behavior toward saturation.

### Slope of the Retention Curve Near Saturation

The asymptotic slope of the retention function near saturation is the most sensitive determinant for conductivity estimations if smooth retention functions (i.e., functions that represent continuous pore-size distributions) are used. This originates from the use of the Hagen-Poiseuille law in the prediction models, which states that the flux density in pores of a certain size is inversely proportional to the square of the pore radius. Consequently, all statistical conductivity prediction methods integrate over the inverse of $\psi$ [*Mualem*, 1992]. The smaller the suction is where changes in the water content take place, the greater is its contribution to the conductivity integral (e.g., (7)). If retention functions with a distinct air entry point are used for the conductivity estimation [*Brooks and Corey*, 1964; *Campbell*, 1974], the integrand in (7), $1/\psi \, dS'_e$, is bounded, since $dS'_e = 0$ between saturation and the air entry pressure. This is different for any retention function which approaches saturation asymptotically. Now the value of the integrand depends on how fast $dS'_e$ approaches zero as $1/\psi$ approaches infinity, i.e., on the slope of the retention function. The absolute sensitivity of $K$ to $S_e$, defined by $s_{\mathrm{abs}} = dK/dS_e$, becomes infinite near saturation. For the closed-form conductivity function of the van Genuchten–Mualem model,

$$K = S_e^{\tau}[1 - (1 - S_e^{1/m})^m]^2, \tag{9}$$

this absolute sensitivity is given by

$$s_{\mathrm{abs}} = \tau S_e^{\tau-1} g(S_e)^2 + \frac{2S_e^{\tau+(1/m)-1} g(S_e)}{(1 - S_e^{1/m})^{1-m}}, \tag{10}$$

where $g(S_e) = [1 - (1 - S_e^{1/m})^m]$. When the effective saturation approaches unity, the first right-hand term and the numerator of the second term in (10) approach finite values, whereas the denominator of the second term becomes zero, because the value of the parameter $m$ is bounded by $0 < m < 1$. This causes $|s_{\mathrm{abs}}|$ to approach infinity. Due to this sensitivity characteristic, even small changes in water content near saturation (indicating the existence of large pores) are very important for the shape of the estimated conductivity function. Measurements close to $\theta_s$ must therefore be taken at small pressure intervals and as accurately as possible.

Reliable conductivity estimations become impossible if measurements near saturation are missing, regardless whether the pore system is heterogeneous or not. To illustrate this, we have fitted three different unimodal functions to hypothetical retention data (Figure 11 (left)). The retention models are the Brooks and Corey function, the van Genuchten function with $m = 1 - 1/n$, and the van Genuchten function with $n = 1.0$. Since there are no measured data between saturation and $S_e = 0.8$ at $pF2$, each function describes the data equally well. However, the corresponding pore-size distributions, which are identical in the fine-pore range, are very different in their asymptotic behavior in the large-pore range. As was discussed above, the Brooks and Corey function (dashed line) restricts the

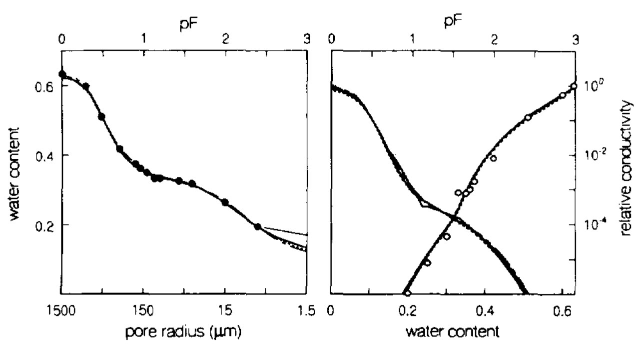


**Figure 10.** Conductivity estimation for Aggregated Loam [*Smettem and Kirkby*, 1990] from four mathematically different retention functions. (Left) Fitted retention models: linear interpolated (solid line), bimodal retention function (equation (4)) with $m_i$ allowed to vary (dotted line), $m_i = 1 - 1/n_i$ (dashed line), and $m_i = 1$ (dashed-dotted line). See Table 1 for coefficients of the models. (Right) Estimated conductivity functions and measured conductivity data. The four retention models yield almost identical estimates. The agreement between estimates and measurements is excellent.

size of the largest pores considered by the conductivity prediction model to the equivalent radius of the air entry pressure ($r \simeq 0.15$ mm in the given example). The two smooth functions represent a certain amount of pores in the large-pore range and can even consider pore sizes that are physically absurd. The conductivity estimates based on the three functions are shifted against each other by orders of magnitude, and without additional measurements between saturation and $pF2$ there is no way to decide which model represents the soil best.

The accuracy of water content measurements is generally limited by the error of the measurement method. Unfortunately, it becomes experimentally more and more difficult to measure the retention characteristic of a soil accurately and reproducibly at very low suctions. It is further questionable whether retention curves, indeed, represent the pore-size distribution of a porous medium at high saturation, where the nonwetting phase is not continuous [*Corey*, 1992]. This means that the conductivity estimation becomes by definition inaccurate when approaching saturation, even if we assume that the predictive model itself is free of error and its applicability does not depend on the pore sizes. As a consequence, conductivity estimations from retention functions that represent a certain pore space in the range of very small suctions (say, below $pF0$) are unreliable, regardless of whether unimodal or multimodal functions are used. This is, for example, generally the case if the parameter $n$ in the constrained van Genuchten equation ($m = 1 - 1/n$) is close to unity.

### Comparisons Between Measured and Estimated Conductivities

To assess whether conductivity estimations from more accurate retention functions are of advantage in practice, comparisons of unimodal and multimodal predictions with experimental data are necessary. To be of statistical significance, such comparisons must rest on a broad database of well-documented measurements of high quality. Existing data have frequently been measured on homogenized and packed soil samples, and a variety of measurement methods have been used. To date, most of the published empirical validation studies on conductivity estimations used relatively small databases of the authors' own measurements. This might be one reason why many of these studies resulted in a new proposed "optimal" value of the tortuosity or pore-interaction factor $\tau$ [e.g., *Kunze et al.*, 1968; *Green and Corey*, 1971; *Jackson*, 1972; *Ghosh*, 1977; *Ragab et al.*, 1981; *Talsma*, 1985; *Alexander and Skaggs*, 1986].

In cases where measured data appear basically reliable, often the retention measurements near saturation are insufficient. Then, the hydrologically important secondary pore system is not strictly determined, as was discussed above. Therefore estimations by a flexible retention function are uncertain, and a better or worse agreement with measurements might be achieved at random. *Durner* [1992] showed for Beit Netofa clay (which served *van Genuchten* [1980] as an example for possible failures of the van Genuchten–Mualem model) that a conductivity estimation based on a bimodal retention function led to a very good agreement with measured data. However, since for this soil no retention measurements are available in the pressure range between saturation and $pF2$, the saturated water content was arbitrarily set 2% larger than the largest measured water content. A different value for $\theta_s$ might have changed the estimation considerably, leading to a bad agreement. Note, however, that it was not possible to come to a satisfactory agreement between measured and estimated conductivities using the unimodal van Genuchten–Mualem model.

Since particularly for heterogeneous soils with secondary pore systems the problem of measurements near saturation is further complicated by macropores, air encapsulations, and hysteresis effects, we do not attempt to compare in this paper unimodal and multimodal conductivity predictions with measurements. It appears doubtful whether a validation attempt in this classical way is viable with presently available data.

## Conclusions

The existence of a secondary pore system greatly affects the shape of the estimated hydraulic conductivity curve in the wet range. Estimation differences due to different retention models can be larger than differences due to the use of alternative prediction models [*Childs and Collis-George*, 1950; *Burdine*, 1953; *Mualem*, 1976]. Consequently, the ignorance of a secondary pore system may lead to large errors. We have shown for soils with heterogeneous pore systems that the commonly applied unimodal retention functions are inadequate for conductivity estimations, because they lack the necessary flexibility in the range of large pores. Their use may lead to wrong results in flow and transport simulations or in parameter estimation procedures where the inverse problem is solved [*Durner*, 1991]. Validation studies of hydraulic conductivity prediction methods should be reevaluated if the applied retention model did not accurately describe the measured data. Particularly for loamy and clayey soils the reasons for the frequent failure of conductivity prediction methods should be reconsidered. In some cases it may not be the failure of the predictive model, but the use of inadequate retention functions which leads to a discrepancy between estimates and measurements. For soils with very wide pore-size distributions, unimodal retention models are sometimes forced to represent a nonnegligible part of the pore space in the range of unrealistically large pore sizes. In such cases (indicated, e.g., by the van Genuchten parameter $n$ being close to unity) the conductivity prediction near saturation is by definition unreliable.

The almost perfect agreement between measured and estimated conductivities for the loamy soil of *Smettem and Kirkby* [1990, Figure 10b] indicates that conductivity prediction methods basing on statistical pore-domain models have a high success potential not only for soils with narrow pore-size distributions, but as well for soils with heterogeneous pore systems. As compared to unimodal retention functions, the use of the multimodal retention function (or of any other flexible retention function) leads to more reliable conductivity estimates if it improves the fit of the measured retention data and if the shape of the fitted retention function in the range of large pores is strictly determined by measurements. Particularly for validations of flow and transport models on laboratory scale, the hydraulic characteristic of the soil sample should be described as accurately as possible.

The slope of the water retention curve near saturation is the most important property in determining the shape of the estimated conductivity function. Even small uncertainties in measured water contents near saturation lead to large estimation uncertainties. When a retention characteristic has no distinct air entry point, the measured saturated conductivity is generally not an appropriate matching value for the predicted conductivity function. This conclusion, which was already stated for unimodal pore systems [e.g., *van Genuchten and Nielsen*, 1985; *Luckner et al.*, 1989; *Nielsen and Luckner*, 1992], is even more important for heterogeneous pore systems. The use of multimodal functions can help to explain this problem; however, it cannot solve it.

We may expect that the basic concepts that underlie the statistical conductivity prediction models generally hold less for secondary pore systems as compared to textural ones. The shape and organization of voids in aggregated soils can be very different, depending on soil genesis and aggregation state [*Wang and Narasimhan*, 1990]. As an example, a net of planar voids will behave hydrologically quite differently from the pore space between spherical aggregates, or the pore space due to microroot channels. Nevertheless, each of these pore systems may have a similarly shaped retention characteristic. Therefore we should regard $\tau$ in the correction function $S_e^\tau$ as a purely empirical fitting parameter [*Roulier et al.*, 1972; *Russo*, 1988]. For use in parameter estimation procedures, *Nielsen and Luckner* [1992] even suggest to decouple the retention and the conductivity function, and to use the closed-form conductivity equation of the van Genuchten–Mualem model (9) as an empirical expression for $K(S_e)$. For soils with heterogeneous pore systems, we expect the best results by still using the shape of the estimated conductivity function while treating the two parameters $K_s$ and $\tau$ as unknowns. By this strategy the information on the pore system contained in the retention function will be used to fullest advantage. Close to saturation the conductivities of soils containing large pores should be directly measured. This means, however, that the attractiveness of the prediction methods is considerably reduced.

Properties of heterogeneous pore systems cannot be identified by parameter estimation techniques where the inverse problem is solved, if a priori unimodal hydraulic properties are assumed. Due to the ill-posedness of the mathematical problem, it appears on the other hand impossible to use more flexible hydraulic functions and to identify the increased number of coefficients by the inverse method. Therefore the retention curves of soils with heterogeneous pore systems should be directly fitted to measured data. Preferably, these measurements are obtained from a transient flow experiment by simultaneously measuring $\psi$ and $\theta$ in high resolution [e.g., *Sobczuk et al.*, 1992]. The flow characteristics of the experiment can then be used to optimize the two conductivity-related unknowns, $K_s$ and $\tau$, by solving the inverse problem.

Finally, we want to recall that the reliability of conductivity prediction methods is generally restricted by some fundamental problems, e.g., the assumption of isotropic organization of pores independent of their size, the validity of the Hagen-Poiseuille law for flow in large pores, the problem of air entrapment, and the problem of hysteresis. The specific findings in this paper for heterogeneous pore systems are nevertheless applicable. The results are further independent of the choice of the particular statistical conductivity prediction model. The extension to the field scale requires the consideration of spatial and temporal variability as well as the consideration of scale problems and errors induced by the measurement method. The further development of suitable measurement methods to identify heterogeneous pore systems appears therefore to be of primary importance.

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