Determination of the Soil Water Retention Curve and the Unsaturated Hydraulic Conductivity from the Particle Size Distribution

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Summary. Because of the complexity of the metrological determination of the soil water retention curve (SWRC), so-called pedotransfer functions (PTF) have been developed for several years. Mostly these PTF are based on a more or less simple regression analysis using a limited set of data. In such methods the SWRC is predicted with data on the amount of soil components sometimes supplemented by values regarding the density or the amount of organic materials. Only few PTF deal directly with the particle size distribution. In many cases empirical factors are necessary to obtain a prediction for the water retention curve. A new method for determining the soil-hydraulic properties using the pore constriction distribution of a soil has been developed, whereby the pore constriction distribution is derived from the particle size distribution depending on the density of the soil. The contribution will present the new pedotransfer method and shows results in comparison to experimental investigations.

Key words: pedotransfer method, soil water retention curve, hydraulic conductivity, pore model

1 Introduction

Different methods have been developed to estimate the SWRC from the particle size distribution. For this purpose different approaches were used. By making estimations using a simple model for the pore structure, the particle size distribution can be separated into fractions of different sizes. Using this information it is possible to incrementally estimate the SWRC for a predefined bedding of particles within a specific size range (Arya and Paris 1981, Fredlund et al. 2002). The analogy between the progression of the particle size distribution and SWRC makes it possible to reach a direct solution using a functional relationship between both curves (Haverkamp and Parlange 1986). Based on the particle size distribution, newly developed methods calculate the capillary and adsorptive bound water separately, which are then summarised in order to receive the SWRC (Schick 2002, Aubertin et al. 2003). However, as a rule, these kinds of solutions require additional empirical information which naturally contains uncertainties. A numerical solution for the calculation of the SWRC and the unsaturated hydraulic conductivity has been given by Kitamura et al. (1998). For the calculation they use a statistical distribution for the pore diameter and the pore inclination, which are both derived from the particle size distribution (cf. Kitamura et al. 2000). On the basis of the consideration of sphere packings Zou (2003, 2004) has developed an elegant solution for the estimation of the SWRC because it is purely analytical. However, for this reason this method can only be used at best for uniform soils.

In the following, a method will be briefly introduced, which uses the pore constriction distribution for the calculation of the SWRC for the case of drainage as well as the relationship for the unsaturated hydraulic conductivity. In this connection, the pore constriction distribution will be calculated from the particle size distribution under consideration of the relative density of the soil.

2 Calculation of the Pore Constriction Distribution

The structure of a pore system depending on the density is the most important factor influencing the soil hydraulic parameters. Another relevant geotechnical question regarding pore structures is the ability of materials to pass through pores in a soil. In this connection the suitability of a soil for grouting purposes (Schulze 1992) or questions concerning geotechnical filters (Wittmann 1980, Witt 1986, Schuler 1997) should be mentioned. However, the direct measurement of the pore size distribution is a challenging undertaking. For this reason very early first approaches have been developed in order to estimate pore size distributions from more easily measurable parameters like the particle size distribution.

A procedure of this kind has been developed by Silveira (1965). It considers a particle group consisting of three touching spherical grains. With this consideration he assumes from the beginning the densest condition of a soil (hexagonal packing). In the space between the grains a spherical pore can be subscribed which touches every three grains representing the pore constriction of this group. As a basis for the selection of the grain sizes Silveira uses the particle size distribution finer by weight, which has been criticised by Ziems (1969) since the introduction of the procedure, because of the underestimation of the finer part of the soil. For a similar procedure Ziems used the particle size distribution finer by amount (quantity distribution).

Schuler (1997) has finally developed the procedure, which is the basis for the calculation of the pore constriction distribution. As a basis for the selection of grains, he uses the particle size distribution finer by surface (surface distribution). Additional modifications carried out by Schuler are as follows:

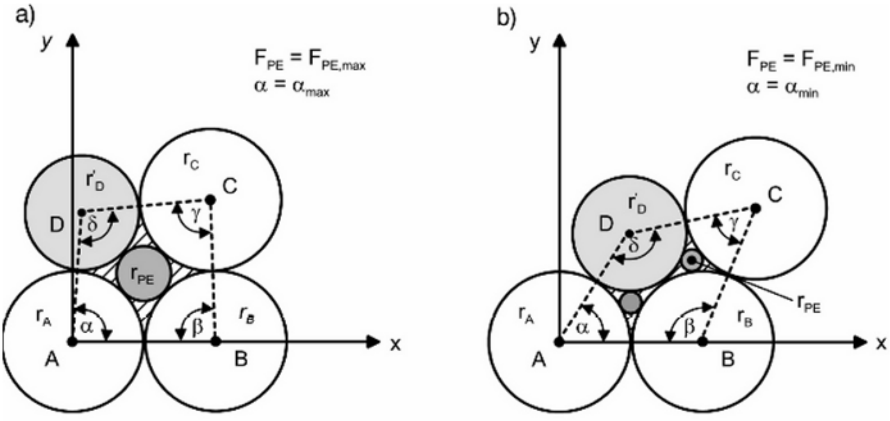

Fig. 1. Calculation of pore constrictions within a pore space consisting of four particles **a**) for the lowest relative density $D = 0$ and b) for the highest relative density $D = 1$

- Experimental investigations have shown that most of the pores are formed by four particles (Witt 1986 (pore imprints) and Glantz 1997 (magnetic resonance imaging)). Due to this observation instead of three particles Schuler considers a group of four particles as shown in Fig. 1.
- When a pore constriction is formed by four particles, the probability that the centre of each spherical grain is located in one intersection is very low, which is verified by observations according to Witt. Due to these observations it is assumed that one particle is shifted in the third dimension, while the radius of this particle is decreased in the two dimensional consideration of Fig. 1 to $r'_D = r_D \cdot (2/3)^{0.5}$ (cf. grey particles (D) in Fig. 1). In Figure 1 it is assumed that all particles have the same radius ($r_A = r_B = r_C = r_D$).
- For a pore constellation (group of particles with specific positions) as shown in Fig. 1 spaces with different sized areas are possible. If particles A and B touch each other, the densest packing of the four particles will be obtained and the angle α as well as the area F_{PE} of the space between the particles then have their lowest values (cf. Fig. 1**b**)). As the values for α increase also the area F_{PE} of the space between the particles grows until F_{PE} reaches a maximum (cf. Fig. 1**a**)). Under this condition the constellation reaches its loosest density. Consequently the constellation of particles takes on different densities according to the area of the space between the particles, which can be assigned to the loosest and densest bedding of the particles. In order to take into account the bedding of the soil for the calculation of the pore constrictions, an analogy is introduced between the area F_{PE} of the space between the particles and the porosity n of the soil as shown in equation (1)

$$D = \frac{n_{\max} - n}{n_{\max} - n_{\min}} = \frac{F_{PE,\max} - F_{PE}}{F_{PE,\max} - F_{PE,\min}} . \tag{1}$$

As mentioned before, the selection of the grains takes place using the surface distribution. For this purpose, the particle size distribution is divided into sections of equal percentage and for every section a mean diameter of the particle is calculated. As a result every particle diameter has the same probability of occurrence. Because of the consideration of four particles and depending on the amount of sections k chosen for the calculation, a total amount of $Z_k = k^4$ constellations has to be considered. Finally, for each pore constellation two pore constriction radii are subscribed and a mean value characterising the pore is calculated.

The subscription of pores into the space between the particles is a purely geometric problem. In order to improve the efficiency of the calculations, an analytical method is used and integrated into a programme. Calculations with $k = 15$ pore sections are possible, which is very important for the consideration of well graded soils.

Figure 2 shows the result of a calculation of a pore constriction distribution with a relative density of $D = 0.8$ in comparison to experimental results from Witt (1986). The solid line on the right shows the particle size distribution, the long dashed line shows the quantity distribution and the line with dashes

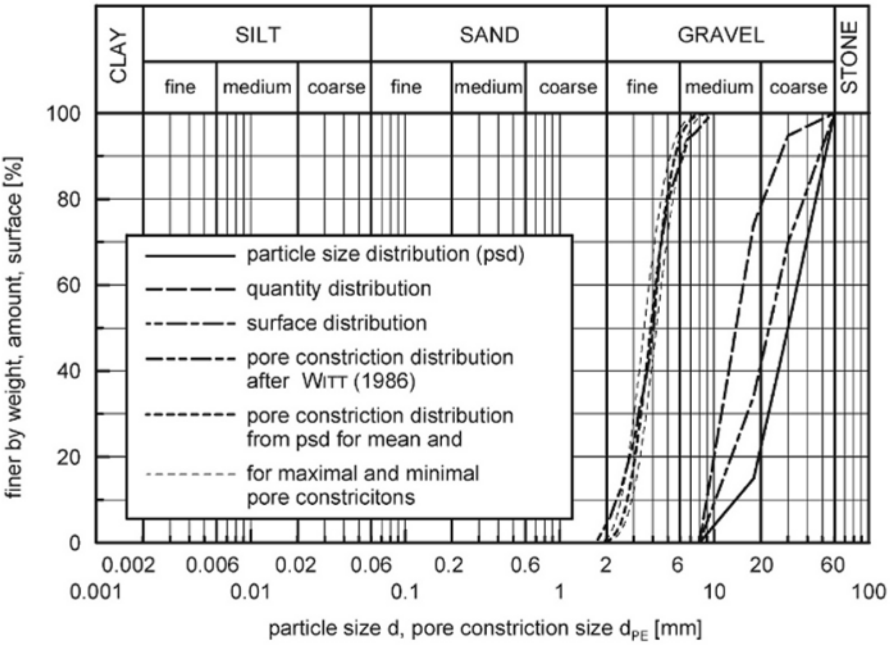

Fig. 2. Comparison between calculated pore constriction distribution and a measured distribution based on silicon pore imprints (according to Witt 1986)

and dots shows the surface distribution. It can be seen from the propagation of the curves that by using the surface distribution the probability of occurrence of finer particles is higher than by using the particle size distribution finer by weight and lower by using the quantity distribution.

The bundle of lines on the left shows the pore constriction distributions finer by amount. The dotted lines represent the results of the calculation. The thick line represents the mean value of the pore constriction and both fine lines represent the limits for maximum or minimum pore constrictions. The experimental result according to Witt is shown by a dashed line with two dots. Witt determined his distribution using silicon imprints of the pores. On the one hand, it is a challenging procedure to assess pore size distributions, but, on the other hand, it is a quite exact one. It can be very clearly recognised that the experimental result is reproduced very well with the calculation, which has already been verified by Schuler (1997). This comparison illustrates the applicability of the introduced procedure for the calculation of the pore constriction distribution depending on the bedding, at least for granular soils.

3 Derivation of Soil Hydraulic Parameters

In the following the required steps for the calculation of the soil hydraulic parameters are presented. The pore constriction distribution constitutes the necessary input data for this calculation, which must be carried out separately. The following calculation examples are presented for a weak gravelly sand, of which the particle size distributions, quantity distribution and surface distribution as well as the calculated distributions for the pore constriction are shown in Fig. 3.

3.1 Soil Water retention Curve (SWRC)

As already mentioned, the SWRC of a soil for the drainage condition is mainly influenced geometrically by the pore constrictions of a soil. The retentive force acting against the drainage of water out of the soil is the capillary force which is activated by the greatest pore with a connection to the free air phase.

Consequently, with the information of the pore constriction distribution, it is possible to determine the capillary forces as isotropic forces acting in a soil. For this purpose the well known equation (2) for the description of the rise of water in a capillary tube is used. In this connection, the so-called capillary rise of water is inversely proportional to the radius of the pore constriction r_{PE}. For the case of drainage (completely wetted surface) it is feasible to assume a value of $\delta = 0°$ for the contact angle (cf. Schubert 1982, Fredlund and Rahardjo 1993). The surface tension σ_{wa} of water to the air phase is a temperature-dependent property, which can be inferred from Table 1. Finally, with the specific weight of water γ_w it is possible to calculate two values for every pore constellation for the capillary rise of water (according to the

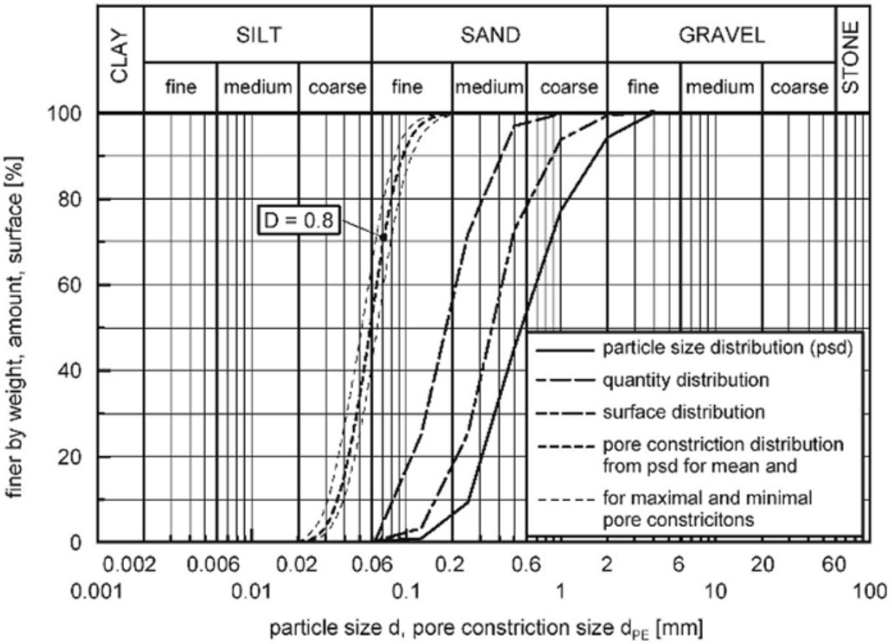

Fig. 3. Particle size distribution, quantity distribution and surface distribution for a weak gravelly sand as well as pore constriction distributions for mean pore constrictions for a relative density of $D = 0.8$ (with variation due to maximal and minimal pore constrictions)

Table 1. Surface tension σ_{wa} of water to air depending on the temperature

Temperature (°C)	10	15	20	30
Surface tension σ_{wa} (N/m)	0.0724	0.0735	0.07275	0.0712

minimum and maximum pore constrictions) as well as a mean value, which is set equal to prevailing capillary forces $|\psi_{PE}|$ due to the a pore constriction:

$$|\psi_{PE}| = \frac{2\sigma_{\text{wa}} \cos \delta}{\gamma_w r_{PE}} \tag{2}$$

The decrease in the water content during drainage is calculated from the loss of water volume, which is set equal to the area loss of the drained pore space for each pore constellation. The sum of the area of all pore spaces equates to $S = 100\%$ saturation. Finally, by presetting the porosity n according to the porosity used for the calculation of the pore constriction distribution (cf. equation (1)), the analogy to the saturated volumetric water content is established.

Without considering water-retention in the pore space, the soil would be completely drained in the calculation. In fact, some water is stored in the contact points or gussets of the particles, which leads to residual water in every pore constellation. However, the water in the gussets of the particles forms a corpus, which is approximated in the 2D-consideration. Furthermore, it is unknown with which radius water is stored in the gussets. Due to these uncertainties, the residual water is considered to be a variable. As an empirical value it is feasible to predefine the residual water content as the sum of all water stored in the gussets of the particles. Another possibility for a predefinition of the water content is the use of a matric suction at which the residual water content will be set (similar to the definition of the field capacity between 60 and 310 hPa). Finally it is also possible to automatically calculate the residual water content using the pore radii of the constrictions of each pore constellation. If the smaller pore constriction of each pore constellation is used for the calculation, an upper limit for the residual water content is obtained and with the use of the smallest pore constriction of all pore constellations, a lower limit is determined. So far adsorptive bound water has been neglected in the calculation.

For a direct estimation of the residual water content or the water content at saturation, data from literature can also be used (e.g. relative values for the water contents by Luckner et al. 1989).

With the procedure presented discrete points of the SWRC are calculated, which can be parameterised using appropriate models like Brooks and Corey (1964) or van Genuchten (1980). Figure 4 shows the result of a calculation (white squares) in comparison to a statically measured SWRC (grey circles) for the weak gravelly sand presented in Fig. 3. Here the saturated water content θ_S was given by the assumed porosity, and the residual water content θ_r was automatically calculated using the smallest pore constriction radius for all pore constellations. Whereas the saturated water content is more or less a given parameter, the residual water content represents a value which can be estimated taking values from experience.

As can be seen in Fig. 4, there is a satisfactorily good match between the measured and the calculated SWRC. In this connection, the calculation of the SWRC was carried out as a prediction for a given porosity n with a resulting relative density D (under consideration of $n_{\max}$ and $n_{\min}$, cf. equation (1)). It can be assumed that the accordance of both curves could be much better with an adapted value for D.

3.2 Unsaturated Hydraulic Conductivity

There are different microscopic approaches for the determination of the unsaturated hydraulic conductivity. Microscopic approaches are based on a pore model and the hydraulic conductivity is calculated by summation of the conductivities of individual capillaries. The most well known model based on a microscopic approach is the model of Mualem (1976) which is the most

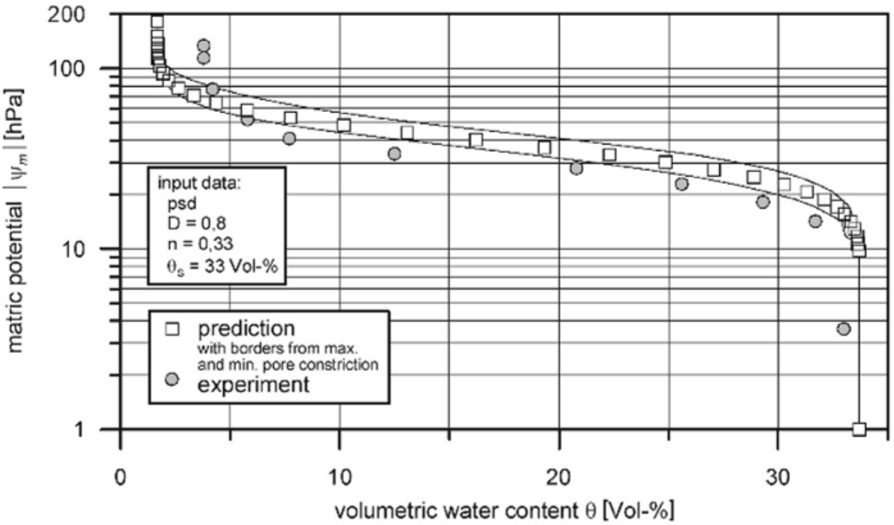

Fig. 4. Comparison between measured and calculated soil water retention curve using the pore constriction distribution for the weak gravelly sand (cf. Fig. 3)

widespread model in combination with the parameterisation of van Genuchten (1980).

For all microscopic approaches specific conditions are assumed which were defined for the first time by Childs and Collis-George (1950):

- The pore size distribution of a soil can be derived from the soil water retention curve.
- For individual pore fragments, the flow model of Hagen-Poiseuille for laminar flow in channel-like capillaries applies (cf. equation (3)).
- Since in the equation of Hagen-Poiseuille the radius of the capillary is used to the power of four, the effective flow resistance in a sequence of pores in series is significantly influenced by the pore with the smallest diameter.
- The total conductivity of a porous media is determined only by sequences of pores in series. Hence a lateral connectivity of pore sequences is neglected.

In this connection, the negative effects of the last two assumptions should counterbalance each other. All microscopic approaches use pore sequences which are combined in a specific way. By the summation of water-bearing pore sequences up to a defined water content or matric suction, it is possible to calculate the unsaturated hydraulic conductivity.

From a statistical point of view, the pore constriction distribution is a representative solution of an arbitrary cut through a soil and, since the pore constriction distribution shows per definition a priori hydraulically active pore openings, it is not necessary to combine them in the sense mentioned above.

This means that for the calculation of the hydraulic conductivity it is feasible to use the equation directly according to Hagen–Poiseuille, as shown in equation (3).

Equation (3) can easily be transformed into a form for the definition of the hydraulic conductivity according to Darcy. Since the term $(\Delta p/l)$ corresponds to the hydraulic gradient i, the flow through a capillary is defined only by the form factor f_{HP} and the dynamic viscosity η. By equitation of equation (3) with the well-known Darcy equation $Q = k_f i A$ equation (4) is obtained, which describes the saturated hydraulic conductivity for all capillaries of number m considered as a bundle representative of a soil with a total surface area of A_B in a representative soil cut.

$$Q = \frac{\Delta V}{\Delta t} = f_{HP} \frac{\Delta p}{l} \frac{1}{\eta} \tag{3}$$

Q	discharge ($\mathrm{m^3/s}$)
ΔV	flow volume ($\mathrm{m^3}$)
Δt	time interval (s)
Δp	pressure difference at the end of the capillary ($\mathrm{kN/m^2}$)
l	length of the capillary (m)
η	dynamic viscosity ($10^{-6}\,\mathrm{kNs/m^2}$) (cf. Table 2)
f_{HP}	form factor ($\mathrm{m^4}$), which is $(r_{PE}^4 \pi)/8$ for circular cross section

Table 2. Dynamic viscosity of water depending on the temperature

Temperature (°C)	10	15	20	30
Dynamic viscosity η ($10^{-6}\,\mathrm{kNs/m^2}$)	1.306	1.138	1.002	0.798

$$k_f = \sum f_{HP,m} \frac{1}{\eta} \frac{1}{A_B} \tag{4}$$

With equation (4) the saturated hydraulic conductivity of a soil considered as a bundle of capillaries is well defined. However, two very important properties of a porous media have been neglected so far, namely the tortuosity of the pore channels and the connectivity among them. In the well known equation according to Mualem, both soil properties are combined in one parameter, for which Mualem originally proposed the constant value 0.5 based on experiments. However, more and more frequently this parameter is being used as a fitting parameter, as a result of which the original physical meaning has been lost. Nevertheless, both the tortuosity and the connectivity are dependent on the water content, which has to be considered in the calculation.

The tortuosity T_0 describes the relationship between the distance of two points L_P and the actual length of the pore channel L_{Pe} between these two points. Most frequently the tortuosity is defined as shown in equation (5) decreasing the saturated hydraulic conductivity (cf. Bear 1972). For a saturated condition it is feasible to use $T_0 = 2/3$ as a constant value for the tortuosity.

$$T_0 = \left(\frac{L_P}{L_{Pe}}\right)^2 \leq 1 \tag{5}$$

When considering the connectivity it is more difficult, because as a topologic property of a porous medium it must be determined based on microstructural investigations or by using the Euler–Poincaré characterisation (cf. Vogel and Roth 1998). However the connectivity K can be considered in context with the relationship between the specific surface of a porous medium and its pore volume (Vasconcelos 1998). Based on this approach, it is possible to assess a constant value for K assuming constant conditions regarding the pore volume. For this a cubic arrangement of same sized particles with the radius r_P resulting in a maximum pore surface is considered. For such a packing of particles the pore constriction between the particles has a radius of $r_{PE} = 0.4142 r_P$. Finally the connectivity results from the relationship between the inner surface of the pore and the pore length, and a value for the connectivity of about $K = 2.6$ is determined.

The tortuosity decreases the hydraulic conductivity, whereas the connectivity has an increasing influence. However, as mentioned before, both are dependent on the water content or the saturation of the soil, whereby the influence of the saturation prevails over the progression of the unsaturated hydraulic conductivity. As a result of this consideration, the factor f_{TK}, as shown in equation (6), takes into account the influence of tortuosity T_0 and connectivity K as the multiplicand for equation (4). A comparison between the calculated curve and a curve determined using the model according to Mualem/van Genuchten based on experimental data is given in Fig. 5.

$$f_{TK} = T_0 K S^2 = 1.73 S^2 \quad \text{with} \quad S = \frac{\theta}{\theta_S} \tag{6}$$

As can be seen from Fig. 5, there is a satisfactorily good match between the progression of the unsaturated hydraulic conductivity determined with the model of Mualem/van Genuchten and the calculated curve based on the pore constriction distribution. But even more astonishing is the direct match of the saturated hydraulic conductivity calculated with the presented procedure. Naturally the hydraulic conductivity depends on the density of the soil. Concerning this additional factor, for the saturated hydraulic conductivity a variance of $10^{-4} \leq k_f \leq 8 \times 10^{-4}$ m/s is obtained, which is a good estimation of this soil property.

4 Summary and Conclusion

A new procedure for the determination of the soil hydraulic properties based on the particle size distribution has been presented. It uses the pore constric-

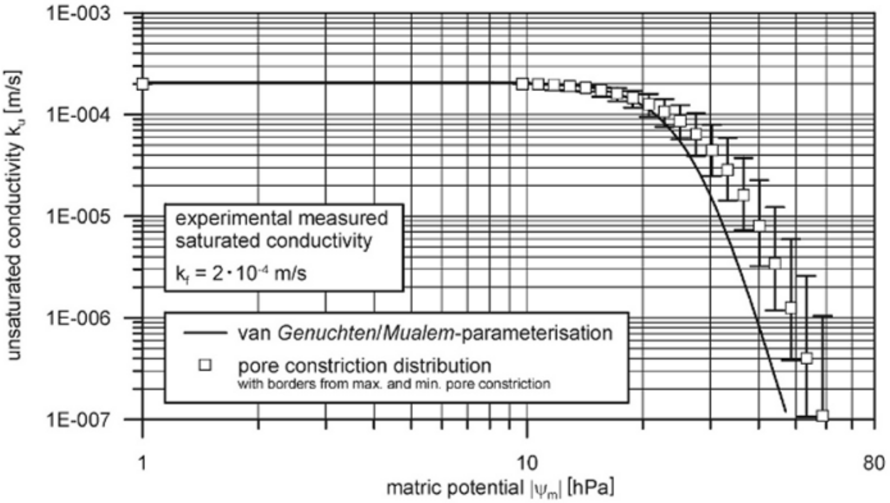

Fig. 5. Progression of the calculated unsaturated hydraulic conductivity from the pore constriction distribution in comparison to the curve determined with the parameterisation according to Mualem/van Genuchten under consideration of the measured saturated hydraulic conductivity of the weak gravelly sand

tion distribution, which has to be calculated separately taking the density of the soil into consideration. Using the equation for the capillary rise of water, the SWRC can be calculated very easily from the pore constriction distribution. The calculation of the unsaturated hydraulic conductivity is based on a consideration of the soil as a bundle of capillaries. In this way it is possible to use the equation according to Hagen-Poiseuille for the flow in capillary tubes, in order to determine the hydraulic conductivity of the soil. However, for this purpose the influence of tortuosity and connectivity must be taken into account.

The comparisons between calculated and measured curves matched satisfactorily well. The introduced procedure was also tested with other granular materials up to silty materials and it was also compared with other pedotransfer functions based on the particle size distribution (cf. Scheuermann 2005). Thus this procedure has proved to be in constant accordance over the range of tested materials.

One great advantage of the procedure presented is its independence from empirical parameters. The shape of both curves of the soil hydraulic properties is the result of the pore constriction distribution, which is directly influenced by the assumed density of the soil. The saturated water content of the SWRC is given by the porosity of the soil, and the residual water content can be automatically calculated or predefined using a measured residual water content or an estimated matric suction.

Furthermore, this procedure also provides a possibility to determine the imbibition SWRC. A concluding step in this connection could be the investigation of the hysteresis of the soil hydraulic parameters.

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