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Abstract

So-called characteristic relations, or retention curves, quantify relations between capillary pressure, water saturation and relative permeability. Parameters for traditional characteristic relations, such as the most widely used van Genuchten (vG) model, can be determined from laboratory measurements in undisturbed soil samples. Similar measurements are in most cases unfeasible in fractured media. An alternative is then to use aperture-based characteristic relations, which are based on parameters that can be determined in the field, for instance from hydraulic testing of rock fractures. However, a main drawback with using aperture-based relations is that their parameters differ from the vG-type of parameterizations that are integrated in most state-of-the art numerical codes for unsaturated flow. Departing from the observed range of fracture transmissivities and (estimated) fracture aperture characteristics for the Forsmark site, we here show that site-relevant aperture-based characteristic relations are very similar in shape to the traditional vG-curves. By matching the vG-curves to the fracture aperture based characteristic curves, we furthermore show how values for the vG-parameters δ and n (reflecting the bubble pressure and the width of the pore size distribution) could be unambiguously determined from the fracture characteristics $\mu_{\ln a}$ and $\sigma_{\ln a}$ (mean value and standard deviation of a log-normal fracture aperture distribution).

Sammanfattning

Så kallade karakteristiska kurvor för omättat flöde beskriver relationer mellan kapillärtryck, vattenmättnad och relativ permeabilitet. Parametrar för traditionella karakteristiska kurvor, såsom exempelvis van Genuchten (vG) modellen, kan bestämmas genom laboratoriemätning i ostörda jordprover. Liknande mätningar är i de flesta fall ogenomförbara i sprickiga medier. Ett alternativ är då att använda aperturbaserade karakteristiska kurvor, som bygger på parametrar som kan bestämmas i fält, till exempel genom hydrauliska tester i bergsprickor. En nackdel med att använda aperturbaserade kurvor är att deras parametrar skiljer sig från vG-typen av parametriseringar, vilka är integrerade i de flesta numeriska koder för omättat flöde. Med utgångspunkt i observerade transmissiviteter och (uppskattad) aperturstatistik för Forsmark, visar vi här att aperturbaserade karaktäristiska kurvor är mycket lika traditionella vG-kurvor till formen. Genom att matcha vG-kurvor till de aperturbaserade karaktäristiska kurvorna visar vi hur värden för vG-parametrarna δ och n (som återspeglar bubbeltryck och porstorleksfördelning) entydigt kunde bestämmas från sprickparametrarna $\mu_{\ln a}$ och $\sigma_{\ln a}$ (medelvärde och standardavvikelse för en log-normal aperturfördelning).

Contents

1 Background

In order to predict repository performance and understand the consequences of repository malfunction, including accidental release of radionuclides into the deep groundwater surrounding the repository, key processes that can influence the transport processes and the transport time-scales need to be well understood. The prevalence of unsaturated conditions in porous and fractured media generally has a considerable influence on water flow and thereby also on water-borne transport of substances. Specifically, the occurrence of mixed gas-water flows may influence the environment near the deposition holes as well as the physical and biogeochemical processes along the transport pathways from the repository. For instance, Rutqvist and Tsang (2008) point out that such unsaturated conditions can be caused by tunnel ventilation. Unsaturated conditions may also prevail in the backfill material for an extended period of time if the re-saturation process is slow, which can be the case if a relatively low suction of the bentonite and/ or the backfill causes a desaturation of the ambient rock fractures.

2 Statement of the problem

The intrinsic properties of the porous or fractured medium with regard to unsaturated flow are usually quantified through so-called characteristic relations, or retention curves, which show the relations between capillary pressure, water saturation and relative permeability. Such constitutive relations provide a necessary basis for all state-of-the art numerical continuum models and represent processes at a sub-grid scale. Parameters for traditional constitutive relations, such as the most widely used van Genuchten (vG) model (van Genuchten 1980) can be determined from laboratory measurements in undisturbed soil samples. However, this is in most cases not possible in fractured media, because it is extremely hard to sample fractures and re-assemble them in the laboratory, in such a way that the original unsaturated hydraulic conditions in the field are reproduced (see, e.g. review by Jouanna 1993).

Aperture-based characteristic relations developed by Jarsjö et al. (2001) were shown to be consistent with a series of experimental observations of two-phase flow in transparent replicas of actual rock fractures from the Äspö HRL and the Stripa mine, as well as field observations of two-phase flow at 460 metres depth in the Äspö HRL (Jarsjö and Destouni 2000). In contrast to the parameters of the van-Genuchten relation, the parameters of aperture-based constitutive relations can be determined from measurements in the field, either from direct measurements (Hakami 1995, Jarsjö and Destouni 1998, Lanaro 2001) or by inferring information on fracture aperture(s) from e.g. hydraulic test results, as further outlined in Chapter 6.

3 Objectives

The objectives of the performed work were to:

1) Derive fracture aperture distributions for the Forsmark area, e.g. through synthesis of available hydrological test data from the site investigation programme,
2) Use the derived aperture distributions for estimation of a set of characteristic curves that are relevant for the Forsmark area,
3) Translate the parameters of these (aperture-based) characteristic curves into parameters used by the traditional vG-relation, i.e. presenting the results in a form that currently is required by most existing numerical codes for unsaturated flow.

4 Considered fracture geometry and basic flow relations

We consider fractures with a log-normal aperture distribution, which is consistent with in-situ measurements of fracture aperture distributions at Äspö Hard Rock Laboratory (Hakami 1995). The hydraulic aperture of the fracture is determined from measured transmissivity values T (see Chapter 5) according to the cubic law, which has in many cases proven to be a useful approximation for the relation between local fracture transmissivity and local aperture value (e.g. Murphy and Thomson 1993):

$$a_h = \sqrt[3]{\frac{12\,\mu_l T}{\rho g_0}} \tag{4-1}$$

where μ_l is the liquid viscosity, ρ is the liquid density and g_0 is the gravitational constant. The (arithmetic) mean aperture is estimated from the hydraulic aperture according to

$$\overline{a} = Ca_h \tag{4-2}$$

where C was reported to be between 1.1 and 1.7 in the experiments of Hakami (1995). Jarsjö and Destouni (1998) reported C-values of 2.1 and 2.4 in fracture replicas from Stripa and Äspö, respectively. In the here considered base scenario we use a C value of 1.7 (in the middle of the above range). Finally, we consider the relation between $\overline{a}$ and the mean value of ln a, $\mu_{\ln a}$:

$$\mu_{\ln a} = \ln(\overline{a}) - \sigma_{\ln a}^2/2 \tag{4-3}$$

Given the assumed $\sigma_{\ln a}$-value and the estimated, fracture specific $\mu_{\ln a}$-value, the lognormal pdf is given by:

$$f_{\ln}(a;\mu_{\ln a},\sigma_{\ln a}) = \frac{1}{a\sigma_{\ln a}\sqrt{2\pi}}\exp\left(-\frac{1}{2\sigma^2}\left(\ln a - \mu_{\ln a}\right)^2\right) \tag{4-4}$$

The relative transmissivity of water as a function of capillary pressure (the characteristic relation for fractured rock), $T_{rel}(p_c) = T_{us}(p_c)/T_s$, where $T_{us}(p_c)$ is the unsaturated fracture transmissivity as a function of capillary pressure and T_s is the saturated fracture transmissivity, is now given by (modified from equation (2-19) in Jarsjö et al. 2001):

$$T_{rel}(p_c;\mu_{\ln a},\sigma_{\ln a}) = \frac{\int_0^\infty a^3 f_{\ln}(a;\mu_{\ln a},\sigma_{\ln a})da - \int_{2\sigma_w/p_c}^\infty a^3 f_{\ln}(a;\mu_{\ln a},\sigma_{\ln a})da}{\int_0^\infty a^3 f_{\ln}(a;\mu_{\ln a},\sigma_{\ln a})da} \tag{4-5}$$

where σ_w is the surface tension of water. The equation is solved numerically using MathCad, see Chapter 6 for details.

5 Considered transmissivity data

We consider transmissivity data from Posiva Flow Log (PFL) tests that were conducted at the Forsmark site, as reported in Tables 5-1 to 5-20 of Follin et al. (2007). Since PFL-measurements are performed for a relatively long time period (about one week; see Follin et al. 2007), reported transmissivities reflect average transmissivities along considerable distances. Therefore, they can represent fracture properties relatively far away from the borehole (in contrast to e.g. traditional withdrawal tests), where commonly less is known about contributing fractures or fracture networks. Through scenario analyses, we will quantify potential impacts of uncertainties related to fracture geometry and configuration, see further Chapter 6.

6 Methods

We used the following main steps and assumptions in the present analyses:

Step 1. Hydraulic apertures were calculated using reported T-values from the PFL-measurements. In many cases, more than one flow anomaly was reported per measurement section (Follin et al. 2007). Since the relative contribution of these anomalies is unknown, the calculations were made in two different ways:

a) Assuming that one anomaly (or "fracture") per measurement section has much larger flow than the others, the cubic law for flow in a single fracture (Equation (4-1)) was applied to calculate equivalent hydraulic apertures from the measured T-values;

b) Assuming that all anomalies (or "fractures") within a measurement section contribute equally to the measured T-values, the T-values were first divided by the number of anomalies before applying the cubic law.

Step 2. Arithmetic mean apertures were estimated based on the calculated hydraulic apertures (Equation (4-2); assuming $C = 1.7$ in a base scenario and $C = 1.1$ in an alternative scenario). Assuming also that the aperture distribution is log-normal, the mean value of $\ln a$ was calculated (Equation (4-3)). We further assumed $\sigma_{\ln a} = 0.8$ for these fractures which represents relatively rough fractures, however well within the range of fracture roughness characteristics observed by Hakami (1995). In a second set of calculations, we relaxed this assumption and considered the full range of fracture roughness – as reflected by the standard deviation of the fracture aperture – measured by Hakami (1995). Combined, **Step 1** and **Step 2** address **objective (1)** of this report.

Step 3. Calculated values of $\mu_{\ln a}$ and $\sigma_{\ln a}$ for assumed log-normal aperture distributions were used to determine corresponding aperture-based characteristic curves from Equation (4-5), addressing **objective (2)**.

Step 4. Soil-based characteristic relations for unsaturated flow of van Genuchten (vG; Equation (6-1)) were matched with aperture-based characteristic curves, and the best-fit vG-parameters were determined, addressing **objective (3)**. More specifically, in the vG-relations, the hydraulic conductivity K is expressed either as a function of saturation or the water pressure potential head h (being related to the capillary pressure p_c as $h = -p_c/\rho g$). We considered the vG-relation between K and h, which is:

$$K(h) = K_s \frac{\left(1-(\delta|h|)^{n-1}\left(1+(\delta|h|)^n\right)^{-(1-1/n)}\right)^2}{\left(1+(\delta|h|)^n\right)^{m(1-1/n)}} \quad \text{for } h < 0 \qquad (6\text{-}1)$$

$$K(h) = K_s \quad \text{for } h \geq 0$$

where δ is a (fitting) parameter that is inversely related to the bubble pressure head value, n is a (fitting) parameter that reflects the width of the soil pore size distribution, and m is an additional fitting parameter. For soil samples, the vG-parameters are commonly determined by fitting the functional vG-relation (6-1) to experimentally determined relations between capillary pressure and water saturation (S), or capillary pressure (p_c) and hydraulic conductivity (K). The number of fitting parameters is then commonly reduced by assigning m the value of 0.5 as we do in this study; Mualem (1976) and van Genuchten (1980) found that this value provided the best match with a set of experimental data from 45 soils.

As briefly mentioned above, we determined the vG-parameters by fitting (6-1) to the fracture aperture based relation (4-5). The sum of the squares of the deviations were minimized using the Levenberg-Marquardt method in MathCad (version 1.4; Parametric Technology Corporation). In all cases, the optimization was performed for the part of the curve where $T_{rel} > 0.05$. This yields a good fit to the part of the curve that represents the main drainage of the fracture, see example in Figure 6-1. If a (considerably) larger part of the tail, which is infinitely long, would be included in the optimization, the main drainage part of the curve may not be well represented in the corresponding optimal solution.

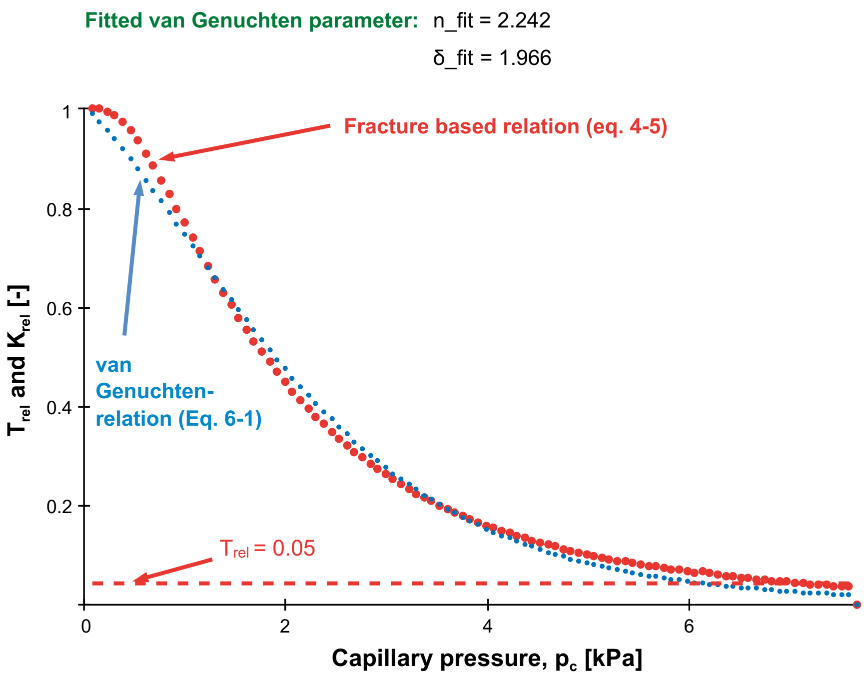


Figure 6-1. *Example match between the van Genuchten relation and the part of the fracture aperture based relation where* $T_{rel} > 0.05$.

The fracture aperture based relation (4-5) needs to be solved numerically before performing the above-described curve fitting procedure. Through a criterion-based choice of a value *inf* representing "infinity" in the integrals of (4-5), we reduce instabilities that are reported to arise in most state-of-the art numerical integration procedures as $a \rightarrow \infty$ when integrating expressions of form $f(a) \times f_{ln}(a)$ (e.g. Gubner 2006). The value *inf* was here chosen such that it fulfils the condition

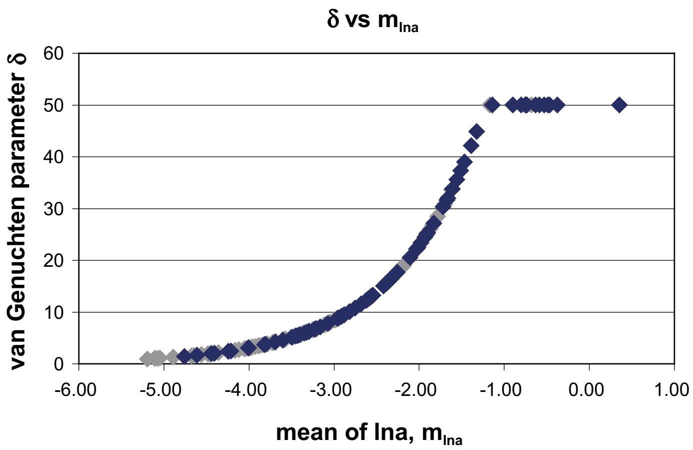
$$\int_0^{\inf} f_{\ln}(a; \mu_{\ln a}, \sigma_{\ln a}) da = 1. \quad (6\text{-}2)$$

7 Results

The dark blue diamonds in Figure 7-1 show the vG-parameters (a) δ and (b) n as functions of the mean value of ln *a* (which in turn is related to the fracture transmissivity according to Equations 4-1 to 4-3). Each blue diamond corresponds to a mean aperture that was estimated (see above steps 1 and 2) from a reported T-value of a PFL-measurement at the Forsmark site, assuming that the T-value reflects a single fracture (Step 1a). Figure 7-1 shows that the mean value of ln *a* of the estimated fracture apertures in Forsmark range between −5 and 0, which corresponds to *a*–values between approximately 0.007 and 1 mm. The grey diamonds show mean apertures derived from the same data, using the alternative assumption (Step 1b) that all identified flow anomalies contribute equally to the measured T-value. The alternative assumption implies that that there is a higher number of fractures, each with a lower transmissivity and mean aperture value than assumed in Step 1a (resulting in lower values of mean ln *a*; this is primarily reflected by the grey diamonds in the leftmost part Figure 7-1). The difference in outcome between these two scenarios is however modest; the tightest fractures are estimated to have a mean value of ln*a* of about −5 in both cases.

Figure 7-1a clearly shows that the vG-parameter δ can be related to the mean value of ln *a*, at least under the used assumption $\sigma_{\ln a} = 0.8$ (reflecting the fracture roughness). In contrast, the vG-parameter n is essentially not related to (or only partially related to) the mean value of ln*a* (Figure 7-1b), which is further explored in the next paragraph, where both ln*a* and $\sigma_{\ln a}$ are varied in the curve-fitting procedure.

a)



b)

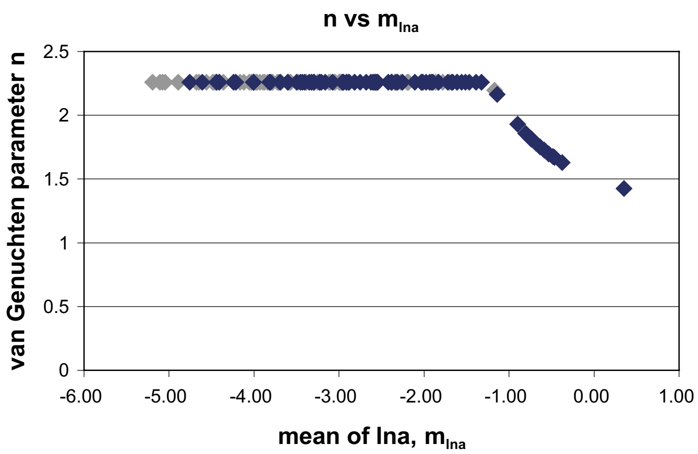


Figure 7-1. *van Genuchten parameters (a) δ and (b) n as a function of the mean value of ln a (defined in Equation 4-3), assuming that σlna is constant and equal to 0.8. The fracture aperture a is given in mm.*

More generally, Figure 7-2 shows matched van Genuchten parameters δ (Figure 7-2a) and n (Figure 7-2b) to fractures of different mean aperture ($\mu_{\ln a}$ or $m_{\ln a}$; x-axis) and standard deviation ($\sigma_{\ln a}$ or sd(lna); coloured lines). The figure illustrates that relatively simple patterns emerge from the matching of seemingly complex curves (Equations 4-4, 4-5 and 6-1). For instance, whereas the δ-value depends on both $\mu_{\ln a}$ and $\sigma_{\ln a}$, the n-value is independent of $\mu_{\ln a}$. Hence, regardless of $\mu_{\ln a}$, the results show that the rougher (with higher $\sigma_{\ln a}$) the fracture is, the lower is the matching n-value. The results for $\sigma_{\ln a} = 0.8$ (blue lines of Figure 7-2) coincide with those shown in Figure 7-1 for $-6 < \mu_{\ln a} \leq -1$. Note in particular that the curve of Figure 7-1a becomes linear when the y-axis is plotted on a log-scale (Figure 7-2a; dark blue line). For $-1 < \mu_{\ln a} \leq 0$, the δ and n results differ between Figure 7-1 and Figure 7-2. This is because we used a more strict convergence criterion when producing the results of Figure 7-2 (compared to the results of Figure 7-1), which confirms that n is indeed independent of $\mu_{\ln a}$. The numerical data that were used for creating the graph of Figure 7-2 are given in Appendix A. Specifically, we there display the best matching values of the van Genuchten parameters n and δ ($m = 0.5$ in all cases), for reproducing unsaturated flow characteristics of variable fractures with different mean values $\mu_{\ln a}$ and standard deviations $\sigma_{\ln a}$ of the fracture aperture a

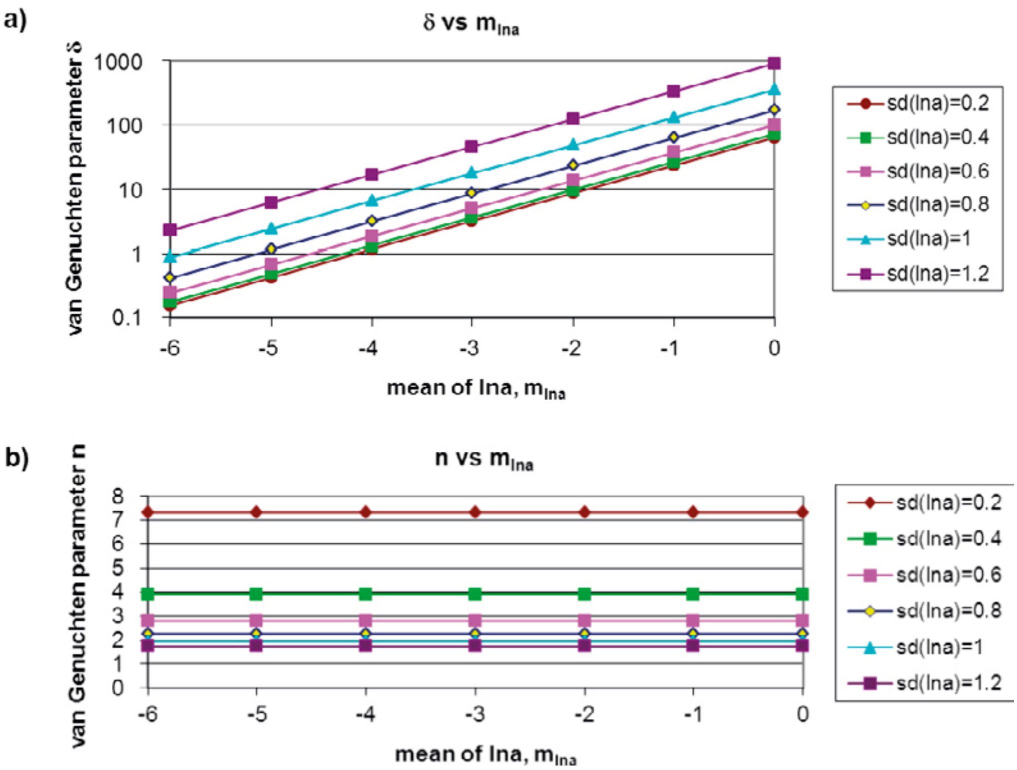


Figure 7-2. *van Genuchten parameters (a) δ and (b) n versus $m_{\ln a}$ (denoted $\mu_{\ln a}$ in the main text) and sd(lna) (denoted $\sigma_{\ln a}$ in the main text). The fracture aperture a is given in mm.*

8 Conclusions

We synthesise and interpret T-values derived from Posiva Flow Log (PFL) tests that were conducted at the Forsmark site (Follin et al. 2007). We conclude that the T-values reflect fractures that are approximately between 0.007 and 1 mm wide on average. Furthermore, previous results of Hakami (1995) showed that fractures frequently follow a log-normal aperture distribution, and that a reasonable range for the fracture "roughness", or the aperture variability around the mean value, is $0.2 \leq \sigma_{\ln a} \leq 1.2$.

Given these physical constraints on fracture geometry (which should be relevant for the Forsmark site), present results show that the fracture aperture based characteristic curves, developed specifically for rock fractures by Jarsjö and Destouni (2001), are very similar in shape to the van Genuchten curves for unsaturated flow. The latter curves have been widely used to characterize unsaturated flow in porous media and are therefore available by default in most existing numerical codes for unsaturated flow.

By matching the fracture aperture based characteristic curves with the vG-curves, we showed that the relation between the mean aperture *a* and the van Genuchten parameter δ is linear in log-log space, and that the value of the van Genuchten parameter n can be directly determined from the value of $\sigma_{\ln a}$, independent of the mean aperture value *a.* Our results specifically show how values of δ and n could be unambiguously determined from the fracture characteristics $\mu_{\ln a}$ and $\sigma_{\ln a}$, if a constant value of 0.5 is assumed for the van Genuchten parameter m (which is a frequently used assumption in soil literature).

Our results are logical from the viewpoint that the van Genuchten parameter δ is viewed as being related to the bubble pressure, which also should be the case for $\mu_{\ln a}$. Furthermore, the van Genuchten parameter n is related to the soil pore size distribution, which in the rock aperture case should correspond to the fracture aperture distribution (or standard deviation $\sigma_{\ln a}$/variation around the mean aperture).

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Appendix A

Best matching values of the van Genuchten parameters n and δ (m = 0.5 in all cases), for reproducing unsaturated flow characteristics of variable fractures with different mean values $\mu_{\ln a}$ and standard deviations $\sigma_{\ln a}$ of the fracture aperture a (given in mm). The tabulated data are illustrated in Figure 7-2.

Mean of ln a	σ of ln a	Parameter n	Parameter δ
−6	0.2	7.331	0.157
−5	0.2	7.331	0.426
−4	0.2	7.331	1.158
−3	0.2	7.331	3.147
−2	0.2	7.331	8.554
−1	0.2	7.331	23.253
0	0.2	7.331	63.209
−6	0.4	3.917	0.178
−5	0.4	3.917	0.483
−4	0.4	3.917	1.313
−3	0.4	3.917	3.57
−2	0.4	3.917	9.706
−1	0.4	3.917	26.382
0	0.4	3.917	71.715
−6	0.6	2.802	0.247
−5	0.6	2.802	0.67
−4	0.6	2.802	1.822
−3	0.6	2.802	4.952
−2	0.6	2.802	13.46
−1	0.6	2.802	36.588
0	0.6	2.802	99.458
−6	0.8	2.257	0.419
−5	0.8	2.257	1.139
−4	0.8	2.257	3.095
−3	0.8	2.257	8.414
−2	0.8	2.257	22.871
−1	0.8	2.257	62.169
0	0.8	2.257	168.993
−6	1	1.938	0.875
−5	1	1.938	2.378
−4	1	1.938	6.463
−3	1	1.938	17.57
−2	1	1.938	47.759
−1	1	1.938	129.823
0	1	1.938	352.896
−6	1.2	1.732	2.252
−5	1.2	1.732	6.121
−4	1.2	1.732	16.638
−3	1.2	1.732	45.227
−2	1.2	1.732	122.939
−1	1.2	1.732	334.182
0	1.2	1.732	908.401

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