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3.3.5 Property-Transfer Models

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As defined in the previous sections of this chapter, the water retention curve expresses the relation between soil water matric head (h_m) and volumetric soil water content (θ). Its highly nonlinear shape very much depends upon the particle-size distribution, which determines the *soil texture*, and the arrangement of the solid particles referred to as *soil structure* (e.g., Richards & Weaver, 1944; Croney & Coleman, 1954; Salter & Williams, 1965; Sharma & Uehara, 1968; Reeve et al., 1973). Other soil properties, such as organic matter content and soil water composition, also influence the behavior of the water retention curve, but to a lesser extent.

The water retention curve is commonly expressed in terms of a parametric water retention function. All of these parametric models (e.g., Brooks & Corey, 1964; Brutsaert, 1966; van Genuchten, 1980) involve fitting parameters to soil water retention data (Section 3.3.4). Aside from the question of whether these parameters are physically meaningful or not, a full description of the water retention function, $h_m(\theta)$, requires at least three parameters: one or more dimensionless shape parameters and two dimensional scale parameters (one for water content and one for matric head). As explained in the previous sections, several methods exist for the estimation of water retention parameters from either laboratory measurements (Section 3.3.2) or field measurements (Section 3.3.3). However, both laboratory and field procedures are highly time-consuming, and their extrapolation to large areas is rather unrealistic. This has motivated numerous attempts in the last three decades to predict soil water characteristic curves from more easily accessible field data, such as textural information, organic matter content, and bulk density.

Prediction models can be grouped into two classes, which are (i) empirically or (ii) physically based:

First, the empirical approach consists of relating the different soil characteristic parameters to textural and structural soil properties by the use of statistical regression analysis (e.g., Ghosh, 1976; Clapp & Hornberger, 1978; Gupta & Larson, 1979a; Bloemen, 1980; Brakensiek et al., 1981; McCuen et al., 1981; Rawls & Brakensiek, 1982; Cosby et al., 1984; Puckett et al., 1985; Wösten & van Genuchten, 1988; Vereecken et al., 1989; Schaap et al., 1998). Although most empirical models clearly show correlations between water retention and textural or structural soil data, valid application is in general restricted to the soil tested. Hence, the results are site- and data-specific and predictions may contain important errors in water content, especially at the wet end of the $h_m(\theta)$ relationship, which is dominated by soil structural parameters.

Second, the few physically based models proposed in the literature (e.g., Arya & Paris, 1981; Haverkamp & Parlange, 1986) postulate a fundamental relationship between the water retention curve and measurable properties like the cumulative particle-size distribution. The Arya–Paris (1981) model, the most commonly used, divides the particle-size distribution into a number of fractions, assigning a pore volume and volumetric water content (θ_i) to each fraction, on the basis of the bulk density and the weight percentage of particles in each fraction. A corresponding matric head value, $(h_m)_i$, is computed using capillary theory to obtain h_m from the average pore size of the fraction. To move from particle size to pore size and from pore size to matric head, an empirical parameter (α), later interpreted as the fractal dimension of a tortuous pore (Tyler & Wheatcraft, 1989), was introduced. A second physically based model, proposed by Haverkamp and Parlange (1986), allows for a direct estimation of the parameters for the Brooks and Corey (1964) water retention function for sandy soils in the absence of organic matter. The predicted $h_m(\theta)$ curve is associated with the boundary (main) wetting curve of the hysteresis family. Coupled with the hysteresis model proposed by Parlange (1976), the full family of wetting curves can be predicted.

The physically based models are conceptually the most appealing. The underlying hypothesis of shape similarity (different from shape identity) between the shape of the cumulative particle-size distribution function and that of the water retention curve, was recently confirmed by an analysis of the soil database GRIZZLY (Haverkamp et al., 1998). Defining the shape of water retention curves by the shape indicator mn and cumulative particle-size functions by the shape indicator MN (both parameters are addressed in more detail in Section 3.3.5.1), the positive correlation between mn and MN is clearly shown in Fig. 3.3.5–1. This result confirms the fact that for a large number of soils the water retention shape parameter mn depends

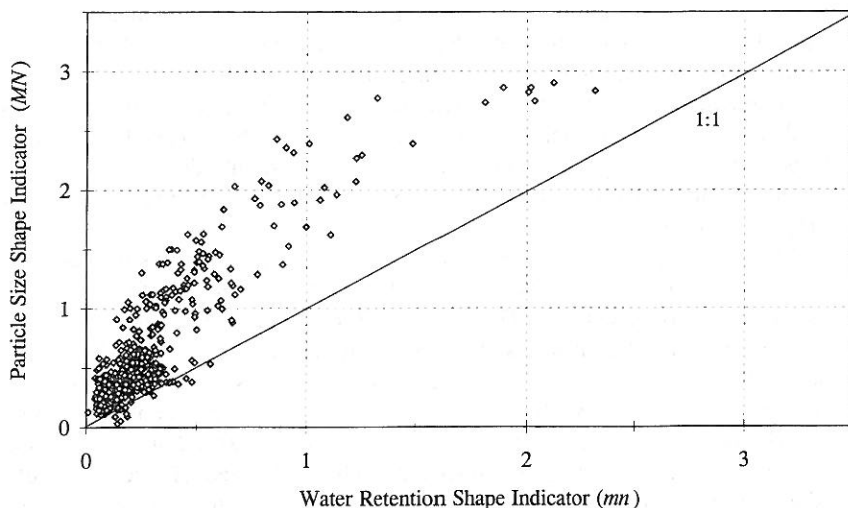


Fig. 3.3.5–1. The particle-size shape indicator (MN) as a function of the water retention shape indicator (mn) calculated for the 660 soils of the GRIZZLY soil database (Haverkamp et al., 1998).

mainly on texture. A similar analysis for a particle-size scale parameter (D_g) and matric head scale parameter (h_g) shows no correlation (Fig. 3.3.5-2). This observation highlights the danger of predicting the soil structure-dependent scale parameters from soil textural information alone. The two texture-based models considered here (Section 3.3.5.1) take account of the soil structural effect only through the dry bulk density (ρ_b) embedded in the definition of the parameter (α) for the Arya-Paris model (1981) or through the proportionality factor between pore size and associated particle diameter for the Haverkamp-Parlange model (1986).

When soil structure is significant, the pore space defined by the size distribution of the basic soil particles (conveniently referred to as the *textural pore space*) is not the dominant characteristic that defines the water retention scale parameters. When soil particles are bound together to form clods and crumbs, the position and orientation of these aggregates with respect to each other define an interaggregate pore space (referred to as *structural pore space*), which is more significant than the textural pore-size distribution for the determination of the structure-dependent scale parameters for soil water content and matric head. To take this effect of the structural pore space into account, Nimmo (1997) proposed a water retention prediction model that considers a soil water retention curve as the sum of two components, one textural (θ_{te}) and the other structural (θ_{st}). The structural part of this model operates like a texture-based model that is based on aggregate sizes rather than particle sizes.

Section 3.3.5.1 describes the principles of the two texture-based prediction models of Arya and Paris (1981) and Haverkamp and Parlange (1986), with the procedures of application and comments on the pros and cons of the models. Section 3.3.5.2 describes the texture- and structure-based prediction model of Nimmo (1997), with discussion of procedures and comments.

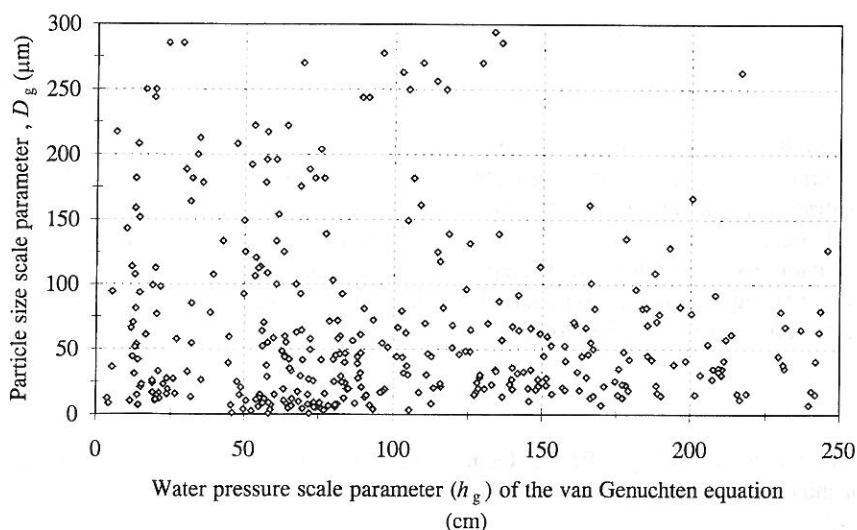


Fig. 3.3.5-2. Matric head scale parameter h_g as a function of the particle-size scale parameter D_g calculated for the 660 soils of the GRIZZLY soil database (Haverkamp et al., 1998).

3.3.5.1 Physically Based Water Retention Prediction Models

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3.3.5.1.a Introduction

Even though both the Arya–Paris (1981) and the Haverkamp–Parlange (1986) model are based on the same hypothesis of shape similarity between the cumulative particle-size distribution function and the water retention curve, the routing procedures used to navigate from the cumulative particle-size distribution to the cumulative pore-size distribution, and subsequently to the water retention curve, are different. While the Arya–Paris model uses discrete equations giving point values of the water retention curve, the Haverkamp–Parlange model uses functional forms leading directly to a parametric water retention function. The second fundamental difference between the two models is that the Haverkamp–Parlange model has attempted to take into account the problem of hysteresis. As the cumulative particle-size distribution is unique for a given soil, only one associated water retention curve can be predicted. In reality water retention is represented by a family of different wetting and drying curves (hysteresis; Section 3.3.1). Hence, from a purely conceptual point of view, it is necessary to choose whether the particle-size distribution function is associated with a wetting curve of the hysteresis loop or a drying curve. Haverkamp and Parlange (1986) decided upon the main wetting curve for reasons which will be explained in Section 3.3.5.1.c. The only simple but precise hysteresis model available in the literature at that time (1986) was the prediction model of Parlange (1976), which obliged the authors to consider a parametric water retention function without inflection point, for example, the Brooks and Corey (1964) water retention function:

$$\begin{aligned}\theta/\theta_s &= (h_{bc}/h_m)^\lambda & \text{for } h_m \leq h_{bc} \\ \theta &= \theta_s & \text{for } h_{bc} \leq h_m \leq 0\end{aligned}\quad [3.3.5-1]$$

where θ is volumetric water content ($L^3 L^{-3}$); θ_s is the volumetric water content at natural saturation, chosen as the water content scale parameter; h_m (L) is soil water matric head taken to be negative and expressed in centimeters of water; h_{bc} is the soil specific Brooks and Corey matric head scale parameter (L); and λ is the dimensionless water retention shape parameter (see Section 3.3.4.a for more details). A more adequate choice would have been the S-shaped van Genuchten (1980) water retention function (see Section 3.3.4.b):

$$\theta/\theta_s = [1 + (h_m/h_g)^n]^{-m} \quad [3.3.5-2]$$

where h_g is the soil specific van Genuchten matric head scale parameter (L), and m and n are the dimensionless water retention shape parameters assumed to be linked by:

$$m = 1 - (k_m/n) \quad [3.3.5-3]$$

Van Genuchten (1980) introduced k_m to calculate closed-form analytical expressions for the hydraulic conductivity function using the predictive conductivity model of Burdine (1953), when $k_m = 1$, or Mualem (1976), when $k_m = 2$. When other conductivity functions, such as the one of Brooks and Corey (1964), are chosen, there is no need to impose, a priori, an integer value of k_m . For large negative matric head values the van Genuchten water retention equation (Eq. [3.3.5-2]) behaves like the Brooks and Corey equation (Eq. [3.3.5-1]) with $\lambda = mn$. However, it should be noted that this identity has only been confirmed for soils with $mn \leq 0.8$ while using the Burdine mode of the van Genuchten equation (Haverkamp et al., 1998). The curvature of the van Genuchten relation for large $|h_m|$ values thus depends on the product mn , rather than on one of the individual parameters m or n . The product mn is referred to as the *water retention shape indicator* (see also Fig. 3.3.5-1).

The choice of a parametric water retention function, for example, the Brooks and Corey equation (Eq. [3.3.5-1]) or the van Genuchten equation (Eq. [3.3.5-2]) is not without consequences. As will be shown below, the type of equation to be used for the cumulative particle-size distribution function is fully conditioned by the choice of the expression used for the water retention curve. For example, starting with the van Genuchten water retention equation requires using a van Genuchten type of equation for the cumulative particle-size distribution function. Unfortunately, the model of Haverkamp and Parlange (1986) had to compromise on this consistency criterion. While for reasons of hysteresis (explained above) the authors had to choose a Brooks and Corey expression for the water retention curve, they preferred for reasons of best fit a van Genuchten type-equation for the cumulative particle-size distribution function.

3.3.5.1.b Arya-Paris Model: Principles

This model involves dividing the cumulative particle-size distribution function into a number of class fractions with an average particle-size and fraction weight assigned to each class. Assuming that the particles are spherical and the pores cylindrical, the number of particles (n_i) in each class is determined by:

$$n_i = (6W_i)/(\pi D_i^3 \rho_s) \quad [3.3.5-4]$$

where D_i is the mean particle diameter (L) of the i th size fraction, W_i is the corresponding solid mass per unit sample mass (M), and ρ_s is the particle density (generally taken equal to $\rho_s = 2.65 \text{ g cm}^{-3}$ when C content is negligible). The values of W_i are chosen in such a way that the sum of all W_i is unity.

The pore volume dVp_i (L^3) associated with each size fraction is defined by:

$$dVp_i = \pi R_i^2 Le_i \quad [3.3.5-5]$$

where R_i is the mean pore radius (L) and Le_i is the effective pore length (L) of size class i . In the absence of tortuosity the apparent pore length (L_i) can be estimated as the product of the number of particles in size class i and the mean particle diameter (D_i) of that class. However, for field soils the effect of tortuosity should not be ignored. Therefore, Arya and Paris (1981) defined the effective pore length (Le_i) as:

$$Le_i = n_i^\alpha D_i \quad [3.3.5-6]$$

where α is a tortuosity correcting parameter ($\alpha \geq 1$). When tortuosity effects are negligible the value of α equals 1. Applying the tortuosity (T) concept used by most capillary models to express the apparent flow velocity per volume unit as a function of the flow velocity in soil pores (e.g., Burdine, 1953; Brooks & Corey, 1964; Dullien, 1979), Eq. [3.3.5-6] gives:

$$(T_i)^p = Le_i/L_i = n_i^{\alpha-1} \quad [3.3.5-7]$$

where p is a tortuosity parameter. Although p should be considered as a soil specific variable defined for values of $p > 0$, some authors proposed a constant value based on the capillary model of choice. For example, Brooks and Corey (1964) and Dullien (1979) suggested $p = 0.5$, whereas Burdine (1953) used $p = 1$. Obviously, when $p = 0$ there is no tortuosity and the effective pore length is equal to the apparent pore length (Eq. [3.3.5-7]). The model of Arya and Paris sets $p = 1$, independent of the soil in question. Arya and Paris then derived a nonlinear relation between the mean pore radius (R_i) and the corresponding mean particle diameter (D_i) of the form:

$$R_i = 1/2 D_i [(2en_i^{1-\alpha})/3]^{0.5} \quad [3.3.5-8]$$

where e is the void ratio defined as the ratio of the void volume fraction or porosity, ϵ ($L^3 L^{-3}$), and the solid volume fraction:

$$e = \epsilon/(1 - \epsilon) \quad [3.3.5-9]$$

Equation [3.3.5-8] results from the argument that a pore length can be estimated by the number of particles that lie along the pore path times the length contributed by each particle (i.e., the particle diameter). For the sake of simplicity the void ratio (e) and hence the soil porosity were considered to be constant for all particle-size classes. This global porosity value for the total soil sample is referred to hereafter as the *apparent soil porosity*, $\tilde{\epsilon}$. The parameter α was determined experimentally through fitting and was found to vary between 1.31 and 1.43. An average value of 1.38 yielded satisfactory results (Arya & Paris, 1981).

Once the mean pore radius (R_i) is defined (Eq. [3.3.5-8]), the corresponding matric head, $(h_m)_i$, is determined by the classical capillary rise equation written in its simplified form by (see Sections 3.3-1 and 3.3-2):

$$(h_m)_i = -(0.149/R_i) \quad [3.3.5-10]$$

where the soil water matric head, $(h_m)_i$, and the mean pore radius, R_i , are both expressed in centimeters.

Finally, the volumetric water content values are calculated from the pore volumes dVp_i (Eq. [3.3.5-5]). In doing so, it is assumed that the pore volumes generated by each size fraction are progressively accumulated, from smallest to largest size fraction, and filled with water. The volumetric water content values at the upper bounds of successive particle-size fractions are then calculated by:

$$\tilde{\theta}_i = \sum_{j=1}^{j=i} dV p_j \rho_b \quad [3.3.5-11]$$

where $\tilde{\theta}_i$ is the volumetric water content represented by a pore volume for which the largest size pore corresponds to the upper limit of the i th particle-size range, and ρ_b is the dry soil bulk density ($M L^{-3}$) related to the apparent soil porosity (ϵ) by:

$$\epsilon = 1 - (\rho_b / \rho_s) \quad [3.3.5-12]$$

Note that the use of ρ_b in Eq. [3.3.5-11] is justified by the fact that the sum of all weight fractions W_i is chosen equal to unity. Moreover, the use of Eq. [3.3.5-11] implies that the maximum volume to be filled with water equals the porosity (ϵ). The influence of air entrapment (with $\theta_g < \epsilon$) is not taken into account by the model. Finally, the average volumetric water content corresponding to the midpoint of a given particle-size fraction is given by:

$$\theta_i = (\tilde{\theta}_i + \tilde{\theta}_{i+1})/2 \quad [3.3.5-13]$$

Hence, the minimum input data necessary to operate the Arya-Paris prediction model are the cumulative particle-size distribution curve and the dry bulk density or soil porosity.

Procedure

1. Divide the cumulative particle-size distribution curve into a number of fractions starting from the end representing the smallest-size particle. Arya and Paris suggested 20 as an optimum number of fractions, with upper size limits for particle diameter at 1, 2, 3, 5, 10, 20, 30, 40, 50, 70, 100, 150, 200, 300, 400, 600, 800, 1000, 1500, and 2000 μm . An average particle diameter value (D_i) is assigned to each particle-size fraction. The steps described hereafter are then applied to each D_i -value.
2. Calculate the fraction weights (W_i) from the cumulative particle-size distribution curve. The differences in cumulative percentages corresponding to successive particle sizes divided by 100 give values of W_i such that the sum of all W_i is unity.
3. Calculate the number of soil particles (n_i) of the i th particle-size class by using Eq. [3.3.5-4].
4. Calculate the mean pore radius (R_i) by using Eq. [3.3.5-8] with the tortuosity parameter α equal to 1.38 and the void ratio (e) calculated from Eq. [3.3.5-9].
5. The pore volume fraction ($dV p_i$) of the i th particle-size class is calculated by the combined use of Eq. [3.3.5-5] and [3.3.5-6], with the values of n_i and R_i given by the previous Steps 3 and 4.
6. The soil water matric head value, $(h_m)_i$, is calculated from Eq. [3.3.5-10] using the mean pore radius, R_i , expressed in centimeters.
7. Finally, the volumetric water content value (θ_i), corresponding to the midpoint of the i th particle-size class, is calculated by the combined use of Eq. [3.3.5-11] and [3.3.5-13].

3.3.5.1.c Haverkamp–Parlange Model: Principles

Similar to the above prediction model, the Haverkamp–Parlange (1986) approach is based on the hypothesis of shape similarity between cumulative particle-size distribution and water retention curves. However, instead of working with a discrete formulation as used by the Arya–Paris model, the Haverkamp–Parlange model is expressed in functional form. The model is composed of two submodules, one that describes the routing procedure from particle size to water retention and another that deals with the coupled hysteresis model.

Starting with the first module, the cumulative particle-size distribution function is expressed in the form of a van Genuchten type of equation (similar to Eq. [3.3.5–2]):

$$F = [1 + (D_g/D)]^{-M} \quad [3.3.5-14]$$

where F is the cumulative distribution of particle weight per unit sample mass ($M M^{-1}$), D is the particle diameter (L), D_g is a particle-size scale parameter (L), and M and N are the particle-size shape parameters assumed to be linked by an expression similar to Eq. [3.3.5–3]:

$$M = 1 - (k_m/N) \quad [3.3.5-15]$$

The integer k_m is chosen identical to that used by the van Genuchten (1980) water retention equation (Eq. [3.3.5–2]) with $k_m = 1$. The product MN is referred to as the *shape indicator of the cumulative particle-size distribution* (Fig. 3.3.5–1). The values of D_g and M (and/or N) are calculated by fitting Eq. [3.3.5–14] to the experimental cumulative particle-size data using a classical least-squares technique (e.g., Marquardt, 1963). With the cumulative particle-size distribution function defined, the routing procedure between $F(D)$ and the water retention curve is then to relate the shape and scale parameters of $h_m(\theta)$ to the parameters used for the description of $F(D)$.

Haverkamp and Parlange suggested a linear relationship between the pore radius, R , (L) and the corresponding particle diameter, D , of the form:

$$R = \gamma D \quad [3.3.5-16]$$

where γ is a soil specific tortuosity parameter.¹ The estimation of γ will be addressed later in this section. Even though the $R(D)$ relation given by Eq. [3.3.5–16] is quite crude for general field soils, its use was assumed to be reasonable when structural characteristics become independent of the degree of saturation, which is the case for soils with relatively uniform particles. For these reasons the model was explicitly recommended for sandy soils. Combining Eq. [3.3.5–16] with the capillary rise equation (Eq. [3.3.5–10]) gives:

¹ The particle-size/pore-size relation (Eq. [3.3.5–16]) was originally presented by Haverkamp and Parlange (1986) in the form of D as a function of R rather than R as a function of D . Consequently, we should read γ^{-1} instead of γ when comparing the packing coefficient values with those given by Haverkamp and Parlange. It is only for reasons of consistency that we have chosen to write the particle-size/pore-size relation (Eq. [3.3.5–16]) in a similar form as that used before in the context of the Arya–Paris model (Eq. [3.3.5–8]).

$$h_m = 0.149/\gamma D \quad [3.3.5-17]$$

which permits the direct calculation of the matric head h_m as a function of D , once the value of γ is known.

It follows from the $R(D)$ relationship, given by Eq. [3.3.5-16], that the relative pore fraction and the relative solid fraction are equal. When defining the degree of saturation, S , as the ratio of water content, θ , and porosity, ϵ , the degree of saturation can be set equal to the cumulative particle-size distribution (where the particle density ρ_s is considered to be constant). However, due to air entrapment, the water content at natural saturation (θ_s) seldom reaches saturation of the total pore space. If we assume that air is contained not only in the largest pores, but in a distribution of pores representative of the total pore system (Lenormand, 1981), it follows:

$$\theta = \theta_s F(D) \quad [3.3.5-18]$$

or

$$\theta/\theta_s = [1 + (h_m/h_e)^N]^{-M} \quad [3.3.5-19]$$

Comparing Eq. [3.3.5-19] with the van Genuchten water retention equation (Eq. [3.3.5-2]), it follows that the shape parameters of the water retention equation become identical to those used for the particle-size distribution function; that is, $m = M$ and $n = N$. Obviously, such shape identity is generally not realistic for field soils ($mn < 1$) and is in disagreement with the experimental results shown in Fig. 3.3.5-1. Even for pure sand soils with $mn > 2$ the shape identity is not observed. To account for this problem, Haverkamp and Parlange (1986) suggested correcting the water retention shape indicator mn by relating it to the dry bulk density. However, before doing so they had to adapt the water retention equation to the conditions imposed by the hysteresis model chosen.

When coupling the water retention prediction model with the hysteresis concept of Parlange (1976), the particle-size distribution curve is supposed to be associated with the main wetting (mw) curve [$h_m(\theta_{mw})$]. For reasons inherent to the rational extrapolation technique used by the Parlange hysteresis model the main wetting curve can only be expressed by an equation that does not exhibit an inflection point. Hence, it excludes use of the van Genuchten water retention equation. Consequently, Haverkamp and Parlange chose a Brooks and Corey type of equation (Eq. [3.3.5-1]):

$$\begin{aligned} \theta_{mw}/\theta_{ac} &= (h_{ae}/h_m)^\lambda & \text{for } h_m \leq h_{ae} \\ \theta_{mw}/\theta_{ac} &= [1 + \lambda - \lambda(h_m/h_{ae})] & \text{for } h_{ae} \leq h_m \leq 0 \end{aligned} \quad [3.3.5-20]$$

where h_{ae} is the matric head value (L) associated with the air-entry matric head value, and θ_{ac} is the water content on the main wetting curve corresponding with h_{ae} (Fig. 3.3.5-3). The wetting branch of $h_m(\theta_{mw})$ for $h_{ae} \leq h_m \leq 0$ represents a straight line passing through the points (θ_{ac}, h_{ae}) and $(\epsilon, 0)$ and is defined by the continuity in slope at (θ_{ac}, h_{ae}) . The value of θ_{ac} is determined by the straight part of the water retention curve (Eq. [3.3.5-20]):

$$\theta_{ae} = \epsilon / (1 + \lambda)$$

$$[3.3.5-21]$$

Before going into detail on the hysteresis module (the second part of the Haverkamp–Parlange model), estimations of the shape parameter (λ) and the tortuosity correction factor (γ) are addressed. The calculation of the matric head scale parameter (h_{ae}) is given in the second part dealing with the hysteresis concept.

When working with functional forms for $F(D)$ and $h_m(\theta_{mw})$ the obvious means for the determination of λ would be to use an identification procedure based on the hypothesis of shape similarity between both functions. However, when

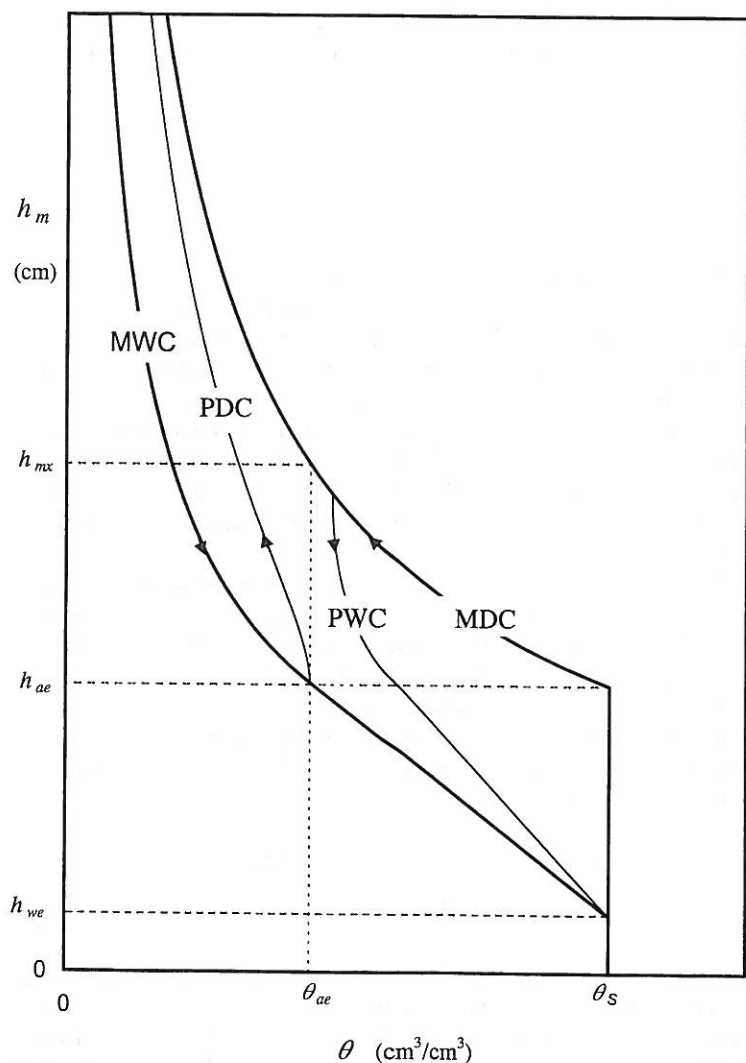


Fig. 3.3.5-3. Schematic diagram of the Parlange (1976) hysteresis model with the main wetting curve (MWC), the main drying curve (MDC), a primary drying curve (PDC), and a primary wetting curve (PWC).

going from the cumulative particle-size distribution function to the van Genuchten water retention curve and subsequently to the Brooks and Corey water retention curve, two difficulties arise. The first one, explained above, concerns the fact that mn becomes equal to MN when using a linear $R(D)$ relationship. This is obviously not realistic as even for pure sands this hypothesis is not justified. The second difficulty concerns the geometrical difference between the two water retention equations of van Genuchten (Eq. [3.3.5-2]) and Brooks and Corey (Eq. [3.3.5-20]). Even though both expressions describe the same water retention characteristic, they are formulated in different ways with different shape parameters (e.g., an apple and a pear are both fruits but they do not necessarily have the same form). While for large negative matric head values the van Genuchten water retention equation (Eq. [3.3.5-2]) behaves like the Brooks and Corey equation (Eq. [3.3.5-20]) with $\lambda = mn$, this quasi-identity is only valid for small values of mn (i.e., $mn < 0.8$). For pure sands, with $mn \approx 2$, the van Genuchten shape indicator (mn) is systematically smaller than that of the Brooks and Corey (1964) equation. Using the collation of soils of the GRIZZLY database, Haverkamp et al. (1998) determined the following polynomial regression equation (Fig. 3.3.5-4):

$$\lambda = 0.911mn - 0.076(mn)^2 \quad [3.3.5-22]$$

with a squared correlation coefficient of $r^2 = 0.9801$. Equation [3.3.5-22] was calculated over the interval $0 \leq mn \leq 6$. Beyond this interval the equation may be inadequate.

Because of the two problems, information on shape similarity between the two functions $F(D)$ and $h_m(\theta_{mw})$ could not be used to its full advantage for the shape parameter identification procedure. Consequently, Haverkamp and Parlange (1986) chose to correlate the particle-size shape indicator (MN) directly to the Brooks and

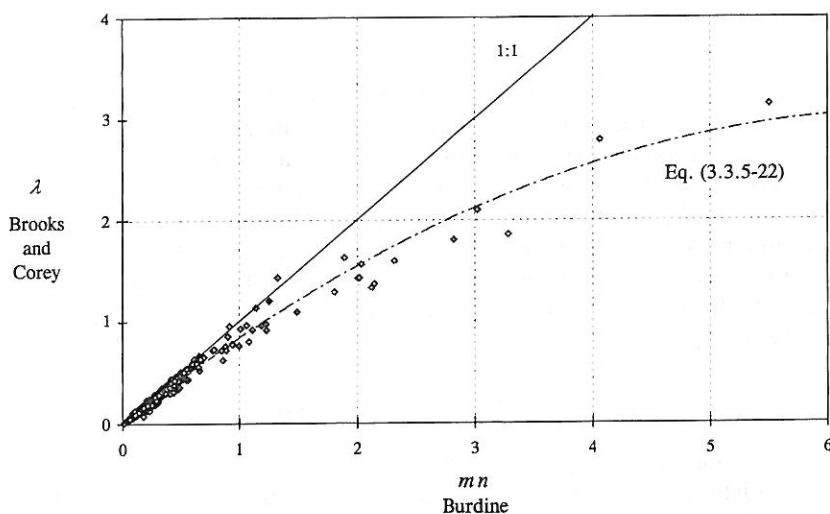


Fig. 3.3.5-4. The Brooks and Corey shape parameter (λ) as a function of the van Genuchten shape indicator (mn) calculated for the 660 soils of the GRIZZLY soil database, together with the regression line (dashed) given by Eq. [3.3.5-22]; taken from Haverkamp et al. (1998).

Corey shape parameter (λ) by the use of an empirical regression equation with the dry bulk density (ρ_b) as the independent variable:

$$\lambda = 0.0723MN(\rho_b)^{3.8408} \quad [3.3.5-23]$$

where the regression parameters were determined over a population of 10 sand soils.

The next step concerns the determination of the tortuosity parameter γ . Its theoretical value can only be calculated for very particular packing arrangements; for example, for a completely stable tetrahedral particle arrangement γ equals 0.112 (Gupta & Larson, 1979b). In the case of field soils, Haverkamp and Parlange (1986) used a polynomial regression equation expressed as a function of λ :

$$\gamma = (17.1736 - 4.7043\lambda + 0.1589\lambda^2)^{-1} \quad [3.3.5-24]$$

where the regression parameters were again calculated for a population of 10 sand soils.

So far only the main wetting curve has been defined (Eq. [3.3.5-20]). The second part of the Haverkamp-Parlange model deals with the hysteresis link. As our discussion is focused on the physically based property-transfer models rather than on the problem of hysteresis (Section 3.3.1), we present here only the development of the main drying curve (MDC). For the description of the respective wetting and drying scanning curves we refer the reader to the articles of Parlange (1976) and Haverkamp and Parlange (1986).

To define the main drying curve (MDC) a similar matric head scale parameter is introduced as for the main wetting curve (MWC) (Eq. [3.3.5-20]), namely, the water entry matric head value h_{we} , which is assumed to be different from h_{ae} . The value of h_{we} is defined by the straight part of the MWC for $\theta = \theta_s$ (Fig. 3.3.5-3):

$$\theta_{ae} = \theta_s [1 + \lambda - \lambda(h_{we}/h_{ae})]^{-1} \quad [3.3.5-25]$$

Both values of h_{ae} and h_{we} occur for the same water content (θ_s) and, hence, are linked by a functional relationship. Considering a uniform-sized particle system, for example, glass beads, one can derive the relationship (Gupta & Larson, 1979b) $h_{ae} = 1.84h_{we}$, which is very close to the estimate given earlier by Bouwer (1966), namely, $h_{ae} = 2h_{we}$. However, such a constant relationship is physically unrealistic for natural packing arrangements because one may expect that the water entry matric head tends to zero when the pore space becomes totally saturated, that is, when θ_s tends to the porosity ϵ . Use of the latter condition, together with Eq. [3.3.5-21] and [3.3.5-25] gives:

$$h_{we}/h_{ae} = [(1 + \lambda)/\lambda][1 - (\theta_s/\epsilon)] \quad [3.3.5-26]$$

which fixes the value of h_{we} once h_{ae} is known.

With the parameter h_{we} defined, the MDC is calculated from the rational extrapolation equation of the Parlange (1976) hysteresis model:

$$h_m - h_{std}(d\theta_{mw}/dh_m) = \theta_{mw} - \theta_{md} \quad \text{for } \theta_{md} \leq \theta_{std} \quad [3.3.5-27]$$

which permits the estimation of the MDC starting at a matric head h_{std} on the main wetting curve. The subscript "md" refers to the main drying curve. Substitution of the main wetting curve (Eq. [3.3.5-20]) into Eq. [3.3.5-27] with $h_{std}(\theta_{std}) = h_{we}(\theta_s)$ gives the following main drying equations:

$$\theta_{md}/\theta_s = (h_{ae}/h_m)^\lambda$$

$$\{[1 + \lambda - \lambda(h_{we}/h_m)]/[1 + \lambda - \lambda(h_{we}/h_{ae})]\} \quad \text{for } h_m \leq h_{ae}$$

$$\theta_{md} = \theta_s \quad \text{for } h_{ae} \leq h_m \leq 0 \quad [3.3.5-28]$$

Equations [3.3.5-20] and [3.3.5-28] are the final expressions used to describe the main wetting and main drying water retention curves.

The last point to solve is the calculation of the air-entry matric head value h_{ae} . Haverkamp and Parlange (1986) used an identification procedure based on the comparison between the matric head values on the main wetting curve and main drying curve calculated for the same water content. Defining h_{mx} as the matric head value on the main drying curve corresponding to the water content value θ_{ae} (Fig. 3.3.5-3), the combination of Eq. [3.3.5-21], [3.3.5-26], and [3.3.5-28] yields the implicit equation:

$$\frac{h_{ae}}{h_{mx}} = \left\{ (1 + \lambda) \left[1 - \left(1 - \frac{\theta_s}{\varepsilon} \right) \frac{h_{ae}}{h_{mx}} \right] \right\}^{-1/\lambda} \quad [3.3.5-29]$$

which can be easily solved for the ratio h_{ae}/h_{mx} in an iterative way. This ratio is then used for the final calculation of the matric head value h_{ae} by combining Eq. [3.3.5-14], [3.3.5-17], and [3.3.5-18]:

$$h_{ae} = (0.149/\gamma D_g)[(\theta_{ae}/\theta_s)^{-1/M} - 1]^{1/N}(h_{ae}/h_{mx}) \quad [3.3.5-30]$$

The minimum input data necessary to operate the Haverkamp-Parlange prediction model are the cumulative particle-size distribution curve, the dry bulk density or soil porosity, and the water content at natural saturation.

Procedure

1. Fit the cumulative particle-size distribution function $F(D)$, Eq. [3.3.5-14], with $k_M = 1$, through the experimental data. This yields values of M and D_g . The corresponding value of N is estimated from Eq. [3.3.5-15].
2. Calculate the Books and Corey shape indicator λ from Eq. [3.3.5-23] using M and N determined in Step 1.
3. Calculate the parameter γ from Eq. [3.3.5-24] with λ determined in Step 2.
4. Determine the water content value θ_{ae} from Eq. [3.3.5-21] with ε calculated from the dry bulk density ρ_b (Eq. [3.3.5-12]). The particle density may be taken as $\rho_s = 2.65 \text{ g cm}^{-3}$.
5. The ratio h_{ae}/h_{mx} is computed iteratively from Eq. [3.3.5-29] with a λ value determined in Step 2.
6. The matric head value h_{ae} is calculated from Eq. [3.3.5-30] using M , N , D_g , γ , θ_{ae} , and h_{ae}/h_{mx} values determined in Steps 1, 3, 4, and 5.

7. Finally the main wetting and drying water retention curves are calculated from Eq. [3.3.5–20] and [3.3.5–28], respectively.

3.3.5.1.d Comments

Generally speaking, both prediction models presented above are based on the assertion that the size of the soil particles (textural property) and the dry bulk density to which they are packed (structural property) are the primary determinants of the pore-size distribution and, hence, of the water retention curve. Even though this is not entirely the case, both models correctly predict the shape of many water retention curves. In some way this is not surprising as both models are based on the experimentally verified hypothesis (Haverkamp et al., 1998) of shape similarity between the cumulative particle-size distribution curve and the water retention curve. On the other hand, both models lack precision in the prediction of the soil structural dependent water content and matric head scale parameters for most field soils. This shows that the dry bulk density is not the only determinant of the pore-size distribution and/or water retention curve. Even though the Haverkamp–Parlange model seems to be less affected by this soil structure dependent scale problem, one should bear in mind that this model is only valid for the very limited range of field soils of pure sands that generally are considered as quasi-nonstructured soils. As far as the Arya–Paris prediction model concerns, Arya et al. (1999) have recently reformulated the tortuosity parameter α by including the effect of soil structure in a more satisfying way (details given below).

Of the two prediction models, the Arya–Paris model is definitely the more user-friendly. Even though the concept of the Haverkamp–Parlange model is simple, its description is more complicated to follow because the authors choose to incorporate the concept of hysteresis. Moreover, and independent from the question whether hysteresis effects are important under field conditions or not, the use of the Arya–Paris model is not restricted to a small group of soil types. On the contrary, the Haverkamp–Parlange model is only valid for sandy soils in the absence of organic matter. This certainly explains the fact that the Arya–Paris model is the most widely used. Aside from these general qualitative remarks, we believe it is useful to describe in more detail the different conceptual problems inherent in the two models.

The Arya–Paris Model. A first difficulty of the Arya–Paris model is that it does not account for trapped air (Arya & Paris, 1981, p. 1029). As the water content of field soils at natural saturation (θ_s) is rarely identical to the porosity (ϵ), it follows that the water content scale parameter is systematically overestimated. This obviously induces errors in the predicted water content values; these errors are most visible at the wet end of the water retention curve. As indicated by Arya and Paris (1982), this effect could be accounted for in the model at the cost of additional soil information. In a later study, Arya et al. (1999) introduced a correction factor θ_s/ϵ in front of the sum term in Eq. [3.3.5–11]. However, the presence of trapped air translates in a disguised way the problem of tortuosity and, consequently, not only affects the water content scale parameter but also the matric head scale parameter of the water retention curve. From a conceptual point of view this implies that the classical capillary rise equation (Eq. [3.3.5–10]) should also be adjusted in order to ac-

count for the effect of trapped air. While the water retention scale parameters have a dominant effect on the description of vadose zone water movement (which obviously is the final goal of our compulsive attempts to predict hydraulic soil characteristics) the problem of trapped air should not be overlooked.

This brings us to the second difficulty of the Arya-Paris model: the definition of the parameter α , which relates the particle size to the pore radius. Arya and Paris (1981) proposed an average value of $\alpha = 1.38$, calculated for a limited number of soils. However, several researchers (e.g., Schuh et al., 1988; Mishra et al., 1989; Gupta & Ewing, 1992) have suggested that predictions of the water retention curve could be improved if α is allowed to vary over the range of particle sizes. As most model users employ the constant α value (i.e., $\alpha = 1.38$), Haverkamp et al. (1999) have tested the validity of a constant α for more than 1000 soils taken from the UNSODA database (Leij et al., 1996). For the reported soils, both the water retention and particle-size distribution curves are available and the value of α can easily be calculated. Defining the normalized water content as $\theta_i^* = \theta_i/\theta_s$, a series of θ_i^* values was chosen at various intervals between zero and unity. Subsequently, for each soil a value α_i was calculated for each θ_i^* . The results, shown in Fig. 3.3.5-5, challenge the validity of a constant α . The values vary not only as a function of soil type, but also as a function of water content. Neither at the wet nor at the dry end of the water retention curve is the average value for $\alpha = 1.38$ satisfied. From Eq. [3.3.5-8] we observe that the ratio R_i/D_i is proportional to a power function in n_i with an exponent of $(1 - \alpha)/2$. Hence, when calculating R_i , the uncertainty in α is amplified by a factor of $\ln(n_i)/2$. As the number of particles (n_i) in the small size classes is fairly large (i.e., between 10^6 and 10^9 according to Table 2 of Arya & Paris, 1982) the predicted matric head values at the dry end of the water reten-

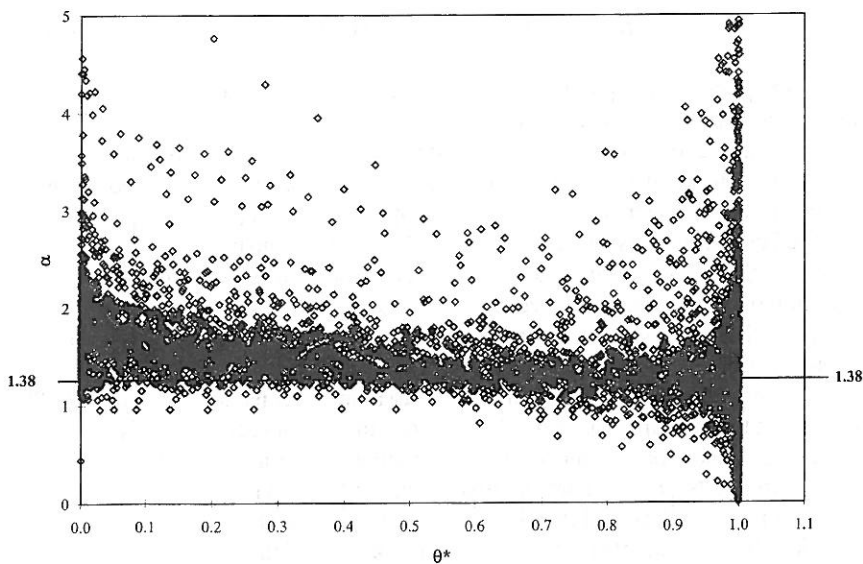


Fig. 3.3.5-5. Evaluation of the tortuosity parameter α of the Arya and Paris (1981) model as a function of θ_i/θ_s calculated for more than 1000 different soils of the UNSODA soil database (Leij et al., 1996) and the GRIZZLY soil database (Haverkamp et al., 1998).

Table 3.3.5-1. Regression parameters according to Eq. [3.3.5-31]; taken from Arya et al. (1999).

Textural class	a_1	a_2
Sand	-1.415	0.489
Sandy loam	-2.353	0.773
Loam	-0.644	0.395
Silt loam	-1.425	0.353
Clay	-1.559	0.305

tion curve are highly sensitive to the precision in α . This explains the important discrepancies between the calculated and the constant α values observed at the dry end (Fig. 3.3.5-5). At the very wet end of the water retention curve, the number of particles (n_i) is small (i.e., $n_i \leq 5$ according to Table 2 of Arya & Paris, 1982) and the erratic behavior of α (Fig. 3.3.5-5) is probably the result of an overestimation of the water content scale parameter.

Prompted by different studies on a nonconstant α value (e.g., Schuh et al, 1988; Mishra et al. 1989), Arya et al. (1999) have recently proposed an empirical method that allows the estimation of the tortuosity parameter α_i as a function of the number of soil particles (n_i) and, hence, as a function of water content (θ_i). The method uses the principle of shape similarity and was developed by the use of "real" soil data taken from the UNSODA database (Leij et al., 1996). For five different soil textural classes, namely, sand, sandy loam, loam, silt loam, and clay (USDA Soil Survey Laboratory Staff, 1992), about five soils were selected for which the linear relationships between $\log(W_i/D_i^3)$ and $\log(N_i)$ have been explored (where N_i is the "real" number of soil particles calculated from the UNSODA water retention data). Arya et al. (1999) established the following regression equation:

$$\alpha_i = 1 + \{[a_1 + a_2 \log(W_i/D_i^3)]/\log(n_i)\} \quad [3.3.5-31]$$

where the parameters a_1 and a_2 are empirical regression parameters with different values for different soil textural classes (Table 3.3.5-1).

For the sake of consistency, we tested the improvement of the new formulation of α on the same soil population as used before for Fig. 3.3.5-5. For each soil and each water content value (θ_i^*), the ratio of the predicted ($(\alpha_i)_{\text{pred}}$ (Eq. [3.3.5-31]) and the best-fit ($(\alpha_i)_{\text{fit}}$) is calculated (Fig. 3.3.5-6). Obviously, when the prediction is perfect the α ratio should be equal to unity. The results show that the new formulation of α systematically overestimates the best-fit α value with roughly 25 to 75%, which is not a serious improvement with respect to the initial definition with a constant α (Fig. 3.3.5-5). However, for each particular soil textural class the scatter between the predicted and calculated α values is considerably reduced. This shows that the principles used for the new formulation of α are basically sound, but that the regression parameters a_1 and a_2 , calculated over a small soil population of roughly five soils, are not representative for the soils taken from the UNSODA database (Leij et al., 1996) and the GRIZZLY soil database (Haverkamp et al., 1998). It evokes the unavoidable problem of transportability of statistically determined regression parameters. For those soils that give values of the α ratio clearly situated outside the bands, that is, $(\alpha_i)_{\text{pred}}/(\alpha_i)_{\text{fit}} > 2$) established for the five soil textural classes (Fig. 3.3.5-6), the quality of soil data may be questioned. Apart from the

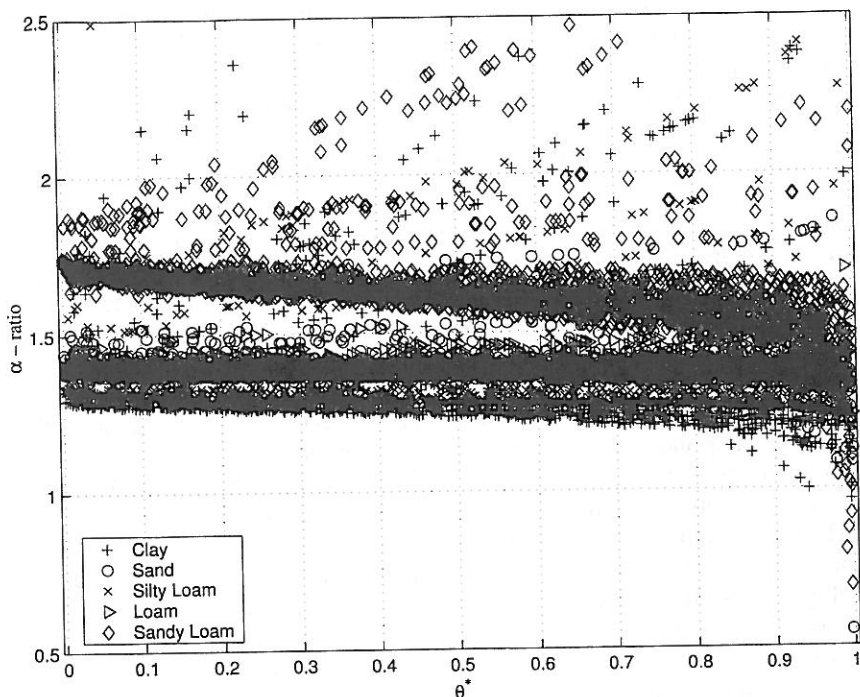


Fig. 3.3.5-6. Evaluation of the predicted $(\alpha_r)_{\text{pred}}$ and the best-fit $(\alpha_r)_{\text{fit}}$ ratio as a function of θ/θ_s calculated for more than 1000 different soils of the UNSODA soil database (Leij et al., 1996) and the GRIZZLY soil database (Haverkamp et al., 1998).

fact that measured water retention curves are most probably affected by measurement errors, they are also quite often influenced by hysteresis effects that are not always recognized as such (Haverkamp et al., 2002).

This brings us to the third difficulty of the Arya-Paris model: the problem of hysteresis. As the cumulative particle-size distribution is unique for a given soil, only one associated water retention curve can be predicted, either the main wetting curve or the main drying curve. To pass from one main curve to the other and/or along scanning curves, the water retention prediction model should theoretically be coupled with a hysteresis model that does not require any supplementary information. Although the discrete equations used by the Arya-Paris model were not formulated to facilitate such coupling, it is feasible to do so. Moreover, it would impose the use of an α value (constant or variable) calibrated on the correct water retention data.

The last remark concerns a slightly more vicious problem related to the non-linear relationship between pore radius and particle size (Eq. [3.3.5-8]). When considering a natural soil sample, we define the total pore volume (L^3) of the sample by V_{p_t} and the total solid particle volume by V_{s_t} (L^3). Both volumes are related by the apparent porosity ($\tilde{\epsilon}$) introduced above:

$$V_{p_t}/V_{s_t} = \tilde{\epsilon}/(1 - \tilde{\epsilon}) \quad [3.3.5-32]$$

When expressing the partial porosity (ϵ_i) for each particular mean pore radius (R_i) and associated particle diameter (D_i), its value is obviously variable and different from the apparent porosity. Using the hypothesis of Arya and Paris (1981), which considers the partial porosity constant over the soil sample (i.e., $\epsilon_i = \tilde{\epsilon}$), we have:

$$dV_p/dV_s = V_{p_i}/V_{s_i} = \tilde{\epsilon}/(1 - \tilde{\epsilon}) = \tilde{\epsilon} \quad [3.3.5-33]$$

where dV_p is the pore volume (L^3) assigned to pores having a radius between R and $R + dR$, and dV_s is the solid particle volume (L^3) assigned to particles having an associated particle diameter between D and $D + dD$. The direct consequence of the constant partial porosity hypothesis (Eq. [3.3.5-33]) is that the relative pore fraction (dV_p/V_{p_i}) and the relative particle fraction (dV_s/V_{s_i}) are equal. Hence, the cumulative pore fraction can be set equal to the cumulative distribution of particle weight (F), such as assumed by the prediction models of both Arya and Paris (1981) and Haverkamp and Parlange (1986). However, the validity of Eq. [3.3.5-33] is also conditioned by the relation $R(D)$. The identity of Eq. [3.3.5-33] is only justified when R is directly proportional to D such as suggested by Eq. [3.3.5-16] and used in the Haverkamp–Parlange model. On the contrary, when the relation $R(D)$ is not linear (e.g., a power function such as used by the Arya–Paris model) the postulate of Eq. [3.3.5-33] becomes erroneous; that is, $dV_p/V_{p_i} \neq dV_s/V_{s_i}$ and the partial porosity (ϵ_i) may not be set constant any more. In spite of this compatibility problem, the Arya–Paris model uses the hypothesis of constant partial porosity together with a non linear $R(D)$ relationship.

The Haverkamp–Parlange Model. The first comment made regarding the Arya–Paris model also applies to the Haverkamp–Parlange model; the matric head scale parameter is not corrected for trapped air.

The second drawback of the model is the use of a linear $R(D)$ relationship. As shown above, this hypothesis leads to the unrealistic condition of shape identity (instead of shape similarity) between the cumulative particle-size distribution function and the water retention curve. Even though the authors have overcome this problem by introducing, a posteriori, a regression equation relating both the shape indicators of $F(D)$ and $h_m(\theta_{mw})$ as a function of dry bulk density (Eq. [3.3.5-23]), they compromised, by doing so, on the consistency criterion and introduced empiricism. The direct consequence of choosing a linear relationship between R and D is that the model can only be applied to pure sands, which covers a very limited range of field soils. The parameter γ , used to equate R as a function of D , is comparable to α of the Arya–Paris (1981) model. The γ value is considered constant for a given soil and is calculated empirically (Eq. [3.3.5-24]). Even though it was shown for the Arya–Paris model that these assumptions led to serious errors in the prediction of the α parameter, the problem is less crucial for the Haverkamp–Parlange model, as it is only applicable to pure sand soils.

The definite positive aspect of the Haverkamp–Parlange (1986) model is the fact that the authors coupled the water retention prediction model with a hysteresis model. Unfortunately, the hysteresis concept obliged the authors to choose different type-equations for $F(D)$ and $h_m(\theta_{mw})$, which, together with the postulate on a linear $R(D)$ relationship, made it impossible to take full advantage of the shape

similarity hypothesis. To overcome the problem the authors had to introduce empiricism (see remark above), which to some extent compromised the advantage of using the coupled hysteresis model. Moreover, the introduction of the hysteresis concept complicated the model description, hence making it more difficult to follow and less user-friendly.

In conclusion, in spite of the progress made with these prediction models and in our understanding of the complexity of pore structures, there is still a need for a physically based hysteresis-coupled prediction model that allows for an accurate estimation of the soil characteristic shape and scale parameters without empirical calibration. This need is particularly great in modeling vadose zone transfer processes at large scales. However, one should not overlook the danger inherent in such types of models. Owing to their simplicity, one may believe that they closely approximate reality, the "actual" pore structure. In fact, nothing could be farther from the truth.

3.3.5.2 Property Transfer from Particle and Aggregate Size to Water Retention

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3.3.5.2.a Principles

As discussed in the previous section, it is frequently desirable to predict soil water retention from more easily measured properties. This section addresses the situation where the available measured data include particle-size distributions, but where this alone does not lead to an adequate prediction. For many soils, macropores and other structural features significantly influence the hydraulic properties. Thus, water retention curves may not be well predicted on the basis of particle-size distributions alone. A model with assumptions that relate the aggregate-size distribution to these features and their effect on retention can produce better predictions. The model of Nimmo (1997) considers the volumetric water content (θ) as the sum of two components, one textural (θ_t) and the other structural (θ_s):

$$\theta(\psi) = \theta_t(\psi) + \theta_s(\psi) \quad [3.3.5-34]$$

where ψ is the pressure potential (Pa). The porosity (ϕ) is similarly divided into components for texture and structure:

$$\phi = \phi_t + \phi_s \quad [3.3.5-35]$$

Figure 3.3.5-7 shows an example of this partitioning. To estimate $\theta_t(\psi)$, the Arya-Paris (1981) model can be applied using particle-size distribution (Section 3.3.5.1), but with an assumed value of ϕ_t instead of ϕ . For the texture-based porosity, ϕ , the value 0.3 is used for all media (Nimmo, 1997). This value is chosen because it is the approximate porosity for a wide range of media with a nearly random structure. The estimation of $\theta_s(\psi)$ requires additional data. Gupta and Ewing (1992) and Rieu and Sposito (1991a) have used aggregate data for similar reten-

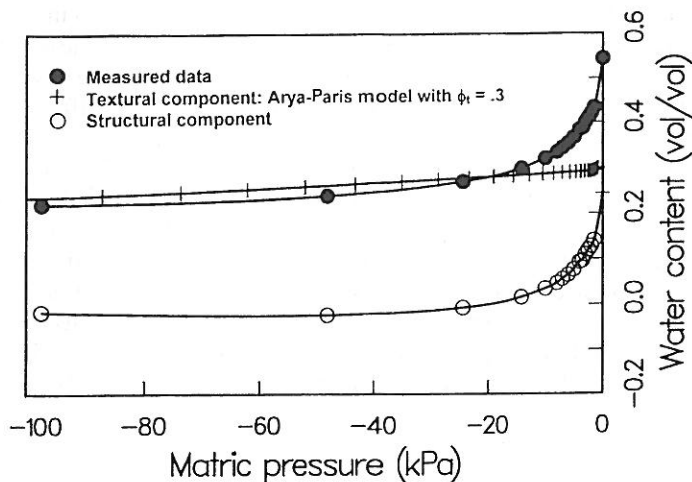


Fig. 3.3.5-7. Separation of a retention curve into textural and structural components as illustrated for a core sample with a silt loam structure.

tion predictions. Soil aggregates can be related to large pores that contribute to ϕ_s and $\theta_s(\psi)$. In effect, this is like a texture-based model that is based on aggregate sizes rather than particle sizes.

To predict $\theta_s(\psi)$ from a size distribution, it is necessary to relate aggregate size to pore size, and to relate pore size to pore opening or effective capillary radius. Relating aggregate size to pore size can be done analogously to the capillary theory relation of particle size to pore size for a randomly structured medium, and modified for the distinctive features of interaggregate as opposed to intraaggregate pores. Each interaggregate pore is taken to have a volume proportional to an aggregate volume so the volumes scale as

$$v_{\text{pore}}/v_{\text{agg}} = \phi_s/(1 - \phi_s) = \eta_s \quad [3.3.5-36]$$

where η_s is the structural void ratio. If both v_{pore} and v_{agg} vary as the cube of the effective radii of the pore and grain, then

$$r_{\text{pore}}/r_{\text{agg}} = \eta_s^{1/3} \quad [3.3.5-37]$$

Capillary theory relates the size of the pore opening r to the matric pressure at which the pore drains:

$$r = -(C/\psi) \quad [3.3.5-38]$$

where C equals about 0.13 mm kPa^{-1} for small contact angles and a surface tension 10% less than that of pure water.

In general the pore opening is smaller than the main body of the pore, which is represented in the model by a factor β (> 1), which equals the ratio of pore body

radius/pore opening radius for pores defined by adjacent basic particles, not aggregates. Typically, β would have a value of 2 or more (Nimmo, 1997). For a randomly structured medium a value of 2.2 is reasonable, and the model assumes this value for intraaggregate pores.

Aggregates generally fit together better than individual particles because they form in situ and also because they are more malleable. The model accounts for this with the additional assumption that the lognormal standard deviation (σ) of the aggregate-size distribution can serve as an index of the orderliness of the medium, indicative of the width (per unit length) of interaggregate pores. Defined in terms of logarithms, σ ranges from 0 to 1. A value of 0 corresponds to perfectly tight aggregates and 1 to a degree of looseness implying randomly structured media. This is algebraically incorporated into the model by taking the ratio of pore/aggregate radius equal to a factor of σ times $\eta_s^{1/3}$, as opposed to equating it directly to $\eta_s^{1/3}$, as in Eq. [3.3.5–37]. Combining these assumptions with Eq. [3.3.5–38] gives a relation of aggregate size to the value of ψ on a drying curve:

$$r_{\text{agg}}(\psi) = -(C\beta)/(\sigma\eta_s^{1/3}\psi) \quad [3.3.5-39]$$

The model uses a fit of Gardner's (1956) lognormal distribution to the aggregate-size distribution:

$$f(\log r_{\text{agg}}) = \frac{1}{\sqrt{2\pi}\log\sigma} \exp \left[\frac{-(\log r_{\text{agg}} - \log r_m)^2}{2(\log\sigma)^2} \right] \quad [3.3.5-40]$$

where f is the relative frequency of occurrence and r_m is the geometric mean radius. The lognormal standard deviation σ , which is used in Eq. [3.3.5–39] and elsewhere, is determined in this lognormal fitting procedure. Incorporating the fit of Eq. [3.3.5–40] and using the normalization described by Nimmo (1997), the model's basic formula is

$$\theta_s(\psi) = \frac{\phi_s}{\sqrt{2\pi}\log\sigma} \int_{-\infty}^{\log r_{\text{agg}}} \exp \left[\frac{-(\log r_{\text{agg}} - \log r_m)^2}{2(\log\sigma)^2} \right] d \log r_{\text{agg}} \quad [3.3.5-41]$$

The modeled $\theta_s(\psi)$ thus has the form of a lognormal distribution, as has been used in other models of soil water retention, for example by Kosugi (1994) and Kosugi and Hopmans (1998). Nimmo (1997) gives additional details of the model's derivation.

An alternative model, similarly based on dual-porosity concepts, and for some media predicting water retention about equally well, uses the Arya-Paris model applied to the aggregate-size distribution (with porosity ϕ_s) as well as to the particle-size distribution (Nimmo, 1997). This is very similar to the Gupta-Ewing (1992) model, but it uses the assumed ϕ_t value to partition the pore space and, therefore, does not require aggregate density data. It may produce essentially the same results, but with the advantage of a lesser data requirement, which widens the available possibilities for testing and application.

3.3.5.2.b Procedure

For the case of most interest, in which no retention data are available, required inputs to the model are the measured porosity (Section 2.3), particle-size distribution (Section 2.3), and aggregate-size distribution (Section 2.6). Steps involved are:

1. Apply the Arya–Paris model to the particle-size data, with porosity equaling the textural porosity of 0.3 and the Arya–Paris α parameter equaling 1.37. The follow-up comment of Arya and Paris (1982) may be helpful in setting up the calculations.
2. Fit the lognormal distribution to the aggregate-size data to obtain values of the parameters r_m and σ . Commercial software packages for statistical applications usually can do this easily. Alternatively, the graphical method used by Gardner (1956) is adequate and practical when data are few.
3. Compute $\theta_s(\psi)$ using Eq. [3.3.5–41] and [3.3.5–39], with ϕ_s taken as 0.3 less than the measured ϕ . Equation [3.3.5–39] converts from r_{agg} on the right side of Eq. [3.3.5–41] to ψ on the left side.
4. Add $\theta_t(\psi)$ and $\theta_s(\psi)$ to predict $\theta(\psi)$.

3.3.5.2.c Comments

Testing this model with data from two sources (Shakofsky, 1995; data of Bousnina cited by Rieu & Spósito, 1991b), Nimmo (1997) found it to fit measured retention data much better than does the texture-based Arya–Paris model alone. For soils that tend to be weakly aggregated and randomly structured, this model is less appropriate, but these are the sorts of media whose water retention relation can often be reasonably predicted with a texture-based model like the Arya–Paris model. For soils with significant aggregation, the texture-based models often give poor predictions, in large part because the greater presence of very fine (e.g., clay) particles promotes aggregation and the formation of large pores, whereas the texture-based models generally assume that the very fine particles are associated only with small pores. Thus, for soils in which the structure is far from random, it is likely to be worthwhile to do the measurements of aggregate size and apply a model that considers both texture and structure, for a better representation of $\theta(\psi)$.

A potential concern arises from the fact that the measurement of aggregate-size distribution is not well standardized and the data are generally less reliable than for particle-size measurement. In terms of effect on the actual form of the predicted retention curve, the model is less sensitive to the values of r_m and σ than to other input values.

For use with wetting rather than drying curves, this model must be modified or supplemented. A wetting curve might be generated by letting β equal 1 instead of 2.2 (Nimmo, 1997). Alternatively, it could be predicted using a separate hysteresis model, though most such models would require additional types of data.

Improvements in fit are likely to be possible by adjusting the values 0.3 and 2.2 used for ϕ_t and β . Although the model may have a nonnegligible sensitivity to these parameters, these designated values have a physical interpretation that makes them reasonable choices for a large number of soils, and there is a practical advantage in not having to optimize them when the model is applied.

3.3.5.3 References

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