

### 3.3.4 Parametric Models

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#### 3.3.4.1 Introduction

Characterization of soils and the vadose zone includes the estimation of the soil water retention and unsaturated hydraulic conductivity relations for a wide range of volumetric water content values. Although occasionally only specific data points are needed, parametric models for both hydraulic properties are preferred. The demand for these expressions is driven by their use in numerical models for simulating fluid flow and mass transport. These models do not necessarily require simple parametric expressions, but can instead use tables of values or spline functions. However, the parametric models are generally well behaved for interpolation purposes and cause fewer numerical problems. The increasing availability of simulation models, their increasing ease of use, and their ability to accurately predict flow and transport has created a need for parametric expressions that describe hydraulic relations for both near-surface soils and deep vadose zones.

Typically, the soils to be characterized exhibit large variations in space and occasionally in time as well. Consequently, techniques need to be developed that allow a physical description of these variations with the least amount of effort. Although scaling techniques are useful in this respect, they generally require parametric models of the soil hydraulic properties. Also, indirect estimation techniques are becoming increasingly popular, so that parameters of soil hydraulic functions can be estimated from other, easier to measure soil physical properties such as particle-size distributions and soil structural characteristics. Alternatively, functional descriptors of water flow and transport can be derived from the parameters of soil hydraulic functions, such as in the use of pedotransfer functions to define land or soil quality indicators. A comprehensive evaluation of indirect estimation techniques is presented in van Genuchten et al. (1992).

The soil water retention function relates the energy state of the soil water to its water content. If the soil pores are represented by an equivalent bundle of capillaries, with identical retention properties as the real soil, a retention function provides the soil's pore-size distribution from which the unsaturated hydraulic conductivity function can be predicted.

We will present the most commonly used parametric models that are available to fit soil water retention data. The function-of-choice depends on soil type,

application, and personal preference. That is not to say that the accuracy of the retention function is not important. On the contrary, deviations between the assumed and true water retention functions are especially critical near saturation and at the dry end of the curve. Moreover, the accuracy of the predictive unsaturated hydraulic conductivity equations is controlled by the adequacy of the soil water retention model over the water content range of interest (van Genuchten & Nielsen, 1985).

In this section we will also briefly introduce the theory of hydraulic conductivity predictions and present the unsaturated hydraulic conductivity models associated with the various soil water retention models. The coupling of soil water retention with unsaturated hydraulic conductivity functions is especially attractive, since it reduces the number of hydraulic function parameters. If the soil is composed of more than one pore-size distribution system, multimodal retention functions can be defined. These will be presented as well, including their incorporation into hydraulic conductivity functions. Finally, we will give a short overview of hysteresis models and their implementation.

### 3.3.4.2 General Characteristics of Water Retention Curves and Important Parameters

We will assume that water and air are the only wetting and nonwetting fluid, respectively, present in the soil. Hence, the notation will pertain to air–water systems only, and might be different for other multi-fluid soil systems, which are described in Chapter 7. We will further assume that the soil is rigid and homogeneous. A schematic representation of a typical soil water retention curve is presented in Fig. 3.3.4–1. By definition, the volumetric water content,  $\theta$ , is equal to the saturated water content,  $\theta_s$ , when the soil matric head,  $h_m$ , is equal to zero. However, only under specific circumstances will the saturated water content be equal to the porosity,  $\phi$ . Due to entrapped air, it generally can be determined that  $\theta_s \approx 0.85 - 0.9\phi$ .

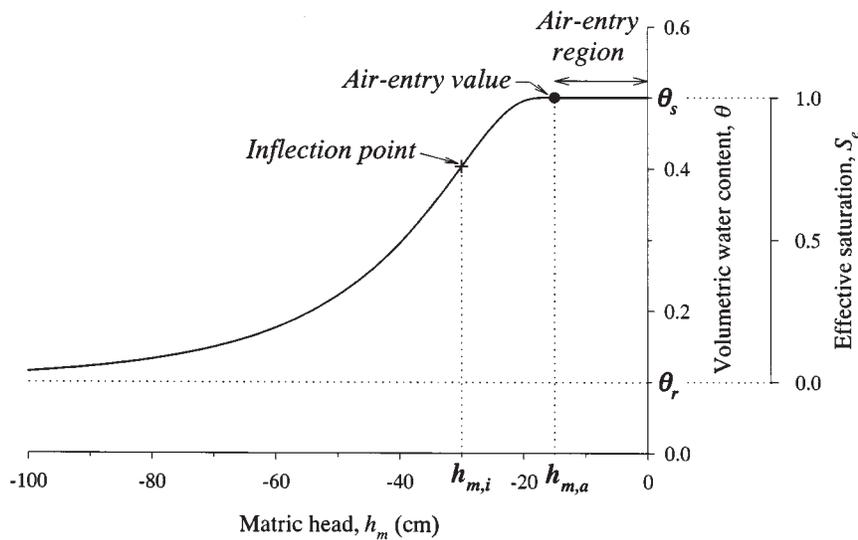


Fig. 3.3.4–1. Schematic of a typical soil water retention curve with definitions of parameters.

For many soils, the value of  $\theta$  will remain at  $\theta_s$  for values of  $h_m$  slightly less than zero. The value of  $h_m$  at which the soil starts to desaturate is defined as the air-entry value,  $h_{m,a}$ . It is assumed to be inversely proportional to the maximum pore size forming a continuous network of flow paths within the soil. As  $h_m$  decreases below  $h_{m,a}$ ,  $\theta$  usually decreases according to a S-shaped curve with an inflection point. In Fig. 3.3.4-1, the matric head at the inflection point is denoted by  $h_{m,i}$ . As  $h_m$  decreases further,  $\theta$  decreases seemingly asymptotically towards a soil-specific minimum water content known as the *residual water content*,  $\theta_r$ . The reason for the finite value of  $\theta_r$  is that the preponderance of historical water content measurements were in the wet range and the typical soil water retention models assumed asymptotic behavior at low water content values. As a result, most retention models describe retention curves in the range of  $\theta_r \leq \theta \leq \theta_s$ . It is convenient to define an effective saturation

$$S_e = (\theta - \theta_r) / (\theta_s - \theta_r) \quad [3.3.4-1]$$

which varies between zero and one. It should be noted that the nature of  $\theta_r$  is still controversial since the water content theoretically goes to zero as  $h_m$  becomes infinitely negative. In practice,  $\theta_r$  is treated as a fitting parameter. Additional comments on  $\theta_r$  can be found in Section 3.3.2.

In addition to the four parameters  $h_{m,a}$ ,  $h_{m,i}$ ,  $\theta_s$ , and  $\theta_r$ , most retention models include a dimensionless parameter, which characterizes the width of the soil pore-size distribution. Many functions have been proposed to relate matric head to volumetric water content. Most of these functional relationships are empirical in nature, but might include parameters that have a physical basis. The following sections include the most widely used expressions.

### 3.3.4.3 Brooks and Corey Type Power Function

Among the earlier models proposed is the Brooks and Corey (1964) water retention model, which expresses the effective saturation,  $S_e$ , as a power function of  $h_m$

$$\begin{aligned} S_e &= (h_{m,a}/h_m)^\lambda && \text{for } h_m < h_{m,a} \\ S_e &= 1 && \text{for } h_m \geq h_{m,a} \end{aligned} \quad [3.3.4-2]$$

As defined above, the parameter  $h_{m,a}$  is the air-entry head value (Fig. 3.3.4-1). The dimensionless parameter  $\lambda$  characterizes the pore-size distribution, and is referred to as the *pore-size distribution index* (Brooks & Corey, 1964). Theoretically, its value approaches infinity for a medium with a uniform pore-size distribution, whereas it approaches a lower limit of zero for soils with a wide range of pore sizes. Usually,  $\lambda$  values are in the range between 0.3 and 10.0. Assuming that soil pore structure satisfies the general fractal geometry conditions, Tyler and Wheatcraft (1990) showed that  $\lambda$  can be determined from the fractal dimension of soil texture. Approximate values of both  $h_{m,a}$  and  $\lambda$  can be obtained by plotting  $\log(S_e)$  vs.  $\log(-h_m)$ . The absolute value of the slope of the resulting straight line is equal to the value of

$\lambda$  and the air-entry value is determined from the intercept. However, a more straightforward estimation of the parameters can be achieved by model fitting (Section 3.3.4.11). Since Eq. [3.3.4-2] does not include an inflection point, but instead identifies a distinct air-entry value, the Brooks and Corey expression usually shows excellent agreement with experimental data for soils with well-defined air-entry values and J-shaped retention curves (Fig. 3.3.4-2a). However, as van Genuchten and Nielsen (1985) and Milly (1987) pointed out, the model may give relatively poor fits for soils with S-shaped retention data (Fig. 3.3.4-2b), such as finer-textured soils and undisturbed field soils.

The retention model used by Campbell (1974) is identical to the power function of Brooks and Corey (Eq. [3.3.4-2]). However, the dependent variable is defined as the degree of saturation, that is,  $\theta/\theta_s$ , instead of effective saturation

$$\begin{aligned} \theta/\theta_s &= (h_{m,a}/h_m)^\lambda && \text{for } h_m < h_{m,a} \\ \theta/\theta_s &= 1 && \text{for } h_m \geq h_{m,a} \end{aligned} \quad [3.3.4-3]$$

### 3.3.4.4 van Genuchten Type Power Function

Brutsaert (1966) proposed the following power function model, which describes an S-shaped retention curve

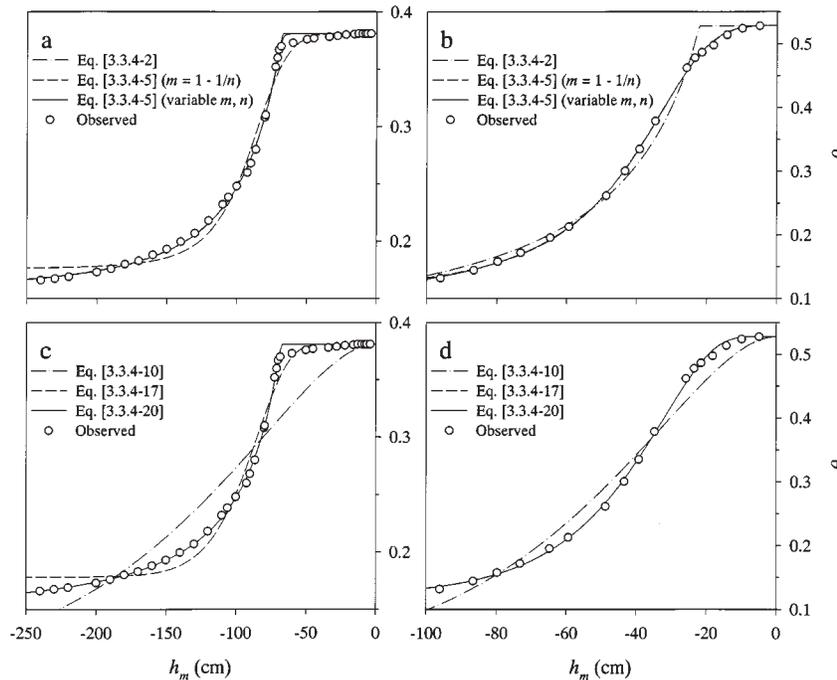


Fig. 3.3.4-2. (a, c) Observed and fitted retention curves for a Rubicon sandy loam, and (b, d) a Touchet silt loam. The observed data were taken from the soil catalog of Mualem (1976b). The saturated water content values,  $\theta_s$ , were fixed as listed in the Mualem catalog.

Table 3.3.4-1. Average values of the parameters in the van Genuchten retention model (Eq. [3.3.4-5] with  $m = 1 - 1/n$ ) and the saturated hydraulic conductivity,  $K_s$ , for soil textural groups according to the USDA classification scheme as estimated by Carsel and Parrish (1988).

Texture	$\theta_s$	$\theta_r$	$\alpha$	$n$	$K_s$
	cm <sup>-1</sup>				cm d <sup>-1</sup>
Sand	0.43	0.045	0.145	2.68	712.8
Loamy sand	0.41	0.057	0.124	2.28	350.2
Sandy loam	0.41	0.065	0.075	1.89	106.1
Loam	0.43	0.078	0.036	1.56	24.96
Silt	0.46	0.034	0.016	1.37	6.00
Silt loam	0.45	0.067	0.020	1.41	10.80
Sandy clay loam	0.39	0.100	0.059	1.48	31.44
Clay loam	0.41	0.095	0.019	1.31	6.24
Silty clay loam	0.43	0.089	0.010	1.23	1.68
Sandy clay	0.38	0.100	0.027	1.23	2.88
Silty clay	0.36	0.070	0.005	1.09	0.48
Clay	0.38	0.068	0.008	1.09	4.80

$$S_e = a/[a + (-h_m)]^b \quad [3.3.4-4]$$

where  $a$  and  $b$  are fitting parameters, which can either be determined from moment analysis (Brutsaert, 1966) or by model fitting (Section 3.3.4.11). The retention model suggested by Ahuja and Swartzendruber (1972) has the same functional form as Eq. [3.3.4-4], whereas Haverkamp et al. (1977) used Eq. [3.3.4-4] to test various numerical algorithms for the solution of one-dimensional infiltration.

A more general version of Eq. [3.3.4-4] was suggested by van Genuchten (1978, 1980) and is currently among the most commonly used soil water retention models

$$S_e = [1 + (-\alpha h_m)^n]^{-m} \quad [3.3.4-5]$$

where  $\alpha$  (L<sup>-1</sup>) is a parameter ( $\alpha > 0$ ) to scale the matric head, and both  $n$  and  $m$  are dimensionless parameters. The  $n$  value is generally restricted to values larger than one, so that the slope of the soil water retention curve,  $d\theta/dh_m$ , is zero as the water content approaches the saturated water content (van Genuchten & Nielsen, 1985). If  $m$  is fixed at a value 1, the model reduces to Eq. [3.3.4-4] where  $a = \alpha^{-n}$  and  $b = n$ .

Instead of using a constant  $m$  value, van Genuchten (1980) proposed the relationship of  $m = 1 - 1/n$  ( $n > 1$ ,  $0 < m < 1$ ). Using this relationship, Eq. [3.3.4-5] does not account for an air-entry value, but does include an inflection point, allowing this model to perform better than the Brooks and Corey type model for soils with S-shaped retention curves as is shown in Fig. 3.3.4-2b. However, the model cannot accurately describe retention characteristics for soils with distinct air-entry regions (Fig. 3.3.4-2a). Table 3.3.4-1 summarizes approximate parameter values for typical soil textural groups as estimated by Carsel and Parrish (1988). Although van Genuchten (1978) provides various graphical and analytical procedures to estimate  $\alpha$  and  $m$ , routinely parameters are obtained using fitting algorithms such as RETC (van Genuchten et al., 1991) and UNSODA (Leij et al., 1996).

Whereas the parameter  $\alpha$  is related to the inverse of the air-entry value (van Genuchten, 1980), the strict definition of this parameter is unclear. Assuming  $m = 1 - 1/n$ , van Genuchten (1978) differentiated Eq. [3.3.4–5] twice with respect to  $h_m$  to obtain the matric head at the inflection point ( $h_{m,i}$ ):

$$h_{m,i} = m^{1-m}/\alpha \quad [3.3.4-6]$$

Inverting this equation with respect to  $\alpha$  and substituting the result into Eq. [3.3.4–5], yields an alternative equivalent expression for the soil water retention curve (Kosugi, 1994):

$$S_e = [1 + m(h_m/h_{m,i})^n]^{-m} \quad [3.3.4-7]$$

where  $m = 1 - 1/n$ .

Although van Genuchten (1980) includes special cases for  $m = 1 - 1/n$  ( $n > 1$ ,  $0 < m < 1$ ) and  $m = 1 - 2/n$  ( $n > 2$ ,  $0 < m < 1$ ), to derive hydraulic conductivity relations, the most general form of Eq. [3.3.4–5] includes the case for which  $m$  ( $m > 0$ ) is independent of  $n$ . Increasing the number of parameters from two to three (excluding  $\theta_s$  and  $\theta_r$ ), allows more flexibility in the fitting of soil water retention data. Van Genuchten and Nielsen (1985) demonstrated that Eq. [3.3.4–5] is almost equivalent to the Brooks and Corey model (Eq. [3.3.4–2]) if  $n$  is increased and  $m$  is simultaneously decreased so that the product  $mn$  remains constant. Under this condition, the values of  $mn$  and  $(-\alpha^{-1})$  of Eq. [3.3.4–5] correspond to  $\lambda$  and  $h_{m,a}$  of Eq. [3.3.4–2], respectively. Therefore, the case with  $m$  independent of  $n$  provides acceptable fits for soils with distinct air-entry values (Fig. 3.3.4–2a), whereas the model simultaneously retains its capability to fit sigmoidal-shaped retention curves as shown in Fig. 3.3.4–2b.

Two other three-parameter related models have been presented that allow the inclusion of an air-entry value, while maintaining the general form of Eq. [3.3.4–5]. First, Vogel and Císlerová (1988) modified Eq. [3.3.4–5] to allow for a non-zero  $h_{m,a}$  value:

$$\begin{aligned} \theta &= \theta_r + (\theta_s' + \theta_r)[1 + (-\alpha h_m)^n]^{-m} & \text{for } h_m < h_{m,a} \\ \theta &= \theta_s & \text{for } h_m \geq h_{m,a} \end{aligned} \quad [3.3.4-8]$$

where  $m = 1 - 1/n$  ( $n > 1$ ), and  $\theta_s'$  ( $\theta_s' \geq \theta_s$ ) is a fitting parameter. The selected value of  $h_{m,a}$  will depend on values of the other parameters to ensure the continuity of the  $\theta$  value at  $h_m = h_{m,a}$ . The case of  $\theta_s' = \theta_s$  leads to  $h_{m,a} = 0$ , so that Eq. [3.3.4–8] is identical to Eq. [3.3.4–5]. The added flexibility of Eq. [3.3.4–8] is included in Šimnek et al. (1998) for the simulation of variably saturated water flow. Second, Kosugi (1994) modified Eq. [3.3.4–7] to include an air-entry head value as well, while maintaining the physical meaning of  $h_{m,i}$  as the matric head at the inflection point:

$$\begin{aligned} S_e &= \{1 + m[(h_{m,a} - h_m)/(h_{m,a} - h_{m,i})]^n\}^{-m} & \text{for } h_m < h_{m,a} \\ S_e &= 1 & \text{for } h_m \geq h_{m,a} \end{aligned} \quad [3.3.4-9]$$

where  $m = 1 - 1/n$  ( $n > 1$ ). Again, if  $h_{m,a} = 0$ , Eq. [3.3.4–9] reduces to Eq. [3.3.4–7], which is equivalent to Eq. [3.3.4–5].

### 3.3.4.5 Exponential Model

Tani (1982), Russo (1988), and Ross and Smettem (1993) proposed a soil water retention model, which reproduces Gardner's (1958) exponential function for unsaturated hydraulic conductivity when incorporated into Mualem's (1976a) conductivity model (Eq. [3.3.4–26]). The model can be written as

$$S_e = [1 + (h_m/h_{m,i})] \exp(-h_m/h_{m,i}) \quad [3.3.4-10]$$

Equation [3.3.4–10] provides reasonable plots for water retention curves by using a single parameter  $h_{m,i}$ , the matric head at the inflection point. However, the model is less accurate than the other two- or three-parameter models (Fig. 3.3.4–2c and 3.3.4–2d).

### 3.3.4.6 Lognormal Distribution Models

Whereas the retention models presented in Sections 3.3.4.3 through 3.3.4.5 are mostly empirical curve-fitting equations, the parameters of the lognormal distribution model are directly related to the statistical properties of the soil pore-size distribution. Gardner (1956) introduced the possibility of characterizing soil structure using a lognormal pore-size distribution. Based upon the fact that many soils show a lognormal particle-size distribution, Brutsaert (1966) proposed a similar approach. In the theory relating pore-size distributions to water retention functions, the valid water content range should be that for which capillary forces solely control soil water retention. In other words, the domain where adsorptive forces dominate ( $h_m$  values  $< -8.5$  m) is not strictly applicable. However, the theory is often extended to the whole range of  $h_m$  values in order to evaluate equivalent pore-size distributions and predict unsaturated hydraulic conductivity values. We will define a volumetric pore-size distribution function,  $g(r)$ , as

$$g(r) = d\theta/dr \quad [3.3.4-11]$$

where the dimension of  $g(r)$  is  $L^{-1}$ . In Eq. [3.3.4–11],  $g(r)dr = d\theta$  represents the contribution of pores with radii  $r \rightarrow r + dr$  to  $\theta$ . Therefore,  $g(r)dr$  is equal to the volume of pores with radii  $r \rightarrow r + dr$  per unit volume of soil. The contribution to the volumetric water content of the water-filled pores with a radius equal to or smaller than  $r_1$  can be computed by integrating Eq. [3.3.4–11], that is,

$$\theta = \int_0^{r_1} g(r)dr + \theta_r \quad [3.3.4-12]$$

When capillary forces operate, the relationship between  $r$  and  $h_m$  is defined by the capillary pressure function of Young and Laplace (Kutílek & Nielsen, 1994)

$$h_m = (-2\sigma_{aw} \cos\beta_c)/(\rho_w g r) = A/r \quad [3.3.4-13]$$

where  $\sigma_{aw}$  is the surface tension of water,  $\beta_c$  is the contact angle,  $\rho_w$  is the density of water,  $g$  denotes the gravitational acceleration, and  $A = -(2\sigma_{aw}\cos\beta_c)/(\rho_w g)$  is a negative constant with an approximate value of  $A = -1.49 \times 10^{-5} \text{ m}^2$  (e.g., Brutsaert, 1966). On the basis of this direct correspondence between  $r$  and  $h_m$ , the integration expressed as Eq. [3.3.4–12] gives the volumetric water content at  $h_m = h_{m,1}$

$$\theta = \int_{-\infty}^{h_{m,1}} g(r)(dr/dh_m)dh_m + \theta_r = \int_{-\infty}^{h_{m,1}} f(h_m)dh_m + \theta_r \quad [3.3.4-14]$$

where  $h_{m,1} = A/r_1$  and

$$f(h_m) = [g(r)dr]/dh_m = d\theta/dh_m \quad [3.3.4-15]$$

In Eq. [3.3.4–15],  $f(h_m)dh_m = d\theta$  represents the volume of pores filled with water, per unit volume of soil, corresponding to soil matric head values varying from  $h_m \rightarrow h_m + dh_m$ . Hence,  $f(h_m)$  can be regarded as the distribution function of the soil matric head. Evidently,  $f(h_m)$  is identical to the water capacity function,  $C$ , defined as the slope of the soil water retention curve. In summary, if the functional form of the volumetric pore-size distribution  $g(r)$  is known, the corresponding soil water retention function can be obtained by integration of Eq. [3.3.4–14].

More recently, Kosugi (1994, 1996) further developed this approach and derived a physically based soil water retention model assuming the pore radii to be lognormally distributed. Applying a lognormal distribution law, the volumetric pore-size distribution function as defined in Eq. [3.3.4–11], is expressed as

$$g(r) = \frac{\theta_s - \theta_r}{\sqrt{2\pi}\sigma r} \exp\left\{-\frac{[\ln(r/\tilde{r})]^2}{2\sigma^2}\right\} \quad [3.3.4-16]$$

where  $\tilde{r}$  is the median pore radius, and  $\sigma$  denotes the standard deviation of the log-transformed soil pore radius ( $\sigma > 0$ ), characterizing the width of the pore-size distribution. Substituting Eq. [3.3.4–16] into [3.3.4–14], while using Eq. [3.3.4–13], leads to the following expression for the soil water retention curve

$$S_e = Q\{[\ln(h_m/\tilde{h}_m)]/\sigma\} \quad [3.3.4-17]$$

where  $\tilde{h}_m$  is defined as the median matric head, that is,  $S_e(\tilde{h}_m) = 0.5$ , corresponding to the median pore radius  $\tilde{r}$  ( $\tilde{h}_m = A/\tilde{r}$  according to Eq. [3.3.4–13]), and  $Q$  denotes the complementary normal distribution function, or

$$Q(x) = [1/(2\pi)] \int_x^{\infty} \exp(-u^2/2) du \quad [3.3.4-18]$$

where  $u$  is a dummy variable. Since  $Q(x)$  can be related to the complementary error function,  $\text{erfc}$ , an alternative equivalent expression for Eq. [3.3.4–17] is

$$S_e = 1/2 \text{erfc}\{[\ln(h_m/\tilde{h}_m)]/2\sigma\} \quad [3.3.4-19]$$

Both Eq. [3.3.4–17] and [3.3.4–19] show that  $S_e$  approaches 1 as  $h_m$  goes to zero. It has been shown that retention data plotted by using Eq. [3.3.4–17] are similar to

those using Eq. [3.3.4–4] (Brutsaert, 1966; Pachepsky et al., 1992) or Eq. [3.3.4–5] with the restriction of  $m = 1 - 1/n$  (Kosugi, 1994, 1996). A comparison of the log-normal distribution model with the various power function models is presented in Fig. 3.3.4–2. Notably, Eq. [3.3.4–17] has difficulty fitting a J-shaped retention curve, as do all other power function models that do not include the air-entry value parameter. However, by including the air-entry head parameter ( $h_{m,a}$ ) in Eq. [3.3.4–17], an adequate description of such retention data is given by (Fig. 3.3.4–2c):

$$S_e = Q\{(1/\sigma)\ln[(h_{m,a} - h_m)/(h_{m,a} - \tilde{h}_m)]\} \quad \text{for } h_m < h_{m,a}$$

$$S_e = 1 \quad \text{for } h_m \geq h_{m,a} \quad [3.3.4-20]$$

### 3.3.4.7 Water Capacity Functions

To solve the unsaturated water flow or Richards equation, a priori knowledge of the water capacity function,  $C$ , is required. For any soil water retention model, the  $C$  function can be computed from the slope of the water retention curve:

$$C = f(h_m) = d\theta/dh_m = (\theta_s - \theta_r)(dS_e/dh_m) \quad [3.3.4-21]$$

In addition to the listed soil water retention models, Table 3.3.4–2 includes the corresponding water capacity functions as derived from Eq. [3.3.4–21].

### 3.3.4.8 Unsaturated Hydraulic Conductivity Functions

In contrast to soil water retention data, unsaturated hydraulic conductivity data are difficult to obtain. Direct measurement methods are presented in Chapter 3.6.1, whereas indirect methods are summarized in Section 3.6.2. Functional unsaturated hydraulic conductivity models, based on pore-size distribution, pore geometry, and connectivity, require integration of soil water retention models to obtain analytical expressions for the unsaturated hydraulic conductivity. The resulting expressions relate the relative hydraulic conductivity  $K_r$ , which is defined as the ratio of the unsaturated hydraulic conductivity  $K$  to the saturated hydraulic conductivity  $K_s$ , to the effective saturation by integrating the contributions of the individual pores according to Poiseuille's flow equation to yield a macroscopic hydraulic conductivity expression. Solutions require the definition of an effective pore radius distribution, validity of the capillary law (Eq. [3.3.4–13]), and incorporation of tortuosity and connectivity as they affect flow. Excellent reviews of independent developments, linking macroscopic flow to microscopic pore geometry using statistical models, were presented by Mualem and Dagan (1978) and Raats (1992). These reviews include the conductivity models of Childs and Collis-George (1950), Burdine (1953), and Mualem (1976a).

Specifically, Mualem and Dagan (1978) summarized Burdine's (1953) and Mualem's (1976a) models to develop a generalized unsaturated conductivity function, which can also be written as (Kosugi, 1999)

$$K_r = S_e^\gamma \left[ \frac{\int_0^{S_e} |h_m|^{-n} dS_e}{\int_0^1 |h_m|^{-n} dS_e} \right]^\gamma \quad [3.3.4-22]$$

Table 3.3.4-2. Commonly used retention models and corresponding water capacity functions,  $C$ , and relative hydraulic conductivity functions,  $K_r$ .

Retention model	Brooks and Corey (Eq. [3.3.4-2])	van Genuchten (Eq. [3.3.4-5])			Exponential (Eq. [3.3.4-10])	Lognormal distribution (Eq. [3.3.4-17])
		$m = 1 - 1/n$	$m = 1 - 2/n$	variable $m, n$		
$S_e$	$(h_{m,a}/h_m)^\lambda$ $h_m < h_{m,a}$ 1 $h_m \geq h_{m,a}$ $\lambda > 0$	$a > 0, n > 1$	$[1 + (-\alpha h_m)^n]^{-m}$ $a > 0, n > 2$	$a > 0, n > 1, m > 0$	$\left(1 + \frac{h_m}{h_{m,i}}\right) \exp\left(-\frac{h_m}{h_{m,i}}\right)$	$S_e = Q\left[\frac{\ln(h_m/\tilde{h}_m)}{\sigma}\right]$ $\sigma > 0$
$C$	$\frac{(\theta_s - \theta_r)\lambda}{-h_{m,a}} \left(\frac{h_{m,a}}{h_m}\right)^{1+\lambda}$ $h_m < h_{m,a}$ 0 $h_m \leq h_{m,a}$	$(\theta_s - \theta_r)mn\alpha(-\alpha h_m)^{n-1}[1 + (-\alpha h_m)^n]^{-m-1}$			$\frac{(\theta_s - \theta_r)(-h_m)}{h_{m,i}^2} \exp\left(-\frac{h_m}{h_{m,i}}\right)$	$\frac{\theta_s - \theta_r}{\sqrt{2\pi}\sigma(-h_m)} \exp\left\{-\frac{[\ln(h_m/\tilde{h}_m)]^2}{2\sigma^2}\right\}$
$K_r$ Burdine model (Eq. [3.3.4-22], $\eta = 2, \gamma = 1$ )	$S_e^{l+1+2/\lambda}$	unused	$S_e^l [1 - (1 - S_e^{1/m})^m]$	$\frac{S_e^l I_{S_e^{1/m}}[m + (2/n), 1 - (2/n)]}{n > 2}$	unused	$S_e^l Q[Q^{-1}(S_e) + 2\sigma]$
$K_r$ Mualem model (Eq. [3.3.4-22]) $\eta = 1, \gamma = 2$	$S_e^{l+2+2/\lambda}$	$S_e^l [1 - (1 - S_e^{1/m})^m]^2$	unused	$\frac{S_e^l \{I_{S_e^{1/m}}[m + (1/n), 1 - (1/n)]\}^2}{2}$	$S_e^l \exp(-2h_m/h_{m,i})$	$S_e^l \{Q[Q^{-1}(S_e) + \sigma]\}^2$
$K_r$ General model (Eq. [3.3.4-22])	$S_e^{l+\gamma+\eta/\lambda}$ $\eta > -\lambda$	$S_e^l \{I_{S_e^{1/m}}[m + (\eta/n), 1 - (\eta/n)]\}$ $-mn < \eta < n$			unused	$S_e^l \{Q[Q^{-1}(S_e) + \eta\sigma]\}^\gamma$

where  $l$  and  $\eta$  are parameters related to the tortuosity of the soil pores, and the value of the parameter  $\gamma$  is determined by the method of evaluating the effective pore radius (Raats, 1992). In the original models of Burdine (1953) and Mualem (1976a), the parameter set of  $(\eta, \gamma)$  is equal to (2, 1) and (1, 2), respectively. Table 3.3.4–2 summarizes the relative hydraulic conductivity functions,  $K_r(S_e)$ , obtained by substituting the listed retention models (Sections 3.3.4.3 through 3.3.4.6) into Eq. [3.3.4–22]. The corresponding  $K_r(h_m)$  functions can be derived by substituting the  $S_e(h_m)$  relationship in each of the listed  $K_r(S_e)$  expressions.

The tortuosity parameter,  $l$ , has been suggested to have a fixed value of 2 by Burdine (1953) or a fixed value of 0.5 by Mualem (1976a). Recent studies suggest that prediction errors based on either the Burdine (1953) or Mualem (1976a) model are partially the result of large variations in the tortuosity parameter  $l$  between soils. For example, Wösten and van Genuchten (1988) showed that  $l$  can vary between  $-16$  and  $>2$ , depending on soil type. They concluded that using a fixed  $l$  value resulted in unacceptable fits, especially for medium- and fine-textured soils. The  $l$  values determined by Schuh and Cline (1990) ranged from about  $-9$  to 15. Subsequent studies (Schaap et al., 1999; Kosugi, 1999) have shown that better  $K$  predictions can be achieved by using  $l$  values different from those proposed by Burdine (1953) or Mualem (1976a). Therefore,  $l$  is treated as a variable in Table 3.3.4–2.

Combining Eq. [3.3.4–5], using the relationship of  $m = 1 - 1/n$ , with Mualem's (1976a) integral model (Eq. [3.3.4–22], with  $\eta = 1$  and  $\gamma = 2$ ) produces the following closed-form equation for  $K_r$ :

$$K_r = S_e^l [1 - (1 - S_e^{1/m})^m]^2 \quad [3.3.4-23]$$

which is one of the most commonly used hydraulic conductivity functions. When the most general form of the van Genuchten retention model (Eq. [3.3.4–5], with  $m$  independent of  $n$ ) is combined with the generalized conductivity model as given by Eq. [3.3.4–22], the resulting  $K_r$  function can be written as (Raats, 1992)

$$K_r = S_e^l [I_{S_e^{1/m}}(m + \eta/n, 1 - \eta/n)]^\gamma \quad [3.3.4-24]$$

where  $I_x(p, q)$  is the incomplete beta function defined as

$$I_x(p, q) = [\int_0^x u^{p-1} (1-u)^{q-1} du] / [\int_0^1 u^{p-1} (1-u)^{q-1} du] \quad [3.3.4-25]$$

Combining the exponential model (Eq. [3.3.4–10]) with Mualem's (1976a) model yields

$$K_r = S_e^l \exp(-2h_m/h_{m,i}) \quad [3.3.4-26]$$

When selecting a tortuosity factor of  $l = 0$ , Eq. [3.3.4–26] becomes identical to Gardner's (1958) exponential model where  $\alpha_{\text{Gardner}} = -2/h_{m,i}$ . If the lognormal distribution model described by Eq. [3.3.4–17] is substituted into Mualem's (1976a) integral model, the derived function for  $K_r$  is (Kosugi, 1996)

$$K_r = S_e^l \{Q[Q^{-1}(S_e) + \sigma]\}^2 \quad [3.3.4-27]$$

where  $Q^{-1}$  denotes the inverse function of the complementary normal distribution function  $Q$ , representing a percentage point of the normal distribution. When Eq. [3.3.4–17] is combined with the generalized integral model (Eq. [3.3.4–22]), the  $K_r$  function becomes (Kosugi, 1999)

$$K_r = S_e^{1/\gamma} Q[Q^{-1}(S_e) + \eta\sigma]^\gamma \quad [3.3.4-28]$$

Additional analysis of Eq. [3.3.4–28] for conductivity fitting can be found in Kosugi (1999).

### 3.3.4.9 Multimodal Retention Functions

So far, it has been assumed that soils are unimodal, characterized by a single pore-size distribution function. However, undisturbed soils may occasionally exhibit retention curves with more than one inflection point. This multimodality of pore-size distribution may be the result of specific particle-size distributions or be due to the formation of secondary pore systems (macroporosity) by various soil genetic processes such as soil aggregation or biological soil forming (Durner, 1994). For these types of soils, the fitting of a single, sigmoidal retention curve model will be unsatisfactory. Othmer et al. (1991), Durner (1992, 1994), Ross and Smettem (1993), and Pachepsky et al. (1992) proposed to describe the retention function of these types of soils by a multi-model function

$$S_e = \sum_{i=1}^N w_i S_{e,i}(h_m) \quad [3.3.4-29]$$

where  $N$  is the number of pore systems from which the total pore-size distribution is determined, and  $w_i$  is the weighting factor for each pore system  $i$ , subjected to the constraint that  $0 < w_i < 1$  and  $\sum w_i = 1$ . Hence, for a bimodal soil system,  $N = 2$ . Any soil water retention model can be substituted into Eq. [3.3.4–29], provided it fits the soil water retention data. For example, Fig. 3.3.4–3 shows excellent results ob-

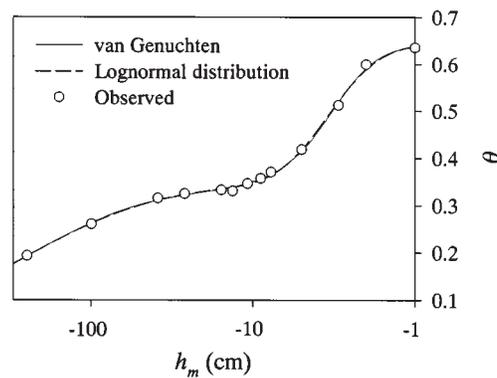


Fig. 3.3.4–3. Soil water retention data for a repacked, aggregated soil (Smettem & Kirkby, 1990), fitted to the bimodal retention model (Eq. [3.3.4–29]) with  $N = 2$ , using both the van Genuchten and lognormal distribution functions. The residual water content  $\theta_r$  was fixed at 0.

tained by fitting bimodal retention functions using both the van Genuchten model (Eq. [3.3.4–5]) and the lognormal distribution model (Eq. [3.3.4–17]) to data for an aggregated soil presented by Smettem and Kirkby (1990). The multimodal approach will obviously increase the number of fitting parameters, but will maintain the functional properties of each specific retention model. However, Durner (1994) cautions that unless the retention data are distinctly multimodal with little overlap of pore-size distributions, physically based parameters might lose their meaning and be considered curve-shape parameters only.

The more complex the form of the soil water retention function is, the less likely a relatively simple functional description of the unsaturated hydraulic conductivity can be derived. Hence, it will require numerical evaluation of Eq. [3.3.4–22]. Durner (1994) concluded that (i) the  $K$  prediction is extremely sensitive to an accurate description of the soil water retention curve, especially near saturation, and (ii) the specific mathematical form of the retention model has no influence on the conductivity prediction as long as it describes soil water retention data accurately.

### 3.3.4.10 Soil Water Hysteresis

Additional complications in the mathematical description of soil water retention curves are caused by hysteresis. As a result,  $\theta$  during drainage is larger than during wetting for the same  $h_m$  value; that is, the soil water retention curve is not unique and is affected by the saturation history. Hysteresis can be attributed to the ink-bottle effect, entrapped air, and the difference in contact angle between an advancing and a receding liquid front over a solid surface (Kutilek & Nielsen, 1994). For a typical hysteretic soil water retention curve (Fig. 3.3.4–4), all soil water retention data are enclosed within a main hysteresis loop, consisting of the main drying curve (MDC) and the main wetting curve (MWC). In this figure, the saturated water content,  $\theta_s$ , is less than the porosity,  $\phi$ , due to entrapped air. Wetting and dry-

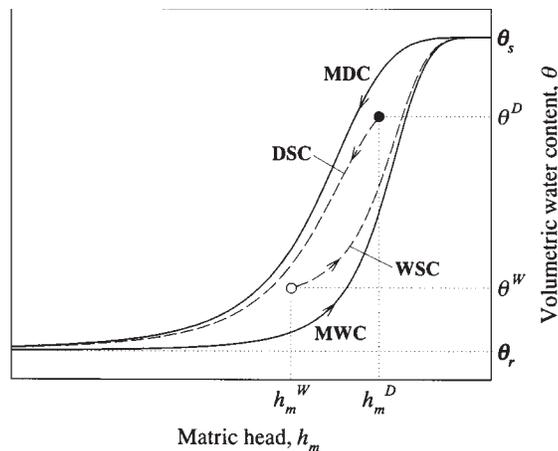


Fig. 3.3.4–4. Typical hysteretic soil water retention curves. MDC is the main drying curve, MWC is the main wetting curve, DSC is a drying scanning curve, and WSC is a wetting scanning curve.

ing cycles that do not initiate at the merger points of  $\theta_s$  and  $\theta_r$ , result in drying and wetting paths within the region enclosed by the main curves and are referred to as *drying scanning curves* (DSC) and *wetting scanning curves* (WSC). Generally, experimental data show that the  $K$ - $\theta$  relation is not affected by hysteresis (Mualem, 1986).

Independent as well as dependent domain models, both of which are independent of the functional relationships used to describe the soil water retention curves, have been developed to model  $\theta$ - $h_m$  hysteresis (e.g., Poulouvasilis, 1962; Philip, 1964; Mualem, 1973, 1974; Mualem & Dagan, 1975; Poulouvasilis & El-Ghamry, 1978). Although the domain models are physically based and the most accurate in predicting scanning curves, their implementation into numerical models of soil water flow is complex, thereby prohibiting their use. More recently, empirical hysteresis models, based on assumptions introduced by Scott et al. (1983), have become more widely used (Kool & Parker, 1987; Parker & Lenhard, 1987; Luckner et al., 1989; Lenhard et al., 1991). These models assume that the main hysteresis loop is expressed by two retention functions with different parameter sets for the MDC and MWC. Most often, hysteretic relationships have been developed using the van Genuchten model (Eq. [3.3.4-5]) under the assumption of  $m = 1 - 1/n$ . The MDC and MWC are then characterized by the parameter sets  $(\theta_{s,d}, \theta_{r,d}, \alpha_d, n_d)$ , and  $(\theta_{s,w}, \theta_{r,w}, \alpha_w, n_w)$ , respectively, whereas the corresponding hydraulic conductivity function is expressed by Eq. [3.3.4-23]. In the simplest case, the effects of entrapped air are neglected and the main hysteresis loop is assumed to be closed at saturation and at the dry end, which leads to  $\theta_{s,d} = \theta_{s,w} = \theta_s$  and  $\theta_{r,d} = \theta_{r,w} = \theta_r$  (Fig. 3.3.4-4). Moreover, it is assumed that the dimensionless  $n$  parameter has identical values for both main curves, yielding nonhysteretic  $K$ - $\theta$  relationships (Eq. [3.3.4-23]). With these assumptions, the resulting expressions for the main retention curves are

$$S_e^{\text{MDC}}(h_m) = [1 + (-\alpha_d h_m)^n]^{-m} \quad [3.3.4-30a]$$

$$S_e^{\text{MWC}}(h_m) = [1 + (-\alpha_w h_m)^n]^{-m} \quad [3.3.4-30b]$$

where  $m = 1 - 1/n$ . Luckner et al. (1989) suggested an approximate relationship of  $\alpha_w \cong 2\alpha_d$ . A drying scanning curve beginning at a reversal point  $(\theta^D, h_m^D)$  is scaled from the MDC, using the same parameters  $\alpha_d$  and  $n$  as the MDC. Assuming that the DSC under consideration merges with the MDC at the residual water content,  $\theta_r$ , the drying scanning curve differs from the MDC only by the saturated water content value (Fig. 3.3.4-4). Based on the requirement that the DSC passes through the reversal point  $(\theta^D, h_m^D)$  the saturated water content,  $\theta_s^*$ , for the scanning curve can be computed directly from:

$$\theta_s^* = \{\theta^D - \theta_r[1 - S_e^{\text{MDC}}(h_m^D)]\} / [S_e^{\text{MDC}}(h_m^D)] \quad [3.3.4-31]$$

so that the  $\theta$ - $h_m$  relationship for the DSC is described by

$$(\theta - \theta_r) / (\theta_s^* - \theta_r) = S_e^{\text{MDC}}(h_m) \quad [3.3.4-32]$$

Note that Eq. [3.3.4-32] is identical to the MDC if  $(\theta^D, h_m^D)$  is equal to  $(\theta_s, 0)$ .

Similarly, a wetting scanning curve (WSC) beginning at a reversal point  $(\theta^W, h_m^W)$  differs from the MWC only in its residual water content,  $\theta_r$  (Fig. 3.3.4–4). Following the same reasoning as for the DSC, the residual water content,  $\theta_r^*$ , for the scanning curve is computed from

$$\theta_r^* = [\theta^W - \theta_s S_e^{\text{MWC}}(h_m^W)] / [1 - S_e^{\text{MWC}}(h_m^W)] \quad [3.3.4-33]$$

so that the  $\theta$ – $h_m$  relationship for the WSC is described by

$$(\theta - \theta_r^*) / (\theta_s - \theta_r^*) = S_e^{\text{MWC}}(h_m) \quad [3.3.4-34]$$

Clearly, if  $(\theta^W, h_m^W)$  is equal to  $(\theta_r, -\infty)$ , Eq. [3.3.4–34] is identical to the MWC.

Equations [3.3.4–30] through [3.3.4–34] provide a comprehensive representation of hysteretic water retention characteristics, using the smallest number of fitting parameters. However, some discrepancies with measured data have been reported. For example, scanning loops are not closed and the effects of entrapped air are ignored. Parker and Lenhard (1987) proposed a modified hysteresis model, in which closure of scanning loops is enforced and the effects of air entrapment are taken into consideration. These improved developments are further presented in Chapter 7 for general multi-fluid soil systems.

### 3.3.4.11 Model Fitting

Fitting of soil water retention and/or unsaturated hydraulic conductivity models through measured data is carried out by means of nonlinear least squares optimization procedures. Parameters are optimized to minimize an objective function,  $\phi(\mathbf{p})$ , which contains the residual sum of squares of observed and fitted water content and/or hydraulic conductivity values:

$$\phi(\mathbf{p}) = \sum_{i=1}^{I_\theta} (\theta_i - \hat{\theta}_i)^2 + w \sum_{i=1}^{I_K} (\log K_i - \log \hat{K}_i)^2 \quad [3.3.4-35]$$

where  $\mathbf{p}$  is the vector containing the fitted parameters,  $\theta_i$  and  $\hat{\theta}_i$  are the observed and fitted water content data, respectively,  $K_i$  and  $\hat{K}_i$  are the observed and fitted unsaturated hydraulic conductivity values, respectively,  $I_\theta$  and  $I_K$  are the number of measured retention and hydraulic conductivity data points, respectively, and  $w$  is a weighting factor to correct for differences in the number of data points and units between  $\theta$  and  $K$  data. In Eq. [3.3.4–35], log-transformed conductivity data are used to compute  $\phi(\mathbf{p})$ , since the largest and smallest  $K$  observations can easily differ several orders of magnitude. If special accuracy is required for the conductivity data in the wet range, one may use untransformed  $K$  data instead of  $\log K$  (Yates et al., 1992). Theory and applications of nonlinear optimization can be found in Section 1.7.

In general, one must try to reduce the number of fitted parameters, thereby minimizing nonuniqueness of the optimized parameters. For example, the saturated water content,  $\theta_s$ , can be easily measured independently and is preferably excluded as a fitting parameter. All fitting results presented in Fig. 3.3.4–2 were obtained in this way. One may also choose to fix the saturated hydraulic conductivity,  $K_s$ , to its

measured value. However, as was pointed out by Luckner et al. (1989),  $K_s$  values measured in the field under a slightly positive water pressure are generally dominated by soil structural properties and may have little relation to the hydraulic conductivity in the unsaturated water content range. Hence, it is usually recommended to consider  $K_s$  as a fitting parameter. Alternatively, one may select a measured unsaturated hydraulic conductivity value in the relatively wet range as a matching point for the conductivity function.

As was pointed out above, many algorithms are currently available for parameter optimization. In addition to RETC (van Genuchten et al., 1991) and UNSODA (Leij et al., 1996), many commercial spreadsheet software programs such as Quattro Pro (Corel Corp., Ottawa, ON Canada), Excel (Microsoft Corp., Seattle, WA), Lotus 1-2-3 (IBM Software Group, Cambridge, MA), and MATLAB (The MathWorks, Inc., Natick, MA) can also be used (Wraith & Or, 1998).

### 3.3.4.12 Comments

The concept of residual water content,  $\theta_r$ , is an essential but potentially problematic element in soil water retention models. Its value is required to improve model fitting in relatively wet soils. Luckner et al. (1989) suggested a physically based definition of this parameter such that  $\theta_r$  is the water content at which films of wetting liquid coating the soil particles are reduced to the point where “all or parts of the connecting films become so thin, and hence so strongly adsorbed onto the solid phase, that the wetting fluid loses its ability to respond to hydraulic gradients.” However, as pointed out by Nimmo (1991), this definition is not well supported by observations, since its fitted value depends on the water content range of the fitted retention data. Because the water content theoretically goes to zero as the matric head becomes infinitely negative, retention models that contain  $\theta_r$  as a fitting parameter tend to cause discrepancies with measured data in the low matric head range ( $h_m < -10^3$  cm). To maintain the physical meaning of  $\theta_r$  as a measurable quantity, Šir et al. (1985) introduced a water content  $\theta_b$  ( $\theta_b \leq \theta_r$ ), which is a fitting parameter without physical significance (Kutilek & Nielsen, 1994). Fayer and Simmons (1995) proposed modified parametric soil water retention functions that adequately represent retention across the whole soil water matric head range of 0 to  $-10^7$  cm. Combinations of power functions and logarithmic functions were used by Rossi and Nimmo (1994) to characterize soil water retention from saturation to oven-dryness.

In addition to the presented parametric models for the soil water retention relation, many other functional forms have been suggested. We emphasize that any of these other models may describe measured soil water retention data equally well, but are much less widely used. When retention and conductivity functions are coupled through mutual parameters, the shape of the retention function has a large influence on the prediction of the unsaturated hydraulic conductivity, especially near saturation. We surmise that the consideration of a bimodal soil water retention function, allowing the formulation of a secondary macroporous pore system, can improve the unsaturated hydraulic conductivity prediction near saturation for structured soils.

Finally, it should be understood that values of the parameters occurring in retention models are based on a range of input values of water content and pressure

head. Extrapolation of model values outside the range of input data should only be done with caution. Moreover, any model is only as good as the input data on which it is based, emphasizing the consideration of uncertainty analysis in the model output data.

### 3.3.4.13 References

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