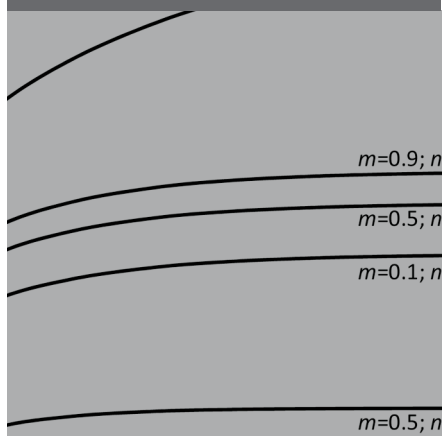


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Alternatives for the van Genuchten hydraulic conductivity equations are presented using approximations of infinite series of hypergeometric functions. These approximations match very closely to the analytical results and allow the use of independent parameter values in the soil water retention model for subsequent prediction of the hydraulic conductivity.

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Alternative Analytical Expressions for the General van Genuchten–Mualem and van Genuchten–Burdine Hydraulic Conductivity Models

The van Genuchten expressions for the unsaturated soil hydraulic properties, first published in 1980, are used frequently in various vadose zone flow and transport applications assuming a specific relationship between the m and n soil hydraulic parameters. By comparison, probably because of the complexity of the hydraulic conductivity equations, the more general solutions with independent m and n values are rarely used. We expressed the general van Genuchten–Mualem and van Genuchten–Burdine hydraulic conductivity equations in terms of hypergeometric functions, which can be approximated by infinite series that converge rapidly for relatively large values of the van Genuchten–Mualem parameter n but only very slowly when n is close to one. Alternative equations were derived that provide very close approximations of the analytical results. The newly proposed equations allow the use of independent values of the parameters m and n in the soil water retention model of van Genuchten for subsequent prediction of the van Genuchten–Mualem and van Genuchten–Burdine hydraulic conductivity models, thus providing more flexibility in fitting experimental pressure-head-dependent water content, $\theta(h)$, and hydraulic conductivity, $K(h)$, or $K(\theta)$ data.

The unsaturated hydraulic conductivity is a key property for modeling water flow in the vadose zone. This property can be measured directly (Klute and Dirksen, 1986) or indirectly (van Genuchten and Leij, 1992) or estimated implicitly using inverse methods (Hopmans and Šimůnek, 1999; Butters and Duchateau, 2002). Based on pore size distribution theories proposed by Childs and Collis-George (1950), Burdine (1953), and Mualem (1976), among others, several approaches for predicting the unsaturated hydraulic conductivity from measured soil water retention data have been presented in the literature. These theories produced predictive expressions for the relative hydraulic conductivity, K_r , which is the ratio between the hydraulic conductivity, K , at a certain water content, θ , or pressure head, h , and the hydraulic conductivity at saturation, K_s :

$$K_r(\theta, h) = \frac{K(\theta, h)}{K_s} \quad [1]$$

A frequently used equation for describing the soil water retention curve is (van Genuchten, 1980)

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[1 + (\alpha |h|)^n \right]^{-m} \quad [2]$$

where S_e is the effective saturation, θ_s and θ_r are the saturated and residual soil water contents, respectively, and α , m , and n are empirical parameters. As shown by van Genuchten (1980) and van Genuchten and Nielsen (1985), Eq. [2] may be combined with the pore size distribution models of Burdine (1953) or Mualem (1976) to lead to predictive expressions for the relative hydraulic conductivity of unsaturated soils. The Burdine (1953) and Mualem (1976) models differ in the manner in which effective pore radii are estimated (Vereecken, 1995). The model of Mualem (1976) is given by

$$K_r(S_e) = \frac{S_e' \left\{ \int_0^{S_e} [1/h(S_e)] dS_e \right\}^2}{\left\{ \int_0^1 [1/h(S_e)] dS_e \right\}^2} \quad [3]$$

where l is a mostly empirical pore-connectivity or tortuosity parameter. Its value was initially estimated by Mualem (1976) to be 0.5, although widely different values have since been reported, generally between about -6 and 6 (e.g., Yates et al., 1992; Schaap and Leij, 2000; Wösten et al., 2001).

Following the theory of Burdine (1953), another equation for K_r is given by

$$K_r(S_e) = S_e^\lambda \frac{\int_0^{S_e} [1/b(S_e)]^2 dS_e}{\int_0^1 [1/b(S_e)]^2 dS_e} \quad [4]$$

where λ , similar to l in Eq. [3], is a pore-connectivity or tortuosity parameter, generally assumed to be 2.0. Modifications of Eq. [3] and [4], including the use of other values for l or λ , have been proposed by Marshall (1958), Wyllie and Gardner (1958), Millington and Quirk (1961), Kunze et al. (1968), and Farrell and Larson (1972), among others.

The combination of Eq. [2] with either Eq. [3] or [4] allows direct evaluation of the integrals in the $K_r(S_e)$ expressions. Closed-form equations for K_r were derived by van Genuchten (1980) by expressing m in Eq. [2] as a function of n . Van Genuchten and Nielsen (1985) later presented solutions for $K_r(S_e)$ without assuming a dependency between the m and n parameters. These solutions contained the incomplete beta function, which they evaluated numerically using continued fractions. Probably because of computational demands (Ross, 1992), the general solutions have been used only rarely in vadose zone hydrologic applications. One recent exception was given by Regalado (2005). The predictive qualities of the equations with m expressed as a function of n were evaluated by Stephens and Rehfeldt (1985), Yates et al. (1992), Khaleel and Relyea (1995), and Cornelis et al. (2005), among others.

In the following, we revisit the general solutions of van Genuchten and Nielsen (1985), show that it is feasible to derive alternative formulations for the closed-form K_r expressions, and provide analytical approximations that are very easy to evaluate.

Theory The Original van Genuchten–Mualem Equations

We first briefly review the original approach followed by van Genuchten (1980) and van Genuchten and Nielsen (1985). Inverting Eq. [2] and substitution into Eq. [3] leads to

$$K_r(S_e) = S_e^l \left[\frac{f(S_e)}{f(1)} \right]^2 \quad [5]$$

where

$$f(S_e) = \int_0^{S_e} \left(\frac{S_e^{1/m}}{1 - S_e^{1/m}} \right)^{1/n} dS_e \quad [6]$$

Using the substitution $y = S_e^{1/m}$ in Eq. [6] yields a more tractable form:

$$f(S_e) = m \int_0^{S_e^{1/m}} y^{m-1+(1/n)} (1-y)^{-1/n} dy \quad [7]$$

In van Genuchten (1980), m and n were assumed to be related by

$$m = 1 - \frac{1}{n} \quad [8]$$

so that Eq. [7] simplifies to

$$f(S_e) = m \int_0^{S_e^{1/m}} (1-y)^{-1/n} dy \quad [9]$$

which can be integrated immediately to yield

$$f(S_e) = 1 - (1 - S_e^{1/m})^m \quad [10]$$

Substitution of Eq. [10] into [5] leads then to the following expression for K_r :

$$K_r(S_e) = S_e^l \left[1 - (1 - S_e^{1/m})^m \right]^2 \quad (n > 1) \quad [11]$$

General van Genuchten–Mualem Equations with Independent m and n Values

The more general approach with independent values of m and n in Eq. [2] was considered in detail by van Genuchten and Nielsen (1985). They were able to integrate Eq. [7] to obtain

$$f(S_e) = m I_\zeta \left(m + \frac{1}{n}, 1 - \frac{1}{n} \right) B \left(m + \frac{1}{n}, 1 - \frac{1}{n} \right) \quad [12]$$

where I_ζ and B are the regularized incomplete and complete beta functions, respectively (Abramowitz and Stegun, 1972), and $\zeta = S_e^{1/m}$. Because $f(1) = mB(m + 1/n, 1 - 1/n)$, the general van Genuchten–Mualem equation with independent m and n becomes

$$K_r(S_e) = S_e^l \left[I_\zeta \left(m + \frac{1}{n}, 1 - \frac{1}{n} \right) \right]^2 \quad [13]$$

which holds for values of m and n restricted by $m > 0$ and $n > 1$.

Equation [13] contains the regularized incomplete beta function, I_ζ , evaluated by van Genuchten and Nielsen (1985) using a continued fraction approximation. They found the approximation to require, in most cases, five terms in the expansion to obtain accuracy in K_r of at least four significant digits. A few more terms were recommended for relatively large values of the parameter m .

We revisited Eq. [7] and found an alternative formulation for Eq. [12], in terms of the hypergeometric function F (Abramowitz and Stegun, 1972, p. 558):

$$f(S_e) = \frac{mn S_e^{1+(1/mn)} F\left[m + (1/n), (1/n); m + (1/n) + 1; S_e^{1/m}\right]}{mn + 1} \quad [14]$$

with $m > -1/n$ and $n > 1$. Equations [12] and [14] are completely equivalent (cf., Abramowitz and Stegun, 1972, p. 263, Eq. 6.6.8) in that for any $r = m + 1/n > 0$ (and hence $m > -1/n$) and $s = 1 - 1/n > 0$ (and hence $n > 1$):

$$r I_\zeta(r, s) B(r, s) = \zeta^r F(r, 1-s; r+1; \zeta) \quad [15]$$

where $\zeta = S_e^{1/m}$.

Abramowitz and Stegun (1972, p. 556, Eq. 15.1.1) presented the following definition for the hypergeometric function:

$$F(a, b; c; z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!} \quad [16]$$

where $(a)_k$, $(b)_k$, and $(c)_k$ are Pochhammer symbols (Abramowitz and Stegun, 1972, p. 256, Eq. 6.1.22) of the form

$$(x)_k = x(x+1)\dots(x+k-1) = \prod_{i=1}^k (x+i-1) \quad [17]$$

Substitution of Eq. [17] with $x = a$, $x = b$, and $x = c$ in Eq. [16] yields

$$F(a, b; c; z) = \sum_{k=0}^{\infty} \frac{z^k}{k!} \prod_{i=1}^k \frac{(a+i-1)(b+i-1)}{(c+i-1)} \quad [18]$$

and hence for $n > 1$

$$F\left(m + \frac{1}{n}, \frac{1}{n}; m + \frac{1}{n} + 1; S_e^{1/m}\right) = \sum_{k=0}^{\infty} \frac{S_e^{k/m}}{k!} \prod_{i=1}^k \frac{\left[m + (1/n) + i - 1\right] \left[(1/n) + i - 1\right]}{m + (1/n) + i} \quad [19]$$

Substituting Eq. [19] into [14] and the result into Eq. [5] yields the general solution

$$K_r(S_e) = \left[\frac{S_e^{(l/2)+(1/mn)+1} [1 + \eta(S_e)]}{1 + \beta} \right]^2 \quad [20]$$

$(0 \leq S_e \leq 1, n > 1 \text{ and } m > 0)$

in which

$$\eta(S_e) = (mn + 1) \sum_{k=1}^{\infty} \left(\frac{S_e^{k/m}}{mn + kn + 1} \prod_{i=1}^k \frac{n^{-1} + i - 1}{i} \right) \quad [21]$$

and

$$\beta = (mn + 1) \sum_{k=1}^{\infty} \left(\frac{1}{mn + kn + 1} \prod_{i=1}^k \frac{n^{-1} + i - 1}{i} \right) \quad [22]$$

Equations [21] and [22] were found to converge rapidly when the parameter n is relatively large; however, convergence of especially Eq. [22] is very slow when n becomes less than about 2 or 3. The convergence of $\eta(S_e)$ given by Eq. [21] can be verified by d'Alembert's ratio test (e.g., Rudin, 1976), which makes use of the parameter L as follows

$$L = \lim_{k \rightarrow \infty} \left| \frac{a_{k+1}}{a_k} \right| \quad [23]$$

where a_{k+1} and a_k are two consecutive terms of the infinite series given by Eq. [21]. Substituting these into Eq. [23] gives

$$L = \lim_{k \rightarrow \infty} S_e^{1/m} \frac{(kn + mn + 2)kn + mn + 1}{(kn + mn + 2n + 1)kn + n(mn + n + 1)} \quad [24]$$

According to d'Alembert's ratio test, a series converges absolutely if $L < 1$ but does not converge if $L > 1$. If $L = 1$ or the limit fails to exist, then the test is inconclusive. In our case, we have $0 \leq L < 1$ for all $0 \leq S_e < 1$, $n > 1$, and $m > 0$, which shows that $\eta(S_e)$ given by Eq. [21] converges.

An analogous procedure for the series in Eq. [22] shows that $L = 1$, which means that d'Alembert's ratio test is inconclusive. In this case, Raabe's test (Rudin, 1976) may be used to prove convergence. Raabe's R test states that if $L = 1$, and if

$$R = \lim_{k \rightarrow \infty} k \left(\left| \frac{a_{k+1}}{a_k} \right| - 1 \right) < -1 \quad [25]$$

then the series will converge. In our case, R is given by

$$R = \lim_{k \rightarrow \infty} k \frac{kn + mn + 1 - 2kn^2 - n(mn + n + 1)}{(kn + mn + 2n + 1)kn + n(mn + n + 1)} \quad [26]$$

$$= \frac{1}{n} - 2$$

which shows that β given by Eq. [22] converges for $n > 1$ (to make $R < -1$).

We calculated values of β for each combination of $n = 1.1, 1.2, \dots, 10.0, 11, 12, \dots, 40$ and $m = 0.05, 0.10, \dots, 0.95$. The number of terms required for each combination was found to depend on the particular n and m values. Relatively small values of n and values of S_e close to 1 in particular required a large number of terms. As a criterion for convergence, we used the parameter δ_β given by

$$\delta_\beta = \frac{\beta(p) - \beta(p-1)}{\beta(p)} \quad [27]$$

where $\beta(p)$ is the value of β after calculating 10^p terms, with p being an integer within the interval $0 \leq p \leq 12$. When, after 10^p terms, δ_β became $< 10^{-4}$, evaluation of the series solution would be terminated. If no convergence was reached after 10^{12} terms ($p = 12$), the calculation was aborted and flagged as inconclusive.

The Original van Genuchten–Burdine Equations

The derivations of the original (restricted) and general van Genuchten–Burdine expressions parallel those of the van Genuchten–Mualem expressions. Inversion of Eq. [2] and substitution into Eq. [4] yields

$$K_r(S_e) = S_e^\lambda \frac{g(S_e)}{g(1)} \quad [28]$$

where

$$g(S_e) = \int_0^{S_e} \left(\frac{S_e^{1/m}}{1 - S_e^{1/m}} \right)^{\lambda/n} dS_e \quad [29]$$

Using again the substitution $y = S_e^{1/m}$, Eq. [29] becomes

$$g(S_e) = m \int_0^{S_e^{1/m}} y^{m-1+(2/n)} (1-y)^{-2/n} dy \quad [30]$$

Assuming that m is related to n by

$$m = 1 - \frac{2}{n} \quad [31]$$

allows the integral in Eq. [30] to be evaluated, resulting in

$$g(S_e) = 1 - \left(1 - S_e^{1/m} \right)^m \quad [32]$$

Substituting Eq. [32] into [28] yields

$$K_r(S_e) = S_e^\lambda \left[1 - \left(1 - S_e^{1/m} \right)^m \right] \quad (n > 2) \quad [33]$$

General van Genuchten–Burdine Equations with Independent m and n Values

Following van Genuchten and Nielsen (1985), direct integration of Eq. [29] for independent values of m and n (restricted to $m > 0$ and $n > 2$) leads to

$$g(S_e) = m I_\zeta \left[m + (2/n), 1 - (2/n) \right] B \left[m + (2/n), 1 - (2/n) \right] \quad [34]$$

which, when substituted into Eq. [28], gives

$$K_r(S_e) = S_e^\lambda I_\zeta \left[m + (2/n), 1 - (2/n) \right] \quad [35]$$

Equation [34] can also be formulated in terms of the hypergeometric function as follows:

$$g(S_e) = \frac{mn S_e^{1+(2/mn)} F_{m+(2/n), (2/n); m+(2/n)+1; S_e^{1/m}}}{mn+2} \quad (n > 2) \quad [36]$$

Substituting Eq. [36] into [28] and evaluating the hypergeometric functions analogously as shown for the Mualem case (Eq. [16–19]) yields the general van Genuchten–Burdine solution:

$$K_r(S_e) = \frac{S_e^{\lambda+(2/mn)+1} [1 + \zeta(S_e)]}{1 + \chi} \quad (0 \leq S_e \leq 1, n > 2, \text{ and } m > 0) \quad [37]$$

in which

$$\zeta(S_e) = (mn+2) \sum_{k=1}^{\infty} \left(\frac{S_e^{k/m}}{mn+kn+2} \prod_{i=1}^k \frac{2n^{-1}+i-1}{i} \right) \quad [38]$$

$$\chi = (mn+2) \sum_{k=1}^{\infty} \left(\frac{1}{mn+kn+2} \prod_{i=1}^k \frac{2n^{-1}+i-1}{i} \right) \quad [39]$$

Analogous to the case of $\eta(S_e)$ (Eq. [21]), it can be shown that d'Alembert's L parameter for $\zeta(S_e)$ (Eq. [38]) equals $S_e^{1/m}$, which indicates that Eq. [38] converges. For χ (Eq. [39]), $L = 1$ and Raabe's R parameter becomes $2/n - 2$; R is less than -1 for $n > 2$, which shows that Eq. [39] then converges also.

Values of χ (Eq. [39]) were calculated for each combination of $n = 2.1, 2.2, \dots, 10.0, 11, 12, \dots, 40$ and $m = 0.05, 0.10, \dots, 0.95$. Analogously to the invoked procedure for β , we used as a criterion of convergence for χ the parameter $\delta\chi$ given by

$$\delta_\chi = \frac{\chi(p) - \chi(p-1)}{\chi(p)} \quad [40]$$

where $\chi(p)$ is the value of χ after calculating 10^p terms, with p being an integer. The remaining calculations were similar to those for β as described above.

Results

Equations [20] and [37] are equivalent to the general van Genuchten–Mualem and van Genuchten–Burdine expressions (Eq. [11] and [33], respectively) for the unsaturated soil hydraulic conductivity assuming independent m and n values. Generally, only a few terms were needed when n was relatively large ($n > 5$).

The variables η (Eq. [21]) and ζ (Eq. [38]) were found to converge within 1000 terms for $0 < S_e \leq 0.99$ for all combinations of n and m analyzed, using as a criterion that the relative change in η or ζ became $<10^{-4}$ compared with the 10,000-terms estimate. The β (Eq. [22]) and χ parameters, however, converged very slowly, especially for values of n close to 1 and 2, respectively. As an example, Fig. 1 shows the convergence of β for several combinations of n and m . Notice that an inordinate number of terms are needed when n becomes relatively small (approaching the lower limit of 1.0). Convergence of χ was found to be even slower.

Using an efficient Fortran routine running on a state-of-the art microcomputer, it took >12 h to evaluate 10^{12} terms of Eq. [22] for each combination of m and n . For $n \leq 1.5$, convergence of β evaluated with Eq. [22] and invoking the described criteria would take even more terms (i.e., at least 10^{13} terms or >120 h of computing time); the corresponding values were therefore not calculated. For $1.6 \leq n \leq 40$ and $0.05 \leq m \leq 0.95$, we evaluated β using 2185 combinations of m and n , and fitted to the results the equation

$$\tilde{\beta} = a + bL(n; n_0, \nu) + cL(m; m_0, \mu) + dL(n; n_0, \nu)L(m; m_0, \mu) \quad [41]$$

where $\tilde{\beta}$ is the fitted approximation of β , L is the cumulative Cauchy distribution function defined by

$$L(f; f_0, \phi) = \frac{1}{2} + \frac{1}{\pi} \arctan\left(\frac{f - f_0}{\phi}\right) \quad [42]$$

and $a, b, c, d, n_0, m_0, \nu$, and μ are adjustable parameters. Of several alternative expressions we examined, Eq. [41] gave by far the best fit to the 2185 points ($R^2 = 0.9995$; $F = 6.0 \times 10^5$). Values and standard errors of $a, b, c, d, n_0, m_0, \nu$, and μ are listed in Table 1.

A similar approximation $\tilde{\chi}$ for χ was derived using 1900 values of χ calculated with Eq. [39] for various combinations of m and n across the interval $3.1 \leq n \leq 40$ and $0.05 \leq m \leq 0.95$:

$$\tilde{\chi} = p + qL(n; n_1, \tau) + rL(m; m_1, \rho) + sL(n; n_1, \tau)L(m; m_1, \rho) \quad [43]$$

where L is defined by Eq. [42] as before. Values and standard errors of the parameters $p, q, r, s, n_1, m_1, \rho$, and τ for the best fit ($R^2 = 0.9997$; $F = 8.9 \times 10^5$) are shown in Table 2.

Together with a computer routine to evaluate the relatively quickly converging η (Eq. [21]) or ζ (Eq. [38]) (we suggest 1000 terms for a $<0.01\%$ error), Eq. [41] or [43] can be used to estimate the slowly converging β or χ functions, respectively, thus allowing calculation of K_r for any combination of the n and m parameters with an insignificant computing time. Figure 2 shows an example of K_r calculated as a function of S_e for $n = 4$, $l = 0.5$, and $\lambda = 2$, assuming five values for m : 0.05, 0.25, 0.5, 0.75, and 0.95. For the Mualem case, $m = 0.75$ corresponds to Eq. [11] with $m = 1 - 1/n$. For the Burdine calculations, $m = 0.5$ corresponds to Eq. [33] with $m =$

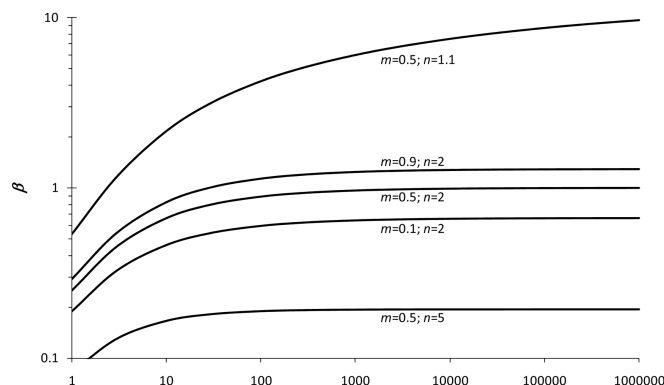


Fig. 1. Estimate of parameter β as a function of the number of terms evaluated in Eq. [22].

Table 1. Values and standard errors of fitting parameters of Eq. [41] for estimation of β (Eq. [22]) for $1.6 \leq n \leq 40$ and $0.05 \leq m \leq 0.95$.

Parameter	Value	SE
a	0.09389	0.01607
b	16.92	1.688
c	-0.2923	0.06759
d	-30.77	7.103
n_0	1.325	0.0032
m_0	-0.3778	0.32359
ν	-0.3958	0.00301
μ	-1.790	0.2700

Table 2. Values and standard errors of fitting parameters of Eq. [43] for estimation of χ (Eq. [39]) for $3.1 \leq n \leq 40$ and $0.05 \leq m \leq 0.95$.

Parameter	Value	SE
p	0.1282	0.01706
q	19.43	1.481
r	-0.3891	0.06589
s	-33.87	5.718
n_1	2.561	0.0052
m_1	-0.3047	0.22473
τ	-0.7068	0.00512
ρ	-1.821	0.2187

$1 - 2/n$. Values calculated with these equations (thick lines in Fig. 2) showed an essentially perfect match to those obtained with the approximate equations.

Concluding Remarks

The general expressions of van Genuchten and Nielsen (1985) for predicting the unsaturated hydraulic conductivity based on the theories of Burdine (1953) and Mualem (1976) can be formulated in terms of hypergeometric functions. The hypergeometric functions can be approximated by infinite series, which converge very

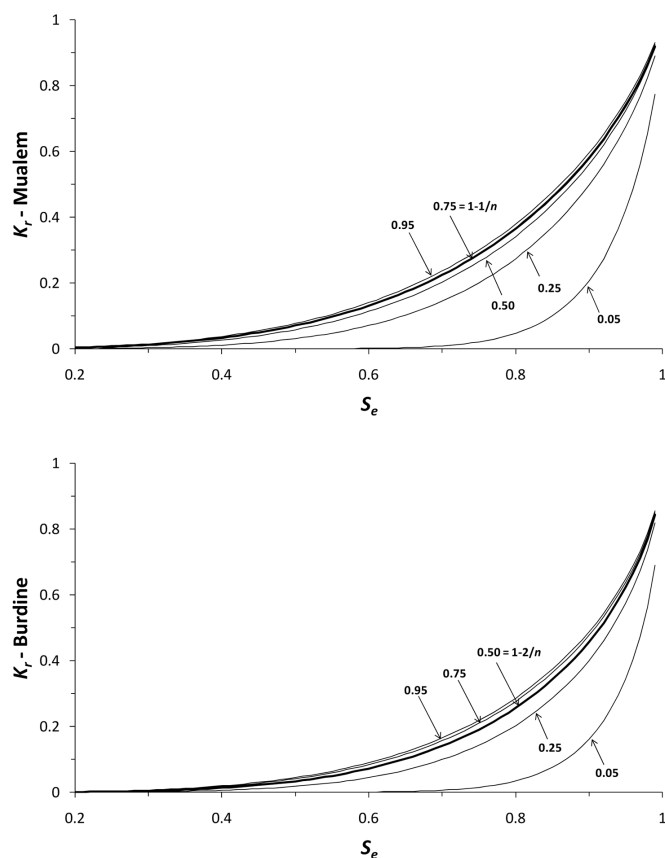


Fig. 2. Relative hydraulic conductivity (K_r) as a function of the effective saturation (S_e) evaluated for $n = 4$, $l = 0.5$, and $\lambda = 2$ by the Mualem Eq. [20] and the Burdine Eq. [37] (thin lines) and for $m = 0.05, 0.25, 0.50, 0.75$, and 0.95 by Eq. [11] and [33] (thick lines).

slowly when the parameter n is close to 1 or 2 for the Mualem and Burdine solutions, respectively. Alternative equations may be used to obtain very close approximations of the infinite series for selected values of the van Genuchten m and n parameters, thus allowing the use of the general expressions without a need for time-consuming computational processes.

The newly proposed equations permit the use of independent values of the parameters m and n in the soil water retention model of van Genuchten (1980) for subsequent prediction of the van Genuchten–Mualem and van Genuchten–Burdine hydraulic conductivity models. Thus, more flexibility is allowed in fitting experimental $\theta(h)$ and $K(h)$ or $K(\theta)$ data.

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