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TECHNICAL NOTE

Modified expression for hydraulic conductivity according to Mualem–van Genuchten to allow proper computations at low-pressure heads

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Abstract

Water retention and hydraulic conductivity characteristics are key input data in studies on soil water dynamics in the vadose zone. The most well-known analytical functions to describe these characteristics are those given by Mualem and van Genuchten, where van Genuchten showed that both can be described by a limited set of shared parameters. Analytically, there are no restrictions on the range of pressure heads for which these characteristics can be used. Experience, however, has shown that for certain sets of parameters, the hydraulic conductivity cannot be computed accurately at low-pressure heads. This is due to the accuracy of (double precision) floating point operations in computer code. It is shown that for low-pressure heads, the Mualem function approaches a power function. An adapted version of the Mualem–van Genuchten (MvG) expression for the hydraulic conductivity is proposed: between saturation and a soil-dependent critical pressure head, the classical Mualem expression is valid and below this critical pressure head a power function is used. The power function is defined such that it matches the Mualem value at the critical pressure head. No accuracy problems will occur when using the power function until the result approaches the smallest possible (double precision) floating point value that significantly differs from zero.

1 | INTRODUCTION

Perhaps the most well-known and often used mathematical descriptions for the water retention and hydraulic conductivity characteristics are those given by Mualem (1976) and van Genuchten (1980). The water retention characteristic is given by

$$\theta(h) = \begin{cases} \theta_s & 0 \le h \\ \theta_r + \frac{(\theta_s - \theta_r)}{(1+|\alpha h|^n)^m} & h < 0 \end{cases}. \quad (1)$$

Abbreviation: MvG, Mualem–van Genuchten.

The hydraulic conductivity characteristic is given by (provided $m = 1 - 1/n$)

$$K(h) = \begin{cases} K_s & 0 \le h \\ K_s \frac{\left[(1+|\alpha h|^n)^m - |\alpha h|^{n-1}\right]^2}{(1+|\alpha h|^n)^{m(\lambda+2)}} & h < 0 \end{cases}. \quad (2)$$

Here, θ is the volumetric water content (cm^3 cm^{-3}), h is the pressure head (cm; $h < 0$ when unsaturated), K is the hydraulic conductivity (cm day^{-1}), θ_r is the (asymptotic) residual θ (cm^3 cm^{-3}), θ_s is θ at saturation (cm^3 cm^{-3}), K_s is K at saturation

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(cm day^{-1}), and α (cm^{-1}), n, m, and λ (all three dimensionless) are curve shape parameters. Except for λ, all parameters are positive, with $0 \leq \theta_r < \theta_s \leq 1$, and $n > 1$. Parameter λ can be negative, zero, or positive; however, there is a restriction on its lower bound as discussed later. The beauty of these combined relationships is that they share parameters and in total a full description is thus given by the set of parameters θ_r, θ_s, a, n, λ, and K_s (Mualem–van Genuchten [MvG] parameters). Both physically and mathematically, there are no restrictions on the magnitude of h. Computationally in computer code, however, we have experienced problems in calculating $K(h)$ at low h. This technical note describes our findings and provides an alternative expression for $K(h)$.

Core Ideas

- Computer calculated hydraulic conductivities K can show anomalous behavior at low-pressure heads h.
- Double precision floating point constraints are the main cause.
- The Mualem–van Genuchten K expression can be approximated by a power function at low h.
- An extended expression for the Mualem–van Genuchten $K(h)$ equation is proposed.
- With the extended expression, K can be computed to values as low as floating point precision allows.

2 | HYDRAULIC CONDUCTIVITY AT LOW-PRESSURE HEAD

Under unsaturated conditions in soils h and K vary several orders of magnitude. For that reason, one often plots the $K(h)$ relationship on log-log scales. These plots have typical shapes of being concave near saturation, monotonically decreasing and approaching a linear decrease at low h. For certain sets of MvG parameters for individual soil samples and one soil textural class of the Dutch Staring series (Heinen et al., 2022), we observed that at certain low values of h this pattern was violated, and the decrease of $K(h)$ no longer followed the anticipated linear decrease in a log-log plot. Figure 1 provides an example for soil sample 10134, a coarse sand, where the $K(h)$ data were computed either using Fortran (Intel OneAPI HPC Toolkit Fortran version 2023; https://www.intel.com/content/www/us/en/developer/tools/oneapi/toolkits.html) or R (R Core Team, 2023) with double precision. The MvG parameters for this sample are as follows: $\theta_r = 0.03539$ cm^3 cm^{-3}, $\theta_s = 0.36683$ cm^3 cm^{-3}, $\alpha = 0.02135$ cm^{-1}, $n = 7.2372$, $\lambda = 0.0001$, $K_s = 101.3839$ cm day^{-1}.

Such a violation of the general concave shape of the curve was observed earlier. According to Peters et al. (2011), the monotonicity demand requires that $\lambda > -2/m$ (with $m = 1 - 1/n$) and the concavity demand requires that $\lambda > 1 - 2/m$. The concavity demand is more strict. With $n > 1$, we have $0 < m < 1$, so that no problems will ever occur in case $\lambda > -1$; however, depending on the magnitude of n, more negative values for λ are still valid without violating the monotonicity and concavity demands. Since for soil sample 10134 λ is greater than the most strict demand for both monotonicity and concavity ($\lambda = 0.0001 > -1$), the $K(h)$ curves should not show the upward curvature as obtained from the Fortran and R double precision calculated $K(h)$ data for any h. When quadruple precision (Fortran) was used, we obtained the expected linear decrease on the log-log scale (Figure 1; Fortran, quadruple), at least for the range in h considered in Figure 1. Apparently, for this sample, and a few other samples (data not shown), we have reached the limits of floating point precision on the double precision calculated $K(h)$ function in computer code. In general, these are all samples with relatively high values for the n parameter, and large values for n mean that $|h|^n$ becomes large. For example, for the 999 samples used in the derivation of the Staring series (Heinen et al., 2022), there were 18 samples with $n > 4$, of which 10 samples belong to the soil textural class of coarse sand and seven to the soil textural class of weak loamy sand.

Not only for individual soil samples this phenomenon is observed, it is also seen for some class-averaged soils in the Dutch Staring series (coarse sand subsoil O05; Heinen et al., 2022), Rosetta (sand; Schaap, 2002), and Hypres (coarse sand subsoil; Wösten et al., 1999; Figure 2). For these three soil classes, the λ-criterion for monotonicity and concavity ($\lambda > -1$), as described above, is always satisfied: Staring series O05: $\lambda = 0.0736$; Rosetta sand: $\lambda = -0.93$; Hypres coarse sand: $\lambda = 1.25$.

The pressure head where this deviation occurs differs between soil samples and soil classes, that is, it is dependent on the MvG parameter set. However, it appears that the corresponding K-values are of the order of 10^{-20}–10^{-40} cm day^{-1} (double precision; or 10^{-40}–10^{-75} cm day^{-1} in quadruple precision). These K-values are still much larger than the theoretical smallest value that can be represented by double precision floating point representation, that is approximately 2.23×10^{-308} (better: 2^{-1022}).

3 | POWER FUNCTION APPROXIMATION

As mentioned above, the MvG relationship for $K(h)$, when plotted on log-log scale, approaches a linear decrease with decreasing h. This indicates that for decreasing h, the $K(h)$

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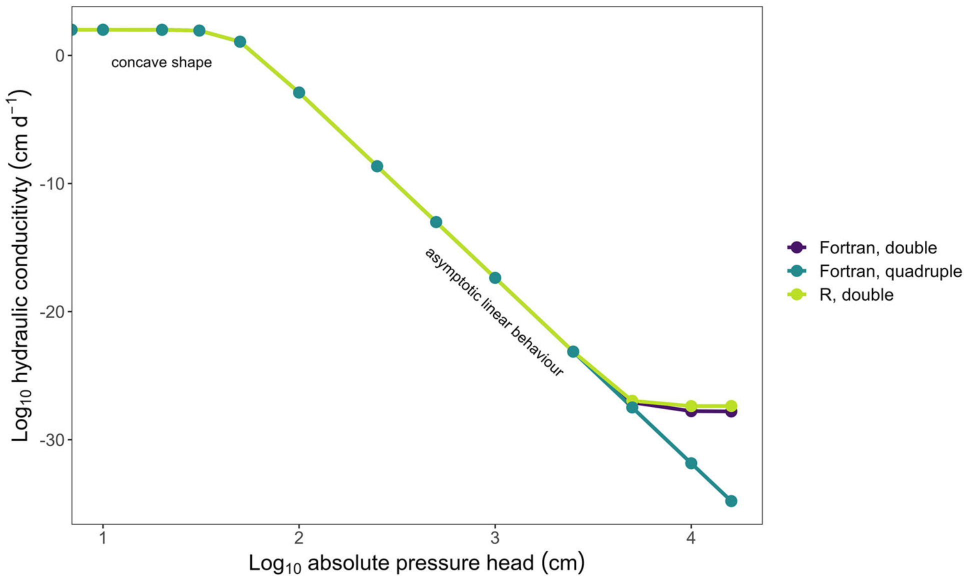

FIGURE 1 The $K(h)$ relationship plotted on log-scales for soil sample 10134 computed with double precision Fortran and R and with quadruple precision Fortran. See text for further explanation. *Source*: Heinen et al., 2022.

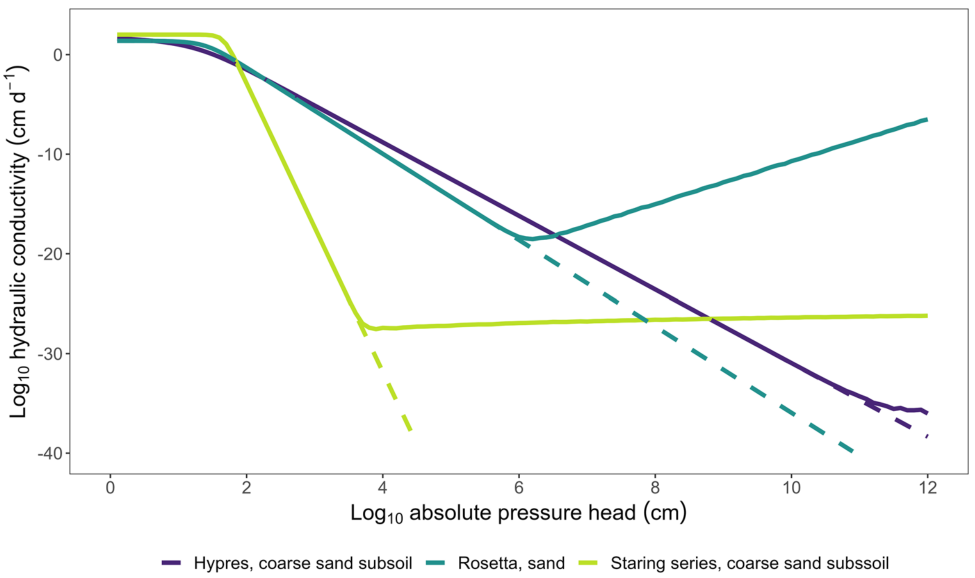

FIGURE 2 The $K(h)$ relationship plotted on log-scales for selected soil classes of the data bases Staring series (Heinen et al., 2022), Rosetta (Schaap, 2002) and Hypres (Wösten et al., 1999). The solid lines refer to the computed data using the double precision calculations with Equation (2), whereas the broken lines refer to the quadruple precision calculations.

relationship should approach some power expression for $K(h)$. de Willigen and Heinen (2014) showed that this can be derived from Equation (2) as follows. The unsaturated part of Equation (2) can be rewritten as

$$y = \frac{K}{K_s} = \left(|\alpha h|^n + 1\right)^{-m\lambda}\left(|\alpha h|^n + 1\right)^{-2m}\left[\left(|\alpha h|^n + 1\right)^m - |\alpha h|^{\frac{m}{1-m}}\right]^2, \tag{3}$$

where y is the relative hydraulic conductivity and, as before, $m = (n-1)/n$. Introducing the substitute variable $s = 1 + |\alpha h|^n$ (with $|\alpha h| = (s-1)^{1/n}$), we obtain

$$y = s^{-m\lambda} s^{-2m} s^{2m}\left[1 - \left(\frac{s-1}{s}\right)^m\right]^2 = s^{-m\lambda}\left[1 - \left(\frac{s-1}{s}\right)^m\right]^2. \tag{4}$$

Note that s is related to the effective degree of saturation $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ as $s = (S_e)^{-1/m}$. If we now define a new

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variable x as

$$x = \frac{s-1}{s} = \frac{|\alpha h|^n}{|\alpha h|^n + 1} \tag{5}$$

with inverse $s = 1/(1-x)$, we find

$$y = (1-x)^{m\lambda}(1-x^m)^2 \tag{6}$$

Since $s \geq 1$, it follows that $0 \leq x < 1$. The term x^m can be written as a Taylor expansion around $x = 1$ yielding

$$x^m = 1 + m(x-1) + O(x-1)^2, \tag{7}$$

then it follows that

$$(1-x^m)^2 \approx \{1 - [1 + m(x-1)]\}^2 = [-m(x-1)]^2 = m^2(x-1)^2. \tag{8}$$

Substituting Equation (8) in Equation (6) then yields

$$y = (1-x)^{m\lambda}(1-x^m)^2 \approx m^2(1-x)^{2+m\lambda} \tag{9}$$

For low values of h, $(1-x)$ can be approximated as

$$(1-x) = 1 - \frac{|\alpha h|^n}{|\alpha h|^n + 1} = \frac{1}{|\alpha h|^n + 1} \approx |\alpha h|^{-n}. \tag{10}$$

So, for sufficiently low-pressure heads, $K(h)$ can thus be approximated by substituting Equation (10) in Equation (9), yielding (substituting y by K/K_s)

$$K(h) = K_s m^2 |\alpha h|^{-(2+m\lambda)n} \tag{11}$$

This means that there is a linear relation between ln(K) and ln(h) according to

$$\ln(K) = \ln\left(K_s m^2 \alpha^{-(2-m\lambda)n}\right) - (2-m\lambda)\, n \ln(h). \tag{12}$$

A power type function for $K(h)$ was earlier proposed by Wind (1955) and Brooks and Corey (1964), and here it is shown that for large absolute values of h, the MvG $K(h)$ relationship approaches such a power type function. In some studies and models, the matric flux potential M (cm^2 day^{-1}), defined as the integral of the $K(h)$ relationship, is needed. For the power function according to Equation (11), this is given by

$$M(h) = K(h)\frac{h}{1-(2+m\lambda)\, n}. \tag{13}$$

This is a much more simple form then M for the original MvG $K(h)$ relationship as given by de Jong van Lier et al. (2009) and Heinen and Bakker (2016).

In the derivations above, two approximations have been applied, one for x^m and other for $(1-x)$. The question now is: for what range of h values are these approximations justified? First, we define a maximum relative (to the exact value) deviation that is acceptable, here denoted by ε ($\varepsilon > 0$). For the first approximation, the requirement is then (cf. Equation 7) given as

$$\left|\frac{x^m - [1 + m(x-1)]}{x^m}\right| = \frac{[1 + m(x-1)] - x^m}{x^m} \leq \varepsilon. \tag{14}$$

The corresponding minimum acceptable value of x is thus found by solving

$$-(1+\varepsilon)\, x^m + mx - m + 1 = 0 \tag{15}$$

for $x = x_c$. Since $\varepsilon > 0$, $0 \leq x < 1$, and $0 < m < 1$, the left-hand side of Equation (15) is monotonically decreasing, its first derivative is always < 0, and its second derivative is always $>$ 0, indicating that there exists only one value for x where this function equals zero.

Then from Equation (5), we find the first estimate of the critical pressure head, h_c, below which the approximation holds

$$h \leq h_{c,1} = -\frac{1}{\alpha}\left(\frac{x_c}{1-x_c}\right)^{1/n} \tag{16}$$

For the second approximation, the second requirement $h_{c,2}$ is found by

$$\frac{\left|\frac{1}{|\alpha h|^n+1} - \frac{1}{|\alpha h|^n}\right|}{\frac{1}{|\alpha h|^n+1}} = \frac{|\alpha h|^n + 1}{|\alpha h|^n} - \frac{|\alpha h|^n + 1}{|\alpha h|^n + 1} = \frac{1}{|\alpha h|^n} \leq \varepsilon \tag{17}$$

This results in

$$h \leq h_{c,2} = -\frac{1}{\alpha}\varepsilon^{-1/n}. \tag{18}$$

For a chosen value of ε, the critical pressure head (h_c) can be taken as the minimum of $h_{c,1}$ and $h_{c,2}$. Table 1 lists the critical pressure head h_c for all soil classes in three data bases

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TABLE 1 The critical pressure heads h_c and corresponding hydraulic conductivities K_c ($\log_{10}$-transformed) for $\varepsilon = 0.01$ and $\varepsilon = 0.05$ below which the Mualem–van Genuchten (MvG) $K(h)$ relationship can be approximated with a power function (Equations 11 and 21) for all soil classes in three data bases.

Data base	Soil class	$\varepsilon = 0.01$		$\varepsilon = 0.05$	
		h_c (cm)	$\log_{10}(K_c)$ (cm day^{-1})	h_c (cm)	$\log_{10}(K_c)$ (cm day^{-1})
Staring series	Sand B01	−656.6	−4.091	−259.6	−2.433
(Heinen et al., 2022)	Sand B02	−1404.4	−6.993	−425.8	−4.346
	Sand B03	−1422.8	−3.767	−488.3	−2.360
	Sand B04	−1816.3	−3.724	−573.9	−2.290
	Sand B05	−298.4	−2.924	−122.5	−1.543
	Sand B06	−1947.0	−2.939	−533.0	−1.720
	Clay-loam B07	−2180.6	−4.624	−600.7	−3.117
	Clay-loam B08	−3504.9	−4.016	−994.8	−2.923
	Clay-loam B09	−5438.2	−4.106	−1527.1	−3.072
	Clay B10	−4501.4	−6.363	−1090.6	−4.612
	Clay B11	−2967.0	−4.165	−693.0	−3.150
	Clay B12	−4117.5	−5.065	−941.4	−3.940
	Loess B13	−2947.5	−2.738	−961.7	−1.643
	Loess B14	−6359.4	−5.168	−1846.6	−3.844
	Peat B15	−1528.7	−2.726	−435.8	−1.571
	Peat B16	−1738.9	−3.703	−493.9	−2.507
	Peat B17	−3015.6	−5.193	−731.9	−3.814
	Peat B18	−2672.9	−4.652	−660.0	−3.273
	Sand O01	−526.0	−6.287	−249.9	−3.864
	Sand O02	−1275.3	−5.258	−443.7	−3.310
	Sand O03	−866.0	−3.682	−336.7	−2.308
	Sand O04	−1617.4	−4.995	−548.6	−3.132
	Sand O05	−162.6	−3.232	−93.1	−1.829
	Sand O06	−2233.2	−3.335	−640.5	−2.112
	Sand O07	−4528.3	−3.649	−1121.3	−2.452
	Clay-loam O08	−2703.4	−3.783	−817.7	−2.565
	Clay-loam O09	−2926.0	−4.002	−908.3	−2.815
	Clay-loam O10	−4012.8	−4.740	−1102.4	−3.469
	Clay O11	−4172.4	−6.109	−999.2	−4.550
	Clay O12	−6050.7	−4.833	−1507.6	−3.750
	Clay O13	−2553.0	−4.376	−575.2	−3.303
	Loess O14	−5251.5	−4.839	−1940.5	−3.331
	Loess O15	−4612.5	−4.862	−1321.2	−3.485
	Peat O16	−3016.3	−4.633	−926.6	−3.378
	Peat O17	−3135.4	−4.280	−884.3	−3.084
	Peat O18	−2613.6	−3.310	−769.4	−2.062
Rosetta	Clay	−2636.3	−4.290	−729.8	−3.128
(Schaap, 2002)	Clay loam	−1635.4	−3.922	−524.7	−2.699
	Loam	−2053.1	−4.187	−688.1	−2.892
	Loamy sand	−402.3	−2.611	−160.0	−1.491
	Sand	−120.9	−1.669	−72.9	−0.735
	Sandy clay	−1354.8	−3.633	−357.4	−2.685
	Sandy clay loam	−1510.9	−3.737	−450.7	−2.577

(Continues)

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TABLE 1 (Continued)

Data base	Soil class	$\varepsilon = 0.01$		$\varepsilon = 0.05$	
		h_c (cm)	$\log_{10}(K_c)$ (cm day^{-1})	h_c (cm)	$\log_{10}(K_c)$ (cm day^{-1})
	Sandy loam	−900.5	−3.299	−296.5	−2.105
	Silt	−2362.2	−4.774	−905.7	−3.228
	Silty clay	−2012.2	−4.105	−595.2	−2.942
	Silty clay loam	−2462.2	−4.481	−854.3	−3.142
	Silty loam	−3150.3	−4.853	−1197.1	−3.380
Hypres	Coarse, top soil	−739.3	−4.038	−229.8	−2.428
(Wösten et al., 1999)	Medium, top soil	−1575.5	−3.838	−403.0	−2.703
	Medium fine top	−4741.8	−4.797	−1313.7	−3.501
	Fine, top soil	−1784.6	−4.319	−413.8	−3.064
	Very fine, top soil	−2451.9	−5.355	−570.1	−3.816
	Coarse, bottom soil	−480.6	−3.949	−166.8	−2.282
	Medium, bottom soil	−2064.5	−4.438	−521.0	−3.133
	Medium fine, bottom soil	−5350.0	−5.077	−1427.1	−3.638
	Fine, bottom soil	−3505.8	−4.687	−796.6	−3.508
	Very fine, bottom soil	−4351.3	−5.424	−971.0	−4.044
	Organic soil	−3526.3	−4.780	−926.3	−3.356

for the case $\varepsilon = 0.05$. For the Staring series, h_c is in the range of [−1941; −93]; in case $\varepsilon = 0.01$, this range equals [−6360; −162].

Thus, Equation (2) can be replaced by

$$K(h) = \begin{cases} K_s & 0 \le h \\ K_s \dfrac{\left[(1+|\alpha h|^n)^m - |\alpha h|^{n-1}\right]^2}{(1+|\alpha h|^n)^{m(\lambda+2)}} & h_c < h < 0 \\ K_s m^2 |\alpha h|^{-(2+m\lambda)n} & h \le h_c \end{cases} \tag{19}$$

Using Equation (19) allows K to reach values close to the smallest value that can be represented by double precision floating point representation, that is approximately 2.23×10^{-308}.

A small discontinuity in monotonicity will exist at and near h_c. The smaller ε is chosen, the smaller this discontinuity will be. In Figure 3, the relationship $h_c(\varepsilon)$ is shown for $0.001 \le \varepsilon \le 0.1$ as well as the corresponding values for K_c at h_c according to Equations (2) and (11) for soil sample 10134. With Equation (11), K_c is always greater than K_c according to Equation (2), with their relative difference more or less linearly increasing with increasing ε: from 0.0019 at $\varepsilon = 0.001$ to 0.19 at $\varepsilon = 0.1$.

To overcome this discontinuity, we shift the power function such that its K-value equals $K(h_c)$ as obtained from Equation (2). This can be achieved by replacing K_s in Equation (11) by K_s^*, which is obtained as follows:

$$K_s^* = K_c \frac{|\alpha h_c|^{(2+m\lambda)n}}{m^2} \tag{20}$$

where $K_c = K(h_c)$ according to Equation (2). Then Equation (19) can be written as

$$K(h) = \begin{cases} K_s & 0 \le h \\ K_s \dfrac{\left[(1+|\alpha h|^n)^m - |\alpha h|^{n-1}\right]^2}{(1+|\alpha h|^n)^{m(\lambda+2)}} & h_c < h < 0 \\ K_s^* m^2 |\alpha h|^{-(2+m\lambda)n} = K_c \left(\dfrac{h_c}{h}\right)^{(2+m\lambda)n} & h \le h_c \end{cases} \tag{21}$$

For $h < h_c$, Equation (21) results in a slight underestimation with respect to the Mualem expression. The maximum underestimation by Equation (21) occurs at $h \to -\infty$ and approaches $K_s^*/K_s (< 1)$. In both cases, the maximum deviation is dependent on K_s^*, and thus on α, n, λ, h_c, and K_c (according to Equation 20). For smaller values of ε, the value for h_c will be lower, so that K_s^*/K_s will be closer to 1.

In Appendix A, some alternative ways how K can be computed according to the MvG model are discussed. These alternatives show similar anomalies in computed K-values as Equation (2) and thus do not perform equal or better than Equation (21). In Appendix B, the anomalous behavior of Equation (2) is visualized by showing the computed K-values in the $h(n)$ plane.

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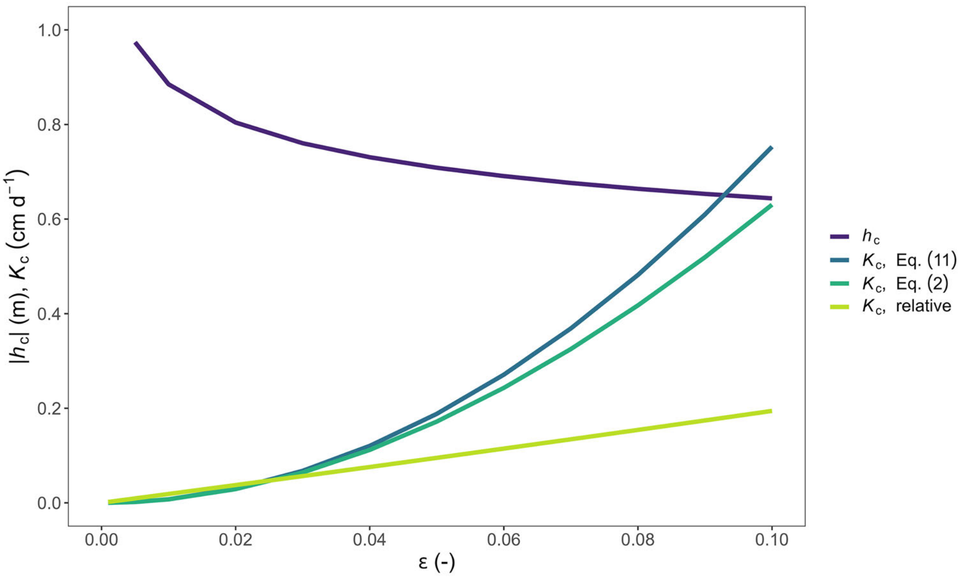

FIGURE 3 Absolute critical pressure head h_c as a function of ε and the corresponding hydraulic conductivities K_c calculated using Equations (2) and (11), and their relative difference for soil sample 10134.

4 | DISCUSSION

This paper focused on the computational problems encountered when the MvG characteristics are evaluated using computer codes. The main issue was the change from a linear decrease in $K(h)$ (when plotted on log-scales) encountered for certain soils at low values of h. This change to a convex shape is purely the result of problems in floating point calculations. However, measured $K(h)$ data have been reported in the literature that showed such convexity at low-pressure heads (e.g., Bakker et al., 2020; Peters & Durner, 2008). In that case, the MvG model will not be able to describe that specific change to a convex shape by definition and one should use alternative models for describing the hydraulic conductivity relationship. For example, Peters (2013), Iden and Durner (2014), and Peters (2014) proposed a model for $K(h)$ consisting of a capillary component (cf. Mualem, 1976), a component accounting for water-film transport, and a component accounting for water-vapor transport. When this model is used in computer code, it may also encounter floating point precision problems at some point. These should be investigated separately. Instead of using an adapted hydraulic conductivity relationship to account for vapor flow, one could also use a coupled model that describes vapor and water flow which are both coupled to heat transport. In such a model, the water flow would still be described using a MvG model. In that case, the same numerical problems would arise, which could be addressed by using the power law approximation.

Modified MvG relationships have been introduced in the past, where modifications were performed near saturation (e.g., Vogel et al., 2000; Ippisch et al., 2006; Schaap & van Genuchten, 2006). Such a modification is due to considering an air-entry pressure head (h_{ae}) near saturation causing a shift in the water retention and hydraulic conductivity characteristics. One could repeat the power function approximation analysis for these modified expressions. However, in case such a modification results in a shift of the curves, a similar power function (with the same slope on log-log scale) will result. A simple approach to obtain h_{c*} for the modified version is to have $K_{c*} = K_c$ from which h_{c*} can be found. As an example, Figure 4 shows the original and a modified Mualem (with h_{ae} $= -40$ cm) curve for a light clay (soil O11 from the Staring series in Heinen et al., 2022) using the modification described by Ippisch et al. (2006) and the power function approximation below h_c and h_{c*}, respectively. Here, $h_c = -4172$ cm (Table 1) and $h_{c*} = -24{,}516$ cm with $K_{c*} = K_c = 7.78 \times 10^{-7}$cm day^{-1}. This example shows that the approximation can also be applied to this kind of other modified MvG relationships. The new parameter h_c and, if applicable, h_{c*} can be precalculated for each soil layer and added as input in computer simulation models.

It is not possible to indicate the practical significance of imprecisions in K on simulation results. This will be a function of the specific soil under consideration (with its own MvG parameters and h_c) and the corresponding boundary and climatic conditions. Academic examples can be given where problems will never be observed or where simulation results will differ between a run using Equation (2) and Equation (21). Equation (2) can easily be replaced by Equation (21) in computer codes at hardly any costs; only one additional input parameter h_c is required. Note that for $h < h_c$, the computational CPU costs decrease, since only one power

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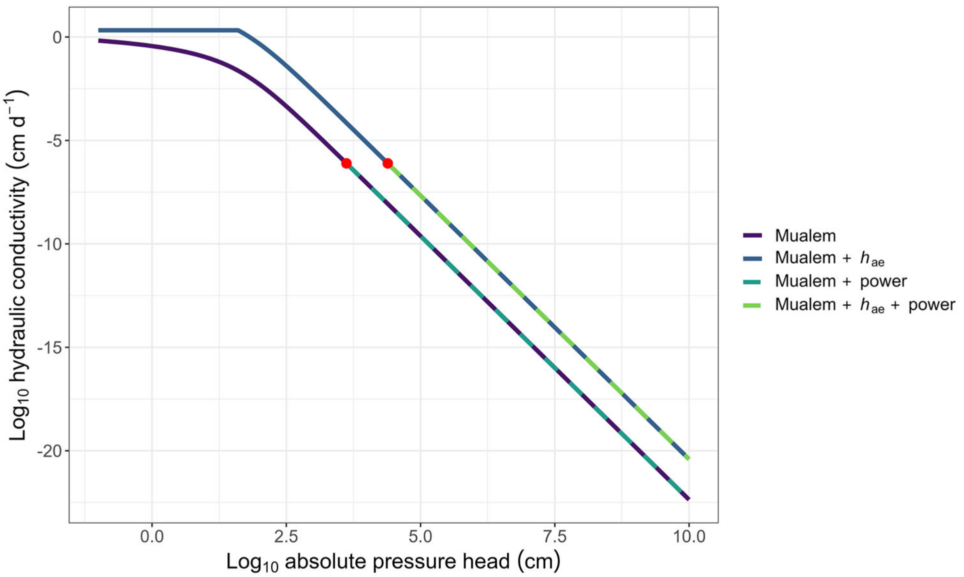

FIGURE 4 Original and modified (including air entry h_{ae}) Mualem relationships for a light clay (soil O11 from the Staring series in Heinen et al., 2022) (solid lines) and the power approximation at dry conditions (dashed lines) which start at the red dots ($K_c(h_c)$ and $K_{c*}(h_{c*})$ with $K_{c*} = K_c$).

operation is required against five power operations according to Equation (2).

5 | CONCLUSION

Physically and mathematically, the MvG relationship for the hydraulic conductivity K has no restrictions (provided that the parameters fulfill their physical constraints). It is valid for all values of pressure head h. However, when we use computer codes to calculate $K(h)$ we may run into problems associated with double precision floating point constraints. This can occur for h-values that are likely to occur in simulation models for water dynamics in unsaturated soils. It has been shown that the MvG expression for $K(h)$ at low values of h approaches a power relationship. An extended expression for the MvG $K(h)$ relationship is proposed where for h less than a certain critical pressure head (h_c), the power function is used (Equation 21). The value for h_c follows from the requirement that the original function and the power function approximation are relatively close to each other. Its value is basically dependent on the α and n parameters for a given measure of acceptable deviation ε (e.g., $\varepsilon = 0.05$ or $\varepsilon = 0.01$).

AUTHOR CONTRIBUTIONS

Marius Heinen: Conceptualization; data curation; formal analysis; methodology; software; validation; visualization; writing—original draft; writing—review and editing.

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CONFLICT OF INTEREST STATEMENT

The author declares no conflicts of interest.

SUPPLEMENTAL MATERIAL

This study does not contain supplemental materials.

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APPENDIX A

During calculations, using Equation (2) apparently rounding errors occur or terms vanish in relation to other terms. Rewriting the unsaturated part in Equation (2) as

$$K(h) = K_s \frac{\left(1+|\alpha h|^n\right)^{2m} + |\alpha h|^{2(n-1)} - 2\left(1+|\alpha h|^n\right)^m |\alpha h|^{n-1}}{\left(1+|\alpha h|^n\right)^{m(\lambda+2)}} \tag{22}$$

or

$$K(h) = K_s \frac{\left[1-|\alpha h|^{n-1}\left(1+|\alpha h|^n\right)^{-m}\right]^2}{\left(1+|\alpha h|^n\right)^{\lambda m}} \tag{23}$$

did not result in proper K-values at low h.

Alternatively, K can also be expressed in terms of θ or S_e ($S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$) according to

$$K(S_e) = K_s S_e^{\lambda}\left[1-\left(1-S_e^{1/m}\right)^m\right]^2 \tag{24}$$

Since in double precision floating point calculations the smallest number that is significantly different from 1 equals 2.22×10^{-16}, $K(S_e)$ becomes zero for $(S_e)^{1/m} \leq 2.22 \times 10^{-16}$. For soil sample 10134, this occurs when K approaches approximately 5×10^{-30} cm day^{-1}.

So, these alternative expressions for the MvG hydraulic conductivity show similar anomalous behavior below a certain pressure head as was observed in Equation (2). These alternatives are, for computational reasons, not performing different from or better than Equation (2).

APPENDIX B

For the MvG parameters of soil sample 10134 (as used in the main text), a sensitivity analysis was performed by computing K in the $h(n)$ plane. This resulted in the contour plots as shown in Figure A1. Based on Equation (2), using double precision, K-values less than approximately 10^{-25} cm day^{-1} cannot be computed accurately; when using quadruple precision, K-values less than approximately 10^{-60} cm day^{-1} cannot be computed accurately. Based on Equation (21), using double precision K-values can be computed for all $h(n)$

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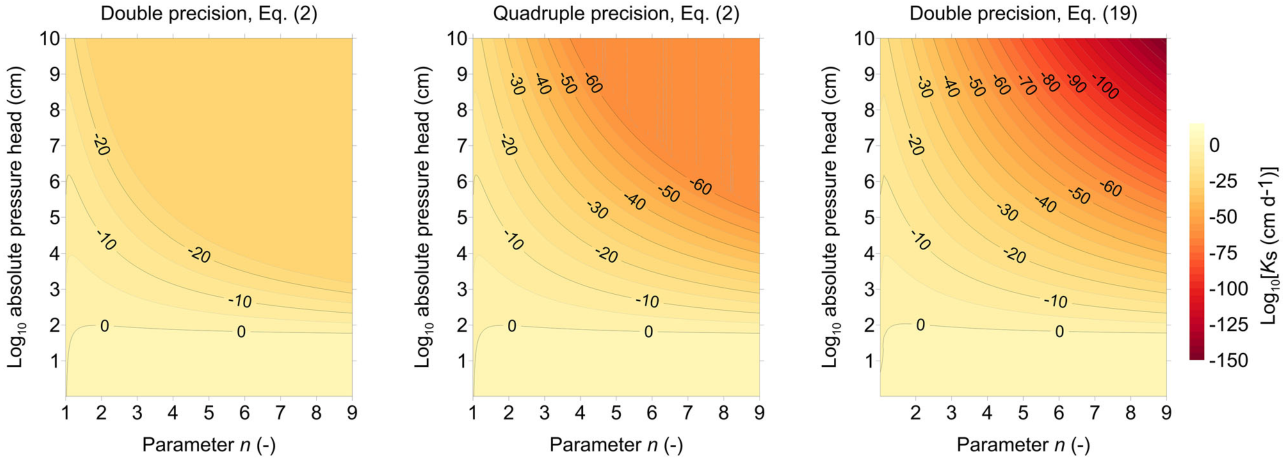

FIGURE A1 Computed values of K as a function of n and h (with $\alpha = 0.02135$ cm^{-1}, $\lambda = 0.0001$, $K_s = 101.3839$ cm day^{-1}) according to Equation (2) using double precision (left) or quadruple precision (middle) and according to Equation (21) using double precision.

considered in this example. For this specific set of parameters and with $n = 7.2372$, K can no longer be computed for $h < -10^{23}$ cm where K is approximately 10^{-307} cm day^{-1}, that is, the theoretical smallest value that can be represented by double precision floating point representation, that is, approximately 2.23×10^{-308} (better: 2^{-1022}). Values for h that are low are not expected in simulation models, whereas values for h in the range -10^4 and -10^7 are more likely to occur in simulation studies which for this soil sample would result in anomalous $K(h)$ behavior when Equation (2) (double precision) is used, and not when Equation (21) is used.

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