Analytical expressions for noncapillary soil water retention based on popular capillary retention models

Thilo Streck | Tobias K. D. Weber

Institute of Soil Science and Land Evaluation, Univ. of Hohenheim, Stuttgart, Germany

Correspondence
Thilo Streck, Institute of Soil Science and Land Evaluation, Univ. of Hohenheim, Stuttgart, Germany. Email: tstreck@uni-hohenheim.de

Funding information
Deutsche Forschungsgemeinschaft, Grant/Award Numbers: SFB1253 CAM-POS, under Grant 281741268

Abstract
Recently, Weber et al. proposed a new model for noncapillary retention of soil water without introducing new parameters. The model is based on the integral of any given saturation function for the capillary part in log space. In the original paper, the integration was carried out numerically. Here, we derive analytical solutions for the most popular soil water retention models (van Genuchten, Kosugi, and Brooks–Corey).

1 | INTRODUCTION

As part of their new modular framework for modeling unsaturated hydraulic properties of soils, Weber, Durner, Streck, and Diamantopoulos (2019) introduced a new model for noncapillary water retention. The commonly adopted approach for modeling the soil hydraulic property functions (Mualem–van Genuchten) is based on completely filled capillaries and is used over the entire range of soil matric potential. However, it has been shown (Diamantopoulos & Durner, 2015; Tuller & Or, 2001) that it fails beyond pF ≈ 2.3, where pF is the common logarithm of soil water suction (absolute value of soil matric potential) given in head units (cm).

The new model has a number of advantages over existing approaches for noncapillary water retention (e.g., Fredlund & Xing, 1994; Peters, 2013). First, it achieves a nearly linear reduction in water content at high, increasing pF; second, a volumetric water content of zero is attained at predefined pF; third, the function is continuously differentiable; and fourth, no extra parameter is introduced. Essentially, this is achieved by integrating the capillary saturation function in pF (log) space. In Weber et al. (2019), the integration was carried out numerically. The purpose of this technical note is to provide analytical solutions for the integrals of the most popular capillary saturation functions—that is, those published by Brooks and Corey (1964), Kosugi (1996), and van Genuchten (1980). To this end, we briefly review the mathematical structure of the model of Weber et al. (2019).

2 | THEORY

The soil water retention curve (WRC) gives the volumetric soil water content, \( \theta (m^3 m^{-3}) \), as a function of soil water suction, \( h \). The WRC is subdivided into a capillary and a noncapillary part:

\[
\theta(x) = \theta_c S^\text{CF}(x) + \theta_{nc} S^\text{NCF}(x)
\]

where \( \theta_c \) and \( \theta_{nc} \) are the maximum capillary and noncapillary volumetric water contents, respectively, whereas \( x = \log_{10}(h) \). \( S^\text{CF}(x) \) and \( S^\text{NCF}(x) \) are the respective saturation functions. These can be derived from the usual
capillary saturation models, $\Gamma_c^{pF}(x)$ (Table 1). Following a proposal by Iden and Durner (2014), the functions $\Gamma_c^{pF}(x)$ are forced to vary between zero and unity by rescaling them:

$$S_c^{pF}(x) = \frac{\Gamma_c^{pF}(x) - \Gamma_0}{1 - \Gamma_0} \quad (2)$$

where $\Gamma_0$ is the saturation at which the soil does not dry out further. Weber et al. (2019) proposed to model the non-capillary part of the WRC by integrating $S_c^{pF}(x) - 1$:

$$S_{nc}^{pF}(x) = \int_{-\infty}^{x} \left(S_c^{pF}(x') - 1\right) dx' \quad (3)$$

where $x'$ is the dummy variable of integration. The integral equals the area between full saturation ($x' = -\infty$, corresponding to $h = 0$ cm) and the capillary saturation at a given pF value. It is slightly different from that given by Weber et al. (2019), who replaced the lower bound of the integral by a finite number to make it numerically tractable. They proposed $pF = -3$ ($h = 0.001$ cm), where the soil is very close to full saturation, as the lower bound.

Subsequently, the result from Equation 3 is rescaled to values between zero and unity by

$$S_{nc}^{pF}(x) = 1 - \frac{S_{nc}^{pF}(x)}{S_{nc}^{pF}(x_0)} \quad (4)$$

where $x_0 = \log_{10}(h_0)$ is the water suction at which the soil is completely dry. Weber et al. (2019) proposed to use $x_0 = 6.8$.

| Name/authors of model, parameters, and label | Saturation function |
|--------------------------------------------|---------------------|
| **Brooks and Corey (1964)**               |                     |
| $\alpha, \beta$                           | Capillary: $\Gamma_c^{pF}(x) = \begin{cases} \left(\alpha^{10^x}\right)^{-\frac{1}{\beta}}, \text{if } \alpha^{10^x} \geq 1 \\ 1, \text{otherwise} \end{cases}$ |
| **A**                                     | Noncapillary: $\Gamma_{nc}^{pF}(x) = \begin{cases} \frac{\beta + \text{ln}(10)}{\text{ln}(10)} \left(\alpha^{10^x}\right)^{-\frac{1}{\beta}} - x, \text{if } \alpha^{10^x} \geq 1 \\ 0, \text{otherwise} \end{cases}$ |
| **Kosugi (1996)**                         | Capillary: $\Gamma_c^{pF}(x) = \frac{1}{2} \text{erfc} \left[\frac{\text{ln}(10^{x-x_m})}{\sqrt{2}x} \right]$ |
|                                           | $\Gamma_{nc}^{pF}(x) = \frac{x-x_m}{2} \text{erfc} \left[\frac{\text{ln}(10^{x-x_m})}{\sqrt{2}x} \right] = \frac{\sigma}{\text{ln}(10)\sqrt{2\pi}} \exp \left[-\frac{\text{ln}^2(10^{x-x_m})}{2\sigma^2}\right] - (x-x_m)$ |
| **B**                                     | Noncapillary: $\begin{cases} \left[1 + (\alpha^{10^x})^{n}\right]^{-\frac{1}{n}} \\ 1 + \frac{\left(\frac{2}{n} - 1\right)}{n}\sum_{k=1}^{\infty} \frac{1}{k(k+1)(nk+1)} \end{cases}$ |
| **van Genuchten (1980)**                  | Capillary: $\Gamma_c^{pF}(x) = \begin{cases} 1 + (\alpha^{10^x})^{n} \\ 1 + \frac{2}{n} - (\frac{2}{n} - 1) \sum_{k=1}^{\infty} \frac{1}{k(k+1)(nk+1)} \end{cases}$ |
| **C1**                                    | Noncapillary: $\begin{cases} \frac{1}{n\text{ln}(10)} \left[B \left[1 + (\alpha^{10^x})^{n}; 1, 0\right] - B \left[1 + (\alpha^{10^x})^{n}; 1, 0\right] \right] \\ + \frac{1}{2} + \left(\frac{2}{n} - 1\right) \sum_{k=1}^{\infty} \frac{1}{k(k+1)(nk+1)} \end{cases}$ |
| **C2**                                    | Noncapillary: $\begin{cases} \frac{1}{n\text{ln}(10)} \left[B \left[1 + (\alpha^{10^x})^{n}; 1, 0\right] - B \left[1 + (\alpha^{10^x})^{n}; 1, 0\right] \right] + \varepsilon - x \end{cases}$ |
Inserting Equation 2 into Equation 3 yields

\[ S_{nc}^{pF}(x) = \int_{-\infty}^{x} \left[ \frac{\Gamma_pF(x') - \Gamma_0}{1 - \Gamma_0} - 1 \right] dx' \]

\[ = \frac{1}{1 - \Gamma_0} \int_{-\infty}^{x} \left[ \Gamma_pF(x') - 1 \right] dx' \]

Upon inserting Equation 5 into Equation 4, the factor \(1/(1 - \Gamma_0)\) cancels out, so that Equation 4 can be rewritten without loss of generality as

\[ S_{nc}^{pF}(x) = 1 - \frac{\Gamma_pF(x)}{\Gamma_pF(x_0)} \]

where we define

\[ \Gamma_pF(x_0) = \int_{-\infty}^{x_0} \left[ \Gamma_pF(x') - 1 \right] dx' \]

Equation 7 contains the selected capillary saturation model, \( \Gamma_pF(x) \). The preceding derivation has shown that rescaling \( \Gamma_pF(x) \) by Equation 2 has no effect on \( \Gamma_{nc}^{pF}(x) \).

Note that the denominator in Equation 6:

\[ \Gamma_{nc}^{pF}(x_0) = \int_{-\infty}^{x_0} \left[ \Gamma_pF(x) - 1 \right] dx \]

is the total area above \( \Gamma_{nc}^{pF}(x) - 1 \) between maximum saturation and maximum dryness.

3 | RESULTS

Table 1 lists the analytical solutions of Equation 7 for the most popular capillary soil water retention models. The derivation is described in the Appendix. The noncapillary saturation function \( S_{nc}^{pF}(x) \) can be calculated from the given solution by applying Equation 6.

Taking the van Genuchten equation as an example, Figure 1 compares the new analytical solution with the numerical solution applied by Weber et al. (2019) and Weber and Diamantopoulos (2019). The difference between the solutions is negligible.
CONFLICT OF INTEREST
The authors declare no conflict of interest.

ACKNOWLEDGMENTS
We thank Lauritz Streck for the fruitful discussion of some mathematical aspects in this paper. This work was prepared within SFB 1253 CAMPOS (Project 7: Stochastic Modeling Framework), funded by Deutsche Forschungsgemeinschaft (DFG) under Grant 281741268.

ORCID
Thilo Streck https://orcid.org/0000-0001-7822-7588
Tobias K. D. Weber https://orcid.org/0000-0002-3448-5208

REFERENCES
Brooks, R., & Corey, T. (1964). Hydraulic properties of porous media. Fort Collins, CO: Colorado State University.
Diamantopoulos, E., & Durner, W. (2015). Closed-form model for hydraulic properties based on angular pores with lognormal size distribution. Vadose Zone Journal, 14(2). http://doi.org/10.2136/vzj2014.07.0096
Fredlund, D. G., & Xing, A. (1994). Equations for the soil-water characteristic curve. Canadian Geotechnical Journal, 31, 521–532. http://doi.org/10.1139/t94-061
Greenspan, H. P., Benney, D. J., & Turner, J. E. (1986). Calculus: An introduction to applied mathematics (2nd ed.). New York: McGraw-Hill.
Hankin, R. K. S. (2016). hypergeo: The Gauss Hypergeometric Function. R package version 1.2-13. Vienna: Comprehensive R Archive Network.
Iden, S., & Durner, W. (2014). Comment on “Simple consistent models for water retention and hydraulic conductivity in the complete moisture range” by A. Peters. Water Resources Research, 50, 7530–7534. https://doi.org/10.1002/2014WR019397
Kosugi, K. (1996). Lognormal distribution model for unsaturated soil hydraulic properties. Water Resources Research, 32, 2697–2703. http://doi.org/10.1029/96WR01776
NIST. (2019). Release 1.0.23 (June 15, 2019). NIST digital library of mathematical functions. Gaithersburg, MD: National Institute of Standards and Technology. Retrieved from http://dlmf.nist.gov/
Peters, A. (2013). Simple consistent models for water retention and hydraulic conductivity in the complete moisture range. Water Resources Research, 49, 6765–6780. http://doi.org/10.1002/wrcr.20548
R Core Team. (2019). R: A Language and Environment for Statistical Computing. Vienna: R Foundation for Statistical Computing.
Tuller, M., & Or, D. (2001). Hydraulic conductivity of variably saturated porous media: Film and corner flow in angular pore space. Water Resources Research, 37, 1257–1276. http://doi.org/10.1029/2000WR900328
van Genuchten, M. Th. (1980). A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Science Society of America Journal, 44, 892–898. https://doi.org/10.2136/sssaj1980.03615995004400050002x
Weber, T. K. D., Durner, W., Streck, T., & Diamantopoulos, E. (2019). A modular framework for modeling unsaturated soil hydraulic properties over the full moisture range. Water Resources Research, 55, 4994–5011. https://doi.org/10.1029/2018WR024584
Weber, T. K. D., & Diamantopoulos, E. (2019). spsh: Estimation and prediction of parameters of various soil hydraulic property models. R package version 1.0.4. Vienna: Comprehensive R Archive Network.

How to cite this article: Streck T, Weber TKD.
Analytical expressions for noncapillary soil water retention based on popular capillary retention models. Vadose Zone J. 2020;19:e20042.
https://doi.org/10.1002/vzj2.20042

APPENDIX
The integration of the Brooks–Corey equation (Brooks & Corey, 1964) is straightforward. Kosugi’s equation (Kosugi, 1996) was integrated by parts. The van Genuchten (1980) equation was integrated as follows. Inserting this equation (see Table 1) into Equation 7 yields

\[ F_{\text{nc}}(x) = \int_{-\infty}^{x} \left[ 1 + \left( \alpha 10^{x/10} \right)^{r} \right]^{n-1} \, dx \]  \tag{9}

Substituting \( x \) by \( y = 1 + \alpha 10^{x/10} \), which implies that

\[ dx = \frac{1}{n \ln(10)} \frac{1}{y-1} \, dy \]  \tag{10}

gives

\[ F(y) = \frac{1}{n \ln(10)} \int_{1}^{y} \frac{1}{y-1} \, dy - \frac{1}{y-1} \, dy' \]  \tag{11}

The integral in Equation 11 is of the Chebyshev type and can be solved in terms of beta functions. The incomplete beta function is defined by (NIST, 2019, 8.17.1):

\[ B(z; a, b) = \int_{0}^{z} s^{a-1}(1-s)^{b-1} \, ds \]  \tag{12}

In case of \( z = 1 \) the incomplete beta function turns into Euler’s beta function, that is, \( B(a, b) = B(1; a, b) \) (NIST, 2019, 5.12.1).

Combining Equations 11 and 12 yields (letting \( a = 1/n \) or \( a = 1 \), respectively, and \( b = 0 \)):

\[ F(y) = -\frac{1}{n \ln(10)} \left[ B\left( y; \frac{1}{n} \right) - B\left( y; 1, 0 \right) + B\left( 1, 0 \right) - B\left( \frac{1}{n}, 0 \right) \right] \]  \tag{13}
The application of Equation 13 is not straightforward because $B(1/n, 0)$ and $B(1, 0)$ are not finite. The difference of the two, however, can be evaluated. To this end, we use the series representation of the beta function (retrieved from http://www.wolframalpha.com/with query [series representation of beta function]):

$$B(a, b) = \sum_{k=0}^{\infty} \frac{(1 - b)_k}{(a + k) k!}$$

where, by definition, $(c)_k = c(c + 1)(c + 2) \ldots (c + k - 1)$, which is known as the Pochhammer notation. Rewriting the difference of the two beta functions from Equation 13 gives

$$B(1, 0) - B\left(\frac{1}{n}, 0\right) = \sum_{k=0}^{\infty} \frac{(1)_k}{(1 + k) k!} - \sum_{k=0}^{\infty} \frac{(1)_k}{\left(\frac{1}{n} + k\right) k!} \quad \text{(15)}$$

$$= \sum_{k=0}^{\infty} \left\{ \frac{1}{1 + k} - \frac{1}{\frac{1}{n} + k} \right\} \quad \text{(16)}$$

$$= \left(\frac{1}{n} - 1\right) \sum_{k=0}^{\infty} \frac{1}{(1 + k)\left(\frac{1}{n} + k\right)} \quad \text{(17)}$$

As can be seen from direct comparison with the convergent series $\sum 1/k^2$ (e.g., Greenspan, Benney, & Turner, 1986, Chapter 4.2), the series in Equation 17 converges. Convergence is rather slow but can be considerably accelerated by rewriting the series as

$$\sum_{k=0}^{\infty} \frac{1}{(1 + k)\left(\frac{1}{n} + k\right)} = n + \sum_{k=1}^{\infty} \frac{1}{(1 + k)\left(\frac{1}{n} + k\right)} \quad \text{(18)}$$

$$= n + \sum_{k=1}^{\infty} \left\{ \frac{1}{k} - \frac{1}{k + 1} - \frac{1}{k(k + 1)(nk + 1)} \right\} \quad \text{(19)}$$

$$= n + 1 - \sum_{k=1}^{\infty} \frac{1}{k(k + 1)(nk + 1)} \quad \text{(20)}$$

where we used the method of telescoping sums (e.g., Greenspan et al., 1986, Chapter 4.6):

$$\lim_{N \to \infty} \sum_{k=1}^{N} \left(\frac{1}{k} - \frac{1}{k + 1}\right) = \lim_{N \to \infty} \left[ 1 - \frac{1}{N + 1} \right] = 1 \quad \text{(21)}$$

Combining Equation 17 with Equation 20, inserting the result into Equation 13 and rearranging yields

$$F(y) = \frac{1}{n \ln(10)} \left[ B(y; 1, 0) - B\left(y; \frac{1}{n}, 0\right) + \frac{1}{n} \sum_{k=1}^{\infty} \frac{1}{k(k+1)(nk+1)} \right] \quad \text{(22)}$$

Resubstitution of $y = 1 + (\alpha 10^n)$ finally yields Equation C1 in Table 1. It is worth noting that even if only the first term of the series is evaluated, the (absolute) error in $\Gamma(x)$ is below 0.01 (for $n \in [1,10]$). Evaluating the first five (ten) terms reduces the maximum error to less than 0.001 (<0.0003).

Alternatively, and from a physical viewpoint sufficient in most cases, the integral in Equation 9 can be evaluated with a finite lower limit $\varepsilon$ (see above). In this case, it is easier to apply the substitution only to the left term in the integral

$$F(x) = \frac{1}{n \ln(10)} \int_{\varepsilon}^{y(x)} \left[ y^{\frac{1}{n} - 1} \right] \frac{1}{y'} \frac{dx'}{x} \quad \text{(23)}$$

Proceeding along the same lines as above yields

$$F(x) = \frac{1}{n \ln(10)} \left[ B\left(y(\varepsilon); \frac{1}{n}, 0\right) - B\left(y(x); \frac{1}{n}, 0\right) \right] - (x - \varepsilon) \quad \text{(24)}$$

and, upon resubstitution of $y$, finally Equation C2 in Table 1.

The solutions presented in Table 1 have been implemented as functions in the R package spsh (https://CRAN.R-project.org/package=spsh; R Core Team, 2019, version 3.6.0). The incomplete beta function in C1 and C2 (Table 1) was computed with the hypergeo package (Hankin, 2016). This required representing it as hypergeometric function (NIST, 2019, 8.17.8).

Equation C2 can be computed faster than Equation C1 but may be difficult to evaluate for large $n$. Presuming that $\varepsilon$ is chosen such that $\varepsilon + \log_{10}(\alpha) = -2$, which should in general be sufficiently accurate, the computation of C2 demands a routine that can evaluate $B[y(\varepsilon); \frac{1}{n}, 0]$ at $y = 1 + 10^{-2n}$.