Derivation of an Explicit Form of the Percolation-Based Effective-Medium Approximation for Thermal Conductivity of Partially Saturated Soils

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Keywords
Thermal conductivity, empirical models, mixing models, percolation-based effective-medium approximation, HYDRUS

Disciplines
Agriculture | Hydrology | Soil Science | Statistical Models

Comments
Derivation of an Explicit Form of the Percolation-Based Effective-Medium Approximation for Thermal Conductivity of Partially Saturated Soils

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Abstract

Thermal conductivity is an essential component in multi-physics models and coupled simulation of heat transfer, fluid flow and solute transport in porous media. In the literature, various empirical, semi-empirical, and physical models were developed for thermal conductivity and its estimation in partially saturated soils. Recently, Ghanbarian and Daigle (GD) proposed a theoretical model, using the percolation-based effective-medium approximation, whose parameters are physically meaningful. The original GD model implicitly formulates thermal conductivity $\lambda$ as a function of volumetric water content $\theta$. For the sake of computational efficiency in numerical calculations, in this study we derive an explicit $\lambda(\theta)$ form of the GD model. We also demonstrate that some well-known empirical models, e.g., Chung-Horton, widely applied in the HYDRUS model, as well as mixing models are special cases of the GD model under specific circumstances. Comparison with experiments indicates that the GD model can accurately estimate soil thermal conductivity.
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1. Introduction

Thermal conductivity ($\lambda$) is a fundamental property of soils required to study heat transfer and non-isothermal water flow in the vadose zone. In partially saturated soils, thermal conductivity depends mainly on soil volumetric water content ($\theta$), and hence, attempts have been made over years to formulate $\lambda$ as a function of $\theta$. Most $\lambda(\theta)$ models existing in the literature are based on empirical relationships or mixing theories. Table 1 summarizes the most common empirical and mixing models of thermal conductivity under partially saturated conditions.

Empirical models commonly include 3 to 5 ad hoc parameters whose values are a priori unknown due to the lack of a solid theoretical concept supporting them. Such parameters, therefore, need to be determined by directly fitting those models to experimental measurements or by inversion of a numerical simulation model.

Towards developing more physics-based models, mixing theories were applied by assuming that components affecting thermal conductivity contribute in series or parallel according to weighted arithmetic or harmonic averaging, respectively. It is well known that weighted arithmetic and harmonic means correspond to upper and lower boundaries of the effective thermal conductivity, respectively. Hashin and Shtrikman (1962) proposed more restricted upper and lower bounds for homogeneous and isotropic media composed of two components (e.g., solid matrix and air or water). Tong et al. (2009) extended the Hashin and Shtrikman work to determine the upper and lower bounds of thermal conductivity in media with three components (e.g., water, air, and solid...
matrix). In any case, mixing models are not physically well-justified, since components contributing to $\lambda$ are arranged neither in parallel nor in series. In reality, typically soils are stochastically complex mixtures of various components.

In order to develop a physics-based model, Ghanbarian and Daigle (2016) applied a theoretical framework from percolation theory and the effective-medium approximation to formulate the $\lambda$-$\theta$ relationship. The main advantages of their model are: (1) its theoretical basis leading to physically meaningful parameters and (2) its ability to describe experimental data from a broad range of porous media, including soils and rocks. One limitation of the model, however, is that thermal conductivity $\lambda$ is an implicit function of volumetric water content $\theta$. In numerical modeling, e.g., simulating coupled heat and water flow, however, the explicit functional form of $\lambda$ in terms of $\theta$ is desired to avoid computational loops for the $\lambda(\theta)$ determination. The explicit $\lambda(\theta)$ form thus results in more computationally-efficient and faster algorithms.

In this study, we derive an explicit form of $\lambda$ in terms of $\theta$ using the percolation-based effective-medium approximation. We also demonstrate that the explicit form reduces to some well-known existing thermal conductivity models, e.g., mixing models as well as the Chung and Horton (1987) model. The latter is widely used in the HYDRUS software (Simunek et al., 2005; 2006). This new linkage provides theoretical insights into such an empirical model and sheds light on its parameters, leading to improved parameterization of that model.

2. Background: Ghanbarian-Daigle (GD) Model

Percolation-based effective-medium approximation is a technique based on concepts from percolation theory and the effective-medium approximation. Within Percolation theory there
exist two frameworks: conductor-insulator and conductor-superconductor, while in the effective-
medium approximation more than one conductor may contribute to flow or transport.
Accordingly, it would be challenging to model thermal conductivity via percolation theory, since
both liquid and solid phases contribute to thermal conductivity under partially saturated
conditions. Using a combination of percolation theory and the effective-medium approximation,
called the percolation-based effective-medium approximation, Ghanbarian and Daigle (2016)
(hereafter GD) developed the following theoretical model for thermal conductivity, $\lambda$, in partially
saturated soils:

\[
(\theta_s - \theta) \frac{\lambda^{1/t_s} - \lambda^{1/t_s}}{\lambda^{1/t_s} + \left[\frac{(\theta_s - \theta_c)}{\theta_c}\right]^{1/t_s}} + \theta \frac{\lambda^{1/t_s} - \lambda^{1/t_s}}{\lambda^{1/t_s} + \left[\frac{(\theta_s - \theta_c)}{\theta_c}\right]^{1/t_s}} = 0
\]  

(1)

where $\theta$ is soil volumetric water content, $\theta_s$ is saturated water content, $\lambda_{\text{sat}} = \lambda(\theta_s)$ and $\lambda_{\text{dry}} = \lambda(0)$
are thermal conductivities under fully saturated and completely dry conditions, respectively, and
$t_s$ is a scaling exponent. $\theta_c$ is the critical water content at which the liquid phase (i.e., water) first
forms a continuous path through the medium. At water contents below $\theta_c$, $\lambda$ is mainly controlled
by $\lambda_{\text{dry}}$, while it is predominantly controlled by $\lambda_{\text{sat}}$ at $\theta > \theta_c$. As Ghanbarian and Daigle (2016)
stated, the concept of the critical water content in the percolation-based effective-medium
approximation is similar to the residual water content frequently applied in the soil physics and
hydrology community. The main difference between the two is that below the residual water
content there is no macroscopic transport, while below the critical water content thermal
conductivity still occurs but mainly through the solid matrix. Ghanbarian and Daigle (2016) also
indicated that the critical water content might be greater/less than or equal to the inflection point
on the $\lambda(\theta)$ curve, depending on the value of $t_s$. $\theta_c$ in Eq. (1) is comparable with $\theta_f$, the volumetric
water content at which the funicular regime is onset, within the Lu and Dong (2015) model. Lu
and Dong (2015) stated that, “The water content where thermal conductivity increases at its maximum rate is herein defined $\theta_f$. Further increasing in the water content in the funicular regime will result in continuous increase in thermal conductivity, but the contribution of heat conduction in pore water becomes less significant.”

Using experimental data, Ghanbarian and Daigle (2016) showed that the critical water content for percolation $\theta_c$ is strongly correlated with clay content [i.e., $\theta_c = 0.0033\text{Clay}($%$)$, $R^2 = 0.91$]. The larger the clay content, the greater the critical volume fraction for percolation, which is in agreement with experimental measurements of Lu et al. (2014), among others.

Compared to empirical models summarized in Table 1, the GD model benefits from a theoretical background and its physically meaningful parameters. In addition, the GD model is more flexible in shape, particularly in fine-textured soils, than most of the empirical models, which are commonly power-law (e.g., Somerton et al., 1974), exponential (e.g., Ewen and Thomas, 1987; Lu et al., 2014) or logarithmic (e.g., Johansen, 1977) in form. The Lu and Dong (2015) model, presented in Table 1, is probably the only empirical model that produces the correct sigmoidal shape of the saturation-dependent thermal conductivity commonly observed in fine-textured soils, while the theoretical GD model fits thermal conductivity measurements in various soil texture classes properly (see Fig. 5-7 of Ghanbarian and Daigle, 2016). One should note that although the Lu and Dong (2015) model returns $\lambda = \lambda_{dry}$ at zero water content ($\theta = 0$), it does not necessarily converge to $\lambda_{sat}$ as water content approaches $\theta_c$.

Equation (1) is general in form and has several special cases. As Ghanbarian and Daigle (2016) pointed out, for $t_c = 1$, Eq. (1) reduces to the weighted arithmetic mean when $\theta_c = 0$, to the weighted harmonic mean when $\theta_c = \theta_s$, to the geometric mean when $\theta_c = \theta = 0.5\theta_s$, and to the Bruggeman (1935) model when $\theta_c = \theta_s/3$. Equation (1) also reduces to the power-law equation
from percolation theory when $\lambda_{\text{dry}} = 0$ (see Table 2). Interestingly, in section 4, we show that under other circumstances the GD model may reduce to the weighted arithmetic, harmonic, and geometric mean models. However, some of those conditions might be unrealistic, as we will discuss.

Although Eq. (1) formulates $\lambda$ implicitly as a function of $\theta$, Ghanbarian and Daigle (2016) derived $\theta$ in terms of $\lambda$ and presented the following explicit $\theta(\lambda)$ form:

$$
\theta = \frac{\left(\lambda^{1/t_s} - \lambda^{1/t_s}_{\text{dry}}\right)\left(\theta_s + (\theta_s - \theta_c)\lambda^{1/t_s}\right)}{\left(\lambda_{\text{sat}}^{1/t_s} - \lambda^{1/t_s}_{\text{dry}}\right)\lambda^{1/t_s}}
$$

(2)

In what follows, we present an explicit solution of Eq. (1) and derive $\lambda$ as a function of $\theta$. One, therefore, might straightforwardly calculate $\lambda$ at different water contents from $\lambda_{\text{dry}}, \lambda_{\text{sat}}, \theta_s, \theta_c$ and $t_s$ values.

3. Explicit $\lambda(\theta)$ form of the GD Model

Although Eq. (1) has 5 physically-meaningful parameters, it can be presented in a form including 4 combined parameters as follows:

$$
\theta = a_1 + a_2 \lambda^{1/t_s} + a_3 \lambda^{-1/t_s}
$$

(3)

in which
\[ a_1 = \frac{\theta c \lambda_{sat}^{1/\tau_s} - (\theta_s - \theta_c) \lambda_{dry}^{1/\tau_s}}{\lambda_{sat}^{1/\tau_s} - \lambda_{dry}^{1/\tau_s}}, \quad a_2 = \frac{\theta - \theta_c}{\lambda_{sat}^{1/\tau_s} - \lambda_{dry}^{1/\tau_s}}, \quad a_3 = \frac{-\theta c \lambda_{sat}^{1/\tau_s} \lambda_{dry}^{1/\tau_s}}{\lambda_{sat}^{1/\tau_s} - \lambda_{dry}^{1/\tau_s}} \] (4)

Multiplying both sides of Eq. (3) by \( \Lambda = \lambda^{1/\tau_s} \), Eq. (3) can be written in the following form of a second order polynomial

\[ a_2 \Lambda^2 + (a_1 - \theta) \Lambda + a_3 = 0 \] (5)

The general solution to Eq. (5) is

\[ \Lambda = \frac{- (a_1 - \theta) \pm \sqrt{(a_1 - \theta)^2 - 4a_2a_3}}{2a_2} \] (6)

Equation (6) can be alternatively written in the following form, yielding the explicit \( \lambda(\theta) \) form of the GD model:

\[ \lambda = \left[ b_1 + b_2 \theta + \text{sgn}(t_s) b_2 \sqrt{b_3 + 2b_2^{-1} \theta + \theta^2} \right]' \] (7)

where sgn is the sign function [i.e., sgn(\( x > 0 \)) = 1, sgn(\( x < 0 \)) = -1] and
\[ b_1 = \frac{-\theta_c \lambda_{\text{sat}}^{1/t_s} + (\theta_s - \theta_c) \lambda_{\text{dry}}^{1/t_s}}{2(\theta_s - \theta_c)}, \quad b_2 = \frac{\lambda_{\text{sat}}^{1/t_s} - \lambda_{\text{dry}}^{1/t_s}}{2(\theta_s - \theta_c)}, \]

\[ b_3 = \frac{\left[ \theta_c \lambda_{\text{sat}}^{1/t_s} - (\theta_s - \theta_c) \lambda_{\text{dry}}^{1/t_s} \right]^2 + 4\theta_c (\theta_s - \theta_c) \lambda_{\text{sat}}^{1/t_s} \lambda_{\text{dry}}^{1/t_s}}{\left( \lambda_{\text{sat}}^{1/t_s} - \lambda_{\text{dry}}^{1/t_s} \right)^2} \]  \quad (8)

Note that since theoretically \( t_s > 0 \), the sign function in Eq. (7) can be disregarded. The four parameters of Eq. (7) can be either calculated directly from Eq. (8) or considered as fitting parameters.

In order to validate the above derivation, Eq. (7) was compared to Eq. (2) using various values of the critical water content \( \theta_c \) and the scaling exponent \( t_s \). Comparisons shown in Fig. 1 verify that Eqs. (2) and (7) are equivalent. It should be noted that for very small \( t_s \) values (i.e., \( t_s \to 0 \)), \( \Lambda \) from Eq. (6) becomes negative, leading to undefined \( \lambda \) in the explicit form of the GD model, Eq. (7). The implicit \( \lambda-\theta \) form, Eq. (2), tends to a step function, as \( t_s \) approaches zero (see Fig. 1).

Although \( t_s \) is assumed to be a positive value according to its physical definition in Ghanbarian and Daigle (2016), the GD model works “mathematically” for \( t_s < 0 \) as well.

4. Special Cases of the GD Model

In what follows, we indicate that the explicit \( \lambda(\theta) \) form derived in this study reduces to some well-known empirical models as well as mixing models presented in the literature.

4.1. Mixing Model (\( \theta_c = 0 \))

For \( \theta_c = 0 \), Eq. (8) becomes
Equation (9) yields 

\[ b_3 = \frac{(b_1/b_2)^2}{2} \]

that results in

\[ b_3 + 2b_1b_2^{-1}\theta + \theta^2 = \left(\theta + b_1b_2^{-1}\right)^2 \]

(10)

By substituting Eq. (10) into Eq. (7), the explicit \( \lambda(\theta) \) form of the GD model reduces to the following model:

\[
\lambda = \left[ \frac{1}{t_s} \frac{\lambda_{\text{dr}}^{1/t_s} + \theta \left( \lambda_{\text{sat}}^{1/t_s} - \lambda_{\text{dr}}^{1/t_s} \right)}{\theta_s} \right]^{t_s} = \left( \frac{\theta - \theta c}{\theta_s} \lambda_{\text{dr}}^{1/t_s} + \frac{\theta}{\theta_s} \lambda_{\text{sat}}^{1/t_s} \right)^{t_s}
\]

(11)

which is a general power mean model and reduces to the weighted arithmetic and harmonic mean models for \( t_s = 1 \) and \(-1 \), respectively. However, we should point out that within the percolation-based effective-medium approximation, negative \( t_s \) is not physically meaningful. The unrealistic negative \( t_s \) value (i.e., \( t_s = -1 \)), may be a consequence of forcing \( \theta c \) to be zero, which can be unrealistic for medium- and fine-textured soils. As Ghanbarian and Daigle (2016) indicated, the GD model reduces to the weighted harmonic mean under other conditions as well, i.e., \( \theta c = \theta s \) and \( t_s = 1 \).

Equation (11) also provides a physical basis for empirical models that relate \( \lambda \) to \( \theta \) by a power function. The empirical model of Chen et al. (2008) presented in Table 1 is a notable example of such models.

It can be indicated that Eq. (11) is also equivalent to the mixing model presented in Table 1 [i.e., equivalent to Eq. (3) of Likos (2015)]:
\begin{equation}
\lambda = \left[ \lambda_{\text{solid}}^{1/p} (1-\theta_s) + \lambda_{\text{water}}^{1/p} \theta + \lambda_{\text{air}}^{1/p} (\theta_s - \theta) \right]^p
\end{equation}

where \( \lambda_{\text{solid}} \), \( \lambda_{\text{water}} \) and \( \lambda_{\text{air}} \) are the thermal conductivities of solid particles, water and air phases, respectively, and \( p \) is the power mean exponent. Equation (12) reduces to the parallel, series, and quadratic-parallel mixing models for \( p = 1, -1, \) and \( 2, \) respectively (Cosenza et al., 2003; Dong et al., 2015).

Assuming that \( \lambda_{\text{air}} \) is negligible, \( \lambda_{\text{dry}} \) and \( \lambda_{\text{sat}} \) can be determined from Eq. (12) as follows:

\begin{equation}
\lambda_{\text{dry}} = \lambda(\theta = 0) = \lambda_{\text{solid}} (1-\theta_s)^p
\end{equation}

\begin{equation}
\lambda_{\text{sat}} = \lambda(\theta = \theta_s) = \left[ \lambda_{\text{dry}}^{1/p} + \lambda_{\text{water}}^{1/p} \theta_s \right]^p
\end{equation}

Combining Eqs. (12), (13) and (14) yields exactly the same \( \lambda(\theta) \) functional relationship as Eq. (11). This verifies the equivalence of Eq. (11) to the mixing model Eq. (12) and provides a new linkage between \( t_s \) and \( p \) (the power mean exponent) that, so far, has been considered mainly equal to 1, \(-1\) or 2 values in the literature. More specifically, we demonstrated that \( p \) is equal to the scaling exponent \( t_s \) defined physically in Ghanbarian and Daigle (2016).

4.2. Chung-Horton Model \((\theta_c = 0, t_s = 1)\)

We indicated above that the GD model reduces to the weighted arithmetic mean model for the case of \( \theta_c = 0 \) and \( t_s = 1 \). Here we show that an approximation of the GD model for this case can also lead to the functional form of the Chung and Horton (1987) (CH) model presented in Table 1. The CH model has been widely applied particularly because the HYDRUS software package implements this model.
For $\theta_c = 0$, the function $(\theta + b_1/b_2)^2$ would be a monotonically increasing function of $\theta$ in the range of 0 and $\theta_s$, and the ratio $b_1/b_2$ would be negligible. It can be indicated that the GD model will reduce to the CH model if one approximates the quadratic function $f = (\theta + b_1/b_2)^2$ by a linear function in the form of $f' = A\theta$, where $A$ is the slope of the line. The best fitting slope $A$ can be analytically derived by minimizing the integrated difference between $f$ and $f'$:

$$\int_0^{\theta_s} (f - f')d\theta = \int_0^{\theta_s} \left[ (\theta + b_1/b_2^{-1})^2 - A\theta \right]d\theta = 0 \quad (15)$$

Solving Eq. (15) gives:

$$A = 0.75\theta_s + 2b_1b_2^{-1} \quad (16)$$

Assuming $f = b_3 + 2b_1b_2^{-1}\theta + \theta^2 = (\theta + b_1b_2^{-1})^2 \approx A\theta$, Eq. (7) reduces to

$$\lambda = \left( b_1 + b_2\theta + b_2\sqrt{A\sqrt{\theta}} \right)^{t_s} \quad (17)$$

Equation (17) is analogous to the empirical Chung and Horton (1987) model, which is

$$\lambda = p_1 + p_2\theta + p_3\sqrt{\theta} \quad (18)$$

Setting $t_s = 1$ in Eq. (17) and comparing Eqs. (17) and (18) provide physical meaning for the empirical constant coefficients $p_1$, $p_2$, and $p_3$ in the CH model. Accordingly, one has

$$p_1 = b_1, p_2 = b_2, p_3 = b_2\sqrt{0.75\theta_s + 2b_1b_2^{-1}} \quad (19)$$

4.3. Comparing the GD Model with its Special Cases
Comparing Eq. (2) with Eq. (11) shown in Fig. 2 verifies that the GD model reduces to the
mixing model for $\theta_c = 0$. As mentioned above, the parallel, series and quadratic parallel mixing
models are obtained when $t_s = 1$, $-1$ and 2, respectively. Figure 2 also illustrates that the CH
model, Eq. (18), is a relatively close approximation of the GD model when $\theta_c = 0$ and $t_s = 1$.
Because the CH model is an approximation of the GD model, dry and saturated soil thermal
conductivities in this model showed to be slightly less than the preset $\lambda_{dry}$ and $\lambda_{sat}$ in the GD
model.

5. Estimating thermal conductivity in soils

5.1. Regression-based Relationships to Determine $t_s$ and $\theta_c$

In this section, we aim to estimate thermal conductivity using the GD model from available soil
textural properties. For this purpose, we propose regression-based relationships to link the
critical water content $\theta_c$ and the scaling exponent $t_s$ to other soil properties. Ghanbarian and
Daigle (2016) fit Eq. (2) to measured thermal conductivity of 17 samples from Lu et al. (2007;
2011; 2013) and reported $\theta_c$, $t_s$, $\lambda_{dry}$ and $\lambda_{sat}$ values for each soil (see Table 3). Using data
reported in Table 3, one finds:

$$\theta_c = 0.0033Clay(\%), \ R^2 = 0.93 \tag{20}$$

$$t_s = -0.0025Clay(\%) + 0.342, \ R^2 = 0.72 \tag{21}$$

Equations (20) and (21) indicate that $\theta_c$ and $t_s$ are strongly correlated to clay content (see Fig. 3).
However, one should apply them with caution to estimate $\theta_c$ and $t_s$ for soils whose clay content is
greater than 40%. Note that although Eq. (20) was previously reported by Ghanbarian and Daigle
(2016), Eq. (21) is presented for the first time here. To derive Eq. (21), we, however, had to remove two outliers (probably due to experimental errors) shown via filled blue circles in Fig. 3 corresponding to soil no. 5 (the first two silty clay loams with $t_s = 0.369$ and 0.351) in Table 3. Given that the pore size distribution index of the Brooks and Corey (1964) soil water retention model is correlated with soil texture, i.e., the finer the texture, the less the pore size distribution index (Brooks and Corey, 1964), one should expect that $t_s$ and $\theta_c$ be correlated to the pore size distribution index. However, this needs to be tested either experimentally or numerically.

We should point out that Eqs. (20) and (21) were derived using only 17 soil samples and, thus, one should not expect them to accurately estimate $\theta_c$ and $t_s$ values and accordingly saturation-dependent thermal conductivity for all types of soils. In the following, we compare thermal conductivity estimates via Eq. (2) with $\theta_c$ and $t_s$ estimated using Eqs. (20) and (21) for four sand packs with various porosities from Chen (2008).

### 5.2. Comparison with Sand Pack Experiments

Chen (2008) measured thermal conductivity at various water contents in four sand packs of various gradations and porosities. Sample A consists of uniform sands of medium size, while sample B incorporates uniform coarse sands. Sample C includes uniform fine sands, and sample D consists of medium sized well-graded sands. All packs have more than 99% quartz sand meaning that their clay content is negligible. We accordingly set clay content equal to zero in Eqs. (20) and (21) and found $\theta_c = 0$ and $t_s = 0.342$ in such sand packs. Using the available and measured porosity $\phi (= \theta_s)$, $\lambda_{dry}$ and $\lambda_{sat}$ values, we then estimated the saturation-dependent thermal conductivity via the GD model. Results shown in Fig. 4 indicate that the greater the
porosity the lower the thermal conductivity. This is because thermal conductivity of quartz is substantially greater than the thermal conductivity of water and air. Figure 4 also demonstrates that the GD model with $\theta_c = 0$ and $t_s = 0.342$ accurately estimates the saturation-dependent thermal conductivity in all sand packs. More specifically, the estimated $\theta_c = 0$ is in good agreement with the experiments. The scaling exponent of 0.342 also provides the correct shape of the thermal conductivity curve. Undoubtedly, one should expect more errors in the estimation of thermal conductivity when $\lambda_{dry}$ and $\lambda_{sat}$ values are roughly estimated from other soil properties, e.g., bulk density and/or porosity (see Lu et al., 2007; 2014).

5.3. Typical Thermal Conductivity Curves for Sand, Loam and Clay

In the previous section, we showed that thermal conductivity could be estimated from clay content, porosity and thermal conductivities measured under completely dry and fully saturated conditions. The main purpose of this section is to determine parameters of the proposed $\lambda(\theta)$ function, Eq. (7), for three main soil texture classes of sand, loam and clay, which are used in the HYDRUS model.

In Table 4 we summarize parameters of the proposed $\lambda(\theta)$ function, assuming three representative soils for sand, loam and clay textures based on the USDA soil classification. Selecting representative clay content for each texture (e.g., 5, 17 and 40% for sand, loam and clay, respectively), we estimated $\theta_c$ using Eq. (20) and $t_s$ using Eq. (21). Specifically, we found $\theta_c = 0.017, 0.056$ and 0.132 and $t_s = 0.330, 0.300$ and 0.242 for sand, loam and clay textures, respectively. As can be observed, $\theta_c$ increases while $t_s$ decreases as clay content increases. We also determined the value of $\theta_s$ for each texture using the data reported in Table 2 from Clapp

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and Hornberger (1978). The values of $\lambda_{\text{dry}}$ and $\lambda_{\text{sat}}$ given in Table 4 for each soil texture were estimated via the following equations from Côté and Konard (2005):

$$\lambda_{\text{dry}} = 0.75 \times 10^{-1.2 \theta_s} \quad (22)$$

$$\lambda_{\text{sat}} = \lambda_{\text{solid}}^{1-\theta_s} \lambda_{\text{water}}^{\theta_s} \quad (23)$$

In Eq. (23), $\lambda_{\text{water}} = 0.6 \text{ W m}^{-1} \text{ K}^{-1}$ and the value of $\lambda_{\text{solid}}$ can be determined using another geometric-mean equation from the quartz content $q$ and thermal conductivities of quartz ($\lambda_{\text{quartz}} = 7.7 \text{ W m}^{-1} \text{ K}^{-1}$) and other minerals ($\lambda_o$) as follows:

$$\lambda_{\text{solid}} = \lambda_{\text{quartz}}^q \lambda_o^{1-q} \quad (24)$$

in which $\lambda_o = 2$ and $3 \text{ W m}^{-1} \text{ K}^{-1}$ for soils with $q > 0.2$ and $q \leq 0.2$, respectively (Lu et al., 2007). Here, we assumed that the quartz content is approximately equal to the representative sand content (see Table 4) and estimated $\lambda_{\text{solid}}$ for each soil texture. Interestingly, $\lambda_{\text{solid}} = 7$ and $2.7 \text{ W m}^{-1} \text{ K}^{-1}$, $\lambda_{\text{dry}} = 0.252$ and $0.198 \text{ W m}^{-1} \text{ K}^{-1}$ and $\lambda_{\text{sat}} = 2.654$ and $1.31 \text{ W m}^{-1} \text{ K}^{-1}$ are close to those values estimated by Côté and Konard (2005) for respectively a sandy and a clayey soil from Kersten (1949). They found $\lambda_{\text{solid}} = 5.5$ and $2.8 \text{ W m}^{-1} \text{ K}^{-1}$, $\lambda_{\text{dry}} = 0.27$ and $0.19 \text{ W m}^{-1} \text{ K}^{-1}$ and $\lambda_{\text{sat}} = 2.42$ and $1.30 \text{ W m}^{-1} \text{ K}^{-1}$ (see Table 3 of Côté and Konard, 2005).

One may notice that the value of $\lambda_{\text{sat}}$ for the sand texture with an average porosity of 0.395 is much greater than that for the clay texture with an average porosity of 0.482 (see Table 4 and Fig. 5). This is in accord with our statement explaining the greater the porosity the smaller the thermal conductivity. One should note that $\lambda_{\text{sat}}$ is a complicated function of several factors such as mineralogy, porosity, and clay content [see Eq. (9) in Ghanbarian and Daigle (2016)]. As a
consequence, a simple geometric relationship linking $\lambda_{\text{sat}}$ to $\lambda_{\text{solids}}$, $\lambda_{\text{water}}$ and $\theta_c$ [i.e., Eq. (23)] only provides a rough approximation.

Using the values given in Table 4 and the GD model, Eq. (2), we determined the saturation-dependent thermal conductivity for the sand, loam and clay textures. Figure 5 shows typical thermal conductivity curves for such soil classes. As can be observed, the clay soil texture has a relatively lower thermal conductivity compared to that of loam and sand. This is mainly because the estimated $\lambda_{\text{sat}}$ value via Eq. (23) is larger in the loam and sand textures. Figure 5 clearly indicates how the value of $\theta_c$ affects the shape of the thermal conductivity curve. Although all curves depicted in Fig. 5 show sigmoidal behaviors, it is more profound in the clay soil texture.

6. Concluding Remarks

In this study, we derived an explicit $\lambda(\theta)$ form of the Ghanbarian and Daigle (2016) physically-based model for thermal conductivity in partially saturated soils. We also demonstrated that the mixing and Chung-Horton models are special cases of the GD model under specific circumstances, e.g., $\theta_c = 0$. Given that $\theta_c$ particularly in fine-textured soils might be significantly greater than zero, the accuracy of the mixing and Chung-Horton models would be questionable. We, therefore, recommend model developers to use the GD model in their numerical codes for improved simulation of water and heat flow in the vadose zone. We believe that the HYDRUS model, which currently implements the Chung-Horton and Campbell (1985) models (see Table 1), could benefit from not only the generality of the GD model and its theoretical basis and physically meaningful parameters, but also its capability in estimating saturation-dependent thermal conductivity. Future investigations are required to possibly link the GD model
parameters to soil hydraulic properties, such as soil water retention curve. This may enhance the GD model parametrization when employed in soil flow models.

Acknowledgement

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References


Kersten, M.S. 1949. Laboratory research for the determination of the thermal properties of soils. Research Laboratory Investigations, Engineering Experiment Station, University of Minnesota, Minneapolis, Minn. Technical Report 23.


Table 1. Mixing model (the first) and empirical models (others) for thermal conductivity of partially saturated soils.

<table>
<thead>
<tr>
<th>Model</th>
<th>No. of param.</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \lambda = \left[ \lambda_{\text{solid}}^{1/p} (1 - \theta_s) + \lambda_{\text{water}}^{1/p} \theta + \lambda_{\text{air}}^{1/p} (\theta_s - \theta) \right]^p )</td>
<td>5</td>
<td>Cosenza et al. (2003); Dong et al. (2013); Likos (2015)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) (\theta / \theta_s)^{0.5} )</td>
<td>3</td>
<td>Somerton et al. (1974)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \left[ 1 + p \ln \left( \theta / \theta_s \right) \right] )</td>
<td>4</td>
<td>Johansen (1977)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{solid}}^{1-\theta_s} \lambda_{\text{water}}^{\theta_s} \left[ p (1 - \theta / \theta_s^2) \right] )</td>
<td>4</td>
<td>Donazzi et al. (1979)</td>
</tr>
<tr>
<td>( \lambda = p_1 + p_2 \theta + p_3 \exp \left[ -\left( p_4 \theta \right)^{p_5} \right] )</td>
<td>5</td>
<td>Campbell (1985)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \left[ 1 - \exp \left( p \theta / \theta_s \right) \right] )</td>
<td>4</td>
<td>Ewen and Thomas (1987)</td>
</tr>
<tr>
<td>( \lambda = p_1 + p_2 \theta + p_3 \sqrt{\theta} )</td>
<td>3</td>
<td>Chung and Horton (1987)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \frac{p \theta / \theta_s}{1 + (p - 1) \theta / \theta_s} )</td>
<td>4</td>
<td>Côté and Konrad (2005)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \left[ 1 - \exp \left( p \theta / \theta_s \right) \right] + \left( \lambda_{\text{sat}} - \lambda_{\text{sat}}^\prime \right) \theta / \theta_s )</td>
<td>5</td>
<td>Markle et al. (2006)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \exp \left{ p_1 \left[ 1 - \left( \theta / \theta_s \right)^{p_2} \right] \right} )</td>
<td>5</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{solid}}^{1-\theta_s} \lambda_{\text{water}}^{\theta_s} \left[ p_1 + (p_1 - \theta / \theta_s)^{p_2} \right] )</td>
<td>5</td>
<td>Chen et al. (2008)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + \exp \left[ p_1 + \theta^{p_2} \right] )</td>
<td>3</td>
<td>Lu et al. (2014)</td>
</tr>
<tr>
<td>( \lambda = \lambda_{\text{dry}} + (\lambda_{\text{sat}} - \lambda_{\text{dry}}) \left{ 1 + \left[ 1 + \left( \theta / \theta_f \right)^p \right]^{1/p-1} \right} )</td>
<td>4</td>
<td>Lu and Dong (2015)</td>
</tr>
</tbody>
</table>

\( \lambda \) is thermal conductivity, \( \theta \) is soil volumetric water content, \( \theta_s \) is saturated water content, \( \theta_f \) is soil water content at which the funicular regime is onset, \( \lambda_{\text{dry}}, \lambda_{\text{sat}}, \lambda_{\text{solid}}, \lambda_{\text{water}} \) and \( \lambda_{\text{air}} \) are \( \lambda \) of dry soil, saturated soil, solid particles, water and air, respectively, \( p, p_1, p_2 \) and \( p_3 \) are model-specific fitting parameters, and \( \lambda_{\text{sat}} \) is \( \lambda(\theta_s) \) from the Ewen and Thomas (1987) model.
Table 2. Special cases of the percolation-based effective-medium approximation thermal conductivity model of Ghanbarian and Daigle (2016), Eq. (1), under various conditions.

<table>
<thead>
<tr>
<th>Description</th>
<th>Model</th>
<th>Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Weighted arithmetic mean</td>
<td>$\lambda = (\theta_s - \theta) \lambda_{\text{dry}} + \theta \lambda_{\text{sat}}$</td>
<td>$t_s = 1$ and $\theta_c = 0$</td>
</tr>
<tr>
<td>Weighted harmonic mean</td>
<td>$\lambda = \left[ (\theta_s - \theta) \lambda_{\text{dry}}^{-1} + \theta \lambda_{\text{sat}}^{-1} \right]^{-1}$</td>
<td>$t_s = 1$ and $\theta_c = \theta_s$</td>
</tr>
<tr>
<td>Geometric mean</td>
<td>$\lambda = \left( \lambda_{\text{dry}} \lambda_{\text{sat}} \right)^{0.5}$</td>
<td>$t_s = 1$ and $\theta_c = 0.5 \theta_s$</td>
</tr>
<tr>
<td>Bruggeman (1935) model</td>
<td>$(\theta_s - \theta) \frac{\lambda_{\text{dry}} - \lambda}{\lambda_{\text{dry}} + 2\lambda} + \theta \frac{\lambda_{\text{sat}} - \lambda}{\lambda_{\text{sat}} + 2\lambda} = 0$</td>
<td>$t_s = 1$ and $\theta_c = \theta_s/3$</td>
</tr>
<tr>
<td>Power-law scaling from percolation theory</td>
<td>$\lambda = \lambda_{\text{sat}} \left( \frac{\theta - \theta_c}{\theta_s - \theta_c} \right)^{t_s}$</td>
<td>$\lambda_{\text{dry}} = 0$</td>
</tr>
</tbody>
</table>
Table 3. Soil physical properties and parameters of the percolation-based effective-medium approximation model (Eq. 2) for 17 soil samples from the literature (after Ghanbarian and Daigle, 2016).

<table>
<thead>
<tr>
<th>Soil No.</th>
<th>Texture</th>
<th>Sand (%)</th>
<th>Silt (%)</th>
<th>Clay (%)</th>
<th>BD* (g cm⁻³)</th>
<th>OM (%)</th>
<th>λ_{dry} (W m⁻¹ K⁻¹)</th>
<th>λ_{sat} (W m⁻¹ K⁻¹)</th>
<th>tₛ</th>
<th>θ_c</th>
<th>R²</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Sand</td>
<td>94</td>
<td>1</td>
<td>5</td>
<td>1.60</td>
<td>0.09</td>
<td>0.253</td>
<td>2.186</td>
<td>0.336</td>
<td>0</td>
<td>0.98</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>2</td>
<td>Sandy loam</td>
<td>67</td>
<td>21</td>
<td>12</td>
<td>1.39</td>
<td>0.86</td>
<td>0.231</td>
<td>1.676</td>
<td>0.307</td>
<td>0.037</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>3</td>
<td>Loam</td>
<td>40</td>
<td>49</td>
<td>11</td>
<td>1.20</td>
<td>0.49</td>
<td>0.215</td>
<td>1.352</td>
<td>0.329</td>
<td>0.032</td>
<td>0.97</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td></td>
<td>Loam</td>
<td>40</td>
<td>49</td>
<td>11</td>
<td>1.30</td>
<td>0.49</td>
<td>0.202</td>
<td>1.617</td>
<td>0.341</td>
<td>0.031</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td></td>
<td>Loam</td>
<td>40</td>
<td>49</td>
<td>11</td>
<td>1.40</td>
<td>0.49</td>
<td>0.203</td>
<td>1.61</td>
<td>0.340</td>
<td>0.032</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>4</td>
<td>Silt loam</td>
<td>27</td>
<td>51</td>
<td>22</td>
<td>1.33</td>
<td>1.19</td>
<td>0.225</td>
<td>1.401</td>
<td>0.256</td>
<td>0.089</td>
<td>0.97</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>5</td>
<td>Silty clay loam</td>
<td>19</td>
<td>54</td>
<td>27</td>
<td>1.20</td>
<td>0.39</td>
<td>0.227</td>
<td>1.366</td>
<td>0.369</td>
<td>0.090</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td></td>
<td>Silty clay loam</td>
<td>19</td>
<td>54</td>
<td>27</td>
<td>1.30</td>
<td>0.39</td>
<td>0.241</td>
<td>1.428</td>
<td>0.351</td>
<td>0.087</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td></td>
<td>Silty clay loam</td>
<td>19</td>
<td>54</td>
<td>27</td>
<td>1.40</td>
<td>0.39</td>
<td>0.305</td>
<td>1.466</td>
<td>0.254</td>
<td>0.102</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>6</td>
<td>Silty clay loam</td>
<td>8</td>
<td>60</td>
<td>32</td>
<td>1.30</td>
<td>3.02</td>
<td>0.243</td>
<td>1.337</td>
<td>0.289</td>
<td>0.099</td>
<td>0.98</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>7</td>
<td>Clay loam</td>
<td>32</td>
<td>38</td>
<td>30</td>
<td>1.29</td>
<td>0.27</td>
<td>0.222</td>
<td>1.367</td>
<td>0.279</td>
<td>0.101</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>8</td>
<td>Sand</td>
<td>93</td>
<td>1</td>
<td>6</td>
<td>1.60</td>
<td>0.07</td>
<td>0.301</td>
<td>2.129</td>
<td>0.313</td>
<td>0.006</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>9</td>
<td>Sand</td>
<td>94</td>
<td>1</td>
<td>5</td>
<td>1.60</td>
<td>0.09</td>
<td>0.272</td>
<td>1.735</td>
<td>0.337</td>
<td>0</td>
<td>0.99</td>
<td>Lu et al. (2013)</td>
</tr>
<tr>
<td>10</td>
<td>Sand</td>
<td>92</td>
<td>7</td>
<td>1</td>
<td>1.58</td>
<td>0.6</td>
<td>0.229</td>
<td>2.283</td>
<td>0.324</td>
<td>0.028</td>
<td>0.98</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>11</td>
<td>Loam</td>
<td>50</td>
<td>41</td>
<td>9</td>
<td>1.38</td>
<td>0.25</td>
<td>0.225</td>
<td>1.769</td>
<td>0.296</td>
<td>0.036</td>
<td>0.99</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>12</td>
<td>Silt loam</td>
<td>11</td>
<td>70</td>
<td>19</td>
<td>1.31</td>
<td>0.84</td>
<td>0.287</td>
<td>1.587</td>
<td>0.291</td>
<td>0.071</td>
<td>0.96</td>
<td>Lu et al. (2007)</td>
</tr>
<tr>
<td>13</td>
<td>Silty clay</td>
<td>7</td>
<td>50</td>
<td>43</td>
<td>1.29</td>
<td>2.09</td>
<td>0.163</td>
<td>1.001</td>
<td>0.225</td>
<td>0.135</td>
<td>0.97</td>
<td>Lu et al. (2011)</td>
</tr>
</tbody>
</table>

* BD is bulk density, and OM is organic matter.
Table 4. Parameters of the proposed $\lambda(\theta)$ function, Eq. (7), for three main soil textures assumed based on the USDA soil classification.

<table>
<thead>
<tr>
<th>Texture</th>
<th>Sand (%)</th>
<th>Clay (%)</th>
<th>$\theta_s$</th>
<th>$\theta_c$</th>
<th>$\lambda_{dry}$</th>
<th>$\lambda_{sat}$</th>
<th>$t_s$</th>
<th>$b_1$</th>
<th>$b_2$</th>
<th>$b_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand</td>
<td>93</td>
<td>5</td>
<td>0.395</td>
<td>0.017</td>
<td>0.252</td>
<td>2.654</td>
<td>0.330</td>
<td>-0.4253</td>
<td>25.4496</td>
<td>0.0003</td>
</tr>
<tr>
<td>Loam</td>
<td>38</td>
<td>17</td>
<td>0.451</td>
<td>0.056</td>
<td>0.216</td>
<td>1.534</td>
<td>0.300</td>
<td>-0.2921</td>
<td>5.2621</td>
<td>0.0032</td>
</tr>
<tr>
<td>Clay</td>
<td>23</td>
<td>40</td>
<td>0.482</td>
<td>0.132</td>
<td>0.198</td>
<td>1.310</td>
<td>0.242</td>
<td>-0.5749</td>
<td>4.3583</td>
<td>0.0175</td>
</tr>
</tbody>
</table>

$\theta_s$ (cm$^3$/cm$^3$) is the average value from Clapp and Hornberger (1978), $\theta_c$ (cm$^3$/cm$^3$) and $t_s$ were determined from clay content and respectively Eqs. (20) and (21), $\lambda_{dry}$ (W m$^{-1}$ K$^{-1}$) was estimated from saturated water content using Eq. (22), $\lambda_{sat}$ (W m$^{-1}$ K$^{-1}$) was determined via Eqs. (24) having $\lambda_{water} = 0.6$ W m$^{-1}$ K$^{-1}$ and $\lambda_{solid}$ calculated from Eq. (23) (= 7.0, 3.3, and 2.7 W m$^{-1}$ K$^{-1}$ for sand, loam, and clay, respectively), and final parameters of Eq. (7), $b_1$, $b_2$ and $b_3$, were calculated from Eq. (8).
Figure 1. Thermal conductivity $\lambda$ as a function of volumetric water content $\theta$ for various values of the critical water content $\theta_c$ (a) and the scaling exponent $t_s$ (b) obtained from the original Ghanbarian-Daigle (GD) model, Eq. (2), represented by solid lines, and the explicit $\lambda(\theta)$ solution derived here, Eq. (7), denoted by unfilled circles, for a soil sample with parameters shown.
Figure 2. Thermal conductivity $\lambda$ as a function of volumetric water content $\theta$ for the critical water content $\theta_c = 0$ and various values of the scaling exponent $t_s$ obtained from the original Ghanbarian-Daigle (GD) model, Eq. (2), represented by solid lines, the mixing model, Eq. (11), denoted by unfilled circles, and the Chung-Horton (CH) model, Eq. (18). The empirical parameters of the CH model were calculated directly from Eq. (19).
Figure 3. (a) Critical water content $\theta_c$ and (b) scaling exponent $t_s$ versus clay content (%) for 17 soil samples from Lu et al. (2007, 2011, 2013). Filled blue circles identify outliers in plot (b), which were eliminated to fit a linear function.
Figure 4. Thermal conductivity $\lambda$ as a function of water saturation $S_w = \theta/\phi$ for four sand packs i.e., samples A, B, C and D from Chen (2008). Filled circles and curves represent measured data points and estimated thermal conductivity for each sand pack. The critical water content $\theta_c = 0$ and the scaling exponent $t_\theta = 0.342$ were estimated from clay content using Eqs. (20) and (21), respectively.
Figure 5. Typical saturation-dependent thermal conductivity curves determined via the GD model (Eq. 1) for sand, loam and clay soil texture classes. The GD model input parameters are given in Table 4.