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An Empirical Model for Estimating Soil Thermal Conductivity from Texture, Water Content, and Bulk Density

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Soil thermal conductivity (λ) models are needed frequently in studying coupled heat and water transfer in soils. Several models are available, but some are complicated and some produce relatively large errors. In this study, we developed a simple model for estimating λ from soil texture, bulk density (ρ_b), and water content (θ). Three parameters, α, β, and λ_{dry}, are included in the model, where λ_{dry} is determined by ρ_b and α and β are shape factors estimated from soil texture and ρ_b. Empirical relations were developed for α and β by fitting the model to heat-pulse (HP) measurements of $\lambda(\theta)$ on seven soils of various textures. The model performance was evaluated with independent $\lambda(\theta)$ data from independent HP measurements and literature values. The results show that the model is able to express the $\lambda(\theta)$ curves from oven dry to saturation at fixed ρ_b values. When ρ_b is varied, the estimated λ data agree well with measured values. The root mean square errors are <0.15 W m^{-1} K^{-1}, and the bias is within 0.10 W m^{-1} K^{-1}. The new model has the potential for use in studying heat movement in soils of varying texture, bulk density, and water content and can be incorporated into numerical algorithms for describing coupled heat and mass transfer processes.

Abbreviations: HP, heat pulse; PSD, particle size distribution; RMSE, root mean square error.

Soil thermal conductivity (λ), a measure of the ability of a soil to conduct heat, is needed frequently in soil science (Horton and Ochsner, 2011). The magnitude of λ depends largely on soil texture, mineral composition, water content (θ), and bulk density (ρ_b) (de Vries, 1963; Campbell, 1985). At similar θ and ρ_b values, a sandy soil usually has a higher λ value than a clay soil. A soil with higher quartz content (f_q) usually has greater λ because quartz has a λ value two times that of most other soil minerals (Campbell, 1985). Larger ρ_b, or smaller porosity, leads to greater λ, as more solid matter per unit volume results in better contacts between soil particles (Farouki, 1986). The arrangement of soil particles and soil microstructure also influences λ significantly (Kohout et al., 2004; Ju et al., 2011).

Under field conditions, soil λ is strongly affected by θ, which changes dynamically with time and depth. Several semi-theoretical and empirical models have been developed to estimate λ from θ or the degree of saturation (S_r). De Vries (1963) presented a physically based model that treated soil as a mixture of ellipsoidal particles in the continuous media of air and water. This model has been used widely for modeling soil λ with considerable accuracy (Wierenga et al., 1969; Campbell et al., 1994). Farouki (1986) indicated that the major er-

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rors of the de Vries (1963) model came from the assumption that soil particles were not in contact with each other, and a 25% increase from the original λ estimations was suggested on dry soils. The approximation procedure in de Vries (1963) for estimating particle shape factors also produces errors in λ estimations. Johansen (1977) proposed an empirical function for estimating λ of unfrozen and frozen soils. The normalized λ (i.e., Kersten's number K_e) was introduced to relate λ with S_r and soil mineral composition for the entire soil water content range. Recently, the Johansen (1977) model was improved by reducing the λ estimation errors effectively at lower water contents (Côté and Konrad, 2005; Lu et al., 2007).

Although the normalized λ(θ) models give considerable accuracy for estimating λ, it has been demonstrated that the Johansen (1977) model is sensitive to soil porosity when used for estimating soil heat fluxes (Peters-Lidard et al., 1998). A few θ-based λ relations, e.g., Campbell (1985) and Chung and Horton (1987), have also been used and even been incorporated into models such as the Soil–Vegetation–Atmosphere Scheme (SVATS) and HYDRUS (Šimůnek et al., 2005). The drawback of the Campbell (1985) model are that it is difficult to determine the five model parameters. The λ(θ) relation of Chung and Horton (1987) is represented by a polynomial expression with only a single set of parameters each for sand, loam, and clay. Compared with experimental data, the λ(θ) relations of Chung and Horton (1987) are not able to fully express the λ(θ) relations for soils with various soil textures and different ρ_b. In addition, the Chung and Horton (1987) equation was developed for water contents between the residual water content and the saturated water content and thus is not valid for water contents less than the residual water content. Poor soil λ estimations are bound to cause large biases in surface energy balance studies and in predicting soil temperature (Peters-Lidard et al., 1998).

Many researchers have investigated the effect of the quartz (or sand) fraction on λ estimations, but no existing λ model considers the influence of soil clay content on λ, especially at low and intermediate water contents. Lu et al. (2007) presented thermal conductivity equations for "coarse-" and "fine-textured" soils, further confirming the importance of the soil clay content for estimating soil λ values. Tarnawski and Leong (2012) reported that the diverse trends of λ vs. S_r could be attributed to the difference in soil water retention in the miniscule pore space, which in turn, was influenced by soil texture. Few studies are available that have evaluated the effects of various ρ_b values on λ estimations. Thus, there is a need to develop a relatively simple and accurate λ(θ) function for different soil textures and ρ_b values.

In this study, we have developed a simple λ(θ) model with three empirical parameters that can be easily derived from soil texture and ρ_b. The model was established using heat-pulse (HP) λ(θ) data, and the model performance was examined using comprehensive data sets from additional, independent λ(θ) measurements and literature values.

MATERIALS AND METHODS

Soil Samples

Seventeen mineral soils were used in this study (Table 1): four from Ochsner et al. (2001), 11 from Lu et al. (2007), one from Lu et al. (2011), and one from Lu et al. (2013). Table 1 lists the particle size distribution (PSD), organic matter content, and ρ_b of the repacked soils. The soil samples were air dried, ground, and sieved through a 2-mm screen. Soil PSD was determined with the pipette method (Gee and Or, 2002), and the soil organic matter content was determined with the Walkley–Black titration method (Nelson and Sommers, 1982).

Heat Pulse Measurement of Soil Thermal Conductivity

The λ values of Soils 1 to 13 were determined with the HP method on repacked soil columns with fixed ρ_b and θ from air dry to saturation (Ochsner et al., 2001; Lu et al., 2007, 2013). For Soils 14 to 17, HP measurements were performed on soil samples repacked with various ρ_b and θ values (Ochsner et al., 2001).

Prescribed amounts of water were added to air-dried soil samples, which were then mixed thoroughly and packed into cylinders (50.2-mm inner diameter and 50.2 mm high) at the desired ρ_b. The packed soil columns were placed in a temperature-regulated room (20 ± 1°C) for 24 h before making the HP measurements. A thermo-time domain reflectometry probe (Ren et

Table 1. The soils used for calibrating and evaluating the new model, as well as the bulk density ranges for repacking the soil samples.

Soil	Texture	Particle size distribution			Bulk density	Organic matter content	Source
		2–0.05 mm	0.05–0.002 mm	<0.002 mm			
		%			g cm^{-3}	%	
1	sand	94	1	5	1.60	0.09	Lu et al. (2007)
2	sandy loam	67	21	12	1.39	0.86	Lu et al. (2007)
3	loam	40	49	11	1.20/1.30/1.40	0.49	Lu et al. (2007)
4	silt loam	27	51	22	1.33	1.19	Lu et al. (2007)
5	silty clay loam	19	54	27	1.20/1.30/1.40	0.39	Lu et al. (2007)
6	silty clay loam	8	60	32	1.30	3.02	Lu et al. (2007)
7	clay loam	32	38	30	1.29	0.27	Lu et al. (2007)
8	sand	93	1	6	1.60	0.07	Lu et al. (2007)
9	sand	94	1	5	1.50	0.09	Lu et al. (2013)
10	sand	92	7	1	1.58	0.60	Lu et al. (2007)
11	loam	50	41	9	1.38	0.25	Lu et al. (2007)
12	silt loam	11	70	19	1.31	0.84	Lu et al. (2007)
13	silty clay	7	50	43	1.29	2.09	Lu et al. (2011)
14	sandy loam	66	23	11	0.95–1.69	2.3	Ochsner et al. (2001)
15	clay loam	37	35	28	0.85–1.52	2.3	Ochsner et al. (2001)
16	silt loam	23	64	13	0.91–1.45	0.9	Ochsner et al. (2001)
17	silty clay loam	12	56	32	1.05–1.47	1.1	Ochsner et al. (2001)

al., 1999) was used for measuring soil λ with the HP method. For details about the theory, equipment, and procedures of measuring soil thermal properties with the HP method, please refer to Ren et al. (1999) and Ochsner et al. (2001). The HP measurements were repeated three times, and average λ values were calculated. The soil samples were oven dried at 105°C to constant mass, and ρ_b and θ were determined.

For Soils 1 to 13, the recorded temperature data with time were analyzed with MATLAB software (The MathWorks) with consideration of finite probe effects following Lu et al. (2013). For Soils 14 to 17, the original λ(θ) data and soil properties of Ochsner et al. (2001) were used, where the λ values were calculated following the pulsed infinite line source theory.

Model Evaluation

The root mean square error (RMSE) and bias of the estimations were calculated to evaluate the performance of the new model:

$$\mathrm{RMSE}=\sqrt{\frac{\sum\left(\lambda_m-\lambda_e\right)^2}{n}} \quad [1]$$

$$\mathrm{bias}=\frac{\sum\left(\lambda_m-\lambda_e\right)}{n} \quad [2]$$

where n is the number of data points, λ_m is the measured λ, and λ_e is the λ estimated by the models.

MODEL DEVELOPMENT

General Characteristics of the Water-Content-Based Thermal Conductivity Curve

Soil thermal conductivity as a function of soil water content [i.e., the λ(θ) curve] has been investigated extensively (Farouki, 1986). Generally, the λ(θ) curve is divided into different zones with respect to various water domains, with each domain having a specific feature. For example, Tarnawski and Gori (2002) split the λ(θ) curve into four zones representing residual, transitory meniscus, micro/macroporous capillary, and superfluous water. In the residual water domain, water is held tightly on a soil particle surface by adhesion force, and the soil λ remains almost constant because water has an insignificant contribution to heat conduction. When the surfaces of all soil particles are coated, water bridges are formed between solid particles. As a result, heat conduction between soil particles is improved and λ increases sharply with the increasing θ (Ewing and Horton, 2007). After most soil capillaries are wetted, additional water fills the larger pores between soil particles. At this stage, λ increases with linearly θ but with a smaller slope than for the capillary water domain because the contribution of the water supply to thermal conductivity mainly stems from replacing air with water. Finally, λ hardly changes with θ in the superfluous water domain, where capillary and drainable water fills almost all of the pores.

Key Soil Factors Determining the Shape of the Water-Content-Based Thermal Conductivity Curve

The nonlinear behavior of λ as a function of θ varies mainly with the soil mineral composition, ρ_b, and the soil structure (de Vries, 1963; Farouki, 1986; Lu et al., 2007; Ju et al., 2011). Figure 1 shows the λ(θ) data of a sand soil, a sandy loam soil, and a silt loam soil across the entire θ range. The data were adopted from Tarnawski and Leong (2012) and Tarnawski et al. (2013). The sand is Toyoura sand, while the sandy loam and silt loam are Canadian field soils that were denoted as Cumberland and Acadia soils in Tarnawski and Leong (2012). Toyoura sand has been reported to be 100% sand. The sandy loam and silt loam were reported to contain 61 and 33% sand, respectively. The clay fractions (f_{cl}) are 0, 5, and 10% for the sand, sandy loam, and silt loam, respectively. It is evident that the λ(θ) curves vary significantly for the different soils. The Toyoura sand has the largest λ values across the entire θ range, and λ increases dramatically with θ, while only a gradual increase is observed for the silt loam. The diverse λ(θ) trends among these soils of different texture can be attributed to the differences in the sand fraction f_{sa} (or f_q) and the formation of water bridges between soil particles. The f_q for sand, sandy loam, and silt loam are 0.9, 0.7, and 0.5, respectively. Quartz has a λ of 7.7 W m^{-1} K^{-1}, which is much larger than that of most other soil minerals (with an average λ of 2.13 W m^{-1} K^{-1}, Tarnawski et al., 2012). It is expected that soils with a relatively large f_{sa} have relatively large λ values and a sharply increasing rate as θ increases. For fine-textured soils with relatively large clay fractions (thus, large specific areas), a relatively large water content is required to form the water bridges, which determines the efficiency of heat transfer through both soil solids and liquid (Lu et al., 2007; Tarnawski and Leong, 2012), thus a more gradual λ change with θ is observed.

Soil ρ_b influences the λ(θ) curves by modifying the amount of contacts between soil solids and the ratio of soil solids in the bulk soil. As shown in Fig. 1, larger λ values are recorded

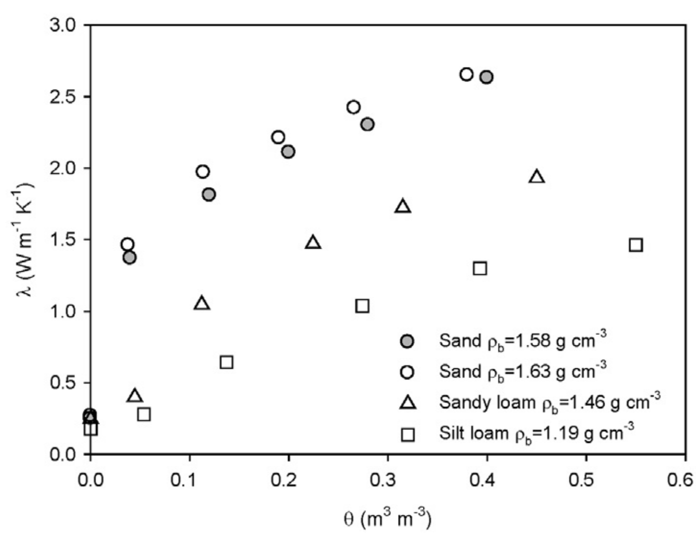

Fig. 1. The thermal conductivity (λ) vs. water content (θ) data for three soils with different bulk densities (ρ_b) from Tarnawski and Leong (2012) and Tarnawski et al. (2013).

when the ρ_b of the sand is increased from 1.58 to 1.63 g cm^{-3}. Analysis by Ochsner et al. (2001) indicated that soil λ values decreased linearly with increasing air-filled porosity, which was inversely related to ρ_b.

General Features of the New Model

Tarnawski and Gori (2002) applied linear functions to depict the dependence of λ on θ in the four water domains. Several studies of the published $\lambda(\theta)$ curves (e.g., de Vries, 1963; Ochsner et al., 2001), however, have indicated that for mineral soils at moderate temperature, a complete $\lambda(\theta)$ curve resembles the shape of an exponential curve. Lu et al. (2007) successfully improved the normalized $\lambda(S_r)$ relation using an exponential equation. In this study, we propose the following exponential function to express the nonlinear behavior of λ as related to soil θ, texture, and ρ_b:

$$\lambda = \lambda_{dry} + \exp\left(\beta - \theta^{-\alpha}\right) \qquad \theta > 0 \qquad [3]$$

where λ_{dry} is the thermal conductivity of an oven-dried soil sample (W m^{-1} K^{-1}), and parameters α and β are shape factors of the $\lambda(\theta)$ curve, which are related to soil texture and ρ_b. Mathematically, the term λ_{dry} represents the intercept (i.e., λ at zero θ), thus it has no influence on the shape of the $\lambda(\theta)$ curve. The linear equation of Lu et al. (2007) can be applied to estimate λ_{dry} from the soil porosity (τ):

$$\lambda_{dry} = -0.56\tau + 0.51 \qquad [4]$$

The influence of parameters α and β on the shape of the $\lambda(\theta)$ curve are illustrated in Fig. 2, where λ_{dry} is set at 0.2 W m^{-1} K^{-1}. In Fig. 2a, α is a constant, fixed at 0.3, and β is increased from 1.0 to 1.6. Generally, the model produces larger λ values with increasing β across the entire θ range, and the gaps between the neighboring $\lambda(\theta)$ curves become larger with increasing θ (Fig. 2a). Therefore parameter β modifies the rate of λ change with θ, but it has a more significant effect on the magnitude of λ at higher θ values. A larger β indicates a greater λ value near saturation and a relatively faster increase in λ with θ.

In Fig. 2b, β is a constant, fixed at 1.5, and α varies from 0.2 to 0.8. The four curves vary greatly in their sharpness, as indicated by the larger differences in λ scales and the rates of λ increase at lower θ values. Mathematically, the curves representing different α values converge toward the end, indicating that the extent of α effects on the $\lambda(\theta)$ curves becomes less near saturation. Thus, parameter α characterizes the sensitivity of λ to the change in θ. A large α value indicates that λ is impervious to θ change, especially at lower water contents.

Relating Parameters α and β to Soil Texture and Bulk Density

Our analysis shows clearly that the response of λ to changing θ is sensitive to parameters α and β: both affect the shape and scale of the $\lambda(\theta)$ curve, but the effect of α has more weight on the curvature of the curve (i.e., the rate of change at lower water contents) and β has greater influences on the magnitude of λ, especially at higher water contents. Meanwhile, we have demonstrated that soils with coarse textures and higher ρ_b values tend to have greater λ values and sharply increasing rates as θ is increased, while fine-textured soils usually show lower λ values and more gradual responses to θ changes (Fig. 1). Therefore, it is reasonable to assume that parameters α and β are related to soil texture (e.g.,f_{sa} and f_{cl}) and ρ_b. We hypothesize that curvature of the $\lambda(\theta)$ curve is controlled mainly by parameter α and is related to f_{cl}, while the scale of the $\lambda(\theta)$ curve is determined by parameter β, which is a function of f_{sa} and ρ_b.

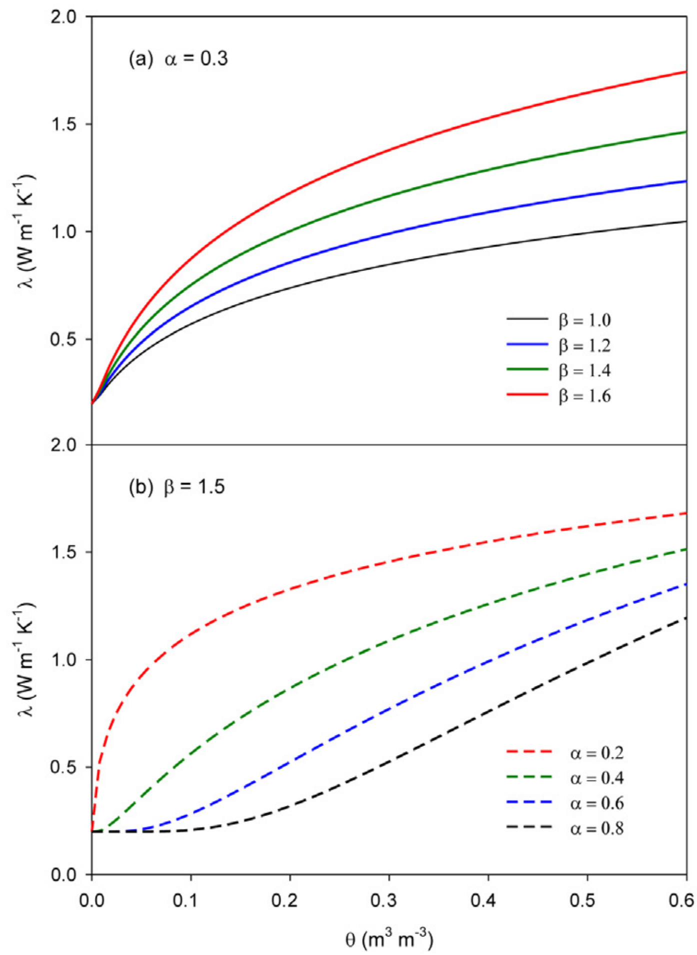

Fig. 2. The effects of the parameters (a) β and (b) α on thermal conductivity (λ)–water content (θ) curves obtained with Eq. [3]. The thermal conductivity of dry soil samples was set at 0.20 W m^{-1} K^{-1}.

Lu et al. (2007) established and tested a thermal conductivity model using measured $\lambda(\theta)$ data for 12 soils across the entire water content range. Soil texture ranged from sand to clay loam, and soil ρ_b varied from 1.20 to 1.60 g cm^{-3}. Lu et al. (2007) demonstrated that the $\lambda(\theta)$ curves differed considerably between coarse- and fine-textured soils. In this work, we recalculated the soil λ using the raw data of Lu et al. (2007) by accounting for the influences of the finite probe body on HP measurements (Lu et al., 2013). The recalculated λ data were used to develop the new model (Eq. [3]). To estimate α

and β for these soils, we first calculated λ_{dry} using the linear relationship between λ_{dry} and soil porosity τ from Eq. [4]. Soil porosity τ was calculated with the measured ρ_b values, assuming a soil particle density of 2.65 g cm^{-3}. For each soil, α and β were estimated by fitting Eq. [3] to the HP λ(θ) data using a nonlinear optimization procedure (Wolfram, 2003). The results are presented in Fig. 3 and Table 2. The new model was able to describe the λ–θ relation across the entire θ range for seven soils (Fig. 3). For soils with a relatively large quartz fraction (fine sands), relatively large λ values were calculated and the λ(θ) curves display dramatically increasing trends at lower and intermediate water contents (Fig. 3a), while the λ(θ) curves for loamy and clayey soils tend to show relatively slow λ changes in response to θ increases (Fig. 3b).

It can be seen from Table 2 that the fitted α values for coarse soils (Soils 1 and 2) are smaller than those for medium-textured (Soils 3 and 4) and fine-textured soils (Soils 5, 6, and 7), indicating an increasing α trend with respect to f_{cl}. This is reasonable because the soils with higher f_{cl} require more water to form water bridges between solid particles. Based on the results presented in Table 2, we established the following linear relationship between f_{cl} and α:

$$\alpha = 0.67 f_{cl} + 0.24 \quad [5]$$

The trend of β is more complicated because it generally increases with soil ρ_b as well as f_{sa}. Because β is influenced by ρ_b and f_{sa}, we used a multiple regression method to determine the dependence of β on ρ_b and f_{sa} using the results in Table 2. Using the multiple regression method with data analysis in Excel, we obtained the following relationship for β, with a coefficient of determination of 0.98 ($n = 7$):

$$\beta = 1.97 f_{sa} + 1.87\rho_b - 1.36 f_{sa}\rho_b - 0.95 \quad [6]$$

Therefore, as long as soil texture (e.g., f_{sa} and f_{cl}) and ρ_b data are available, soil λ can be estimated as a function of θ using Eq. [3–6].

RESULTS AND DISCUSSION

Model Evaluation with Heat-Pulse Water-Content-Based Thermal Conductivity Data Measured under Fixed Bulk Density

We first tested the performance of the new model on Soils 8 to 13, where λ(θ) measurements were obtained at a fixed ρ_b value for each soil. Equations [3–6] were applied to estimate soil λ values from f_{sa}, f_{cl}, ρ_b, and θ. In Eq. [4], soil porosity τ was calculated from ρ_b, taking the soil particle density as 2.65 g cm^{-3}.

Figure 4 presents the λ(θ) measurements (symbols) along with the model estimations (curves) for the six soils. The measured values had the following characteristics:

1. The λ_{dry} values, ranging from 0.22 (Soil 13) to 0.29 (Soil 8) W m^{-1} K^{-1}, were quite similar for soils with different textures.
2. At lower and intermediate θ ranges, λ increased with θ, but the rates of increase varied considerably among the soils. Sands (Soils 8–10) had sharp increases, while loamy soils (Soils 11 and 12) and a clayey soil (Soil 13) had more gradual increases.
3. At θ near saturation, the sandy soils had higher λ values

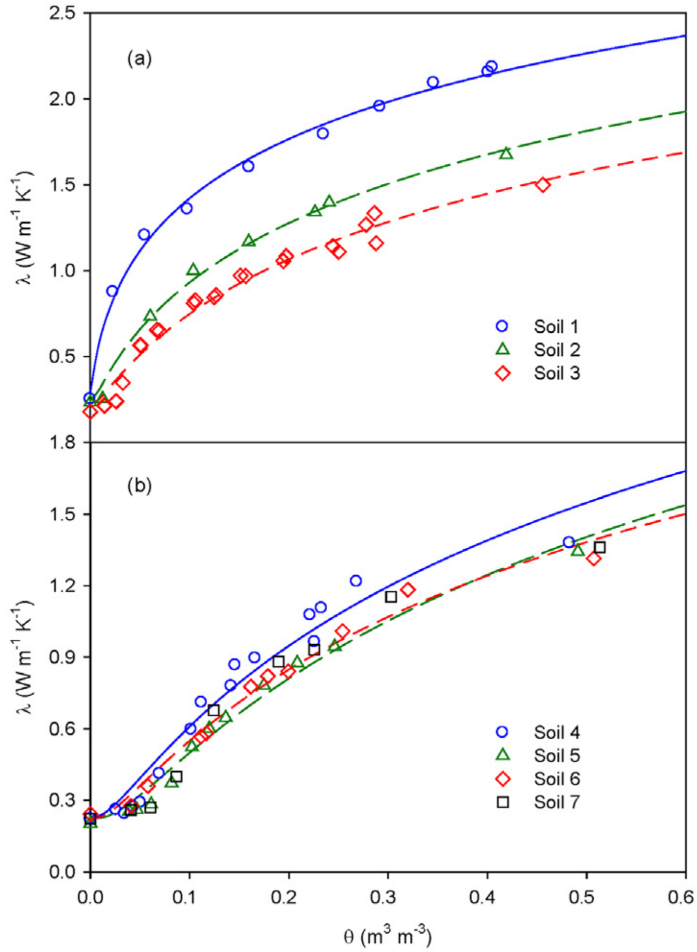

Fig. 3. Heat-pulse measured (symbols) and fitted (curve) thermal conductivity (λ) vs. water content (θ) data for (a) coarse-textured soils and (b) fine-textures soils. The curves were obtained by fitting Eq. [3] to the measured λ(θ) data using a nonlinear optimization procedure (Wolfram, 2003).

Table 2. Soil porosity (τ) and estimated model parameters for the seven soils used for model calibration. The thermal conductivity of oven-dry soil samples (λ_{dry}) was calculated with Eq. [4], and the shape factors α and β were obtained by fitting Eq. [3] to heat-pulse-measured thermal conductivity vs. water content.

Soil	τ	λ_{dry}	α	β
		W m^{-1} K^{-1}		
1	0.40	0.29	0.24	1.86
2	0.48	0.24	0.32	1.70
3	0.51	0.23	0.35	1.58
4	0.50	0.23	0.41	1.61
5	0.51	0.23	0.45	1.53
6	0.51	0.23	0.42	1.48
7	0.51	0.22	0.44	1.54

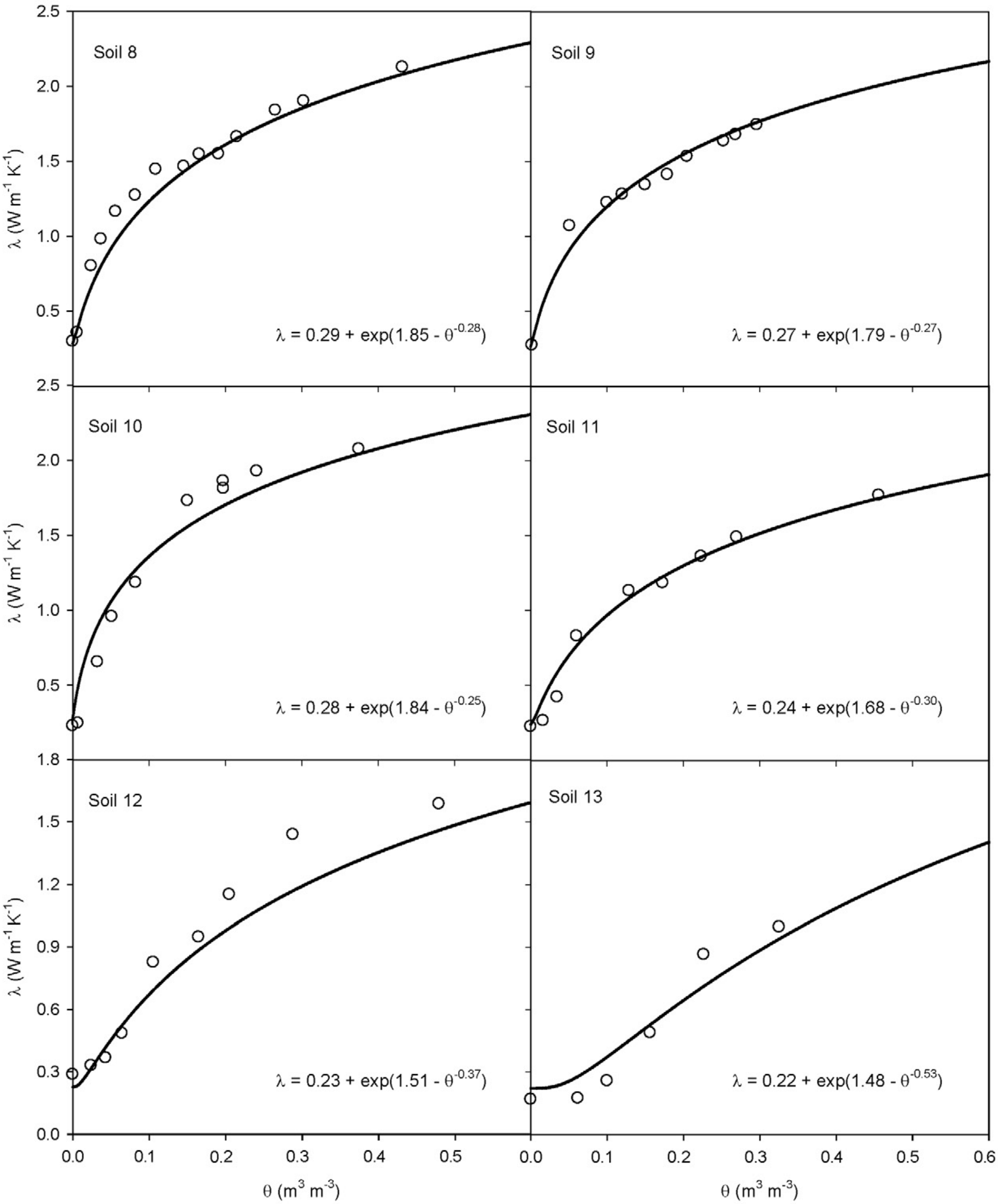

Fig. 4. Measured (symbols) and estimated (lines) thermal conductivity (λ) vs. water content (θ) data for six soils. The estimations were obtained with Eq. [3], where the parameters α and β were calculated using Eq. [5] and [6] and the thermal conductivity of an oven-dried soil sample (λ_{dry}) was calculated using Eq. [4]. The λ(θ) equation for each soil is included.

(about 2.0 W m^{-1} K^{-1}) than did the loamy and clayey soils (about 1.5 W m^{-1} K^{-1}).

The new model captured these features of the λ(θ) curves with relatively constant λ_{dry} and variable shape parameters α and β (Fig. 4). Compared with the sandy soils, the loamy and clayey soils had greater α values and smaller β values, which produced slower λ responses to changes in θ and relatively lower λ values near saturation.

The estimation accuracies of the new model, as expressed by the RMSE and bias, are presented in Table 3. The new model generally gave reliable λ estimations, with RMSE ranging from 0.07 to 0.15 W m^{-1} K^{-1} and bias ranging from −0.01 to 0.08 W m^{-1} K^{-1}. For the three sandy soils with similar ρ_b values, the bias of the λ estimations ranged from −0.01 (Soil 10) to 0.07 W m^{-1} K^{-1} (Soil 8). For loamy and clayey soils, except for Soil 12, the new model gave λ estimates with fairly good accuracy across the entire θ range. Bristow (1998) and Tarnawski et al. (2012) reported that using f_{sa} instead of f_q for λ estimations produces significant errors in λ. Mineral composition analysis using the X-ray diffraction technique showed that these soils contained abundant amounts of quartz (data not shown). However, the dominant mineral for Soil 12 was moganite, while it was α-quartz for the other soils. The deviation of λ for Soil 12 may be caused by the differences in crystal structure and other physical properties between moganite and α-quartz (Zhang and Moxon, 2014).

The positive or negative bias values in model predictions indicate that soil λ may be over- or underestimated by the empirical model. Heat-pulse measurement errors, originating from the non-uniformity of repacked soil columns at different water contents, may also produce uncertainties in bias estimation. For example, a fixed ρ_b value (1.50 g cm^{-3} for Soil 9) was used in the model, but the actual ρ_b (e.g., 1.51 or 1.49 g cm^{-3}) for a specific packed column may differ slightly from this value.

Model Evaluation Using Heat-Pulse Water-Content-Based Thermal Conductivity Data Measured under Variable Bulk Density

As discussed above, the soil ρ_b influences λ by modifying the soil solid particle contacts in the bulk soil. In moist soil samples, ρ_b and θ interactively determine the degree of particle-to-particle contacts and the effectiveness of heat transfer. Figure 5 presents HP measurements of the λ(θ) curves of Soils 3 and 5 with three different ρ_b values (1.20, 1.30, and 1.40 g cm^{-3}). Soil 3 has a larger f_{sa} value, thus it exhibits larger λ than Soil 5 for a given θ. For both soils, increasing ρ_b generally leads to an increase in λ. However, the magnitude of λ change in response to increasing ρ_b is insignificant in the dry range, becoming apparent in the intermediate and high θ regions. The threshold water contents are about 0.10 and 0.15 m^3 m^{-3} for Soils 3 and 5, respectively (Fig. 5).

Ochsner et al. (2001) presented HP measurements for complete θ ranges of four soils with various textures and a large range in ρ_b (Table 1). Ochsner et al. (2001) provided a comprehensive data set for evaluating the performance of λ(θ) models. In this study, we evaluated the new model by comparing its λ(θ) estimates with those of the Lu et al. (2007) model. The input parameters for the Lu et al. (2007) model are λ_{dry}, λ_{sat}, and S_r, where λ_{dry} was estimated with Eq. [4], λ_{sat} was determined with the geometric mean equation, and S_r was calculated from τ and θ data.

Figure 6 compares the measurements of Ochsner et al. (2001) vs. the estimations from the new model and from the Lu et al. (2007) model. Measured and estimated values are distributed randomly along the 1:1 line, the slopes of the regression lines are close to unity, and the coefficients of determination were >0.90. Thus, the new model provided relatively accurate λ estimates, and the new model estimates were similar to those of the Lu et al. (2007) model. Error analysis showed that the RMSEs of λ estimates from the new model and the Lu et al. (2007) model were within 0.15 and 0.17 W m^{-1} K^{-1}, respectively, and the corresponding bias of λ estimates were in the range of −0.06 to 0.10 and −0.11 to 0.11 W m^{-1} K^{-1}, respectively (Table 4). Clearly, the λ estimation errors of the new model are acceptable and are slightly lower than those of the Lu et al. (2007) model. Thus, the new model is simpler and easier to use than the Lu et al. (2007) model.

It should be pointed out that the λ results of Ochsner et al. (2001) may be slightly biased toward underestimation of the actual λ values because their calculation procedure did not account for influences of soil–probe contact resistance and the finite radius and heat capacity of the HP probe. The RMSE and bias of the model estimates would be smaller if those influences were accounted for in data processing (Lu et al., 2013).

Table 3. Root mean square error (RMSE) and bias of thermal conductivity estimations with the new model for Soils 8 to 13.

Soil	RMSE	Bias
	W m^{-1} K^{-1}	
8	0.10	0.07
9	0.07	0.00
10	0.15	−0.01
11	0.08	−0.02
12	0.13	0.08
13	0.10	−0.02

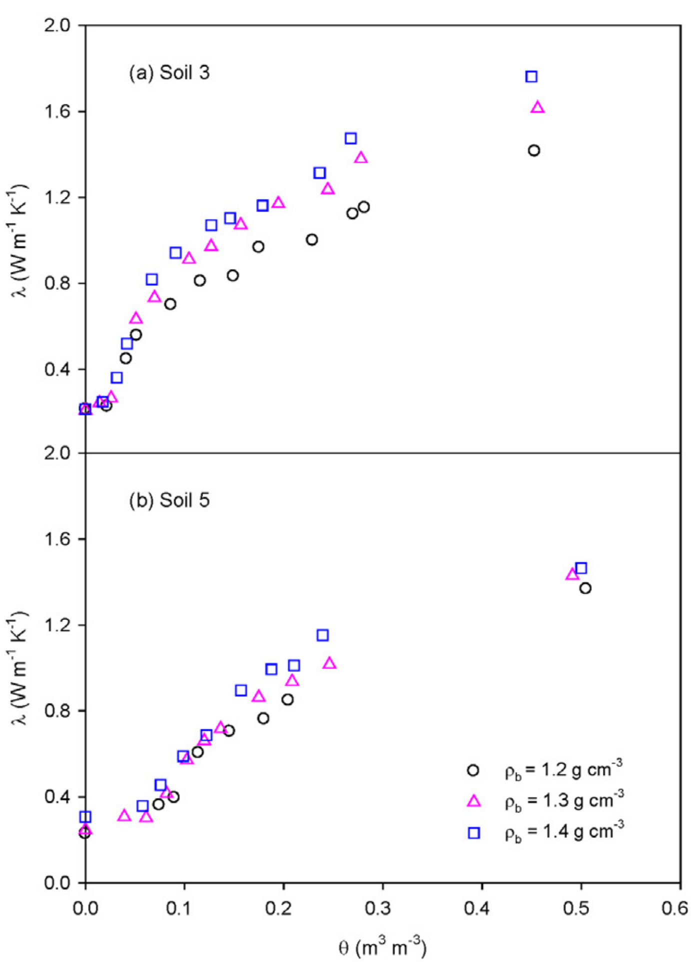

Fig. 5. Measured thermal conductivity (λ) vs. water content (θ) data with different soil bulk densities (ρ_b) for (a) Soil 3 and (b) Soil 5.

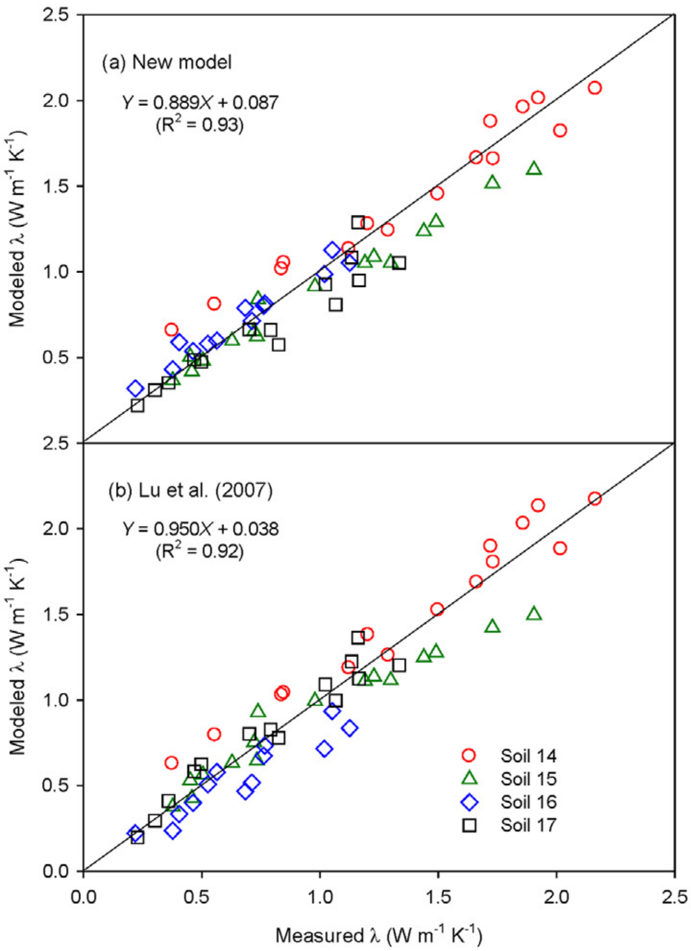

Fig. 6. Comparison of soil thermal conductivity (λ) measurements from Ochsner et al. (2001) with estimated values using (a) the new model and (b) the Lu et al. (2007) model. The regression equations and coefficients of determination for the measured vs. estimated λ are included.

Potential Limitations and Solutions

Our analysis indicated that the new model generally provides reliable λ estimations with information on the soil θ, texture, and ρ_b. However, like many other pedotransfer functions that estimate soil properties from PSD information, the new model is not expected to give accurate λ estimations for every soil and in all circumstances. This is caused by the fact that, in addition to soil PSD, θ, and ρ_b, λ is also influenced by other factors such as particle shape, mineral composition, temperature, organic matter content, and soil structure. It may be necessary to correct the model for particular soils with significant amounts of clay and organic matter, and under conditions when soils show abnormal thermal behaviors (e.g., high temperature and apparent structure formation).

Table 4. Root mean square error (RMSE) and bias of the new model and the Lu et al. (2007) model for four soils from Ochsner et al. (2001).

Soil	RMSE		Bias	
	New model	Lu et al. (2007)	New model	Lu et al. (2007)
	W m^{-1} K^{-1}			
14	0.15	0.15	−0.06	−0.11
15	0.15	0.17	0.10	0.07
16	0.08	0.15	−0.06	0.11
17	0.15	0.09	0.09	−0.03

For λ_{dry} estimation, we used the linear relationship between the λ of dry samples and the soil porosity τ (i.e., Eq. [4]), which was established by Lu et al. (2007) using measurements on 18 mineral soil samples. The applicability of this equation to soils with particular compositions (e.g., higher ratios of quartz, expansive clay, and organic content) requires further validation. In addition, the information on soil ρ_b and particle density (ρ_s) is necessary for estimating the soil porosity τ. Although ρ_b can be measured accurately, it shows strong spatial and temporal variability in the tilled layer (Liu et al., 2014), which is usually ignored because of difficulties in determining in situ ρ_b continuously. For ρ_s, we assumed a value of 2.65 Mg m^{-3}. In reality, depending on the soil composition, the ρ_s of mineral soils may vary from 2.50 to 2.80 Mg m^{-3} (Sumner, 1999). Inaccurate ρ_b and ρ_s data will cause further uncertainties in λ_{dry} estimates with the new model.

The shape factor α of the new model is related linearly to the soil f_{cl} (Eq. [3]). Any error in f_{cl} will transfer directly to α and then affect the rate of λ change in response to θ. Because Eq. [3] was established based on f_{cl} measurements with the pipette method (Gee and Or, 2002), it is advisable to use f_{cl} data measured following the same procedure. There are reports that particle size analysis with the laser technique tends to underestimate f_{cl} (Konert and Vandenberghe, 1997; Gee and Or, 2002), which will result in smaller α values than the pipette method.

The new model uses a nonlinear equation (Eq. [6]) for estimating shape factor β from soil ρ_b and f_{sa} with the assumption that the PSD is representative of the soil mineralogy. This is a simplified approximation because quartz has a significantly higher λ than most other minerals of similar particle size (de Vries, 1963). Bristow (1998) illustrated that a change in the ratio between quartz and other minerals could cause λ to vary by a factor greater than two across a large part of the water content. Lu et al. (2007) also demonstrated that using f_{sa} instead of f_q yielded biased soil λ.

Considering the fact that f_q is often unknown and could occur in all particle sizes (Balland and Arp, 2005), here we propose a single-point correction method to estimate β, especially for coarse-textured soils. For a soil of known PSD and ρ_b, the parameters α and λ_{dry} are calculated with Eq. [5] and [4], respectively. Assuming that a single-point measurement of λ_i is made at a specific water content θ_i (preferably at an intermediate water content where the largest changes related to β occur), then β can be determined using the following equation (obtained by rearrangement of Eq. [3]):

$$\beta = \ln\left(\lambda_i - \lambda_{dry}\right) + \theta_i^{-\alpha} \quad [7]$$

We expect that when soil PSD and ρ_b information are available, together with a measured data point (θ_i, λ_i), the new model should be able to provide accurate λ values as a function of θ.

Model Applications

Under field conditions, λ is a key property influencing heat exchange between the soil and atmosphere and between top and deep soil layers. It has been well established that the spatial and temporal changes of λ are controlled mainly by soil texture, ρ_b, and f_q (de Vries, 1963; Bristow, 1998). Due to the complicated mechanisms involved, however, there is a lack of quantitative information. The new model provides the opportunity to investigate the collective effects of the PSD, ρ_b, and θ on λ. Figure 7 presents three-dimensional $\lambda(\theta, \rho_b)$ graphs obtained using the new model applied to three hypothetical soils with distinct textures (Table 5). The θ data extend from dry to saturation, and ρ_b covers a typical range for a tilled soil layer (1.0–1.6 Mg cm^{-3}). For dry conditions, the three soils display similar patterns with changes in ρ_b (as determined by Eq. [4]). However, with increasing ρ_b and θ, the λ of the sand rose sharply at lower θ values and became flat at intermediate water contents, while the λ changes of the clay were slow at lower θ values and only became significant at θ values near saturation. It should be noted that for illustration purposes, the same θ and λ scales were used for the three soils, which produced different maximum λ values (about 2.09, 2.01, and 1.62 W m^{-1} K^{-1} for the sand, loam, and clay soils, respectively). In reality, the clay soil may have a higher porosity than loamy and sandy soils. It is expected that, at saturated water contents, λ differences among the soils will not be as large as those shown in Fig. 7.

Information on λ dynamics is required for many comprehensive models (e.g., HYDRUS, SVATS, and the Root Zone Water Quality Model [RZWQM; Ahuja et al., 2000]) that simulate heat exchange between the soil and atmosphere and/or coupled heat and water flow processes within soil profiles. In these models, the PSD, ρ_b, and θ data are usually available. Therefore, Eq. [3–6] can be incorporated into these models for estimating λ with soil texture, ρ_b, and θ under different management systems.

CONCLUSIONS

In this study, we developed a new model for estimating soil λ values at room temperature. The model has three parameters: λ_{dry}, α, and β. The parameter λ_{dry} was related to soil porosity (which was estimated from soil ρ_b), and empirical relationships were developed to calculate the shape factors α and β with PSD information and the soil ρ_b.

Model evaluations using heat-pulse measurements and literature data revealed that the new model could

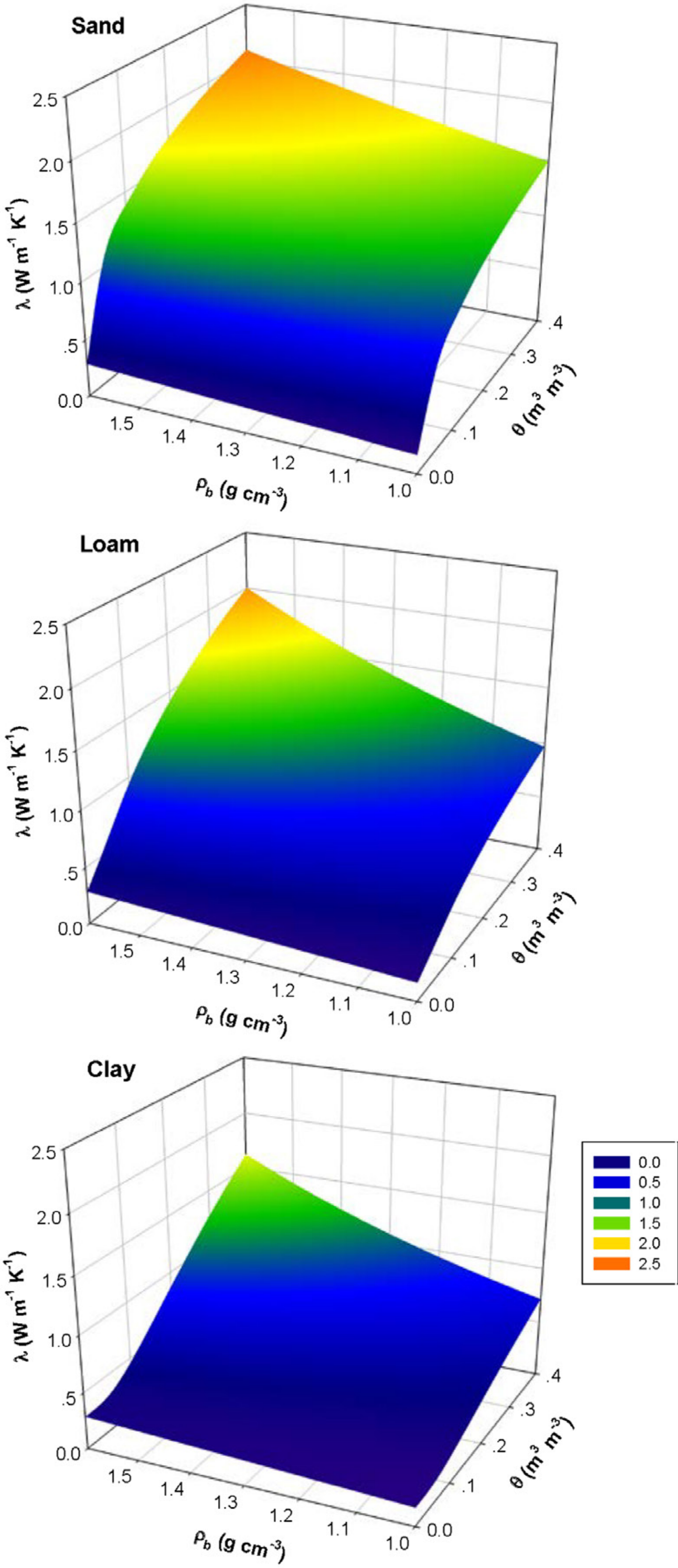

Fig. 7. The effects of soil water content (θ) and bulk density (ρ_b) on thermal conductivity (λ) for three hypothetical soils.

Table 5. Hypothetical texture and bulk density for three soils used to illustrate the interactive effects of water content and bulk density on thermal conductivity with the new model.

Soil texture	Particle size distribution			Bulk density range
	2–0.05 mm	0.05–0.002 mm	<0.002 mm	
	——— % ———			g cm^{-3}
Sand	100	0	0	1.00–1.60
Loam	45	35	20	1.00–1.60
Clay	30	20	50	1.00–1.60

provide reliable λ estimations, with results were comparable to those obtained by the Lu et al. (2007) model. The new model can be incorporated in simulation software packages for studying coupled heat and water processes in soils.

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