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An Empirical Model for Estimating Soil Thermal Diffusivity from Texture, Bulk Density, and Degree of Saturation

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An Empirical Model for Estimating Soil Thermal Diffusivity from Texture, Bulk Density, and Degree of Saturation

Abstract
Soil thermal diffusivity $\kappa$ is an essential parameter for studying surface and subsurface heat transfer and temperature changes. It is well understood that $\kappa$ mainly varies with soil texture, water content $\theta$, and bulk density $\rho_b$, but few models are available to accurately quantify the relationship. In this study, an empirical model is developed for estimating $\kappa$ from soil particle size distribution, $\rho_b$, and degree of water saturation $S_r$. The model parameters are determined by fitting the proposed equations to heat-pulse $\kappa$ data for eight soils covering wide ranges of texture, $\rho_b$, and $S_r$. Independent evaluations with published $\kappa$ data show that the new model describes the $\kappa(S_r)$ relationship accurately, with root-mean-square errors less than $0.75 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$. The proposed $\kappa(S_r)$ model also describes the responses of $\kappa$ to $\rho_b$ changes accurately in both laboratory and field conditions. The new model is also used successfully for predicting near-surface soil temperature dynamics using the harmonic method. The results suggest that this model provides useful estimates of $\kappa$ from $S_r$, $\rho_b$, and soil texture.

Disciplines
Agricultural Science | Hydrology | Soil Science | Statistical Models

Comments
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An empirical model for estimating soil thermal diffusivity from texture, bulk density, and degree of saturation

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Soil thermal diffusivity (κ) is an essential parameter for studying surface and subsurface heat transfer and temperature changes. It is well understood that κ mainly varies with soil texture, water content (θ), and bulk density (ρ_b), but few models are available to accurately quantify the relationship. In this study, an empirical model is developed for estimating κ from soil particle size distribution, ρ_b, and the degree of water saturation (S_r). The model parameters are determined by fitting the proposed equations to heat-pulse κ data for eight soils covering wide ranges of texture, ρ_b and S_r. Independent evaluations with published κ data show that the new model describes the κ(S_r) relationship accurately, with root mean square errors less than 0.75 × 10^-7 m^2 s^-1. The proposed κ(S_r) model also describes the responses of κ to ρ_b changes accurately in both laboratory and field conditions. The new model is also used successfully for predicting near-surface soil temperature dynamics using the harmonic method. The results suggest that this model provides useful estimates of κ from S_r, ρ_b and soil texture.
1. Introduction

Soil thermal diffusivity ($\kappa$) describes the speed of soil temperature wave transmission and determines the depth of soil influenced by diurnal surface heating and cooling. Knowledge of $\kappa$ is essential for modeling coupled heat and water transfer in soils and ground energy budgets, and for predicting soil temperature in land surface models (Xia et al. 2013; Koch et al. 2016). Furthermore, $\kappa$ has been used for estimating soil heat flux (de Silans et al. 1996; Roxy et al. 2014), an important component of land surface energy balance that influences the energy exchange between land surface and the atmosphere (Heusinkveld et al. 2004).

Only a few methods are available for measuring $\kappa$ directly. The surface step change in temperature method, which estimates $\kappa$ using the analytical solution to the one-dimensional heat conduction equation (Jackson and Taylor 1986; Horton 2002), works only on laboratory soil columns. Recently, heat pulse (HP) probes have been accepted as reliable tools for in situ measurement of soil thermal properties. A heat pulse is introduced into the soil, and $\kappa$ is determined from the temperature changes at a distance from the heater according to the pulsed line heat source theory (Bristow et al. 1994; Kluitenberg et al. 1995; Liu et al. 2017). The small sampling volume and relatively sophisticated equipment setup, however, limit the extensive application of the HP technique in field conditions. An infrared thermal imaging technique has also been proposed for determining field $\kappa$ values, but is limited to the soil surface layers (Kodikara
Numerous studies have focused on determination of apparent $\kappa$ from periodic temperature measurements at multiple depths. Most of the temperature-based approaches use analytical solutions to the heat transfer equation with sinusoidal or Fourier-series upper temperature boundary conditions (Carslaw and Jaeger 1959), assuming a uniform soil profile with conduction as the dominant heat transfer mode (Horton 2002). Among these, the amplitude, phase (Van Wijk and de Vries 1963; Wierenga et al. 1969), arctangent (Nerpin and Chudnovskii 1967) and logarithmic (Seemann 1979) methods, which have explicit forms and use small numbers of temperature data, tend to produce inconsistent or erroneous $\kappa$ values near the soil surface where the temperature dynamics differ from sine-wave curves or two-harmonic functions (Horton et al. 1983). The numerical and harmonic methods, which make use of large numbers of temperature observations to implicitly solve for $\kappa$ values, provide more reliable estimates (Richtmeyer and Mortor 1967; Horton et al. 1983). Evett et al. (2012) reported that the harmonic method-based $\kappa$ and de Vries (1963) model-based soil volumetric heat capacity ($C$) led to better surface heat flux estimates than measurements with heat flux plates. Nonetheless, like other temperature-based methods, the $\kappa$ results from the numerical and harmonic methods are unable to capture the spatial and temporal variations of $\kappa$ (e.g., at various soil depths during wetting/drying periods). Some researchers developed analytical (Lettau 1954) and numerical (Nassar and Horton 1989,
solutions for estimating $\kappa$ of nonuniform soils. These approaches usually fail when an abrupt change occurs in the temperature wave, which can happen during or just after a rainfall event (de Silans et al. 1996). Ross (2013) proposed a Fourier analysis for estimating $\kappa$ by considering in-depth $\theta$ variations and the effects of transient terms. The method, which is relatively complicated and requires soil temperature observations at several depths, has not been applied widely to field conditions.

In meteorological and geophysical applications, $\kappa$ is estimated frequently using soil thermal property models that relate soil thermal conductivity ($\lambda$) and $C$ to volume fractions of the soil particles, $\theta$, and soil bulk density ($\rho_b$) (Wang and Bou-Zeid 2012; Holmes et al. 2008). These models, either empirical (Johansen 1975; McCumber and Pielke 1981; Campbell 1985) or physically based (de Vries 1963), have provided valuable tools for simulating thermal and hydraulic processes that relate to climate change and geophysical flows. However, many studies have demonstrated that the $\lambda$ models are often subject to errors caused by empirical parameters and to ignoring $\lambda$ variability over space and time, which result in misleading $\kappa$ results, and therefore, problematic soil temperature and heat flux estimations (Gao et al. 2017a). For example, the Johansen (1975) $\lambda$ model has been reported to produce erroneous soil heat flux estimates, because it is sensitive to soil porosity and quartz content (Peters-Lidard et al. 1998). Lu et al. (2007) showed that although the Johansen (1975) $\lambda$ model was suitable for coarse-textured soils, it underpredicted $\lambda$ for the entire $\theta$ range on fine-textured soils. The
McCumber and Pielke (1981) λ model, which has been used widely in modeling land surface processes, overestimates λ during wetting and underestimates λ during drying, thus leads to errors in surface heat fluxes (Peters-Lidard et al. 1998). For this reason, some researchers arbitrarily set an upper λ limit of 1.9 W m⁻¹ K⁻¹ (Chen and Dudhia 2001). The five model parameters in the Campbell (1985) λ model vary with soil organic matter (SOM), texture, ρₖ and θ, making it difficult to determine λ accurately. Bristow (1998) showed that inaccurate quartz contents in the Campbell (1985) λ model led to more than 4°C errors in soil temperature predictions.

As an intrinsic soil property, κ is affected by soil mineral composition, porosity, particle arrangement, soil texture and temperature (Ochsner et al. 2001; Roxy et al. 2014), and varies nonlinearly with θ (Campbell 1985). For most mineral soils, κ increases quickly as dry soil wets, reaches the maximum value at a certain θ, and then decreases slowly as θ continues to increase (Ren et al. 1999; Wang et al. 2005; Liu et al. 2008a; Guan et al. 2009; Roxy et al. 2014). Under field conditions, κ shows strong temporal and spatial variability due to changes in θ and ρₖ with depth and time (Gao et al. 2017b). In practice, however, κ is often assumed constant with depth and time when estimating soil heat flux (Wang and Bou-Zeid 2012; Russel et al. 2015). Arkhangel’skaya (2009) used a lognormal function to describe the dependence of κ on θ for relatively fine-textured soils with sand fractions (fₒₘ) less than 0.40. On coarse-textured soils, however, the lognormal function produced large errors. Thus, there is a need for a model that estimates κ with
readily-available physical parameters for applications on various soil types over a range of field conditions.

The objective of this study is to develop an empirical model that is able to describe $\kappa$ as a function of soil texture, $\rho_b$ and degree of saturation ($S_r$). The performance of the model is evaluated by comparing estimated $\kappa$ values with independent $\kappa$ measurements using the HP method under both laboratory and field conditions. The new $\kappa$ model is applied in the conduction heat transfer equation to estimate subsurface soil temperature from harmonic surface temperature. The estimated subsurface temperatures are compared to measured soil temperatures.

2. Datasets for model development and validation

In this study, the $\kappa(S_r)$ data were obtained under laboratory (Soils 1-15) and field conditions (Soil 16) covering a wide range of soil texture, $\rho_b$, and $\theta$. Table 1 lists the particle size distribution (PSD), SOM content and $\rho_b$ range for the soil samples and the data sources. Soil PSD was determined using the pipette method (Gee and Or 2002), and SOM content was determined using the Walkley-Black titration method (Nelson and Sommers 1996). Soils 1-8, with $f_{sa}$ ranging from 19% to 94%, were used to develop the $\kappa$ model. Soils 9-16, with $f_{sa}$ varying from 12% to 93%, were used to validate the model.

2.1 $\kappa$ measurements on repacked soil samples

For Soils 1-8, samples were air-dried, ground and sieved through a 2-mm screen, moistened to the desired water contents, repacked into columns with a volume of 100 cm$^3$.
(5-cm diameter and 5-cm high), sealed with plastic sheets, and then equilibrated in a room at regulated temperature (20 ± 1°C) for 24 h. Soil thermal property measurements were made with a three-needle HP sensor that was inserted into each soil column vertically. The three-needle HP sensor consisted of three parallel stainless-steel needles with 1.3-mm in diameter, 40-mm in length and 6-mm in probe spacing between the heater and sensor probes. The heater probe contained a resistance wire in the heater probe, and a chromel-constantan thermocouple centered in the middle of the three probes for measuring temperature (Ren et al. 1999; Lu et al. 2017). The HP measurements were controlled with a data logger (CR23X, Campbell Scientific, Logan, UT). A 15-s HP was supplied to the heater probe by using a direct current power supply. The datalogger recorded the power input and temperature change of the sensor probe at a 1-s interval. The temperature-by-time data were processed to calculate \( \kappa \) using the nonlinear regression algorithm of Welch et al. (1996). The final \( \kappa \) was the mean value of three repeated measurements. Gravimetric \( \theta \) and \( \rho_b \) of each soil core were determined after making the HP measurements. Before making the HP measurements, the needle-to-needle spacing of the three-needle HP sensor was calibrated in agar-stabilized water (5 g L\(^{-1}\)), assuming that the C of the solution was equal to that of water (4.18 MJ m\(^{-3}\) K\(^{-1}\)).

Thermal properties for Soils 9, 14, and 15 were reported in Liu et al. (2008b) who made HP measurements on repacked soil cores with various \( \theta \) and \( \rho_b \). Thermal properties for Soils 10-13, with a wide range of \( \rho_b \) and \( \theta \) on repacked samples were reported in
Ochsner et al. (2001). Refer to Liu et al. (2008b) and Ochsner et al. (2001) for the details of the sample preparation and the HP measurements for obtaining $\kappa$.

### 2.2 $\kappa$ measurements in field tillage plots

Field measurements were performed on a silt loam soil (Soil 16) at the Luancheng Agricultural Ecosystem Experimental Station of the Chinese Academy of Sciences, Hebei, China. Three contrasting tillage systems were included in the study: Conventional moldboard plow tillage (CT), rotary tillage (RT), and no tillage (NT). For CT and RT, all crop residue was chopped into small pieces (5- to 10-cm long) and then incorporated into the soil after corn harvest. The tillage depth for the CT and RT was about 18 cm and 12 cm, respectively. More than 95% of the surface residue was mixed into the soil. For NT, standing corn stubble was left on the ground surface, and the soil was not disturbed before planting. The amount of returned crop residue was 9.2, 9.2 and 8.5 Mg ha$^{-1}$ yr$^{-1}$ for CT, RT and NT, respectively. After winter wheat harvest in June 2007, in situ HP measurements were made in each tillage plot at three random locations. Four repeated $\kappa$ measurements were performed at each location. Before installing the HP sensors, a small trench (20-cm long, 20-cm wide and 20-cm deep) was dug, and two three-needle HP sensors were pushed horizontally into the soil at depths of 5 cm and 15 cm. The HP data were collected with a datalogger (CR23X, Campbell Scientific, Logan, UT). Undisturbed soil columns were collected nearby with ring samplers (5-cm diameter and 5-cm high) at soil depths of 5 and 15 cm to determine $\rho_b$ and $\theta$ by oven-drying the samples at 105°C for...
To test the model performance, we measured soil temperature on a bare sandy loam soil (79.8% sand and 12.3% clay) at the research farm of China Agricultural University, Beijing, China. Three-wire thermocouples (type E, 50 µm in diameter), which were embedded in stainless-steel needles (4 cm long, and 1.3 mm in diameter), were installed at 14-, 26-, and 66-mm depths, and soil temperatures were recorded at an 1-h interval with a datalogger (CR23X, Campbell Scientific, Logan, UT) during a rain-free period from day of year (DOY) 258 to 264 in 2014. The $\rho_b$ values of the 0- to 50-mm and 50- to 100-mm soil layers were measured with a core sampler (5-cm diameter and 5-cm high) on DOY 258, 260, and 263. Since $\rho_b$ did not vary over time during the observation period, the mean $\rho_b$ values (from 3 repeated measurements) of 1.29 g cm$^{-3}$ and 1.36 g cm$^{-3}$ were used for the 0- to 50-mm layer and 50- to 100-mm layer, respectively. Hourly $\theta$ measurements at the 20- and 60-mm depths were recorded automatically with a time domain reflectometer (TDR100, Campbell Scientific, Logan, UT). Three TDR probes were installed at each depth. The net radiation data were recorded at a 1-h interval with two net radiometers (AV-71NR, Avalon Scientific, Jersey City, NJ) mounted at 0.1 m above the soil surface. Refer to Peng et al. (2017) for the details of field experiment setup.

We applied the harmonic method to predict soil temperature changes at the 26- and
66-mm depths using measured temperatures at the 14-mm depth (boundary temperature) and κ estimates from the new model (Horton et al. 1983). For a uniform soil with the surface subjected to a periodic temperature wave, the daily upper boundary soil temperature dynamics can be described with a Fourier series (Horton et al. 1983),

\[ T(0, t) = \bar{T} + \sum_{n=1}^{M} [A_n \sin(n\omega t + \phi_n)], \quad [1] \]

where \( \bar{T} \) is the average surface temperature for each day (°C), \( t \) represents time (h), \( M \) is the number of harmonics, \( A_n \) and \( \phi_n \) are the amplitude and phase angle of the \( n^{th} \) harmonic, respectively, \( \omega \) is the radial frequency equal to \( 2\pi/P \) with \( P \) being the period of the fundamental cycle (24 h for daily temperature). Accordingly, based on the heat conduction equation with \( M \) harmonics as boundary condition, the temperature at a depth \( z \) (m) below the upper boundary depth is approximated by (Horton et al. 1983),

\[ T(z, t) = \bar{T} + \sum_{n=1}^{M} \left[ A_n \exp\left(-z\sqrt{no\lambda/2\kappa}\right) \sin\left(n\omega t + \phi_n - z\sqrt{no\lambda/2\kappa}\right) \right]. \quad [2] \]

In our study, Eq. [1] was applied to fit the observed boundary temperatures at 14-mm depth, and Eq. [2] was applied to predict subsurface temperatures at depths 26 mm and 66 mm with model-derived κ data. The reliability of the κ model was then evaluated by comparing the measured and predicted temperatures at the two soil depths.

3. Model development

3.1 The empirical soil κ model

According to the linear mixing model, \( C \) is expressed as the sum of heat capacities
of water and soil solids (de Vries 1963; Campbell 1985),

\[ C = \rho_c c_s + \rho_w c_w \theta, \]  

[3]

where \( c_w \) is specific heat of water (4.18 \( \text{J g}^{-1} \text{k}^{-1} \)), and \( \rho_w \) is the density of water (1.0 \( \text{g cm}^{-3} \)).

Lu et al. (2014) present an empirical model that relates \( \lambda \) to \( \theta \), \( \rho_b \) and texture,

\[ \lambda = \exp(\beta - \theta^{-\alpha}) + \lambda_{\text{dry}} \quad \theta > 0, \]  

[4]

where \( \alpha \) and \( \beta \) are shape factors related to \( \rho_b \) and PSD, and \( \lambda_{\text{dry}} \) is the thermal conductivity of dry soils that can be estimated from soil porosity (\( \tau \)).

In this study, we take the forms of the de Vries (1963) C model and the Lu et al. (2014) \( \lambda \) model to establish a general model that estimates \( \kappa \) from other soil physical properties. As the ratio of \( \lambda \) and \( C \), \( \kappa \) is also a function of soil texture, \( \theta \) and \( \rho_b \). Instead of using \( \theta \), we use the dimensionless parameter \( S_r \), which makes it easy to make comparisons between soils of different textures. We propose the following equation that relates \( \kappa \) to soil PSD, \( \rho_b \), and \( S_r \),

\[ \kappa(S_r) = \frac{0.25 + \exp(b - S_r^{-c})}{4.18S_r + c} \quad S_r > 0, \]  

[5]

where \( a, b \) and \( c \) are the shape parameters of the \( \kappa(S_r) \) curve, 4.18 (MJ m\(^{-3}\) K\(^{-1}\)) is the heat capacity of water at room temperature (Campbell et al. 1991), and 0.25 (W m\(^{-1}\) K\(^{-1}\)) is selected to represent the average \( \lambda_{\text{dry}} \) value for mineral soils of different textures (de Vries 1963). Taking soil particle density as 2.65 g cm\(^{-3}\), \( S_r \) is calculated from the ratio of \( \theta \) and \( \tau \).
Figure 1 illustrates the measured (dots) and the fitted (lines) $\kappa$-$S_r$ results using Eq. [5] for Soils 1-8. Except for Soil 2, the $S_r$ on the repacked soil samples ranged from about 0 to 1 (Table 2). In general, the measured $\kappa(S_r)$ data and fitted curves displayed several distinct features across soils. First, $\kappa$ changed dynamically as dry soil wetted. In general, $\kappa$ increased rapidly until $S_r$ reached about 0.2. With further increases in $S_r$, however, the rate of $\kappa$ change was reduced. After reaching a peak value ($\kappa_m$) at a certain $S_r$, $\kappa$ either declined steadily (e.g., Soils 1-5) or leveled off (e.g., Soils 6-8) as $S_r$ increased. Secondly, the magnitude and shape of the $\kappa(S_r)$ curves were strongly related to soil texture, i.e., with increasing $S_r$, $\kappa_m$ was larger and occurred at lower $S_r$ for coarse-textured soils, but was relatively lower and occurred at larger $S_r$ for fine-textured soils. These phenomena can be explained by the fact that: (1) coarse soils (Soils 1–5) usually have more quartz content than fine soils, and the $\kappa$ of quartz ($4.13 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$) is much larger than that of other soil minerals ($1.08 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$, Campbell and Norman 1998), leading to larger $\kappa_m$ values for coarse soils than for fine soils; and (2) fine soils require more water to form water bridges between the solid particles, which leads to smaller changes in fine than in coarse soils in the $\lambda$-$\theta$ curve at the same $S_r$ as dry soil initially wets (Ewing and Horton 2007; Lu et al. 2007), and thus relatively small changes in $\kappa(S_r)$. In addition, an increase in $\rho_b$ results in a greater $\kappa$ value at a specific $S_r$. This was illustrated for the case of Soil 2, where the increase in $\kappa(S_r)$ was found to be as large as $1.60 \times 10^{-7} \text{ m}^2 \text{ s}^{-1}$ when $\rho_b$ was changed from 1.28 to 1.49 g cm$^{-3}$ for the repacked $S_r$ range of 0.02-0.64. This observation
was consistent with the findings of Ochsner et al. (2001) who reported that $\kappa$ decreased linearly with air-porosity (that related inversely to $\rho_b$) on four loamy soils. The coefficients of determination ($R^2$) for the fitted results were all greater than 0.99 (data not shown), and the root mean square error (RMSE) values were within $0.35 \times 10^{-7}$ m$^2$ s$^{-1}$ for the eight soils (Table 2), indicating that the proposed model well described the measured $\kappa(S_r)$ values across the entire $S_r$ range.

3.2 Determination of model parameters $a$, $b$, and $c$

Our earlier analysis indicates that for a specific soil, the $\kappa$ values are well-described by $S_r$, PSD, and $\rho_b$, and the shape and magnitude of the $\kappa(S_r)$ curves are defined by parameters $a$, $b$ and $c$. In this section, we perform a sensitivity analysis to investigate how $a$, $b$ and $c$ influence the $\kappa(S_r)$ curves, and then establish functional relationships among these parameters versus PSD and $\rho_b$.

For Soils 1-8, parameters $a$, $b$ and $c$ varied in the ranges of 0.20–0.46, 4.27–5.35 and 1.28–5.45, respectively (Table 2). To examine the effects of $a$ on the $\kappa(S_r)$ curve, we assigned a value of 4.27 to $b$ and a value of 5.45 to $c$, both corresponded to the lowest fitted values of $b$ and $c$ (Table 2). Then parameter $a$ was varied from 0.20 to 0.46, which covered the fitted $a$ range on Soils 1-8 (Table 2). Similarly, for examination of the effect of parameter $b$ on $\kappa(S_r)$ curve, we assigned a value of 0.46 to $a$ and 5.45 to $c$, while $b$ varied from 4.27 to 5.35. To examine the effect of $c$ on the $\kappa(S_r)$ curve, we set $a$ at 0.46 and $b$ at 4.27, while $c$ varied from 1.30 to 5.50.
The effects of parameter $a$ on the $\kappa(S_t)$ curve were pronounced in the relatively dry region ($S_t < 0.3$), while parameters $b$ and $c$ generally influenced the $\kappa(S_t)$ curve across the entire $S_t$ range (Fig. 2). A higher $a$ value produced a lower rate of $\kappa(S_t)$ increase in the relatively low $S_t$ region (Fig. 2-1). With an increase of parameter $c$, the $\kappa$ value at a specific $S_t$ also decreased, especially in the intermediate $S_t$ region (Fig. 2-3). An opposite trend was observed for parameter $b$, i.e., higher $b$ values led to greater $\kappa$ values, and the change of $\kappa$ was especially significant in the high $S_t$ region (Fig. 2-2). In general, the $\kappa(S_t)$ curve was more sensitive to parameter $a$ in the low $S_t$ region, to $c$ in the intermediate $S_t$ region, and to $b$ in the high $S_t$ region. For example, when $a$, $b$, and $c$ varied in the designated ranges, the maximum changes of $\kappa$ were 1.80, 5.34 and $3.16 \times 10^{-7}$ m$^2$ s$^{-1}$, respectively. At low $\theta$ values (i.e., the dry end of the $\lambda(\theta)$ curve), heat conduction occurs through soil solid particles where soil water exists mainly as water films around the solids (Lu et al. 2007; Lu et al. 2014). Soils with higher clay contents have larger surface areas, and thus, adsorb more water molecules around the solid particles, which leads to a gradual change in the $\lambda(\theta)$ curve in the low $S_t$ region. At intermediate and high $\theta$ values, the magnitude of heat conduction through soil particles depends largely on the capillary bridges among solid particles, which are controlled by soil porosity and pore-size distribution. It appears that parameter $a$, which has significant effects on the $\kappa(S_t)$ curves in the low $S_t$ region, is closely related to the soil clay fraction ($f_{cl}$). Parameters $b$ and $c$
relate mainly to $f_{sa}$ and $\rho_b$, the key factors that determine soil porosity and pore size distribution, and thus the capillary bridges.

To quantify the dependence of parameters $a$, $b$ and $c$ on soil physical properties, we further examined the relations among parameters $a$, $b$ and $c$ and PSD and $\rho_b$ (Fig. 3). The results showed that parameter $a$ increased linearly with $f_{cl}$, and the rate of increase was larger in the $f_{cl}$ range of 0–0.12 than that in the range of $f_{cl} > 0.12$ (Fig. 3-1). Parameters $b$ and $c$ depended largely on $f_{sa}$: with increasing $f_{sa}$, both $b$ and $c$ first decreased and then increased with a splitting point of $f_{sa} = 0.40$ (Figs. 3-2 and 3-3). This is in line with the findings of Johansen (1975) and Lu et al. (2007) who classified the fine-textured and coarse-textured soils using a $f_{sa}$ value of 0.40 in their $\lambda$ models. Hereafter, we will describe soils with $f_{sa} > 0.40$ as coarse-textured soils, and soils with $f_{sa} \leq 0.40$ as fine-textured soils.

Based on the values listed in Table 2, we performed a linear regression analysis to obtain the $a$-$f_{cl}$ and $c$-$f_{sa}$ relationships with piecewise functions,

\[
\begin{align*}
    a & = 3.06 f_{cl} + 0.05 & f_{cl} < 0.12 & R^2 = 0.86 \\
    a & = 0.83 f_{cl} + 0.20 & f_{cl} \geq 0.12 & R^2 = 0.98
\end{align*}
\]

[6]

\[
\begin{align*}
    c & = -12.57 f_{sa} + 6.32 & f_{sa} \leq 0.40 & R^2 = 0.99 \\
    c & = 8.52 f_{sa} - 2.28 & f_{sa} > 0.40 & R^2 = 0.99
\end{align*}
\]

[7]

Parameter $b$ was related to $\rho_b$ and $f_{sa}$ as they both affected the magnitude of the $\kappa(S_t)$ curve. The following relationship was established by applying a multiple regression
algorithm that was included in the Data Analysis of Microsoft EXCEL (version 14 for Windows) to the $b$, $\rho_b$ and $f_{sa}$ values listed in Table 2,

\[
\begin{align*}
\begin{cases}
b = 5.06 + 5.22 f_{sa} \rho_b - 8.73 f_{sa} & f_{sa} \leq 0.40 \quad R^2 = 0.99 \\
b = 3.82 + 1.38 f_{sa} \rho_b - 0.56 f_{sa} & f_{sa} > 0.40 \quad R^2 = 0.99
\end{cases}
\end{align*}
\]  

[8]

Thus, when $f_{sa}$, $f_{cl}$, and $\rho_b$ data are available, the $\kappa(S_t)$ function can be estimated directly by using Eqs. [5-8].

4. Model validation

We evaluated the performance of the new $\kappa$ model (Eqs. [5-8]) by using published datasets on both coarse-textured and fine-textured soils covering wide ranges of $S_t$ and $\rho_b$.

For each soil, parameters $a$, $b$, and $c$ were determined from measured $f_{sa}$, $f_{cl}$, and $\rho_b$ values using Eqs. [6-8]. Then $\kappa$ values were estimated using Eq. [5]. The RMSE and bias of the $\kappa$ estimations were used to indicate model performance,

\[
\text{RMSE} = \sqrt{\frac{\sum (\kappa_{\text{mea}} - \kappa_{\text{est}})^2}{n}},
\]  

[9]

\[
\text{bias} = \frac{\sum (\kappa_{\text{mea}} - \kappa_{\text{est}})}{n}.
\]  

[10]

where $n$ is the number of data points, $\kappa_{\text{mea}}$ and $\kappa_{\text{est}}$ represent the measured and estimated $\kappa$ values, respectively.

4.1 Model evaluation using $\kappa$ measurements on repacked soil samples

Figure 4 presents the measured and estimated $\kappa$ values as a function of $S_t$ for a coarse-textured soil and a fine-textured soil. Soil 10 was a sandy loam soil from Ochsner
et al. (2001) with \( \rho_b \) ranging from 0.95 to 1.69 g cm\(^{-3} \), and Soil 11 was a clay loam soil from Ochsner et al. (2001) with \( \rho_b \) ranging from 0.85 to 1.52 g cm\(^{-3} \). Both measured and estimated \( \kappa(S_t) \) values showed the following characteristics: (1) a soil with a larger \( f_{sa} \) (i.e., Soil 10) had a higher \( \kappa_m \) at a specific \( S_t \), and a sharper \( \kappa \) increase in the low \( S_t \) region (Fig. 4a), while a fine-textured soil (i.e., Soil 11) exhibited more gradual change in this region (Fig. 4b); (2) for a particular soil, a greater \( \rho_b \) produced a larger \( \kappa \) at a specific \( S_t \). In general, the new model provided fairly good \( \kappa \) estimations for variations in \( S_t \) and \( \rho_b \). The RMSE and bias values of \( \kappa \) estimates were within \( 0.75 \times 10^{-7} \) m\(^2\) s\(^{-1} \) and \( 0.54 \times 10^{-7} \) m\(^2\) s\(^{-1} \) on Soils 10 and 11, respectively (Table 3).

The \( \kappa \) model was also tested on one coarse-textured soil and four fine-textured soils (Soils 12 and 13 from Ochsner et al. 2001 and Soils 9, 14 and 15 from Liu et al. 2008b). The repacked soil columns covered a range of \( \rho_b \) conditions (Table 1). The \( \kappa \) estimates agreed closely with the measured values, as indicated by the random distribution of data points along the 1:1 line (Fig. 5), and the low RMSE (within \( 0.64 \times 10^{-7} \) m\(^2\) s\(^{-1} \)) and bias (from -0.39 to \( 0.45 \times 10^{-7} \) m\(^2\) s\(^{-1} \)) (Table 3). Thus, the new model provided accurate \( \kappa \) estimates on both coarse-textured and fine-textured soils over wide ranges of \( S_t \) and \( \rho_b \).

4.2 Model evaluation using in situ \( \kappa \) measurements in tillage plots

Tillage practices alter soil thermal properties, heat transfer in soils and near surface microclimate mainly by changing soil \( \rho_b \) and \( \theta \). For the tillage study on Soil 16, \( \theta \) varied from 0.22 to 0.33 cm\(^3\) cm\(^{-3} \) and the range of \( \rho_b \) was 1.06 to 1.58 g cm\(^{-3} \). In general, the
NT plot had larger $\theta$ and $\rho_b$ values (Figs. 6a and 6b) in the 0- to 10-cm and 10- to 20-cm soil layers, while the differences between CT and RT plots were not significant. As a result, the measured and estimated $\kappa$ values for the NT plot were larger than those for the CT and RT plots (Fig. 6c).

Comparisons between measured and estimated $\kappa$ showed that most of the data distributed randomly along the 1:1 line, and about 80% of the data were within the 10% error lines (Fig. 6d), with an RMSE of $0.54 \times 10^{-7}$ m$^2$ s$^{-1}$ and a bias of $0.27 \times 10^{-7}$ m$^2$ s$^{-1}$ for all of the sampling locations. The new model well captured the $\kappa$ variability in the three tillage systems (Fig. 6c), and the $\kappa$ estimates were consistent with the HP measured values (Fig. 6d). For the CT treatment, $\kappa$ was underestimated slightly (Fig. 6d). The errors might come from: (1) $\kappa$ measurement errors with the HP method due to the presence of crop residue in the soil layer; (2) the point measurements of $\theta$ and $\rho_b$ by core sampling might not fully capture the field variability; (3) the proposed $\kappa$ model ignores soil structural changes caused by tillage practices. Kaune et al. (1993) observed larger apparent $\kappa$ values in structured soils than in disturbed soils; and (4) we ignored the influences of SOM on $\kappa$. Zheng et al. (2015) reported that including SOM content as a thermal property parameter in the Noah land surface model influenced $\lambda$ estimates significantly but had negligible effects on heat flux and temperature simulations. In this study, the soil samples had SOM contents less than 3% (Table 1). Further study is required to investigate the effects of SOM on $\kappa$ for soils with high SOM contents (e.g.,
4.3 Prediction of near-surface soil temperature

In this section, we compare temperature measurements against values estimated with the harmonic method (Eqs. [1] and [2]) over a period of 7 days. The daily average $\theta$, $\rho_b$ and mineral fractions were used to estimate $\kappa$ values (Eqs. [5-8]) of the 0- to 50-mm and 50- to 100-mm soil layers. For each day, we determined $A_n$ and $\phi_h$ by fitting Eq. [1] to the observed soil temperatures at the 14-mm depth using a finite Fourier series with five harmonics (i.e., $M = 5$). The daily $\bar{T}$, $A_n$ and $\phi_h$ values of the 14-mm depth, along with modeled $\kappa$ for each day, were then used as inputs in Eq. [2] for estimating soil temperatures at soil depths of 26 mm and 66 mm. The $\kappa$ values for the 14- to 66-mm soil layer were taken as the weighted averages of those values of the 0- to 50-mm and 50- to 100-mm soil layers.

Figure 7 presents the results of daily mean $\theta$, $\kappa$ estimates, the observed and fitted soil temperatures at the 14-mm depth, the net radiation, and the observed and estimated soil temperatures at the 26- and 66-mm depths during a rain-free period from DOY 258 to 264, 2014. During this period, $\kappa$ varied mainly with $\theta$, because $\rho_b$ values changed little with time. Both $\theta$ and $\kappa$ varied significantly with soil depth (Fig. 7a), i.e., greater $\theta$ and $\rho_b$ values were observed at 60-mm than those at 20-mm, leading to a $\kappa$ difference about 2.0 $\times 10^{-7}$ m$^2$ s$^{-1}$ between the two depths. Under all climatic conditions (cloudy, partially cloudy and clear days, as indicated by the changes in net radiation), harmonic functions
successfully described diurnal soil temperature variations at the 14-mm depth (Fig. 7b).

The estimated soil temperatures at the 26- and 66-mm depths agreed well with the observed values (Fig. 7c), with RMSEs of 0.61°C and 0.58°C for the 26- and 66-mm depths, respectively. This suggested that the new model was capable of providing reliable κ estimates when accurate ρ_b and θ data were available. Thus, the new κ model can be used in heat conduction models to estimate the spatial and temporal patterns of subsurface soil temperature. Further studies are required to evaluate the new κ model in more complicated scenarios, e.g., heat transfer in soils with partial vegetation-cover, and under conditions where latent and convective heat transfer become apparent. Dynamic monitoring of ρ_b is also required where soil structure varies strongly over time.

4.4 Potential limitations of the new model

We demonstrated that the proposed κ(S_r) model was capable of producing acceptable κ data across the entire S_r range for soils with different textures and ρ_b. The deviation of the modeled κ data from the measured κ values might come from several error sources. First, we obtained parameters a, b, and c using PSD rather than soil mineralogical information. Some studies have shown that using PSD instead of soil mineral composition produces biased κ estimations for soils with high fractions of quartz (Bristow 1998; Peters-Lidard et al. 1998; Lu et al. 2014). Second, our model ignores the effects of soil temperature and soil structure on κ values, which merit further study. Third, the κ measurements by the HP sensors are subject to errors associated with probe
deflection, imperfect probe-soil contact, and irregular ambient temperature changes (Liu et al. 2017), which affect the accuracy of the measured $\kappa$ values.

Equation [5] fails in situations where the soils are completely dry (i.e., $S_r = 0$). Based on HP measurements on dry mineral soils, Lu et al. (2013) showed that the $\kappa_{\text{dry}}$ values varied within a small range of $2.18 \times 10^{-7}$ m$^2$ s$^{-1}$ with an average value of $2.41 \pm 0.16 \times 10^{-7}$ m$^2$ s$^{-1}$ for a wide range of textures. Thus, it is recommended to assign a value of $2.41 \times 10^{-7}$ m$^2$ s$^{-1}$ to $\kappa_{\text{dry}}$ for dry soil samples. If $c_s$ value is available, $\kappa_{\text{dry}}$ can be calculated using the following formula:

$$\kappa_{\text{dry}} = \frac{-0.56\tau + 0.51}{c_s}. \quad [11]$$

5. Summary and conclusions

An empirical model for estimating $\kappa$ from soil texture, $\rho_b$ and $S_r$ was developed, in which the shape parameters $a$, $b$ and $c$ were obtained from $f_{\text{sa}}$, $f_{\text{cl}}$ and $\rho_b$. Independent evaluations of the model using published datasets on repacked soil samples as well as a field measured dataset from a tillage experiment showed that the new model could produce acceptable $\kappa(S_r)$ data across the entire $S_r$ range. The model responded well to variable $\rho_b$. The model estimated $\kappa$ values were shown to be useful for estimating near-surface soil temperature dynamics. These promising results indicated that the new $\kappa$ model could potentially be used in soil heat transfer models to make soil temperature and heat flux estimations for meteorological and geophysical applications.
Acknowledgements

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TABLE 1. Soil particle size distribution, soil organic matter (SOM) content, and bulk density ($\rho_b$) for 16 soils used in the study. Soils 1-8, 16 are new measurements, and Soils 9-15 are from the literature.

<table>
<thead>
<tr>
<th>Soil ID</th>
<th>Texture</th>
<th>Particle size distribution</th>
<th>SOM</th>
<th>$\rho_b$</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>2-0.05 mm</td>
<td>0.05-0.002 mm</td>
<td>&lt;0.002 mm</td>
<td>(%)</td>
</tr>
<tr>
<td>1</td>
<td>Sand</td>
<td>94</td>
<td>1</td>
<td>5</td>
<td>0.09</td>
</tr>
<tr>
<td>2</td>
<td>Loamy sand</td>
<td>79</td>
<td>13</td>
<td>8</td>
<td>0.18</td>
</tr>
<tr>
<td>3</td>
<td>Sandy loam</td>
<td>67</td>
<td>21</td>
<td>12</td>
<td>0.86</td>
</tr>
<tr>
<td>4</td>
<td>Loam</td>
<td>50</td>
<td>41</td>
<td>9</td>
<td>0.25</td>
</tr>
<tr>
<td>5</td>
<td>Loam</td>
<td>40</td>
<td>49</td>
<td>11</td>
<td>0.49</td>
</tr>
<tr>
<td>6</td>
<td>Clay loam</td>
<td>32</td>
<td>38</td>
<td>30</td>
<td>0.27</td>
</tr>
<tr>
<td>7</td>
<td>Silt loam</td>
<td>27</td>
<td>51</td>
<td>22</td>
<td>1.19</td>
</tr>
<tr>
<td>8</td>
<td>Silt loam</td>
<td>19</td>
<td>54</td>
<td>27</td>
<td>0.39</td>
</tr>
<tr>
<td>9</td>
<td>Sand</td>
<td>93</td>
<td>0</td>
<td>7</td>
<td>0.06</td>
</tr>
<tr>
<td>10</td>
<td>Sandy loam</td>
<td>66</td>
<td>23</td>
<td>11</td>
<td>2.30</td>
</tr>
<tr>
<td>11</td>
<td>Clay loam</td>
<td>37</td>
<td>35</td>
<td>28</td>
<td>2.30</td>
</tr>
<tr>
<td>12</td>
<td>Silt loam</td>
<td>23</td>
<td>64</td>
<td>13</td>
<td>0.90</td>
</tr>
<tr>
<td>13</td>
<td>Silt clay loam</td>
<td>12</td>
<td>56</td>
<td>32</td>
<td>1.10</td>
</tr>
<tr>
<td>14</td>
<td>Clay loam</td>
<td>31</td>
<td>39</td>
<td>30</td>
<td>0.27</td>
</tr>
<tr>
<td>15</td>
<td>Silt loam</td>
<td>15</td>
<td>65</td>
<td>20</td>
<td>1.46</td>
</tr>
<tr>
<td>16</td>
<td>Silt loam</td>
<td>17</td>
<td>62</td>
<td>21</td>
<td>1.10</td>
</tr>
</tbody>
</table>
TABLE 2. The ranges of degree of saturation ($S_r$), model parameters $a$, $b$ and $c$, and root mean square errors (RMSE) of the new model on Soils 1-8. The model parameters and RMSEs were obtained by fitting Eq. [5] to heat-pulse thermal diffusivity vs. $S_r$ data with a nonlinear regression algorithm (Wolfram, 2003).

<table>
<thead>
<tr>
<th>Soil ID</th>
<th>$S_r$ range</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
<th>RMSE $(10^{-7} \text{ m}^2 \text{ s}^{-1})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.06–1</td>
<td>0.20</td>
<td>5.35</td>
<td>5.45</td>
<td>0.20</td>
</tr>
<tr>
<td>2</td>
<td>0.02–0.46</td>
<td>0.26</td>
<td>4.75</td>
<td>5.08</td>
<td>0.34</td>
</tr>
<tr>
<td>2</td>
<td>0.02–0.64</td>
<td>0.32</td>
<td>4.99</td>
<td>4.42</td>
<td>0.33</td>
</tr>
<tr>
<td>3</td>
<td>0.03–0.89</td>
<td>0.30</td>
<td>4.79</td>
<td>3.16</td>
<td>0.25</td>
</tr>
<tr>
<td>4</td>
<td>0.03–0.95</td>
<td>0.36</td>
<td>4.52</td>
<td>1.74</td>
<td>0.35</td>
</tr>
<tr>
<td>5</td>
<td>0.03–0.89</td>
<td>0.37</td>
<td>4.27</td>
<td>1.28</td>
<td>0.27</td>
</tr>
<tr>
<td>6</td>
<td>0.08–1</td>
<td>0.46</td>
<td>4.47</td>
<td>2.38</td>
<td>0.29</td>
</tr>
<tr>
<td>7</td>
<td>0.05–0.97</td>
<td>0.40</td>
<td>4.58</td>
<td>2.82</td>
<td>0.31</td>
</tr>
<tr>
<td>8</td>
<td>0.08–0.96</td>
<td>0.42</td>
<td>4.68</td>
<td>3.96</td>
<td>0.21</td>
</tr>
</tbody>
</table>
TABLE 3. The root mean square errors (RMSE) and bias of the new model for estimating soil thermal diffusivity on Soils 9-16 with various bulk densities and degree of saturation ($S_r$).

<table>
<thead>
<tr>
<th>Soil ID</th>
<th>$S_r$ range</th>
<th>RMSE ($10^{-7}$ m$^2$ s$^{-1}$)</th>
<th>bias ($10^{-7}$ m$^2$ s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9</td>
<td>0.02–0.50</td>
<td>0.64</td>
<td>0.21</td>
</tr>
<tr>
<td>10</td>
<td>0.19–0.95</td>
<td>0.75</td>
<td>0.64</td>
</tr>
<tr>
<td>11</td>
<td>0.19–0.88</td>
<td>0.54</td>
<td>0.29</td>
</tr>
<tr>
<td>12</td>
<td>0.03–0.43</td>
<td>0.33</td>
<td>0.11</td>
</tr>
<tr>
<td>13</td>
<td>0.08–0.64</td>
<td>0.61</td>
<td>0.45</td>
</tr>
<tr>
<td>14</td>
<td>0.06–0.48</td>
<td>0.53</td>
<td>0.36</td>
</tr>
<tr>
<td>15</td>
<td>0.06–0.52</td>
<td>0.64</td>
<td>-0.39</td>
</tr>
<tr>
<td>16</td>
<td>0.40–0.78</td>
<td>0.54</td>
<td>0.27</td>
</tr>
</tbody>
</table>
Figure Caption List

FIG. 1. Measured (symbols) and fitted (curves) thermal diffusivity ($\kappa$) vs. degree of saturation ($S_r$) for eight soils of various textures. The curves were obtained by fitting Eq. [5] to the measured $\kappa(S_r)$ using a nonlinear curve fitting method (Wolfram, 2003). The fitted equations are presented in the figure.

FIG. 2. The effects of (1) parameter $a$, (2) parameter $b$, and (3) parameter $c$ on soil thermal diffusivity ($\kappa$)--degree of saturation ($S_r$) curves obtained with Eq. [5]. The presented curves have assigned values for parameters $a$, $b$ and $c$.

FIG. 3. Dependence of (1) parameter $a$ on clay fraction ($f_{cl}$), and parameters (2) $b$ and (3) $c$ on sand fraction ($f_{sa}$) for Soils 1-8. The symbols represent the fitted $a$, $b$ and $c$ results in Table 2. The lines are the linear regression results for each domain.

FIG. 4. Measured and estimated soil thermal diffusivity ($\kappa$) vs. degree of saturation ($S_r$) data with the new model for coarse-textured Soil 10 (sand fraction $f_{sa} > 0.40$) (a) and fine-textured Soil 11 ($f_{sa} \leq 0.40$) (b). The repacked soil bulk density ($\rho_b$) ranges are presented in the figure.

FIG. 5. Measured and estimated thermal diffusivity ($\kappa$) using the new model for coarse-textured Soil 9 (sand fraction $f_{sa} > 0.40$) and fine-textured Soils 12-15 ($f_{sa} \leq 0.40$). The solid line is a 1:1 line, and the dashed lines are the 10% error lines.

FIG. 6. The (a) measured soil water content ($\theta$), (b) bulk density ($\rho_b$), (c) measured soil thermal diffusivity ($\kappa$), (d) comparisons between estimated $\kappa$ with the new model and the in situ measured values for the 0- to 10-cm and 10- to 20-cm soil layers in conventional tillage (CT), rotary tillage (RT), and no tillage (NT) treatment plots,
respectively. The bars represent standard deviations of each value.

FIG. 7. Daily mean soil water content (θ) and the estimated soil thermal diffusivity (κ) with the new model for the 20- and 60-mm depths (a); Net radiation, observed and fitted (Eq. [1]) soil temperatures at 14-mm depth (b); and observed and estimated (Eq. [2]) soil temperatures at 26- and 66-mm depths (c) during Day of Year 258 to 264, 2014.
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FIG. 2. The effects of (1) parameter $a$, (2) parameter $b$, and (3) parameter $c$ on soil thermal diffusivity ($\kappa$)–degree of saturation ($S_r$) curves obtained with Eq. [5]. The presented curves have assigned values for parameters $a$, $b$ and $c$. 

[Diagram showing the effects of parameters on soil thermal diffusivity]
FIG. 3. Dependence of (1) parameter $a$ on clay fraction ($f_{cl}$), and parameters (2) $b$ and (3) $c$ on sand fraction ($f_{sa}$) for Soils 1-8. The symbols represent the fitted $a$, $b$ and $c$ results in Table 2. The lines are the linear regression results for each domain.
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