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ORIGINAL ARTICLE

A new empirical model for the estimation of soil thermal conductivity

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Abstract
Soil thermal conductivity (λ) is an important thermal property which serves as an indicator for the coupling of soil, water, heat, and solutes in a numerical model. The objective of this study is to develop a new empirical model for estimating soil thermal conductivity. There are several methods for estimating λ available, but they are complicated and can produce relatively large errors. Using published datasets, the performance of the new estimate was evaluated along with nine other normalized models, and the advantages and disadvantages of each model and its relevant soil types were analyzed and compared. The results showed that the new empirical model is suitable for studying the thermal conductivities of soils of different textures. In the comparisons, it had the best performance among the ten models considered, with a minimum standard deviation (SD) of 0.074 W m^{-1} K^{-1}, the coefficient of determination (R^2) from 0.929 to 0.983 with a mean of 0.964, and relative error (Re), from 5.210 to 9.900% with a mean of 7.335%. The new model has been shown to improve the reliability of estimation of soil thermal conductivity and has application in agricultural science, environmental science, earth science and engineering research.

Keywords Soil · Thermal conductivity · Empirical model · Soil water content

List of symbols

Latin

A, B, C, D, E	Campbell model parameters
C_{clay}	Mass fraction of clay particles
C_{sand}	Mass fraction of sand particles
C_{om}	Mass ratio of organic matter
C_{silt}	Mass fraction of silt particles
n	Soil porosity
a, b, m	Lu et al. (2007) model parameters
c, d, e, f	Su et al. (2016) model parameters
J, L	He et al. (2017) model parameters
O_i,	Measured value
$\bar{O}$	Sample mean
S_i	Model simulated value
N	Number of independent λ records
M	Number of model fitting parameters

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Greek

ξ	Ewen and Thomas model parameters
κ, χ, η	Côté and Konrad model parameters
μ, φ	Lu et al. (2014) model parameters
λ	Soil thermal conductivity (W m^{-1} K^{-1})
θ	Volumetric water content
ρ	Particle density
γ_d	Specific weight
α, β	The new model parameters

Subscripts

b	Bulk
sat	Saturation
dry	Dryness
s	Soil solids
w	Water
o	Other minerals
q	Quartz

Acronyms

S_r	Degree of saturation
Ke	Kersten number
SD	Standard deviation
R^2	Coefficient of determination
Re	Relative error
PSD	Particle size distribution
HP	Heat pulse

Introduction

Soil thermal conductivity (λ) describes the variations in soil temperature and energy transfer. It is the basis of studying other physical processes of soil, such as hydro-thermal coupling transmission (Yosef et al. 2017), gas diffusion (Milly 1984) and materials transportation. It is an important thermophysical value in geotechnical, geothermal, and agricultural and process applications involved in issues such as ground source heat pumps design (Go et al. 2016; Zhang et al. 2015), nuclear waste disposal (Li et al. 2013), heat production in putrefaction (Birkholzer et al. 2018; Faitli et al. 2015), theoretical study of crop growth, and water and fertilizer migration (Phillips et al. 2014; Usowicz et al. 1996).

Although significant progress has been made in soil thermal conductivity measurement technology, with methods such as the heat pulse, line source, and heat plate (Bristow et al. 1994; He et al. 2015), these techniques have other complex problems in the measurement process due to being limited by experimental conditions, such as: susceptibility to the nature of the material, high technical requirements required for testing, and the high accuracy in the testing (Bovesecchi and Coppa 2013; Bovesecchi et al. 2018; Tarnawski et al. 2018); so, processes for rapidly and accurately estimating soil thermal conductivity remain difficult. As a consequence, research on soil thermal properties is still the focus of attention.

Soil thermal conductivity (λ) is mainly dependent on soil texture, mineral composition, water content (θ), bulk density (ρ_b) and temperature. To date, many indirect estimation models have been proposed (Campbell 1985; Côté and Konrad 2005; de Vries 1963; Ewen and Thomas 1987; He et al. 2017; Johansen 1975; Kersten 1949; Lu et al. 2007, 2014; Nikoosokhan et al. 2015; Su et al. 2016; Tarnawski and Leong 2016), with the first being an empirical model proposed by Kersten (1949) with only one influencing factor ρ_b. It is one of the earliest methods used to predict the thermal conductivity of frozen soil. In the case of low water content, the model has limited applicability. de Vries (1963) developed a model based on basic parameters of soil physics which treats soil as a mixture of ellipsoidal particles in the continuous media of air and water, and requires various input values (Bachmann et al. 2001a). However, the choice of critical water content and the shape factors greatly affected the estimate of λ (Horton and Wierenga 1984; Ochsner et al. 2001). Johansen (1975) proposed the concept of normalized thermal conductivity which provided an improved prediction of thermal conductivity of soils of different textures. This model has been widely applied (Ewen and Thomas 1987; Young et al. 2002), but its predicted value of soil λ is low for low degrees of water content. Côté and Konrad (2005) modified Johansen's model to eliminate the logarithmic dependence on the saturation ratio, which distorted the results at low degrees of saturation. The model contains three empirical quantities related to particle composition and texture. Lu et al. (2007) based on the Johansen (1975) model, roughly divided the soil into coarse-grained soil and fine-grained soil according to the sand grain content. However, the model does not consider the soil texture, either quantitatively or qualitatively which leads to deviations. Later models (Lu et al. 2014; Nikoosokhan et al.2015; Su et al. 2016; He et al. 2017) changed the rough division of soil texture of the earlier model and the uncertainty value was converted into physical measurements related to the nature of soil. For example, Lu et al. (2014) proposed a model for estimating soil thermal conductivity (λ) using soil water content, porosity, bulk density, and texture, considering the effect of clay content on thermal conductivity, indicating that the grain composition of the soil also affects the thermal conductivity. Nikoosokhan et al. (2015) also developed a model, using soil volumetric water content, sand content, and dry soil specific weight. Forty field soil samples, from nine Canadian provinces, were laboratory tested for their ability to conduct heat [thermal conductivity (λ)] by Tarnawski, using a nonstationary probe technique (Tarnawski et al. 2014). The data were used to verify 13 predictive models; 4 mechanistic, 4 semi-empirical and 5 empirical equations. The applicability of each model was analyzed and compared, and the thermal conductivity models suitable for dry soil and saturated soil were found separately (Tarnawski et al. 2018). In addition to the above models, Tarnawski developed an advanced geometric mean model for predicting the effective thermal conductivity (λ) of unsaturated soils. Three soil structure-based parameters were used in the model, namely an inter-particle thermal contact resistance factor, the degree of saturation of a miniscule pore space, and the bulk thermal conductivity of soil solids. The model is suitable for soils containing less content of quartz and the model estimates were good for all soils in a dry state (Tarnawski and Leong 2016). The inverse modeling was also applied to the λ data of 22 soils from Hokkaido in northern Japan (Tarnawski et al. 2019). Furthermore, Tarnawski also studied the physical and thermal properties of various volcanic soils, frozen and non-frozen soils, as well as the factors affecting the thermal conductivity of each soil. However, further studies have shown that the organic matter content also indirectly affects the thermal conductivity of soil (Abuhamdeh and Reeder 2000), since the organic matter increases the soil's hydrophobicity, which changes the water distribution and hence the thermal conductivity (AbuHamdeh and Reeder 2000; Bachmann et al. 2001b; Gonzalez-Perez et al. 2004; Jaramillo et al. 2000). Still, the previous models rarely consider the influence of organic matter content on λ, and the shape factors used in the models to characterize the growth rate of thermal conductivity and the slope of the curve do not fully consider the effect of soil texture and particle composition. Thus, the prediction accuracy of the previous models is not high. Temperature is also an important factor affecting the thermal conductivity. High temperatures can affect convective water–vapor flow and phase changes or latent heat transfer but, since soil thermal properties are not often affected by temperatures at or below 55 °C (Smits et al. 2013), this paper ignores the influence of temperature on thermal conductivity. Instead, it examines the influence of soil texture and other physical parameters on λ, and develops a new thermal conductivity model with wider applicability and higher simulation accuracy.

The objectives of this study are:

1. To consider the effect of organic matter on thermal conductivity and develop a new empirical model based on the Nikoosokhan et al. (2015) model;
2. To use the new model to simulate the change of thermal conductivity with water content, using published datasets with a wide range of soil types;
3. To evaluate and compare the new model with the nine earlier models to verify the accuracy of the new model.

Nine historical models

Scholars proposed a number of indirect estimation models to describe the relationship between soil λ and other soil properties such as soil texture, bulk density, and water content, which are shown in the following nine models:

The Johansen (1975) model

This model is specific to unsaturated soil and based on dry soil thermal conductivity (λ_{dry}) and saturated soil thermal conductivity (λ_{sat}). Johansen (1975) established the relationship between soil thermal conductivity (λ) and the dimensionless Kersten coefficient (Ke) as:

$$\lambda = (\lambda_{sat} - \lambda_{dry}) \times Ke + \lambda_{dry}. \tag{1}$$

He also proposed a logarithmic relation between Ke and water content (θ) expressed as degree of saturation (S_r) ($S_r = \theta n^{-1}$, where n is the soil porosity):

$$Ke = \begin{cases} 0.7 \log S_r + 1.0, & 0.05 < S_r \le 0.1 \\ \log S_r + 1.0, & S_r > 0.1 \end{cases}, \tag{2}$$

$$\lambda_{sat} = \lambda_s^{1-n} \times \lambda_w^{n}. \tag{3}$$

In Eq. (3), $\lambda_w = 0.598$ W m^{-1} K^{-1} under 20 °C conditions, n is the soil porosity (%), λ_s is obtained by calculation of the quartz content (q) and quartz thermal conductivity $\lambda_q = 7.7$ W m^{-1} K^{-1} as well as the thermal conductivity of other minerals (λ_o) of the whole solid. Specifically given that $\lambda_s = \lambda_q^q \lambda_o^{1-q}$, $\lambda_o = 2.0$ W m^{-1} K^{-1} ($q > 0.2$), $\lambda_o = 3.0$ W m^{-1} K^{-1} ($q \le 0.2$) we have:

$$\lambda_{dry} = \frac{0.135\rho_b + 64.7}{2700 - 0.947\rho_b} \tag{4}$$

where ρ_b is the bulk density of soil or rock (kg m^{-3}).

The Campbell (1985) model

Based on the soil texture, bulk density and water content, Campbell (1985) proposed the empirical formula for calculation of soil thermal conductivity:

$$\lambda = A + B\theta - (A - D)e^{-(C\theta)E}. \tag{5}$$

In the formula, θ is the volumetric water content (cm^3 cm^{-3}) and parameters A, B, C, D and E are calculated according to the soil bulk density and clay content. Specifically,

$$A = 0.65 - 0.78\rho_b + 0.60\rho_b^2, \tag{6}$$

$$B = 1.06\rho_b, \tag{7}$$

$$C = 1 + \frac{2.6}{C_{clay}^{0.5}}, \tag{8}$$

$$D = 0.03 + 0.10\rho_b^2, \tag{9}$$

$$E = 4. \tag{10}$$

In the formula, C_{clay} is the clay particles mass fraction (%).

The Ewen and Thomas (1987) model

Ewen and Thomas (1987) work, based on Johansen (1975) model, proposed the exponential function of Ke:

$$Ke = 1 - \exp(-\xi S_r). \tag{11}$$

In the formula, ξ is a fitted parameter, specifically $\xi = 9.8$. The computational formulas for λ, λ_{sat} and λ_{dry} are (1), (3) and (4), respectively, in Johansen's model.

The Côté and Konrad (2005) model

Côté and Konrad (2005) improved the Johansen (1975) model by introducing a texture-dependent factor, κ to establish the relationship between Ke and S_r using unfrozen and frozen soils of different textures grain sizes based on their own measurements and published datasets:

$$Ke = \frac{\kappa \times S_r}{1 + (\kappa - 1) \times S_r}, \tag{12}$$

where $\kappa = 4.60$, 3.55, 1.90, and 0.60 for gravel and coarse sand, medium and fine sand, silty and clayed soils, and organic fibrous soils, respectively.

Côté and Konrad (2005) conducted an analysis of the relationship between dry soil thermal conductivity and porosity to propose a new computational formula for dry soil thermal conductivity:

$$\lambda_{dry} = \chi \times 10^{-\eta \times n}. \tag{13}$$

In the formula, χ (W m^{-1} K^{-1}) and η are the parameters affected by soil texture. The values of χ and η are shown in Table 1.

The Lu et al. (2007) model

To allow wider applicability of the Johansen (1975) model, Lu et al. (2007) conducted a large number of laboratory experiments investigating thermal conductivity of 12 types of soil under various conditions of water content, using the heat pulse (HP) method. According to the results, and specific to the fine-grained soils, the relationship between *Ke* and degree of saturation (S_r) was found to be somewhat influenced by the soil type. Through experimental data fitting, a simpler linear relationship between dry soil thermal conductivity and porosity was obtained. Finally, on the basis of the Johansen (1975) model, Lu et al. (2007) proposed a new type of exponential function expression of *Ke* and S_r:

$$Ke = e^{m(1-S_r^{m-1.33})}. \tag{14}$$

In Eq. (14), m is an empirical value determined by sand grain content and 1.33 is a shape parameter. The model roughly divides the soil into coarse-texture soil and fine-texture soil. The values of m for coarse-texture soil with sand grain content above 40% and fine-texture soil with sand grain content below 40% are 0.96 and 0.27, respectively. A linear function to predict λ_{dry} from n was introduced:

$$\lambda_{dry} = -a \times n + b, \tag{15}$$

where a and b are the empirical coefficients and n is the porosity (%). When $0.2 < n < 0.6$, the values of a and b are 0.56 and 0.51, respectively.

Table 1 Values of χ and η

Type of soil	χ	η
Crushed rock	1.70	1.20
Mineral soil	1.80	0.30
High organic matter content	0.75	0.87

The Lu et al. (2014) model

On the basis of the Lu et al. (2007) model, Lu et al. (2014) considered the influence of soil clay content on thermal conductivity, and proposed the following exponential function to indicate the non-linear relationship between λ and soil water content, soil texture, and bulk density ρ_b (g cm^{-3}):

$$\lambda = \lambda_{dry} + \exp\left(-\theta^{-\mu}\right), \qquad \theta > 0. \tag{16}$$

In Eq. (16), the parameters μ and φ are the shape factors of the λ (θ) curve related to the sand grain content, clay content and bulk density, and λ_{dry} is calculated from Eq. (15) of Lu et al. (2007).

The linear relationship between μ and the clay particle mass fraction C_{clay} is given as:

$$\mu = 0.67C_{clay} + 0.24. \tag{17}$$

The expression for φ was calculated using multiple regression and is dependent on the sandy soil mass fraction C_{sand}, and the bulk density $\rho_{b:}$

$$\varphi = 1.97C_{sand} + 1.87\rho_b - 1.36C_{sand}\rho_b - 0.95. \tag{18}$$

Hence, when the soil porosity, soil fraction composition (clay and sandy soil content) and ρ_b are known, λ can be estimated through Eqs. (16)–(18).

The Nikoosokhan et al. (2015) model

Nikoosokhan et al. (2015) also adopted the normalized model of Johansen (1975) and proposed two new linear relationships for λ_{sat} and λ_{dry} involving the sandy soil content and dry soil specific weight γ_d which are given by:

$$\lambda_{sat} = 0.53C_{sand} + 0.1\gamma_d, \tag{19}$$

$$\lambda_{dry} = 0.087C_{sand} + 0.019\gamma_d. \tag{20}$$

When the sand content is $0 < C_{sand} < 1$, the dry soil specific weight is $11 < \gamma_d < 20$. The relational expression between γ_d (KN m^{-3}) and ρ_b (g cm^{-3}) is:

$$\gamma_d = g \times \rho_b, \tag{21}$$

where g is the gravity acceleration, $g = 9.8$ m s^{-2}. The relationship between *Ke* and S_r is obtained from Eq. (12) of Côté and Konrad (2005). In this model, the value of k can be calculated from C_{sand} by:

$$k = 4.4C_{sand} + 0.4. \tag{22}$$

The Su et al. (2016) model

To facilitate a more accurate prediction by the Lu et al. (2007) model of soil thermal conductivity and to correctly reflect the influence of soil particle composition, water content, and organic content on the soil thermal conductivity, Su et al. (2016) improved the expression of the shape factor ω:

$$\omega = c \times C_{\mathrm{clay}} + d \times C_{\mathrm{silt}} + e \times C_{\mathrm{sand}} + f \times C_{\mathrm{om}}. \tag{23}$$

In the formula, C_{clay} is the clay particles mass fraction (%), C_{silt} is the silt mass fraction (%), C_{sand} is the sand mass fraction (%), C_{om} is the mass ratio of organic matter (g kg^{-1}) and c, d, e and f are weighting factors ($c = -0.5863$, $d = 0.9451$, $e = 0.1080$, $f = 0.0567$) (Su et al. 2016).

The He et al. (2017) model

He et al. (2017) believed that the computational method of *Ke* can be considered as the numerical interpolation between the value of saturated soil thermal conductivity and the value of dry soil thermal conductivity. Based on the studies by Lu et al. (2007, 2014) and van Genuchten (1980), He et al. (2017) proposed a new type of model for the calculation of *Ke*:

$$Ke = \begin{cases} 0, & \theta = 0 \\ (J \times \exp\left(\theta^{-L}\right), & \theta > 0 \end{cases}, \tag{24}$$

where J and L are the fitting parameters. Notably, the values of J and L are different for different soils, and J and L are not easy to determine (He et al. 2017). The final model is as follows:

$$\lambda = \begin{cases} \lambda_{\mathrm{dry}} & \theta = 0 \\ \lambda_{\mathrm{dry}} + (\lambda_{\mathrm{sat}} - \lambda_{\mathrm{dry}}) \big/ \left[J \cdot \exp(\theta^{-L})\right] & \theta > 0 \end{cases}, \tag{25}$$

where λ_{sat} and λ_{dry} are calculated according to the Eqs. (3) and (15), respectively. And $\lambda_{\mathrm{w}} = 0.598$ W m^{-1} K^{-1}.

The New empirical model

In the Johansen (1975) model, the degree of saturation S_{r} reflects the influence of soil water content, and the soil porosity n reflects the influence of soil bulk density on soil thermal conductivity. However, the influence of soil particle composition on soil thermal conductivity (λ) is not embodied in the Johansen (1975) model. The models by Côté and Konrad (2005) and Lu et al. (2007) are improvements of the Johansen (1975) model. The parameters k and m are utilized to reflect the influence of soil texture on thermal conductivity and the reference values for different soil textures are given. However, the soil type is not adequately classified and errors in simulated results remain. Although later models are continuously improved (He et al. 2017; Lu et al. 2014; Nikoosokhan et al. 2015; Su et al. 2016), there are many factors influencing λ, and each factor is mutually constrained. Thus, errors persist. In this model, the influence of organic matter content and particle composition on thermal conductivity is considered, and a new relationship between *Ke* and θ based on the previous models within the entire range of water content is proposed.

$$Ke = \exp(\alpha - \theta^{-\beta}), \tag{26}$$

where α and β are the shape factors of the $\lambda(\theta)$ curve, Since the values of α and β affect the slope and growth rate of the thermal conductivity curve, the relationship between α and β and soil texture should be considered. Suppose that they satisfy the following linear relationships:

$$\alpha = g \times C_{\mathrm{sand}} + h \times C_{\mathrm{silt}} + i \times C_{\mathrm{om}} + j, \tag{27}$$

$$\beta = p \times C_{\mathrm{clay}} + r \times C_{\mathrm{om}} + s, \tag{28}$$

where ρ_{b} is the bulk density (g cm^{-3}), and g, h, i, p and r are the weighting factors of the physical parameter's effects on λ, j and s are soil particle shape values, and λ_{sat} and λ_{dry} as calculated from Eqs. (19) and (20).

The factors considered by the new model are more comprehensive than that of the previous models. The new model considers the effect of organic matter on soil λ, and the shape factor takes into account the effects of soil texture and particle composition, making it necessary to fit through the measured values to obtain an empirical weighting factors. The fitting results were tested by the Fisher Exact test.

Materials and methods

Soil samples

Nineteen soils were used in this study (Table 2): soils 1–6, 8–14 and 18–19 were from China (Lu et al. 2007; Su et al. 2016; Wang et al. 2012), soil 7 was from Iowa (Lu et al. 2007), soils 15–17 were from Oregon (Cochran 1967). The thermal conductivity values of soils 1–14 and soils 18–19 were measured at 20–25 °C, the thermal conductivity values of soils 15–17 were measured below 20 °C. The 19 soils were divided into two groups, with one group (soils 1–9) used as an integrated dataset to build the new empirical model, while a second group (soils 10–19) was used to verify the accuracy of and to evaluate the performance of the new model.

Table 2 lists the particle size distribution (PSD), organic matter content, and the ρ_{b} for each of the repacked soils. The soil samples were air dried, ground, and sieved through a 2-mm screen. Soil PSD was determined using 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).

Table 2 Physical properties of soils used for calibrating and evaluating of the new model

Soil	Texture	Particle size distribution			Bulk density (g cm^{-3})	Organic matter content (%)	Source
		Sand	Silt	Clay			
1	Sand	0.94	0.01	0.05	1.60	0.09	Lu et al. (2007)
2	Loam	0.40	0.49	0.11	1.20	0.49	Lu et al. (2007)
3	Silt clay loam	0.19	0.54	0.27	1.40	0.39	Lu et al. (2007)
4	Clay loam	0.32	0.38	0.30	1.29	0.27	Lu et al. (2007)
5	Sand	0.93	0.01	0.06	1.60	0.07	Lu et al. (2007)
6	Sand	0.94	0.01	0.05	1.50	0.09	Lu et al. (2007)
7	Sand	0.92	0.07	0.01	1.58	0.60	Lu et al. (2007)
8	Silt loam	0.11	0.70	0.19	1.31	0.84	Lu et al. (2013)
9	Korla sand loam	0.64	0.29	0.07	1.45	0.86	Wang et al. (2012)
10	Sandy loam	0.67	0.21	0.12	1.39	0.86	Lu et al. (2007)
11	Silt loam	0.27	0.51	0.22	1.33	1.19	Lu et al. (2007)
12	Loam	0.50	0.41	0.09	1.38	0.25	Lu et al. (2007)
13	Shenmu sand	0.98	0.01	0.01	1.45	0.53	Wang et al. (2012)
14	Yangling loam clay	0.27	0.43	0.30	1.45	0.27	Wang et al. (2012)
15	AC	0.76	0.21	0.03	0.76	2.66	Cochran (1967)
16	C1	0.94	0.05	0.01	0.44	0.73	Cochran (1967)
17	C2	0.93	0.06	0.01	0.53	0.8	Cochran (1967)
18	Yichuan clay loam	0.49	0.30	0.21	1.34	5.07	Su et al. (2016)
19	Ankang silty loam	0.33	0.39	0.28	1.32	21.65	Su et al. (2016)

Heat pulse measurement of soil thermal conductivity

The λ values of soils 1–14 were determined using the heat pulse (HP) method on repacked soil columns with fixed ρ_b and θ ranging from air dry to saturation (Lu et al. 2007, 2013; Su et al. 2016; Wang et al. 2012). 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 al. 1999) was used for measuring soil λ with the HP method. For further details about the theory, equipment, and procedures of measuring soil thermal properties with the HP method, 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 then oven dried at 105 °C to constant mass, and ρ_b and θ were determined. The λ values of soils 15–17 were determined experimentally with a line heat source. Specific measurement methods can be referred to Cochran (1967).

For soils 18 and 19, the thermal pulse method to measure λ values in the field was used. Soils 15–16 were sampled by the ring knife at the test site, set to 2 columns, 10 measuring points per column, for a total of 20 measuring points, step length 3 m, and 4 kinds of water content for each measuring point. To reduce the error caused by the influence of ambient temperature change on the probe measurement, the measuring point was covered by a shaded plastic canvas. The test was repeated three times, and the average of three tests was taken. Figure 1 shows the measured values of thermal conductivity of the 16 soils with different water contents.

Model evaluation

As shown in Table 2, 10 different types of soil from samples 10–19 which were not involved in the model fitting were selected for the model verification dataset. These samples represented sandy loam, silt loam, loam, Shenmu sand, Yangling loam clay, Yichuan clay loam, Ankang silty loam and three pumice soils (AC, C1, C2), respectively. The thermal conductivities were calculated by putting the physical parameters of the ten samples into the new model as well as into the previous nine models. The study evaluated the simulation precision of each of the ten models using the standard deviation (SD), coefficient of determination (R^2) and relative error (Re):

$$SD = \sqrt{\frac{\sum_1^N \left(O_i - S_i\right)^2}{N - M}}, \tag{29}$$

$$R^2 = 1 - \sum_{i=1}^{N} (O_i - S_i)^2 / \sum_{i=1}^{N} (O_i - \overline{O})^2, \tag{30}$$

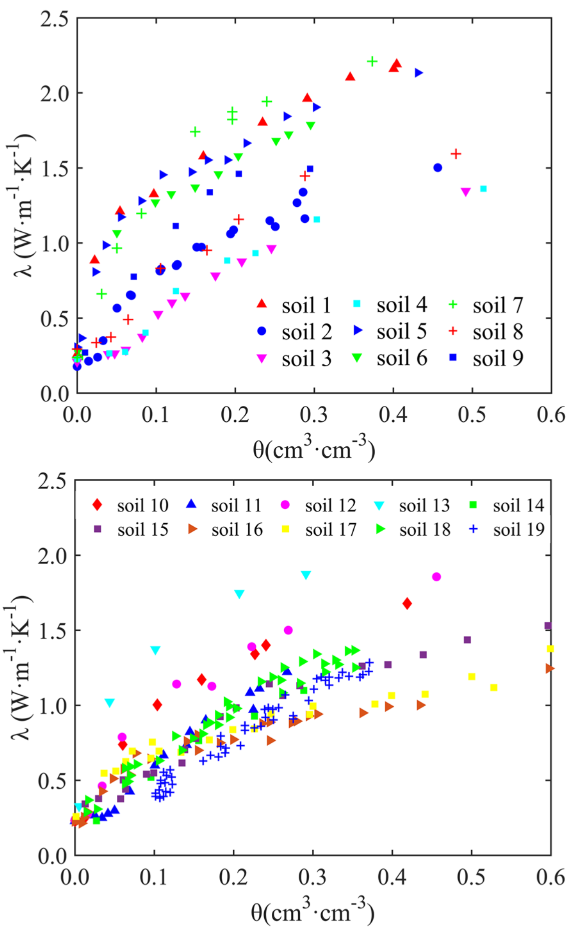

Fig. 1 The measured values of thermal conductivity of 19 soils

$$\mathrm{Re} = \sqrt{\sum_{i=1}^{N} (O_i - S_i)^2 / \sum_{i=1}^{N} O_i^2}, \tag{31}$$

In these equations, O_i is the measured value, S_i is the model simulated value, N is the number of independent λ records, M is the number of parameters in the model used for fitting to measured value and $\bar{O}$ is the sample mean. A smaller SD means a better performance of the predictive model (Tarnawski et al. 2018). The closer the value of the coefficient of determination, R^2, of the linear regression of the measured value versus simulated value is to 1, the more accurate the model (Quinino et al. 2013) and a smaller value of relative error (Re) represents higher model precision (Suñé and Carrasco 2005).

Results and discussion

Determination of α and β for the new model

Soil samples 1–9 were used as an integrated dataset, since the nine soil types provided a good representation of a range of soil types. As such, it provides a useful simulation group to study the effects of soil texture and particle fraction on λ and α and β. The measured values of soil fraction composition, bulk density, porosity and organic matter content, and thermal conductivity are shown in Table 2 and Fig. 1. Using the Curve fitting tool (Cftool) in Matlab, the thermal conductivity of the nine soils was calculated using the new model formulas (26)–(28). The results are shown in Fig. 2. As seen in Fig. 2, the best shape factors α and β for soils 1–9 were compiled, and λ_{sat} and λ_{dry} were calculated using Eqs. (19) and (20), and the results are shown in Table 3.

Looking at Table 3 shows, for example, that the thermal conductivity of sand in dry conditions (soil 1) can reach 0.380 W m^{-1} K^{-1}, while the clay loam (soil 3) is only 0.277 W m^{-1} K^{-1}. From Fig. 1 the thermal conductivity of sand at the same water content is obviously higher than that of sandy loam, followed by loam and the thermal conductivity of clay loam is lowest. Comparing Fig. 2 with Table 2, we see that the higher the sand content, the higher the thermal conductivity of soil, since the sand has a higher content of quartz, and the thermal conductivity of quartz is higher (Johansen 1975; Lu et al. 2007). The trend of thermal conductivity with water content can be described by an exponential function. The value of α ranges from 1.179 to 1.601, and the range of β is 0.250–0.479. Using the best shape factors of the 9 soils, the weighting factors of each particle component were solved by Eqs. (27) and (28).

The following matrices can be formed using multiple linear combinations. The mass fractions of sand (%), silt (%) and clay (%) of the soil types 1–9 (%) are represented by $C_{sand1}-C_{sand9}$, $C_{silt1}-C_{silt9}$ and $C_{clay1}-C_{clay9}$, respectively, the bulk density (g cm^{-3}) by $\rho_{b1}-\rho_{b2}$ and mass ratio of organic matter (g kg^{-1}) by $C_{om1}-C_{om9}$.

$$\begin{pmatrix} C_{sand1} & C_{silt1} & C_{om1} \\ C_{sand2} & C_{silt2} & C_{om2} \\ \vdots & \vdots & \vdots \\ C_{sand8} & C_{silt8} & C_{om8} \\ C_{sand9} & C_{silt9} & C_{om9} \end{pmatrix} \times \begin{pmatrix} g \\ h \\ i \end{pmatrix} + j \times \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_8 \\ \alpha_9 \end{pmatrix}, \tag{32}$$

$$\begin{pmatrix} C_{clay1} & C_{om1} \\ C_{clay2} & C_{om2} \\ \vdots & \vdots \\ C_{clay8} & C_{om8} \\ C_{clay9} & C_{om9} \end{pmatrix} \times \begin{pmatrix} p \\ r \end{pmatrix} + s \times \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_8 \\ \beta_9 \end{pmatrix}. \tag{33}$$

Solving these multivariate equations yielded the values of the empirical weighting factors g, h, i, p and r corresponding to each particle component and soil particle shape values j and s, the Fisher Exact test was carried out, and the test result passed at the confidence level of 0.05, which further

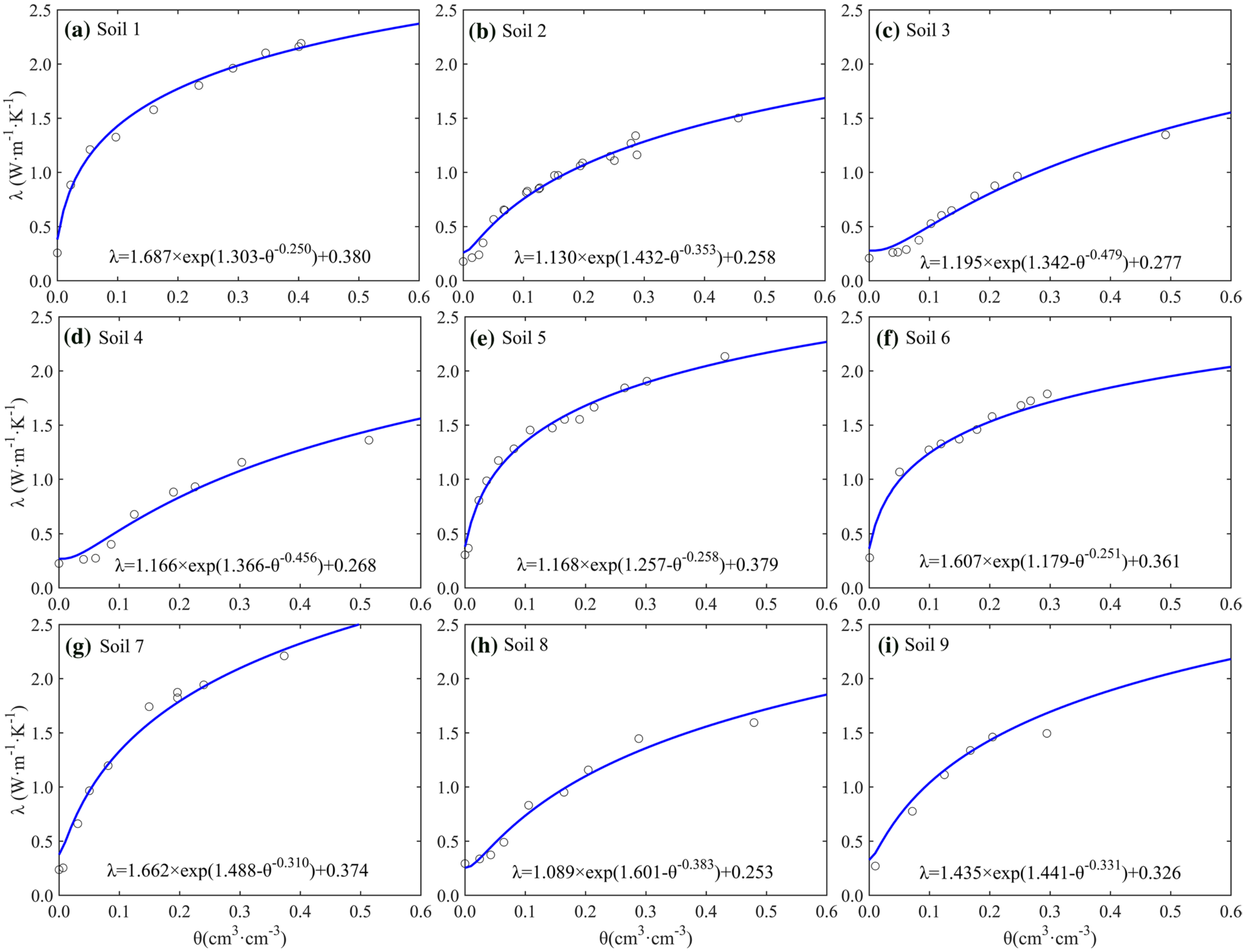

Fig. 2 Fitting results for soil types 1–9

Table 3 Values of the shape factors α and β for soil types 1–9

Soil	Texture	λ_{dry} (W m^{-1} K^{-1})	λ_{sat} (W m^{-1} K^{-1})	α	β
1	Sand	0.380	2.066	1.303	0.250
2	Loam	0.258	1.388	1.432	0.353
3	Silt clay loam	0.277	1.473	1.342	0.479
4	Clay loam	0.268	1.434	1.366	0.456
5	Sand	0.379	2.061	1.257	0.258
6	Sand	0.361	1.968	1.179	0.251
7	Sand	0.374	2.036	1.488	0.310
8	Silt loam	0.253	1.342	1.601	0.383
9	Korla sandy loam	0.326	1.761	1.441	0.331

indicates that the establishment of the new model is meaningful. The shape factors were obtained by substituting into Eqs. (27) and (28). The empirical values for the factors α and β are then:

$$\alpha = 0.493C_{sand} + 0.86C_{silt} + 0.014C_{om} + 0.778, \quad (34)$$

$$\beta = 0.736C_{clay} + 0.006C_{om} + 0.222. \quad (35)$$

Model evaluation and comparison

As discussed previously, eight different types of soil which were not used for fitting the new model were selected from the model verification dataset, specifically, soil types 10–17 representing sandy loam, silt loam, loam, Shenmu sand and Yangling loam clay, and three pumice soils(AC, C1, C2), respectively. The thermal conductivity of these eight soils was calculated using the new model along with the previous nine models. Figure 3a and b show the fit of the new empirical model and other nine soil thermal conductivity models on the soil types 10–17. Table 4 shows the R^2 and Re values in simulated soil conductivity values for different estimation models, Table 5 shows the SD values for different estimation models to evaluate the performance of each model.

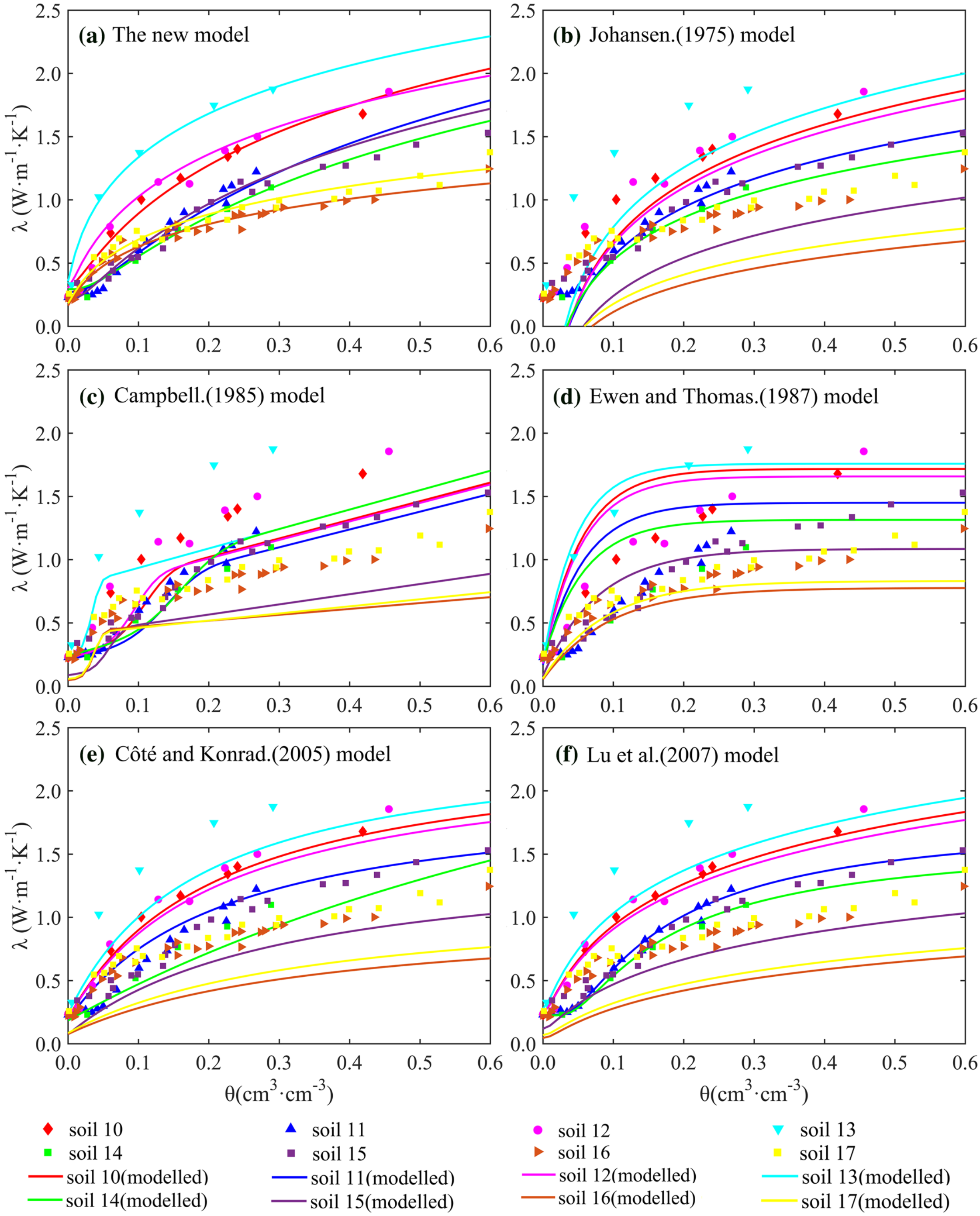

Fig. 3 A comparison of measured and modeled soil thermal conductivity for different water content **a** the new model; **b** the Johansen (1975) model; **c** Campbell (1985) model; **d** Ewen and Thomas (1987) model; **e** Côté and Konrad (2005) model; **f** Lu et al. (2007) model. A comparison of measured and modeled soil thermal conductivity for different water content **g** Lu et al. (2014) model; **h** Nikoosokhan et al. (2015) model; **i** Su et al. (2016) model and; **j** He et al. (2017) model

The main factors influencing soil thermal conductivity are soil water content, porosity, bulk density, mineral composition and organic content. Water content is the most important factor. It can be seen from Fig. 3 that at low water content, the thermal conductivity increases sharply with the increase of water content. When the water content increases to a certain point, the thermal conductivity increases with the increase of water content, and the rate

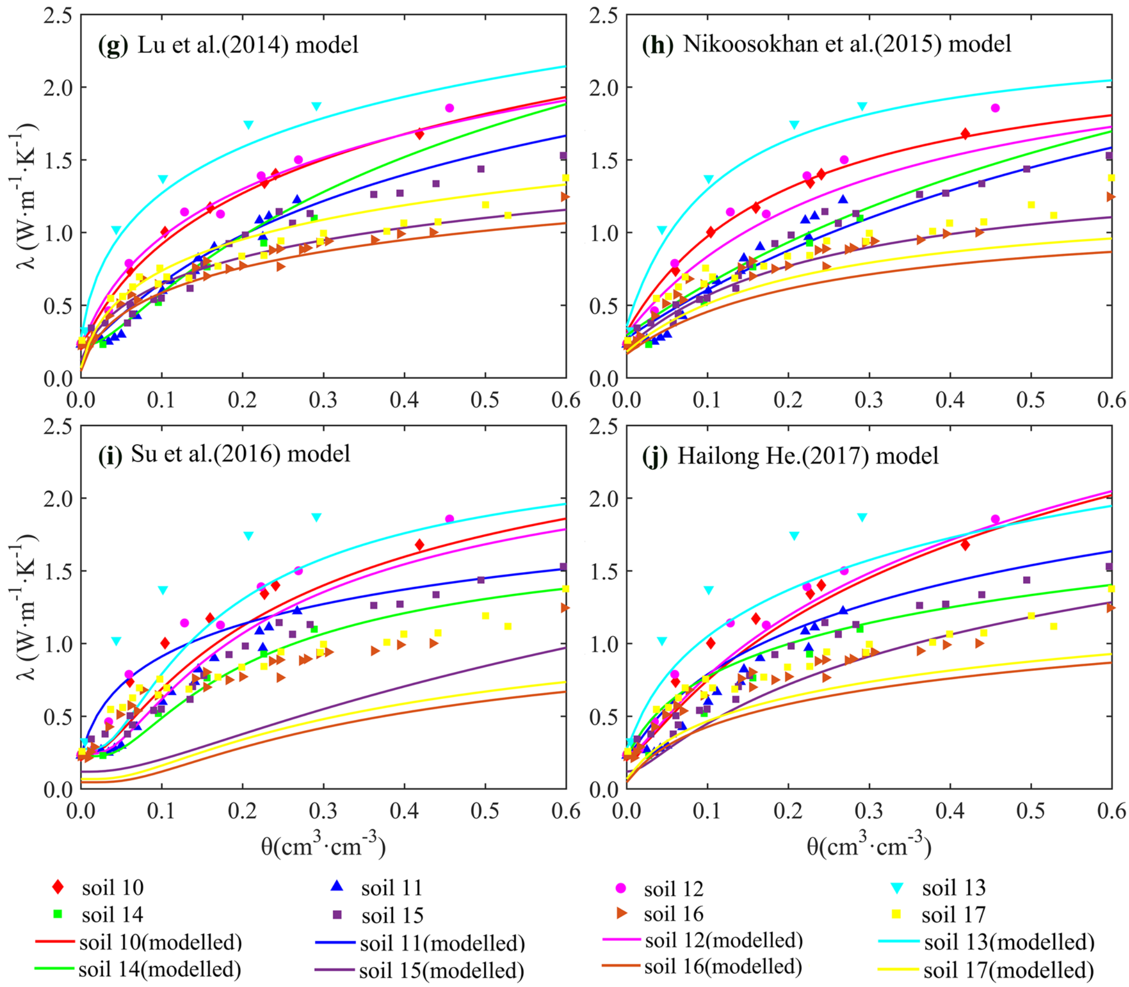

Fig. 3 (continued)

is greatly slowed down. Low effective contact area leads to low thermal conductivity. This is because the thermal conductivity of air is extremely low (only 0.024 W m^{-1} K^{-1}) in the three-phase composition of the soil. Therefore, when the soil is in a dry state, the heat conduction in the soil is mainly through the contact point of soil particles. As the water content increases, the air in the pores of the soil is gradually replaced by water of a relatively high thermal conductivity, since the thermal conductivity of water is 0.605 W m^{-1} K^{-1}, which is 25 times the thermal conductivity of the air. As the soil water content increases, one or more water films are formed between the soil particles, which increases the heat transfer area and also causes an increase in thermal conductivity, However, when the water content increases to a certain point, most of the air in the soil exists in the form of closed bubbles. The heat in the soil can only be transmitted through the water film wrapped around the surface of the particles, and the thermal conductivity of the soil no longer grows with increasing water content. Thermal conductivity values of eight soils at the same water content show that soil 13 (Shenmu sand) > soil 12 (Loam) > soil 10 (Sandy loam) > soil 11 (Silt loam) > soil 14 (Yangling loam clay) > soil 15 (AC) > soil 17 (C1) > soil 16 (C2). Looking at Table 2, it can be seen that the higher the sand content, the lower the clay content, the greater the thermal conductivity of the soil, and the stronger the ability of thermal conductivity. However, the thermal conductivity of pumice soil is generally low, which may be affected by the properties of soil materials and the measurement conditions.

It is obvious from the fitting results that the previous models do not estimate the thermal conductivity of various soil types as well as the new model. The new model achieved a best fit within the entire range of λ (θ) and had better predictive performance. Therefore, it is suitable for application to extensively mineralized soil. Its SD value is the smallest compared to the other models, with the value of 0.074 W m^{-1} K^{-1}, R^2 changes from 0.929 to 0.983, with a mean of 0.964 and Re changes from 5.210

Table 4 Errors in simulated soil thermal conductivity values for different estimation models

Model	Soil 10		Soil 11		Soil 12		Soil 13		Soil 14		Soil 15		Soil 16		Soil 17	
	R^2	Re/%	R^2	Re/%	R^2	Re/%	R^2	Re/%	R^2	Re/%	R^2	Re/%	R^2	Re/%	R^2	Re/%
Johansen (1975)	0.391	18.600	0.923	9.090	0.238	16.400	0.018	62.070	0.745	20.050	0.172	38.330	0.020	53.050	0.080	44.970
Campbell (1985)	0.667	26.160	0.901	14.480	0.686	27.130	0.295	33.790	0.883	13.540	0.189	41.810	0.190	38.070	0.141	39.740
Ewen and Thomas (1987)	0.510	31.760	0.021	66.740	0.660	28.200	0.955	8.570	0.031	54.950	0.699	22.040	0.586	23.580	0.252	24.840
Côté and Konrad (2005)	0.990	4.490	0.851	17.740	0.952	10.580	0.688	22.470	0.822	16.720	0.345	32.490	0.142	48.380	0.135	44.150
Lu et al. (2007)	0.993	3.750	0.988	5.010	0.955	10.280	0.715	21.480	0.994	3.040	0.416	30.690	0.143	48.680	0.133	45.050
Lu et al. (2014)	0.993	3.820	0.956	9.610	0.977	7.410	0.964	7.650	0.900	12.520	0.761	19.640	0.908	11.120	0.812	12.460
Nikoosokhan et al. (2015)	0.978	6.690	0.890	15.260	0.915	14.110	0.972	6.770	0.892	13.010	0.683	22.610	0.507	25.720	0.350	23.160
Su et al. (2016)	0.874	16.110	0.385	36.010	0.798	21.740	0.340	32.680	0.982	5.270	0.162	51.650	0.120	62.150	0.101	56.530
He et al. (2017)	0.925	12.410	0.774	21.830	0.947	11.180	0.734	20.750	0.693	22.000	0.703	21.900	0.332	29.920	0.208	28.410
The new model	0.979	6.560	0.969	8.130	0.962	9.390	0.983	5.210	0.981	5.420	0.939	9.900	0.969	6.400	0.929	7.670

Table 5 The SD value for different estimation models

Model	SD (W m^{-1} K^{-1})
Johansen (1975)	0.308
Campbell (1985)	0.311
Ewen and Thomas (1987)	0.290
Côté and Konrad (2005)	0.295
Lu et al. (2007)	0.289
Lu et al. (2014)	0.115
Nikoosokhan et al. (2015)	0.179
Su et al. (2016)	0.419
He et al. (2017)	0.209
The new model	0.074

to 9.900%, with a mean of 7.335%. The model fit indicators obtained are improvements of those obtained for other models, because the new empirical model more accurately studies the effect of soil texture on thermal conductivity, considering a more comprehensive set of factors and the effect of soil texture on the shape factor of the models. Subsequently, the simulations were obtained using the models of Lu et al. (2014), Nikoosokhan et al. (2015), He et al. (2017) and Lu et al. (2007), with SD values of 0.115, 0.179, 0.209 and 0.289 W m^{-1} K^{-1}, respectively. The model by Côté and Konrad (2005) had SD and mean values for R^2 and Re of 0.295 W m^{-1} K^{-1}, 0.616 and 24.628%. The logarithmic dependence on the saturation ratio in the Johansen (1975) model leads to poor simulated results at low degrees of saturation; it underestimates the thermal conductivity over the entire water content range. It can be seen from Fig. 3a that the Johansen (1975) model has a good fitting effect on soil with high loam content and poor fitting effect on sand. The models of Côté and Konrad (2005), Lu et al. (2007), and Su et al. (2016) underestimate the thermal conductivity of soils with higher sand content. This is because these three models can be seen as a logical extension of Johansen (1975). In these models, Côté and Konrad (2005) and Lu et al. (2007) recommended different parameter values for soil textures, but no quantitative thresholds were given to distinguish boundaries between textures. For example, κ is introduced to distinguish soil texture, where $\kappa = 4.60$, 3.25, 1.40, and 1.12 are used for gravel and coarse sand, medium and fine sand, silty and clayed soils, and the soil with high content of organic matter, respectively by Côté and Konrad (2005), while $m = 0.96$ and 0.27 were suggested for coarse-textured and fine-textured soils, respectively by Lu et al. (2007). However, using two different values of m may result in a similar λ for the same soil which indicates m is difficult to define. Therefore, the fitting effect of these two models is ordinary. The Su et al. (2016) model which is only applicable to soils with high clay content, and has poor fitting effect on other types of soil, had a SD and mean values for R^2 and

Re of 0.419 W m^{-1} K^{-1}, 0.470 and 35.268%. The models by Campbell (1985) and Ewen and Thomas (1987) provided the worst fits. Although the model by Campbell (1985) is simple, it does not consider the effect of sand grain content on thermal conductivity, resulting in a larger simulation error, Specifically, for soil with high sand content, the simulated value and the measured value deviate greatly, The model by Campbell (1985) produced a SD and mean values for R^2 and Re of 0.311 W m^{-1} K^{-1}, 0.494 and 29.340%, respectively. The model by Ewen and Thomas (1987) predicts relatively large values when the soil water content is low and vice versa. On the whole, the model has poor predictive capacity, with mean values for R^2 and Re of 0.464 and 32.585%, respectively. Especially for the three types of pumice soil, except for the new model and Lu et al. (2014) model, each model underestimates the thermal conductivity value of the pumice soil, and the simulated value and the measured value are quite different. The new model has a good fitting effect on the three types of pumice soil, and the simulated value is almost in agreement with the measured value. This further indicates that the new model has better predictive performance and wider application range than other models. The detailed evaluation error results are shown in Tables 4 and 5.

In summary, the smallest error was shown by the new model, mainly because the values of parameters estimated for the other models were not accurate and soil texture was not quantitatively categorized for these models, resulting in uncertain parameter values and larger errors. In addition, the effect of all physical parameters of soil on the thermal conductivity is not comprehensively considered for earlier models. The new model based on the previous models fully accounts for the effects of soil particle composition, water content, bulk density, organic matter content and porosity on thermal conductivity, Furthermore, the relationship between the magnitude of the thermal conductivity λ and the change of water content and the soil texture is studied; so the simulation effect is better, and the scope of application is wider.

Verification of model accuracy

To more clearly compare the error between the simulated and measured values of each model, we verified the model accuracy for soils 10–17 and the other two independently measured soil samples (soil 18 and soil 19). The results of the model verification are shown in Fig. 4a and b.

Figure 4a and b show that the new model performed the best with an R^2 of 0. 98, all fitted values are almost always near the 1:1 line, followed by the models by Lu et al. (2014) and Nikoosokhan et al. (2015) with R^2 values of 0.95 and 0.89, respectively. He et al. (2017) has a good fitting effect, while the Johansen (1975) model obviously underestimates the soil thermal conductivity value, especially when the water content is low, but it fits well to soil 11, soil 14 and soil 18 and soil 19, indicating that the model is suitable for clay loam and soil with high loam content. Similarly, the Campbell model (1985) also underestimates the soil thermal conductivity value, but it also has a high accuracy for soils with high loam content, and the fitting effect is better than the Johansen (1975) model. In contrast, the Ewen and Thomas (1987) model is more likely to overestimate the soil thermal conductivity value.

According to the results shown in Figs. 3 and 4 and Tables 4 and 5, the new empirical model is better able to adapt to most categories of soil texture, has good performance, provides a better fit to observed data and has high prediction accuracy.

Conclusion

For a specific soil, the thermal conductivity depends on the soil texture, porosity, water content, and other parameters. The present study proposes a new empirical model that builds on previous models and is based on various fundamental physical parameters of soil. The new model comprehensively considers the factors influencing soil thermal conductivity. The model simulations of thermal conductivity were verified for 10 types of soil and compared to 9 other models, to evaluate the accuracy of the new model and the following conclusions were drawn:

1. The research proves that the new empirical model does well in simulating the thermal conductivity of different soil textures. Compared to nine other models, the simulation accuracy is higher, and the scope of application is wider. Therefore, it is necessary to consider the influence of organic matter content on the thermal conductivity. The new model could be applied to agricultural science, environmental science, earth science and engineering research.
2. The new model, Lu et al. (2014) and Nikoosokhan et al. (2015) have good fitting effects. The Johansen (1975) model underestimates the thermal conductivity over the entire water content range, because the dependence on the saturation in the model is too large and the fit to sand soil is poor. Lu et al. (2007) and Su et al. (2016) are not suitable for estimating the thermal conductivity of sand, and the fitted value is small. Lu et al. (2007) has a high precision for the thermal conductivity of fine-grained soil and poor for coarse-grained soil. The change law of thermal conductivity simulated by the Ewen and Thomas (1987) model is consistent with the measured value with the change of water content, but the fitting value is larger than the measured value, and the simulation error is larger. In general, the new model showed a wider range of application and smaller errors. One dis-

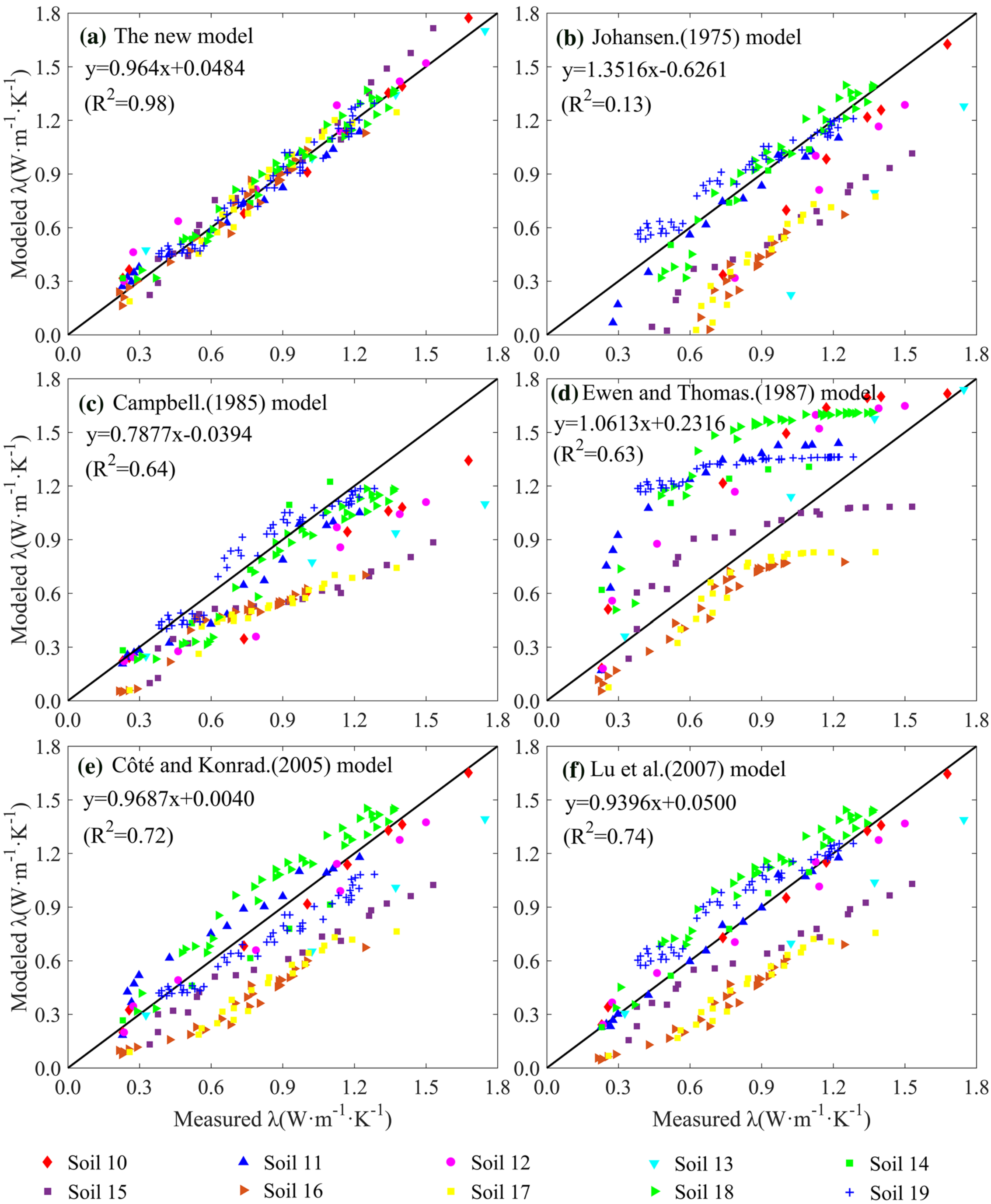

Fig. 4 Comparison of simulated thermal conductivities by various models and measured thermal conductivity using linear regression and coefficient of determination (R^2) **a** the new model; **b** the Johansen (1975) model; **c** Campbell (1985) model; **d** Ewen and Thomas (1987) model; **e** Côté and Konrad (2005) model; **f** Lu et al. (2007) model. **b** Comparison of simulated thermal conductivities by various models and measured thermal conductivity using linear regression and coefficient of determination (R^2); **g** Lu et al. (2014) model; **h** Nikoosokhan et al. (2015) model; **i** Su et al. (2016) model and; **j** He et al. (2017) model

advantage of the model is its requirement of some additional physical parameters. Accordingly, the new model is suitable for estimating soil thermal conductivity when the soil fraction composition, bulk density, porosity and organic matter content of soil are known.

3. Since different models assessed showed both advantages and disadvantages, and the performance of a particular model is dependent on conditions such as soil texture and water content, it is recommended that the model

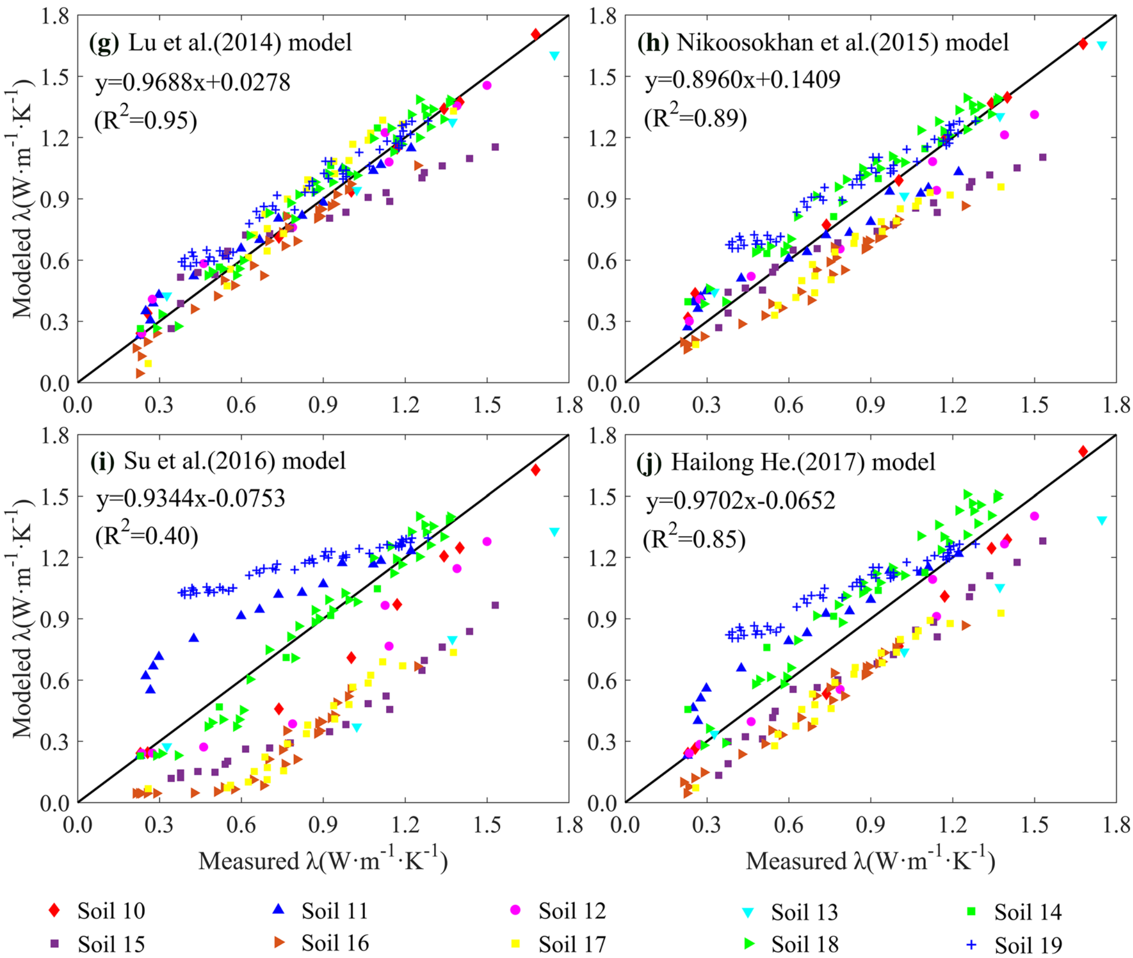

Fig. 4 (continued)

used should be chosen during practical application according to the soil type.

4. In addition to the influence of soil texture and water content, the thermal conductivity of soil will also be affected by the high temperature and soil spatial structure. Therefore, the influence of spatial structure and high temperature on the thermal conductivity of soil should be further studied in the later stage. The thermal characteristics of the soils of special soil types such as volcanic soils and frozen soils and the models they are suitable for should also be further studied.

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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