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A sigmoidal model for predicting soil thermal conductivity-water content function in room temperature

Ali Reza Sepaskhah & Maasumeh Mazaheri-Tehrani

Apparent thermal conductivity of soil (λ) as a function of soil water content (θ), i.e., $\lambda(\theta)$ is needed to determine the heat flow in soil. The function of $\lambda(\theta)$ can be used in heat and water flow models for simplicity. The objective of this study was to develop a sigmoidal model based on logistic equation for entire range of soil water contents and a wide range of soil textures that can be used in simulation of heat and water flow in respected modes. Further, performance of the developed sigmoidal model along with two other models in literature was evaluated. In the proposed sigmoidal model, the constants of this model are estimated based on empirical multivariate equations by using soil sand content and bulk density. The sigmoidal model was validated with good accuracy for a wide range of soil textures, as the relationship between the measured and predicted λ showed slope and intercept values of nearly 1.0 and 0.0, respectively. Comparison of the results obtained by sigmoidal model with those obtained from Johansen and Lu et al. models indicated that, the sigmoidal model was superior to the other two models in prediction of λ for a wide range of soil textures and soil water contents. Furthermore, comparison with a recently proposed model by Xiong et al. indicated that our sigmoidal model is superior. Therefore, our developed sigmoidal model can be used in heat and water flow models to predict the soil temperature and heat flow.

Keywords Logistic equation, Model evaluation, Heat probe, Thermal conductivity measurements, Thermal properties

Heat flow in soil is related to soil thermal conductivity that is used in studying the soil temperature distribution, energy balance at soil surface, the artificial heating of soils for enhanced crop production and heat flow away from industrial installations in the ground¹.

Heat conduction in moist soil (soil solid particle + soil water) is occurred due to heat transfer by soil solid particles and solid-water interaction (liquid and vapor). Therefore, soil thermal conductivity is considered as apparent thermal conductivity (λ). The apparent thermal conductivity of a soil is dependent on the thermal properties of the solid materials, soil texture, pore size distribution, bulk density/porosity, water content, and the temperature of the soil^{2–4}. Among these parameters, soil water content (θ) is varied greatly in field conditions. Accurate values of λ are important for soil heat process determination⁵. However, field measurement of λ as function of θ , i.e., $\lambda(\theta)$ is time consuming and costly efforts and impractical for large-scale application^{3,6}. Therefore, different models have been proposed to predict $\lambda(\theta)$ by many investigators^{1–3,7–10}. The soil thermal conductivity models are classified into two types: physical-based models and empirical models^{1,2,10–12}. A physically based model was developed by de vries². It was used by Campbell et al.¹³ and Sepaskhah and Boersma¹ to predict $\lambda(\theta)$ in different soil temperatures and soil textures. However, it requires appropriate critical soil water content and shape factor for accurate prediction of $\lambda(\theta)$ ^{14,15}. With the continuous development of the model, although the physical mechanism considered by those models are becoming more and more comprehensive, the increase in parameters increases the computational difficulty of the model, limits the use of model in practice and improves the accuracy to a limited extent. Therefore, a new model proposed by Xiong et al.⁵ that described the relationship between soil thermal conductivity and degree of saturation, furthermore, dry soil thermal conductivity and saturated soil thermal conductivity were described using a linear expression and geometric mean model, respectively. Also, a quadratic function with one constant was added to calculate λ beyond the lower

Irrigation Department, Shiraz University, Shiraz, Islamic Republic of Iran. email: sepas@shirazu.ac.ir

λ_{dry} , and upper λ_{sat} limit conditions. However, they used a constant value that should be different for different soil textures that are not given for all different soil textures.

Different empirical models for $\lambda(\theta)$ prediction have been proposed by Kersten¹⁶, Campbell⁸, Johansen⁷, Chung and Horton¹⁸, and Lu et al.¹⁰. Kersten¹⁶ proposed an empirical model that requires bulk density (ρ_b). However, it is not appropriate for prediction of λ at low soil water contents. An empirical model [$\lambda(\theta)$] with two parameters (i.e., soil bulk density and clay content) was proposed by Campbell⁸ to estimate the soil λ for silt, loam soils and forest litter, that is not appropriate for all soil textures. Therefore, as the thermal conductivity accounts for the tortuosity of the soil, it is described with a non-linear simple empirical equation presented by Chung and Horton¹⁷. This equation has been used in models for simulation of heat and water flow in soil such as HYDRUS model¹⁸. In this model, they used soil measured temperature and soil water content to inversely solve for the coefficients of the empirical equation for $\lambda(\theta)$. However, this procedure is required to measure the soil water content and temperature in field that is time consuming and costly for different soil textures.

Johansen⁷ introduced a simple empirical model for $\lambda(\theta)$ that is based on normalized thermal conductivity (K_e), degree of saturation (S_r) and soil mineral compositions. Many investigators used the Johansen⁷ model to predict $\lambda(\theta)$ for many soils accurately^{10,14}. Later on, Cote and Konrad⁹ improved the Johansen⁷ model by using an empirical relationship between K_e and S_r . However, the modified Johansen⁷ model by Cote and Konrad⁹ was not able to predict $\lambda(\theta)$ accurately at lower soil water contents, especially in fine-textured soils¹⁰. Therefore, it was modified further to be applicable for lower soil water contents and fine-textured soils¹⁰. However, the modified model by Lu et al.¹⁰ showed high sensitivity to sand fraction (quartz), especially at soil water content higher than $0.2\text{ cm}^3\text{ cm}^{-3}$. Therefore, this modified model needs further verification for different soil textures.

Sigmoidal model (i.e., logistic growth curve) initially was used for describing population growth. Logistic growth equation is a sigmoidal curve that can be used to model growth that increases gradually at first, more rapidly in the middle, slowly at the end and leveling off at a maximum value after some period of time. It has been widely used in biomass accumulation, crop height, leaf area expansion and crop yield prediction^{19–23}. Also, soil thermal conductivity depends mostly on the soil particles and soil pores size distribution that is filled variably with air and water in different soil water contents. On the other hand, the soil particles and soil pores size distribution follow simple sigmoidal function²⁴. Therefore, the $\lambda(\theta)$ function could be shown by a sigmoidal model^{1,2}. On the other hand, field measurement of $\lambda(\theta)$ is time consuming, costly effort and not practical for large scale application. Therefore, a sigmoidal model should be developed for $\lambda(\theta)$.

The objective of this study was to develop a simple empirical model based on the logistic equation for $\lambda(\theta)$ at room temperature for entire soil water content range and soil textures. Further, the performance of the new empirical model along with Johansen⁷, Lu et al.¹⁰ and Xiong et al.⁵ was evaluated by comparing the predicted thermal conductivity with the measured thermal conductivity for different soil textures.

Method and materials
Soil thermal conductivity measurement

Six soils from Fars province, I.R. of Iran were used in the new model development. The physical properties of these soils are presented in Table 1. Soil particle size distribution was determined by hydrometer method²⁵. Soil textures determined based on soil particle size distribution using USDA procedure.

The soil samples were prepared by adding the amount of water required to bring a pre-packed, air-dried sample to the desired water content. The air-dried soil was packed in glass jars (97 mm in diameter and 100 mm in length, partially filled with soil to a height of 70 mm) which were tapped twice on the top of the laboratory bench with each scoop of sample poured into it. The number of scoop and the filled volume per jar was the same for each sample in order to obtain unique soil bulk density for each soil texture (Table 1). Bulk density of the samples was determined by dividing the weight of dry soil to the soil volume in the jar. Pre-determined quantities of water were applied to the samples such that no water was pond on the soil surface. This method of water application prevented trapping of air in the samples. Soil samples with low water content were prepared by pouring air dried soil on a plastic sheet and spreading it evenly in a thin layer. Required amounts of water were sprinkled onto the soil which was then shaken in a plastic bag to distribute the water uniformly and packed into jars. The containers were capped with a lid to prevent water loss by evaporation during storage. The containers were kept in an empty ice box in laboratory with a room temperature about $20 \pm 1\text{ }^\circ\text{C}$ for 24 h. Thermal conductivity

Study of model	Soil texture	Sand (%)	Silt (%)	Clay (%)	Bulk density (g cm^{-3})	Porosity
Development	Silty clay	10.6	45.4	44.0	1.07	0.596
	Clay loam	35.0	35.0	30.0	1.10	0.593
	Silt loam	24.9	53.3	21.8	1.14	0.578
	Loam	40.0	47.0	13.0	1.15	0.574
	Sandy loam	70.0	18.0	12.0	1.47	0.456
	Loamy sand	85.0	10.0	5.0	1.57	0.419
Validation ^a	Silt loam	2.0	73.0	25.0	1.20	0.556
	Loam	50.0	41.0	9.0	1.38	0.489
	Sand	92.0	7.0	1.0	1.58	0.415

Table 1. Physical properties of soils used in model development and validation. ^aData from Lu et al.¹⁰.

(λ) measurement made at the same time during different days for having similar air temperature during the λ measurement. Apparent thermal conductivity was measured with a cylindrical heat probe with 60 mm length and 1.28 mm diameter (kd2, Decagon Device, Inc, Pullman, WA, USA). The heat probe was inserted in soil samples contained in glass jars. Immediately after removing the cap, the probe was inserted into the soil samples carefully to measure the λ and probe temperature with three replications after 1.5 min. of turning on the kd2 apparatus. The mean values of three replications were considered as soil λ . After λ measurement, soil water contents of samples were measured by gravimetric procedure in oven with 105 °C for 24 h. The gravimetric soil water content was multiplied by soil bulk density to determine the volumetric water content.

Model development

Johansen model

The concept of normalized thermal conductivity, K_e (i.e., the Kersten number) was proposed by Johansen⁷ and he used a relationship between λ and K_e as follows:

$$\lambda = (\lambda_{sat} - \lambda_{dry})K_e + \lambda_{dry} \quad (1)$$

where, λ_{dry} and λ_{sat} are the thermal conductivity of dry and saturated soils ($\text{W m}^{-1} \text{K}^{-1}$), respectively. The values of λ_{dry} and λ_{sat} were determined as follows:

$$\lambda_{sat} = \lambda_s^{1-n} \lambda_w^n \quad (2)$$

and

$$\lambda_{dry} = (0.135\rho_b + 64.7)/(2700 - 0.947\rho_b) \quad (3)$$

where, n is the soil porosity, λ_w is the thermal conductivity of water ($0.594 \text{ W m}^{-1} \text{K}^{-1}$ at 20 °C), ρ_b is the soil bulk density (kg m^{-3}), and λ_s is the effective thermal conductivity of soil solid particles ($\text{W m}^{-1} \text{K}^{-1}$). The values of λ_s are calculated by the following equation as a geometric mean:

$$\lambda_s = \lambda_q^q \lambda_o^{1-q} \quad (4)$$

where, λ_q is the thermal conductivity of quartz (sand) ($7.7 \text{ W m}^{-1} \text{K}^{-1}$), q is the quartz (sand) content (fraction), λ_o is the thermal conductivity of other soil particles content ($2.0 \text{ W m}^{-1} \text{K}^{-1}$ for soils with $q > 0.2$ and $3.0 \text{ W m}^{-1} \text{K}^{-1}$ for soils with $q \leq 0.2$). Furthermore, Johansen (1975) proposed empirical relationships between K_e and normalized soil water content for different soil textures as follows:

$$K_e = 0.7 \log S_r + 1.0 \quad (S_r > 0.05) \text{ for coarse - textured soils} \quad (5)$$

$$K_e = \log S_r + 1.0 \quad (S_r > 0.1) \text{ for fine - textured soils} \quad (6)$$

where, S_r is the normalized soil water content as θ/θ_s where θ and θ_s are the soil water content and saturated soil water content ($\text{cm}^3 \text{cm}^{-3}$), respectively.

Modified Cote and Konrad model

Although Cote and Konrad⁹ improved the Johansen⁷ model, however their modified model was not accurate in λ prediction for fine-textured soils at lower water contents. Therefore, Lu et al.¹⁰ proposed the following equation for K_e estimation across the entire range of soil water content:

$$K_e = \exp\left\{\alpha \left[1 - S_r^{(\alpha-1.33)}\right]\right\} \quad (7)$$

where, α is the soil texture dependent parameter ($\alpha = 0.96$ for coarse-textured soils and $\alpha = 0.27$ for fine-textured soils, respectively) and 1.33 is a shape factor.

Furthermore, Lu et al.¹⁰ used a simple empirical linear relationship between λ_{dry} and soil porosity (n) as follows:

$$\lambda_{dry} = -an + b \quad (8)$$

where a and b are constants as $a = 0.56$ and $b = 0.51$ for $0.0 < n < 0.6$, and n is the soil porosity. The value of λ_{sat} was calculated according to Eq. (2) used in Johansen⁷ model.

New Xiong et al. model

The proposed model by Xiong et al.⁵ is as follows:

$$\lambda = P + QS_r^R + S\{\exp[S_r(1 - S_r)]\} \quad (9a)$$

$$P = \lambda_{dry} = 0.51 - 0.6n \quad (9b)$$

$$Q = \lambda_{sat} - \lambda_{dry} = (\lambda_q^q \lambda_o^{1-q})^{1-n} (\lambda_w)^n (0.51 - 0.6n) \quad (9c)$$

$$S = 1.5(S_r - S_r^2)$$
 (9d)

where, n is the soil porosity (-), S_r is the degree of soil saturation as θ/θ_s (%), λ_q is the thermal conductivity of quartz (sand) ($7.7 \text{ W m}^{-1} \text{ K}^{-1}$), q is the quartz (sand) content (fraction), λ_o is the thermal conductivity of other soil particles content ($2.0 \text{ W m}^{-1} \text{ K}^{-1}$ for soils with $q > 0.2$ and $3.0 \text{ W m}^{-1} \text{ K}^{-1}$ for soils with $q \leq 0.2$), λ_w is the thermal conductivity of water ($0.594 \text{ W m}^{-1} \text{ K}^{-1}$) and the value of R is 1.2 for sand, 1.5 for the fine-textured soils, and 2.0 for clay. However, the values of R for fine-textured soils are not well designated for different fine-textured soils.

Sigmoidal model

Sigmoidal model (i.e., logistic equation) to describe the soil thermal conductivity as a function of soil water content is as follows:

$$\lambda = K/[1 + Aexp(-B\theta)]$$
 (10)

where, λ is the soil thermal conductivity ($\text{W m}^{-1} \text{ K}^{-1}$), θ is the soil volumetric water content ($\text{cm}^3 \text{ cm}^{-3}$), K is the upper most asymptote implies the upper limits of soil thermal conductivity, and A and B are coefficients as taken of initial stage and total accretion rate.

Measured soil thermal conductivities at different soil water contents for six soils with different textures were used in Eq. (10) to determine the values of K , A , and B by Solver tool in EXCEL software. Then, the values of K , A , and B were used in multiple linear regression analysis in EXCEL software to obtain an empirical model to estimate the values of K , A , and B based on soil physical parameters. These parameters were sand, silt, and clay contents, soil bulk density, soil porosity. Among these parameters sand content and soil bulk density entered in the empirical multiple linear regression as follows:

$$K = a_o + a_1q + a_2\rho_b$$
 (11)

$$A = b_o + b_1q + b_2\rho_b$$
 (12)

$$B = c_o + c_1q + c_2\rho_b$$
 (13)

where, a_o , a_1 , a_2 , b_o , b_1 , b_2 , c_o , c_1 , and c_2 are constants, q is the sand particle content (%), and ρ_b is the soil bulk density (g cm^{-3}). The entrance of soil bulk density and sand content is due to the fact that the thermal conductivity of sand (instead of quartz) is much higher than the clay and silt particles and it contributes much more to the λ value of soil, and value of bulk density indicates the compaction of soil, soil pores distribution and extend the contact of the soil particles to cause the soil thermal conductance.

Using the measured values of λ in sigmoidal model (Eq. 10) and Solver tool in EXCEL software, the values of K , A , and B were determined for six different soil textures (Table 2). These values were used in Eq. (10) to estimate $\lambda(\theta)$ for different soil water contents.

Sigmoidal model validation

For validation of the new model, measured data from Lu et al.¹⁰ for three different soil textures are used (Table 1). By use of the empirical multi-linear equations (Eqs. 11, 12, and 13), the values of the empirical-logistic constants (K , A , and B) were estimated. Based on these coefficients the values of $\lambda(\theta)$ were estimated. Then, the estimated values of $\lambda(\theta)$ were compared with the measured values reported by Lu et al.¹⁰.

Statistical analysis

The outputs of the model were compared by the measured values using following statistical parameters:

$$NRMSE = (1/N \sum_{i=1}^n (X_i - Y_i)^2)^{0.5} / O$$
 (14)

Study of model	Soil texture	K	A	B
Development	Silty clay	1.000	6.82	13.96
	Clay loam	1.047	4.86	10.24
	Silt loam	1.073	5.60	14.52
	Loam	1.073	5.91	15.97
	Sandy loam	1.501	3.93	20.78
	Loamy sand	1.649	4.23	20.60
Validation	Silt loam	1.060	8.76	21.98
	Loam	1.361	5.63	20.05
	Sand	1.663	3.20	20.38

Table 2. The estimated values of the logistic equation (K , A , and B) for the sigmoidal model development and model validation.

where, NRMSE is the normalized root mean square error, N is the number of observations, X is the measured values, Y is the estimated values and O is the mean values of measured data. The value of NRMSE approaches 0.0 for the accurate estimation. The closer the NRMSE is to 0, the model is more accurate. Linear relationship between the measured and predicted values is compared with 1:1 line with slope and intercept of 1.0 and 0, respectively by using Fisher F-test.

Results and discussion

Measured thermal conductivity

Measured λ as a function of θ for six different soil textures are shown in Fig. 1. The values of λ for different soil textures are different. For given value of θ , the values of λ for coarse-textured soils (sandy loam, and loamy sand) are higher than those values for medium-textured soil (loam) and λ of medium textured soil are higher than those for fine-textured soils (silty clay). The main reason for this finding is greater soil porosity in fine-textured soil (Table 1). By increasing porosity, λ is decreased due to higher air and water content in fine-textured soils with much lower λ value for air and water¹. Of course, the sand content (quartz) in coarse-textured soil is higher with higher λ values than those in fine-texture soil with low values of sand/higher values of clay with lower values of λ (Table 1). Therefore, the values of λ in coarse textured soils are higher than those in fine-textured soils.

Furthermore, for given soil texture, λ value increased by increasing soil volumetric water content. However, the value of λ remained unchanged as the θ values increased from zero to 0.05–0.06 cm³ cm⁻³ for medium textured soil (loam) to fine-textured soils (silt loam, clay loam, and silty clay) (Fig. 1). This is occurred because the fine-textured soils showed large surface area²⁶, therefore higher water content is needed to form water bridge between soil particles. By increasing the soil water content higher than the critical soil water content, the λ was increased faster as θ was increased. This increase in λ was higher in coarse-textured soils than in fine-textured soils. This increase in λ is due to the formation of wedges of water at the points where soil particles make contact. With further addition of water, soil pores gradually are filled and the increase of λ with each increment of water added becomes smaller. Furthermore, it is indicated that λ is increased by soil bulk density due to increase in number of soil particles in unit volume of soil and consequently increase in the number of contacts between soil particles that increase the heat conduction.

Figure 1 indicated that $\lambda(\theta)$ curve could be grouped into two different soil textures as coarse-textured soils (sandy loam, and loamy sand) with sand content > 40%, and fine-textured soils (loam, silty loam, clay loam, and silty clay) with sand fraction of $\leq 40\%$ that is corresponding to those findings reported by Lu et al.¹⁰.

Sigmoidal model development

The estimated $\lambda(\theta)$ and the measured λ are shown in Fig. 2. It is indicated that the estimated values of λ by logistic equation are very close to those of measured values, especially in low and high soil water content, that the accuracy of estimation is higher.

The values of K, A, and B for six different soils were used to develop linear-multiple regression equation to relate these values to different soil physical properties, i.e., sand, silt, clay, bulk density, porosity, geometric mean diameter, and geometric standard deviation by multiple regression analysis. According to the ANOVA Table and probability level statistics for the coefficients of linear multiple regression (data not shown), the sand particle content and soil bulk density were included in the linear-multiple regression as follows:

$$K = 0.0035q + 0.878\rho_b \quad (15)$$

$$N = 6, R^2 = 0.999, SE = 0.028, p < 0.0001$$

$$A = -0.0935q + 7.458\rho_b \quad (16)$$

$$N = 6, R^2 = 0.990, SE = 0.666, p = 0.0007$$

$$B = -34.66 - 0.219q + 47.56\rho_b \quad (17)$$

$$N = 6, R^2 = 0.956, SE = 1.277, p = 0.009,$$

where, q is the sand content (%), ρ_b is the bulk density (g cm⁻³), N is the number of observations, R² is the coefficient of determination, SE is the standard error, and p is the level of probability. The statistical parameters indicated that Eqs. (15)–(17) have acceptable accuracy. Therefore, by using these equations and sand content and soil bulk density of different soils, the values of K, A, and B can be estimated. Then, by using these constants

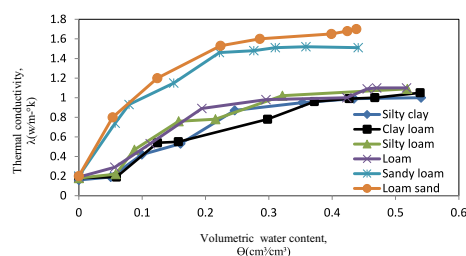


Figure 1. Measured soil thermal conductivity at different water contents for different soil textures.

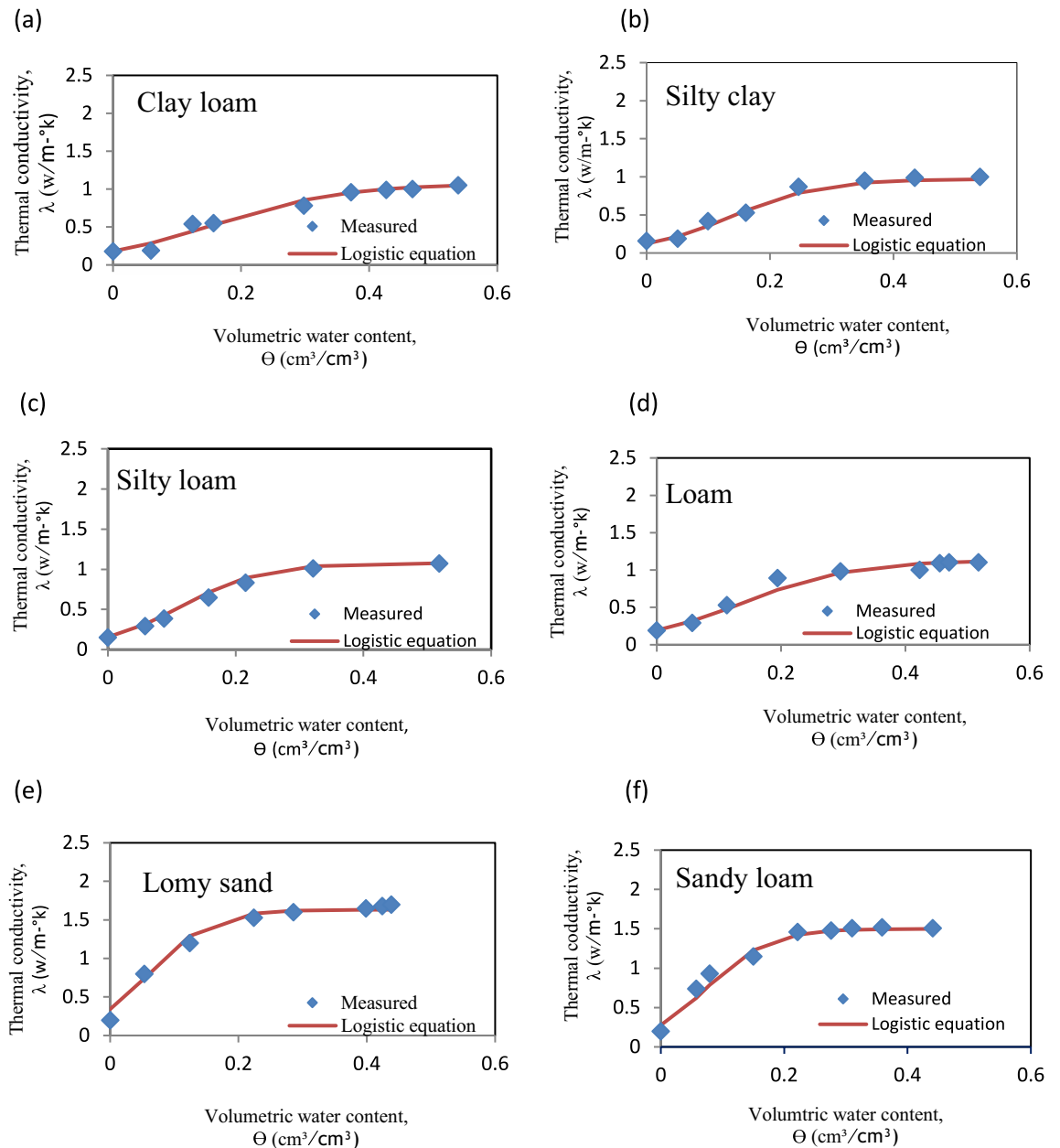


Figure 2. Measured and predicted soil thermal conductivity with logistic equation (Eq. 10) for different soil textures: (a) Clay loam, (b) Silty clay, (c) Silty loam, (d) Loam, (e) Loamy sand, (f) Sandy loam.

in Eq. (10), the values of λ for different soil water contents can be estimated. To show the accuracy of these estimations, the estimated λ and the measured λ for the six different soils used in the model development are presented in Fig. 3. In this Figure, relationship between the measured λ (λ_m) and the predicted λ (λ_p) were compared with 1:1 line by Fisher F-test. It is indicated that the slope and intercept of the linear relationships are close to 1.0 and 0.0, respectively and the estimation of λ are accurate.

Sigmoidal model validation

For validation of the sigmoidal model, the measured $\lambda(\theta)$ of three different soil textures presented by Lu et al.¹⁰ was used. The physical properties of these soils are shown in Table 1. Initially, the values of K , A , and B were estimated by the sand content and ρ_b of the soils presented by Lu et al.¹⁰, then the estimated values of K , A , and B (Table 2) were used in Eq. (10) and $\lambda(\theta)$ was estimated. The estimated $\lambda(\theta)$ and the measured values of λ by Lu et al.¹⁰ are shown in Fig. 4. It is shown that in a wide range of soil water contents the estimated values of λ are very close to the measured values. However, in saturation water content the estimated λ is lower than the measured values. This difference is more pronounced in coarse-textured soil (sand), however this difference is not significant. Relationship between the measured and estimated λ was compared with 1:1 line in Fig. 5.

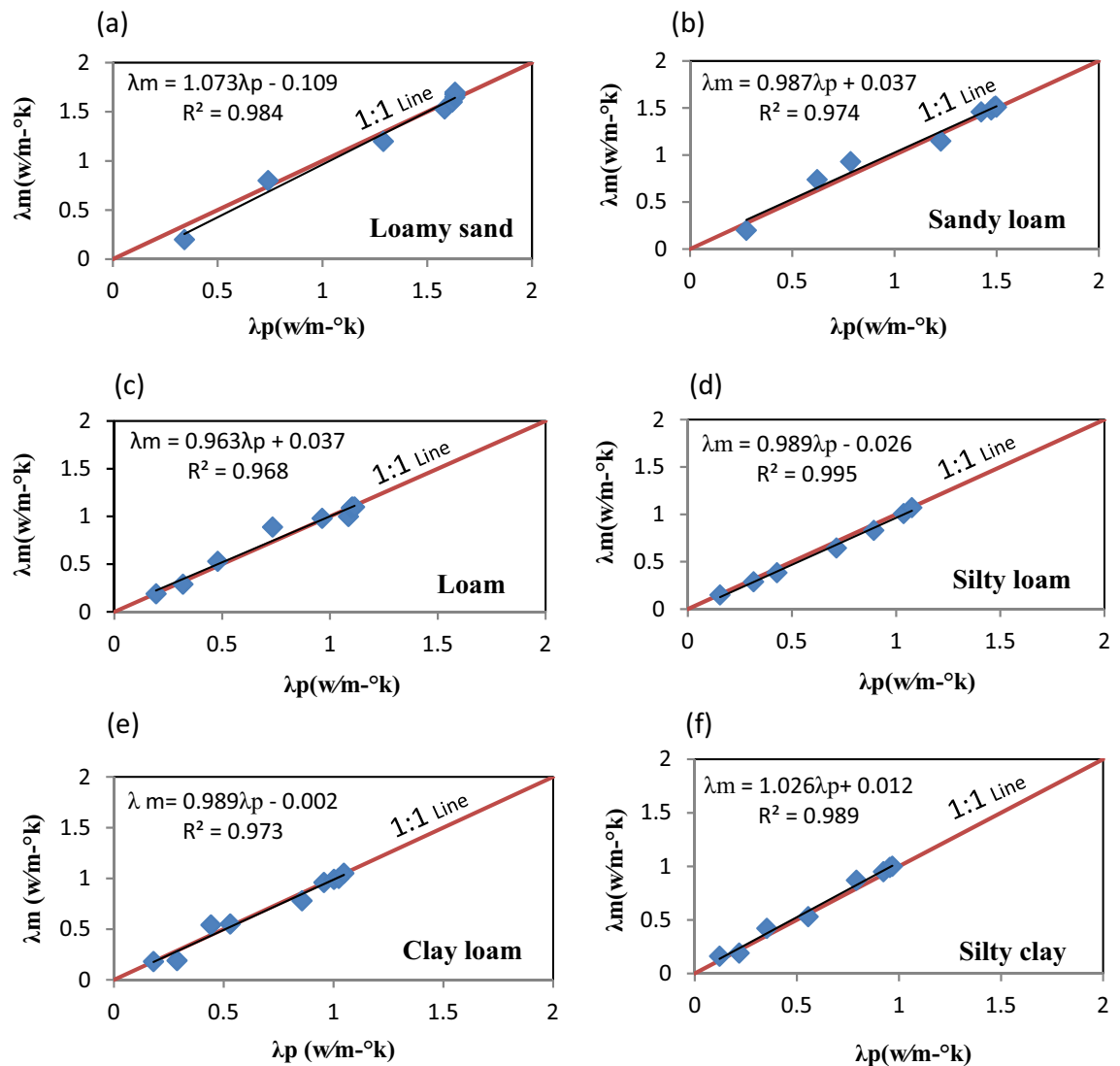


Figure 3. Comparison between measured soil thermal conductivity (λ_m) and predicted values (λ_p) by the sigmoidal model for different soil textures: (a) Loamy sand, (b) Sandy loam, (c) Loam, (d) Silt loam, (e) Clay loam, (f) Silty clay.

Comparison between the slopes and intercepts by Fisher F-test indicated that there are non-significant differences between the slope and 1.0 and the intercept and 0.0 ($p > 0.05$). The linear relationships are as follows:

$$\lambda_m = 1.03\lambda_p, \quad R^2 = 0.993 \quad \text{For silt loam soil} \quad (18)$$

$$\lambda_m = 1.05\lambda_p, \quad R^2 = 0.988 \quad \text{For loam soil} \quad (19)$$

$$\lambda_m = 1.16\lambda_p, \quad R^2 = 0.991 \quad \text{For sand soil} \quad (20)$$

where λ_m and λ_p are the measured and predicted λ , respectively ($\text{W m}^{-1} \text{K}^{-1}$). Therefore, the estimated λ are accurate, however there is 16% under-estimation of λ by the sigmoidal model for sand soil at soil water content near saturation (Figs. 4, and 5).

Evaluation of different models

The physical parameters of six soils used in developing the new model (Table 1) and three soils used in Lue et al.¹⁰ (Table 1) were used to evaluate the models of Johansen⁷ [Eqs. (1)–(6)], Lu et al.¹⁰ [Eqs. (7)–(8)] and the sigmoidal model proposed in this study [Eqs. (10)–(13)]. Classification of soil texture as coarse or fine is critical in Johansen⁷ and Lu et al.¹⁰ models to estimate K_e . Therefore, in this evaluation the loam soil was considered as coarse/fine texture to evaluate the suitability of this selection. Results of these evaluations are presented in Figs. 6, and 7. Comparison between the measured and predicted λ is evaluated by NRMSE (Eq. 14) (Table 3).

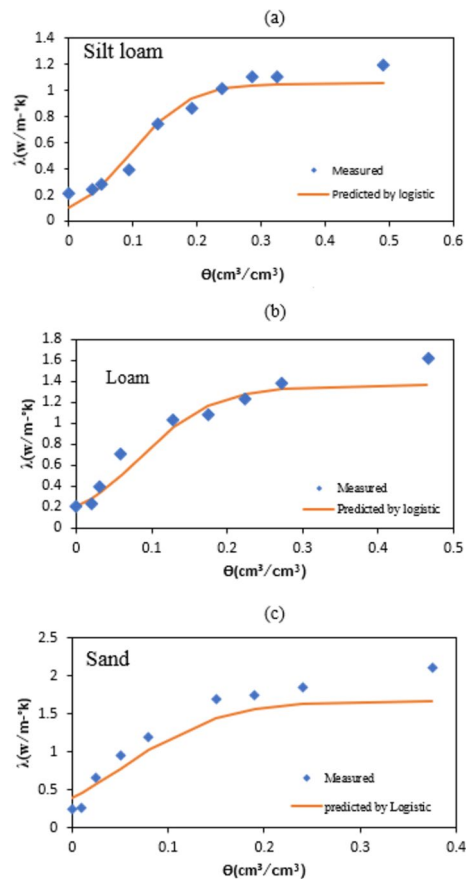


Figure 4. Measured soil thermal conductivity (λ_m) by Lu et al.¹⁰ and predicted values (λ_p) for validation of the sigmoidal model for different soil textures: (a) Silt loam, (b) Loam, (c) Sand.

Classification of loam soil in Johansen⁷ and Lu et al.¹⁰ models as a fine-textured soil for estimation of K_e value indicated that NRMSE of this selection is lower as 0.107. Whereas, based on classification as coarse-textured soil, this selection is more critical in Johansen⁷ model with higher value of NRMSE as 0.916 for coarse-textured selection in comparison to 0.107 for fine-textured soil selection. However, this classification in Lu et al.¹⁰ model is not very critical due to NRMSE of 0.133 for coarse-textured selection in comparison to 0.107 for fine-textured soil selection.

Johansen⁷ and Lu et al.¹⁰ models resulted in lower λ than the measured values for loam and silt loam soils in a wide range of soil water contents (Figs. 6, and 7), while the sigmoidal model predicted λ accurately. On the other hand, for light-textured soils (sandy loam and loamy sand) the Johansen⁷ and Lu et al.¹⁰ model prediction of λ was higher than the measured values, especially at water contents higher than $0.30 \text{ cm}^3 \text{ cm}^{-3}$, while the sigmoidal model predicted λ with a good accuracy. This difference might be due to the fact that sand particle in soil is assumed as quartz with a higher λ compared with other minerals in soil that is used in prediction of λ . Therefore, small error in this assumption results in higher estimation of λ compared with the measured values.

The values of NRMSE indicated that Lu et al.¹⁰ predicted λ for most of soil textures with higher accuracy than those predicted by Johansen⁷ model (Table 3). For sand, the sigmoidal model was not superior to those of Johansen⁷ and Lu et al.¹⁰ models. In general, the sigmoidal model was superior to the other two models in prediction of λ for wide range of soil textures, except sand.

Results of predicted soil λ values based on Xiong et al.⁵ model for different soil textures are shown in Fig. 8. Also, the measured values are shown in this Figure. It is indicated that for soil textures of loam, silty loam and clay loam Xiong et al.⁵ model predicted λ values accurately. This is shown in Fig. 9 that presented the relationships between the measured and predicted values. These relationships for loam, silty loam and clay loam with slopes of near to 1.0 are similar to 1:1 line with slope of 1.0 and intercept of 0.0. Whereas, for loamy sand, sandy loam and silty clay soils Xiong et al.⁵ model was not able to predict λ values. These discrepancies are mainly due to uncertainties in designating appropriate values of R in Eq. (9a) for different soil textures.

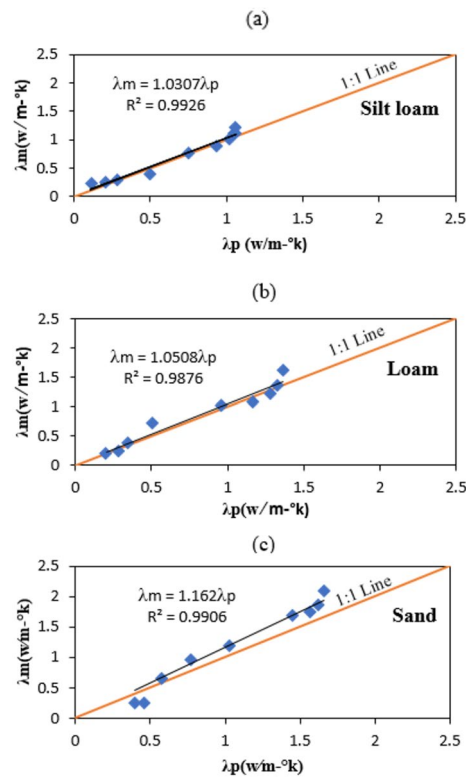


Figure 5. Comparison between measured soil thermal conductivity (λ_m) by Lu et al.¹⁰ and predicted values (λ_p) by the sigmoidal model for different soil texture: (a) Silt loam, (b) Loam, (b) Sand.

Considerations on sigmoidal model

Soil thermal conductivity (λ) is non-linear with many influencing factors, and a simple derivation using only multivariate linear analyses is feasible in some sense, but does not focus on temperature, a factor that has a significant effect. This point may be most valid in high soil temperature condition where water vapor flow occurs in the soil in a greater extent that should be considered in soil thermal conductivity as reported by Sepaskhah and Boersma¹. However, in low soil temperature this phenomenon can be ignored for simplicity.

In Figs. 4 and 5 we validated the performance of the sigmoidal model by using available data from Lu et al.¹⁰ for the given soil textures as silt loam, loam and sand that cover heavy to light textures. In Fig. 5, the linear relationships between λ_m and λ_p [Eqs. (18) (19) and (20)] were compared with the 1:1 line. In these relationships the intercepts are 0.0 and the slopes are close to 1.0 indicated that the λ_m and λ_p values are statistically close together, except for sand soil at soil water content near saturation with 16% under-estimation.

The implications of Multiple Linear Regression may fail to capture nonlinear relationships and performs poorly for complex data patterns. Whether interpolation using multiple linear regression is a reasonable way to derive the proposed model may not be convincing and other methods may be used. In terms of model validation, of course it is better to validate the λ_p by simulation with models such as HYDRUS, however, in our study the soil temperature and water flow such as infiltration rate has not been measured that is required for validation of λ_p in HYDRUS model as reported by Nakhaei and Simunek¹⁸. Therefore, the used procedure in this study is the possible way to validate the λ_p .

Conclusions

A sigmoidal model was developed for predicting soil thermal conductivity from its water content based on a logistic equation that its constants are estimated based on the proposed empirical equations by using soil sand content and bulk density. The sigmoidal model was validated with good accuracy for a wide range of soil textures. Comparison of the sigmoidal model with Johansen and Lu et al. models indicated that the sigmoidal model was superior to the other two models in prediction of λ for a wide range of soil textures and soil water contents. Furthermore, comparison with a recently proposed model by Xiong et al. indicated that our sigmoidal model is superior.

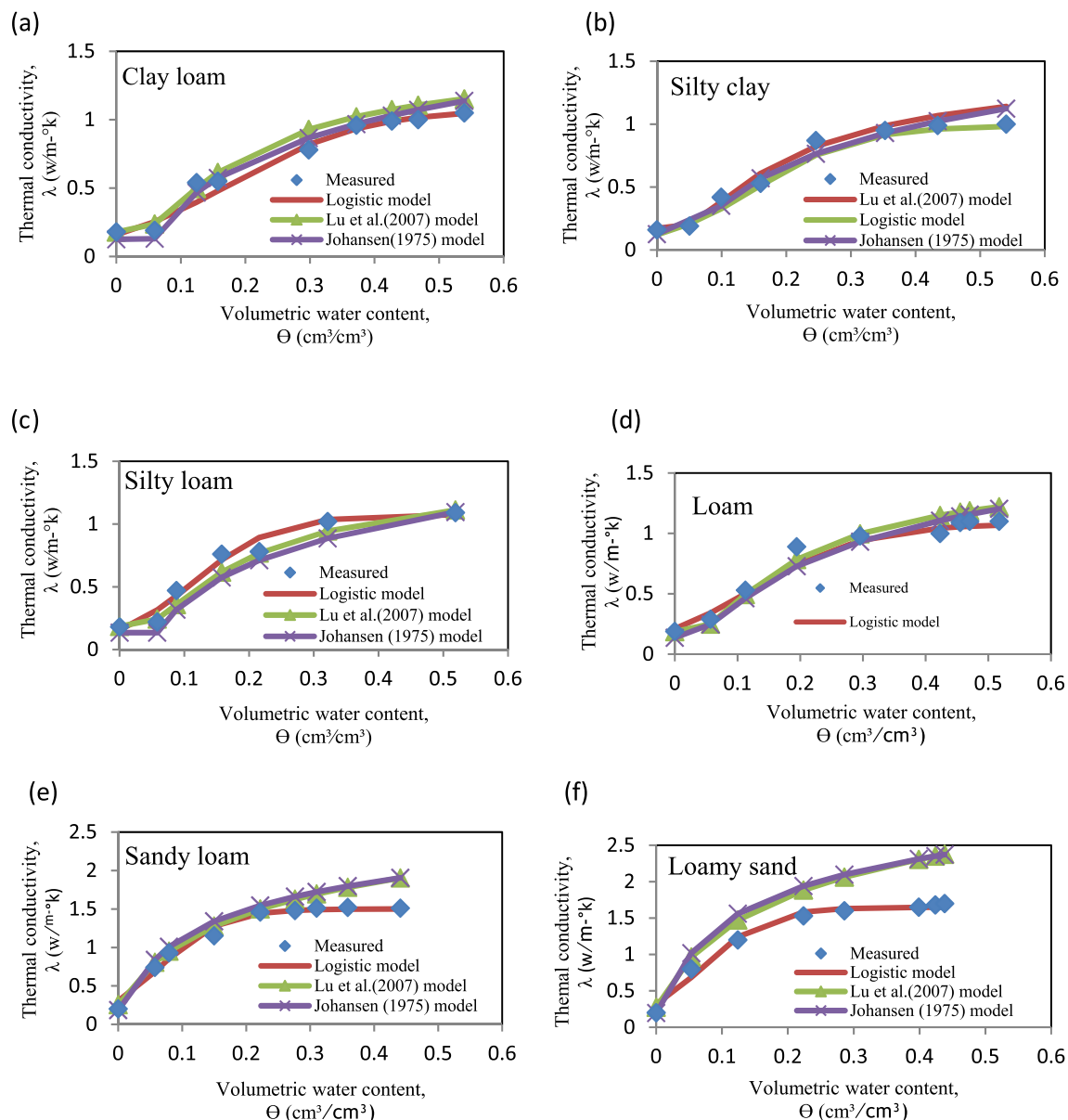


Figure 6. Measured soil thermal conductivity (λ_m) and predicted values (λ_p) by different prediction models for different soil textures: (a) Clay loam, (b) Silty clay, (c) Silt loam, (d) Loam, (e) Sandy loam, (f) Loamy sand.

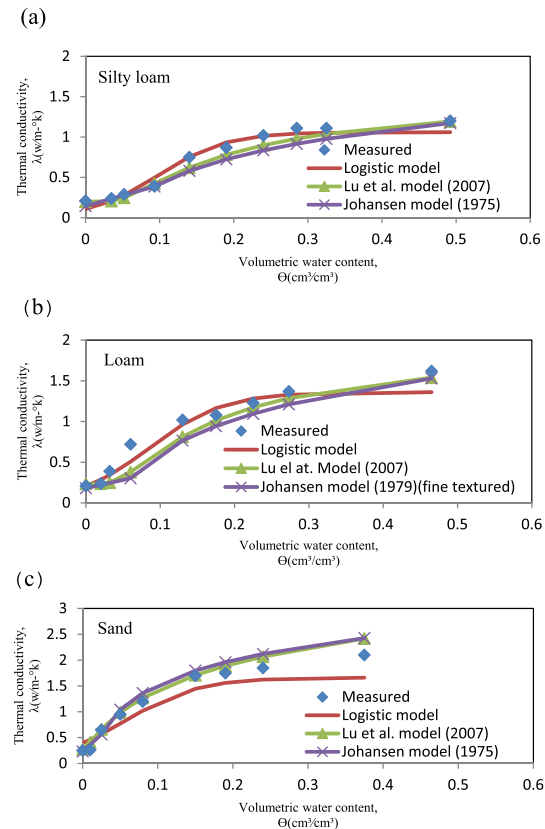


Figure 7. Measured soil thermal conductivity by Lu et al.¹⁰ and predicted values by different prediction models for different soil textures: **(a)** Silt loam, **(b)** Loam, **(c)** Sand.

Study of model	Soil texture	Sigmoidal model	Johansen ⁷ model	Lu et al. ¹⁰ model
Model development	Silty clay	0.0709	0.1112	0.1067
	Clay loam	0.0777	0.0894	0.1206
	Silt loam	0.0998	0.1971	0.1326
	Loam (coarse)	0.0790	0.9161	0.1333
	Loam (fine)	0.0790	0.1069	0.1069
	Sandy loam	0.0633	0.1742	0.1579
	Loamy sand	0.0561	0.3836	0.3693
Validation	Silt loam	0.1026	0.1794	0.1071
	Loam	0.1384	0.2319	0.0902
	Sand	0.1937	0.1378	0.1160

Table 3. Statistical parameter (NRMSE) for evaluation of different model to estimate soil thermal conductivity at different water content.

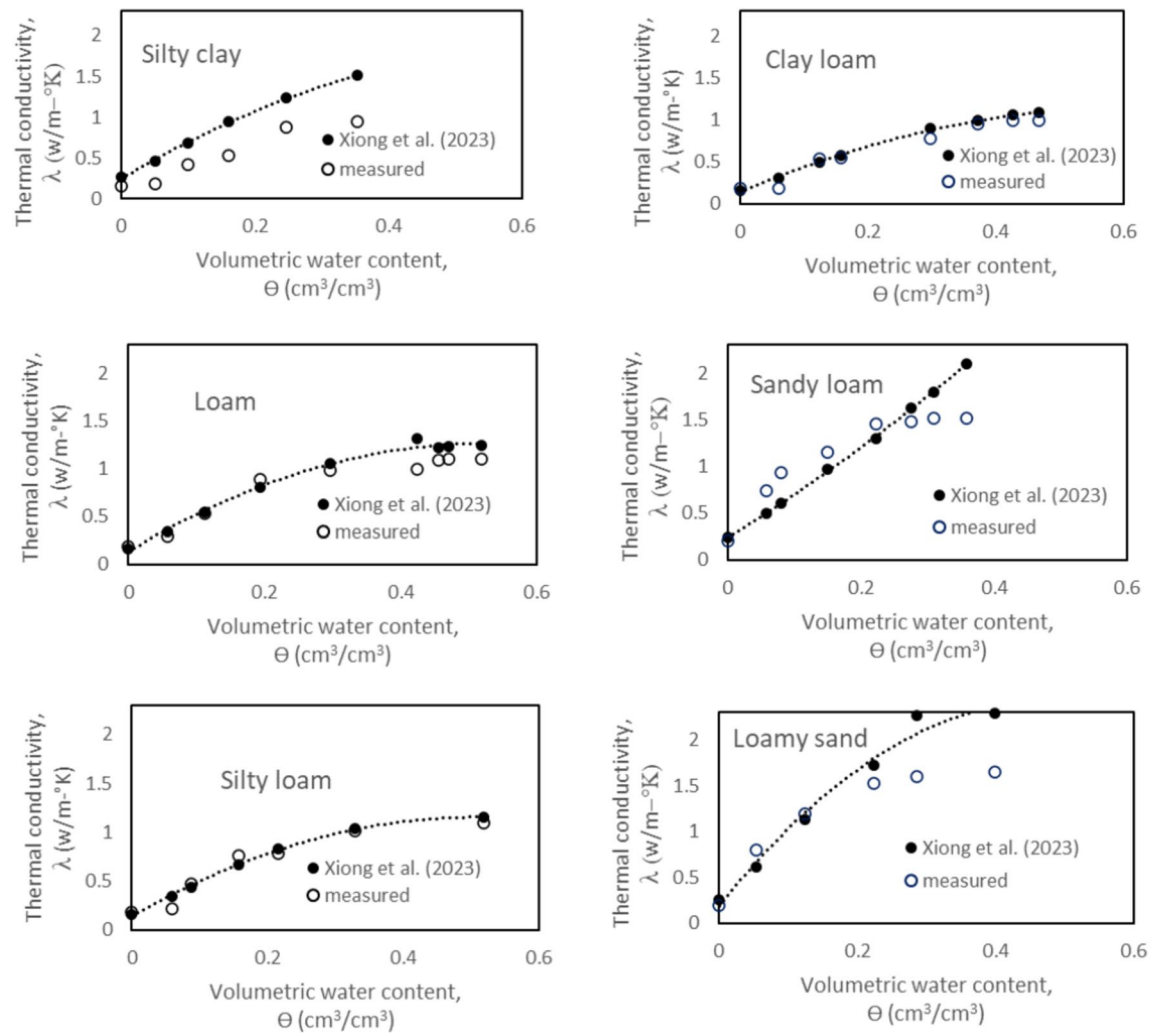


Figure 8. The predicted, λ_p^5 , and measured soil thermal conductivities (λ_m) as a function of soil volumetric water contents.

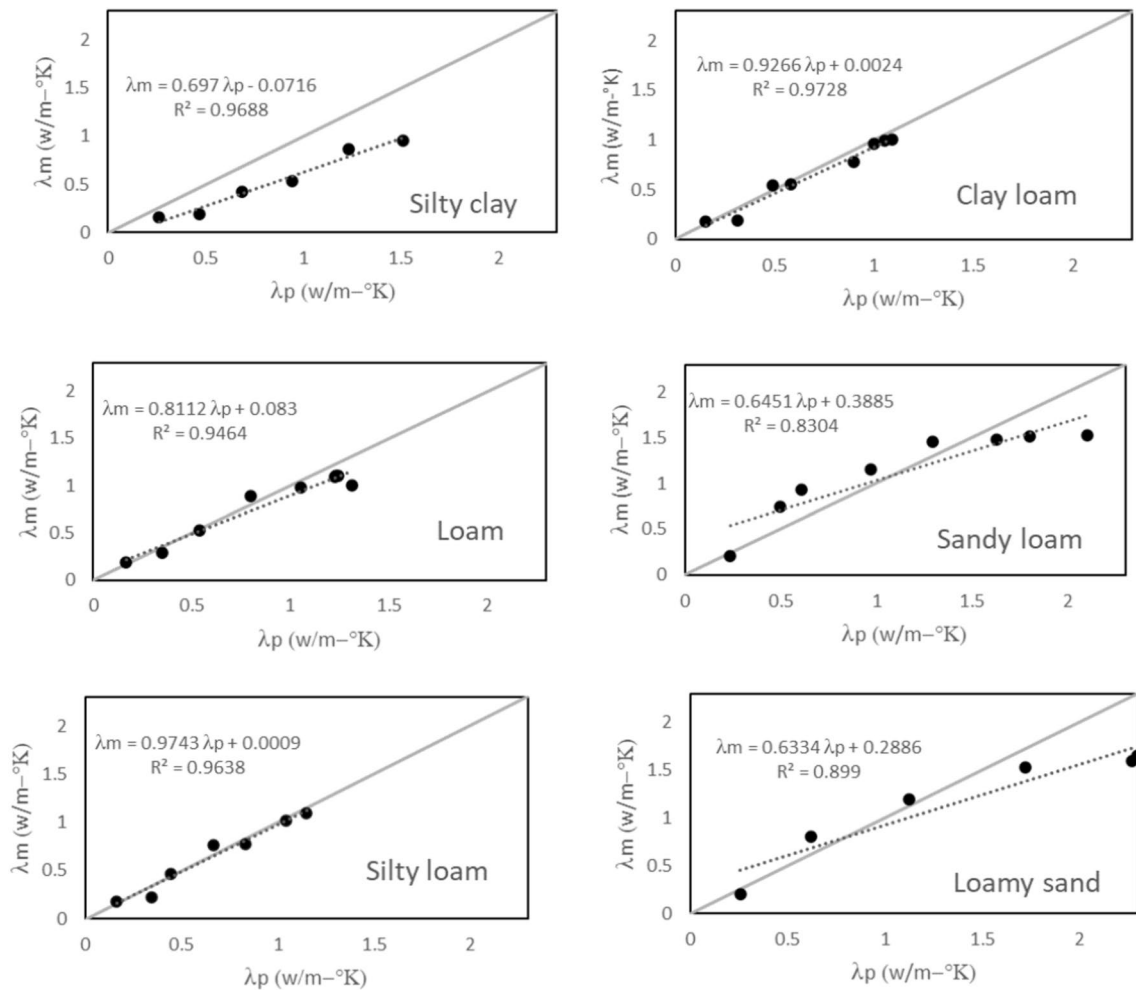


Figure 9. Relationships between the measured (λ_m) and predicted, λ_p , soil thermal conductivities at different soil volumetric water contents.

Data availability

The dataset used and/or analyzed during the current study available from the corresponding author on reasonable request.

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Author contributions

A.R.S. planned the research project and administered the fund, A.R.S. provided the instruments, M.M. and A.R.S. conducted the research, M.M. and A.R.S. analyzed the data, M.M. prepared the first draft in Farsi language, A.R.S. prepared the first draft of manuscript in English language and reviewed the final draft.

Competing interests

The authors declare no competing interests.

Additional information

Correspondence and requests for materials should be addressed to A.R.S.

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