Prediction of Thermal Conductivity of Unsaturated Soils Extending the van Genuchten SWCC Equation

Hao Wang[1], Sai K. Vanapalli*,[2]

[1]*Department of Civil Engineering, University of Ottawa, Ottawa, Canada*

**Corresponding author's email: Sai.Vanapalli@uottawa.ca*

Abstract: Heat and mass transfer processes significantly influence thermal conductivity of porous media such as the soils. The thermal conductivity behavior of unsaturated soils is complex due to interactions between the solids, liquid, and gaseous phases. The dominant factor that influences the thermal conductivity behavior of unsaturated soils is the water saturation. In this study, the soil water characteristic curve (SWCC) model proposed by van Genuchten (1980) is extended as a tool to predict the thermal conductivity of unsaturated soils. The proposed model links pore-scale thermal conductivity to pore size which is upscaled as a relationship to estimate the thermal conductivity of unsaturated soils. The model uses two key parameters, n_1 and η, which are both closely linked to the soil's pore size distribution. The parameter n_1 can be obtained directly from the SWCC data. The proposed model is validated against experimental data with a strong prediction ability. The investigations summarized in this paper are promising for modeling the coupled thermal-hydraulic-mechanical (THM) behavior of unsaturated soils.

Introduction

Heat and mass transfer in porous medium has attracted the attention of many researchers because of its wide application in various fields that include mechanical, chemical, and geotechnical engineering, ceramics, heat exchangers, nuclear reactors, and CO_2 storage [1]. The transfer of heat and mass process requires the porous medium to be investigated considering several coupled phenomena. Therefore, a lot of effort has been put into the Multiphysics simulation and many approaches have been proposed such as the thermal-hydraulic (TH) models, coupled thermal-hydraulic-mechanical (THM) models and the coupled thermo-hydro-mechanical-chemical models (THM-C) to describe the complex mass and heat transfer process and investigate the interaction among physical fields[2-5]. The thermal conductivity, which describes the porous medium's ability to conduct heat is the key property of interest in this study. Compared with metals and mixtures, thermal conductivity of porous medium such as the unsaturated soils is much more complex because there is not only solid phase, but also liquid and gas phases that co-exist in the porous medium. Each of these components is affected by structural conditions (porosity, arrangement of particles) and environmental conditions (temperature and stress and water saturation). For unsaturated soils, the thermal conductivity is significantly influenced by water saturation. Many models have been proposed in the literature to understand the thermal conductivity of unsaturated soils, including those based on empirical relationships, mixing theories, and percolation theory [6, 7]. However, these models have certain limitations. For instance, mixing models perform well for saturated soils but are less accurate for unsaturated soils. Some researchers have developed empirical models by observing the similarity between the SWCC and the variation of thermal conductivity with water saturation [8, 9]. While insightful, these models are empirical in nature and lack a robust theoretical foundation. Due to this reason, such models cannot be used in engineering practice applications. In this paper, a model is proposed based on a rational theoretical framework extending the van Genuchten (VG) model. The proposed model's ability to capture the moisture dependency of thermal conductivity under varying temperature conditions makes it particularly suitable for geotechnical systems involving unsaturated soils. These include energy foundation systems, ground-source heat pumps (GSHPs), borehole thermal energy storage (BTES), and unsaturated soil covers used in landfills and engineered barriers. In such applications, an accurate representation of thermal conductivity as a function of water content is essential for reliable system design, performance prediction, and long-term thermal regulation.

Materials and methods

Unsaturated soils are composed of solid, gas, and liquid phases; these phases change and influence several soil properties including the hydraulic conductivity and the thermal conductivity. The water saturation in soils changes due to variations in air volume during drying-wetting cycles. For instance, during drying, water (liquid phase) with high thermal conductivity is replaced by air (gas phase) with low thermal conductivity in the soil pores [10]. Due to this reason, heat transfer becomes more difficult, and the thermal conductivity decreases during drying. Such a behavior suggests that the thermal conductivity is closely related to the soil components and interaction of the various phases. Therefore, thermal conductivity of unsaturated soils in an unfrozen state may be assumed to be primarily a function of water saturation, if pore structure changes are ignored.

The soil water characteristic curve (SWCC) is defined as the variation of water saturation with respect to suction [11, 12]. A typical SWCC curve is shown in Fig. 1. Since SWCC describes phase changes in a soil, it is reasonable to use SWCC for interpreting the unsaturated soil properties. Several researchers have used the SWCC as a tool for predicting several hydro-mechanical properties of unsaturated soils [13-18]. The advantage of using the SWCC is that they are easier to obtain compared to directly measuring soil properties such as the hydraulic conductivity and shear strength, which not only need expensive equipment, require trained professional to perform, in addition they are also time-consuming. Along similar lines, the SWCC behavior can be reasonably exploited to the predict the complex thermal properties of unsaturated soils.

However, there are limited studies that are based on a theoretical framework using the SWCC as a tool to estimate the thermal conductivity of unsaturated soils.

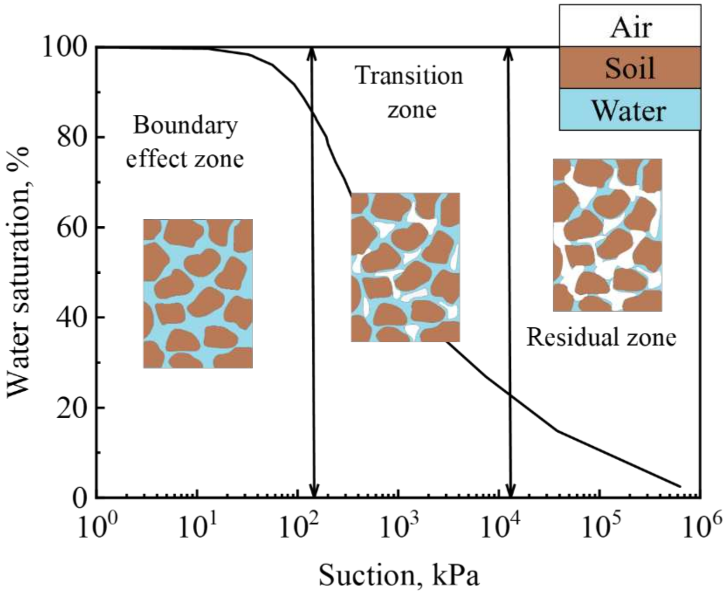

Fig.1 Typical SWCC showing distinct zones of desaturation (modified after Vanapalli et al. [19])

For this reason, in this study, the VG equation [20] is used as a tool for estimating the thermal conductivity of unsaturated soils considering its excellent performance for fitting SWCC of various types of soils:

$$S_e(P_c) = \left[\frac{1}{1+(\alpha P_c)^n}\right]^m \tag{1}$$

where S_e is water saturation; P_c is liquid pressure; α, m, and n are fitting parameters.

Derivation of thermal conductivity model

As previously discussed, the thermal conductivity of unsaturated soils is dependent on the phase transition of soil system. A general thermal conductivity relationship as suggested in [21] is shown below.

$$\lambda = \lambda_{dry} + \lambda_n \cdot (\lambda_{sat} + \lambda_{dry}) \tag{2}$$

For the drying process, the boundary conditions for thermal conductivity are λ_{sat} and λ_{dry}, respectively. A normalized thermal conductivity function, λ_n, in Eq. (2) can be defined to describe the variation of thermal conductivity with water saturation.

The key research objective of the study presented in this paper is directed towards developing an expression of normalized thermal conductivity function, λ_n. First, let us examine the phase transition in soils. During drying process, when air enters into soil pores, it can be related to the pressure difference between air and water. If the pressure reaches the air entry value, air enters into the large pores in soils, which can be described by Young-Laplace equation. Therefore, the phase transition function λ_n should be a function of pore size. At the beginning of drying, the phase transition doesn't happen (i.e., $\lambda_n = 1$), because all the pores are filled with water (i.e., $r = r_{\max}$). During the process that follows during drying, water drains out from soil pores as air enters. For such a scenario, λ_n decreases with a decrease in the pore size. At the end, when all the pores are filled with air, phase transition would be complete and $\lambda_n = 0$.

As a next step, let us introduce the concept of pore-scale thermal conductivity, λ_p. Based on the assumption that soil pores are a collection of spherical pores, some researchers proposed a different approach for modeling pore scale thermal conductivity [22, 23]. For example, Likos [23] proposed a technique for calculating the pore scale thermal conductivity extending mixing models theory and extend it for estimating the thermal conductivity of soil system.

$$\begin{cases} \dfrac{1}{\lambda_p} = x_f \dfrac{1}{\lambda_{sat}} + (1 - x_f)\dfrac{1}{\lambda_{dry}} & \quad Series \\ \lambda_p = x_f + (1 - x_f)\lambda_{dry} & \quad Parallel \\ \lambda_p = \lambda_{sat}^{x_f} \lambda_{dry}^{(1-x_f)} & \quad Geometric \end{cases} \tag{3}$$

where x_f is defined as the fractional area of liquid in a unit cell, dependent on the filling angle. In other words, the pore-scale thermal conductivity is dependent on the phase change in a unit pore.

Eq. (3) is the basis for using pore scale thermal conductivity to derive thermal conductivity of soils. However, the choice of mixing model that should be used in this model is not clear. In addition, determination of x_f that requires the information filling angle is not well defined. Due to these reasons, there are limitations in using Eq. (3). In other words, it is difficult to derive a closed-form function of thermal conductivity for unfrozen soils because of these limitations.

For simplicity, in this study, we consider a horizontal capillary tube with radius R subjected to heat flow in x direction, and the variable r is the radius of the element phase change that ranges from zero to R. For soils that are in an unfrozen state, this element consists of water; however, for frozen state, it's ice. In other words, we assume the heat can only be transferred through pores and the corresponding thermal conductivity is pore-scale thermal conductivity. The relationship between the pore-scale thermal conductivity and the thermal conductivity can be expressed by the mathematical relationship given below.

$$\lambda = \int_{R_{min}}^{R_{max}} \lambda_p f(r)\, dr + \lambda_{dry} \tag{4}$$

From a theoretical standpoint of view, Eq. (4) can be integrated; however, we need a functional relationship for achieving the same for λ_p. At the pore scale level, thermal conductivity is strongly dependent on the pore size. For example, if the capillary pores are filled with water, the thermal conductivity of pore can be treated as pure water, if we ignore the effect of pore wall. However, if the pores are filled with air, the pore scale thermal conductivity is basically equal to the thermal conductivity of air. For such a scenario, we cannot obtain an explicit expression for λ_p. However, pore size, r, and the pore-scale thermal conductivity can be related to the volume fraction of each of the components. The relationship below can be used if we assume the pore-scale thermal conductivity is proportional to the fraction area of the phase change element.

$$\lambda_p \propto \pi r^2 \tag{5}$$

Eq. (5) is valid for capillary tubes assuming that they are of constant pore size.

Eq. (5) was extended by [13], who conceptualized soil pores as capillary tubes with variable radii. A probability function was introduced to describe the likelihood of connecting two pores of different sizes. Accordingly, the function, $a(r, \rho)$ was defined to represent the probability of connection between two pores with radii r and ρ, leading to the definition of an effective radius and effective radius, r_e as given below.

$$a_e(r,\rho) = f(r)f(\rho)drd\rho \tag{6}$$

$$r_e = \sqrt{r\rho} \tag{7}$$

The above relationships suggest that the pore scale thermal conductivity can be expressed in terms of effective radius as given below.

$$\lambda_p \propto \pi r_e^2\, a_e\,(r,\rho)drd\rho \tag{8}$$

The term of $a_e(r, \rho)$ in Eq. (8) represents “effective area” for the corresponding capillary tubes.

By substituting Eqs. (6)–(8) into the general expression for bulk thermal conductivity in Eq. (4), the following relationship is obtained:

$$\lambda \propto \iint rf(r)\,\rho\, f(\rho)drd\rho = \left[\int_{r_{min}}^{r_{max}} rf(r)dr\right]^2 \tag{9}$$

It should be noted that we don’t have an explicit function between the pore-scale thermal conductivity, λ_p, and the pore size, r. In other words, Eq. (9) is not an explicit function, which means that we cannot obtain the thermal conductivity, λ using Eq. (9). Therefore, we use the normalized thermal conductivity, which is the ratio of thermal conductivity to eliminate the constant values in Eq. (9). It is more convenient to use effective water saturation, S_e to define the boundary condition, when $r \rightarrow R_{\max}$, $S_e \rightarrow 1$, and $r \rightarrow R_{\min}$, $S_e \rightarrow 0$. By definition, the relative thermal conductivity can be calculated using the relationship below.

$$\lambda_n = \frac{\lambda - \lambda_{dry}}{\lambda_{sat} - \lambda_{day}} = \left[\frac{\int_0^{S_e} rf(r)dr}{\int_0^1 rf(r)dr}\right]^2 \tag{10}$$

From the Young-Laplace equation [24], the radius of the capillary tube can be related to the capillary pressure, P_c, which is given by:

$$r = \frac{2T_S \cos\beta}{P_c} \tag{11}$$

where T_s is surface tension at the air-water interface; β is the contact angle.

Besides, the pore size can also be expressed by water saturation [25]:

$$dS_e = f(r)dr \tag{12}$$

Substituting Eq. 12 and Eq. 11 into Eq. 10, and replacing the value of 2 in Eq. 10 with a power η to extend it to a more general case, yields:

$$\lambda_n = \left[\frac{\int_0^{S_e} \frac{dS_e}{P_c}}{\int_0^1 \frac{dS_e}{P_c}}\right]^\eta \tag{13}$$

It is difficult to derive an analytical expression of normalized thermal conductivity using Eq. 13 by directly substituting in Eq. 1. Torch [26] proposed a relationship by setting m = 1+ 1/n_1 to replace m = 1- 1/n in the van Genuchten model which yields a closer fit to experimental data for a variety of soil types. The corresponding van Genuchten function is given below.

$$S_e(P_c) = \left[\frac{1}{1 + (\alpha P_c)^{n_1}}\right]^{(1+1/n_1)} \tag{14}$$

Eq. 14 has been validated and applied for the SWCC and relative hydraulic conductivity against published experimental data covering a wide range of soils textures from sand to clay [27, 28]. In our study, the modified van Genuchten model (Eq. 14) is used in the following calculation. Integrating Eq. 13 and inserting Eq. 14 yields a simple closed-form analytical expression with two parameters for predicting the normalized thermal conductivity:

$$\lambda_n = \left[1 - \left(1 - S_e{}^{n_1}\right)^{1+1/n_1}\right]^\eta \tag{15}$$

where m and n_1 are fitting parameters. n_1 can be obtained by fitting the modified SWCC model to experimental data. η comes from the function of pore-scale thermal conductivity which is related to pore size.

Model performance

Data set

To examine the performance of Eq. 15 for the normalized thermal conductivity function, λ_n, a database of the measured thermal conductivity from four soil samples is collected from the literature [29]. The physical properties of the selected soils are summarized in Table 1. In this study, the root-mean-square error (RMSE) were calculated for the new model (i.e., Eq. 15) for evaluating its performance.

$$RMSE = \sqrt{\frac{\sum_{j=1}^{X}\left(\lambda_j^P - \lambda_j^m\right)^2}{X}} \tag{16}$$

where X is the total number of measured data points. λ_j^p and λ_j^m are the j^{th} predicted and measured thermal conductivity values.

Table 1 Soil physical properties and parameters used in the model validation

Soil No.	Texture	Porosity	λ_{sat}	λ_{dry}	n_1	η	RMSE	Reference
1	Granite soil	0.26	3.19	0.302	5.0	0.26	0.0358	[29]
2		0.32	2.56	0.262	3.92	0.28	0.0299	
3		0.36	2.02	0.203	0.85	3.41	0.0240	
4		0.53	1.33	0.213	0.67	5.0	0.0494	

Model performance

Fig. 2 shows the experimental data and fitting results of normalized thermal conductivity, λ_n for granite soils with different porosity values. The results suggest the porosity has a greater influence on the thermal conductivity; for soil with a lower porosity, normalized thermal conductivity, λ_n typically increases linearly with S_e. For soils with a large porosity there is a nonlinear relationship between S_e and normalized thermal conductivity, which can be seen in Fig. 2. The summarized results suggest that there is a good agreement between the experimental data and the calculated results using the proposed model for different trends of the normalized thermal conductivity behavior. The different trends in the normalized thermal conductivity behavior can be explained by the interaction between the thermal conductivity and water saturation. In the wetting process, even when the water is replaced by air, heat is transferred through the air-filled contact points. For such a scenario, the thermal conductivity is mainly dependent on the interparticle contact points. The gas phase is continuous but the fluid phase, which has larger thermal conductivity is not continuous. As water continuously replaces the air, water films begin to form around soil particles. In this stage, both gas and fluid phases are continuous and thus the thermal conductivity of soil increases rapidly following a linear relationship. In the third stage, as the water displaces the less conductive air from pore space, the gas phase is not continuous, but the fluid phase is continuous. The thermal conductivity is nonlinear with water saturation due to this reason. However, for the soils with a lower porosity, the thermal conductivity is governed by the solid matrix and the nonlinear relationship is not obvious. However, as the soil porosity increases, this nonlinear relationship is more obvious.

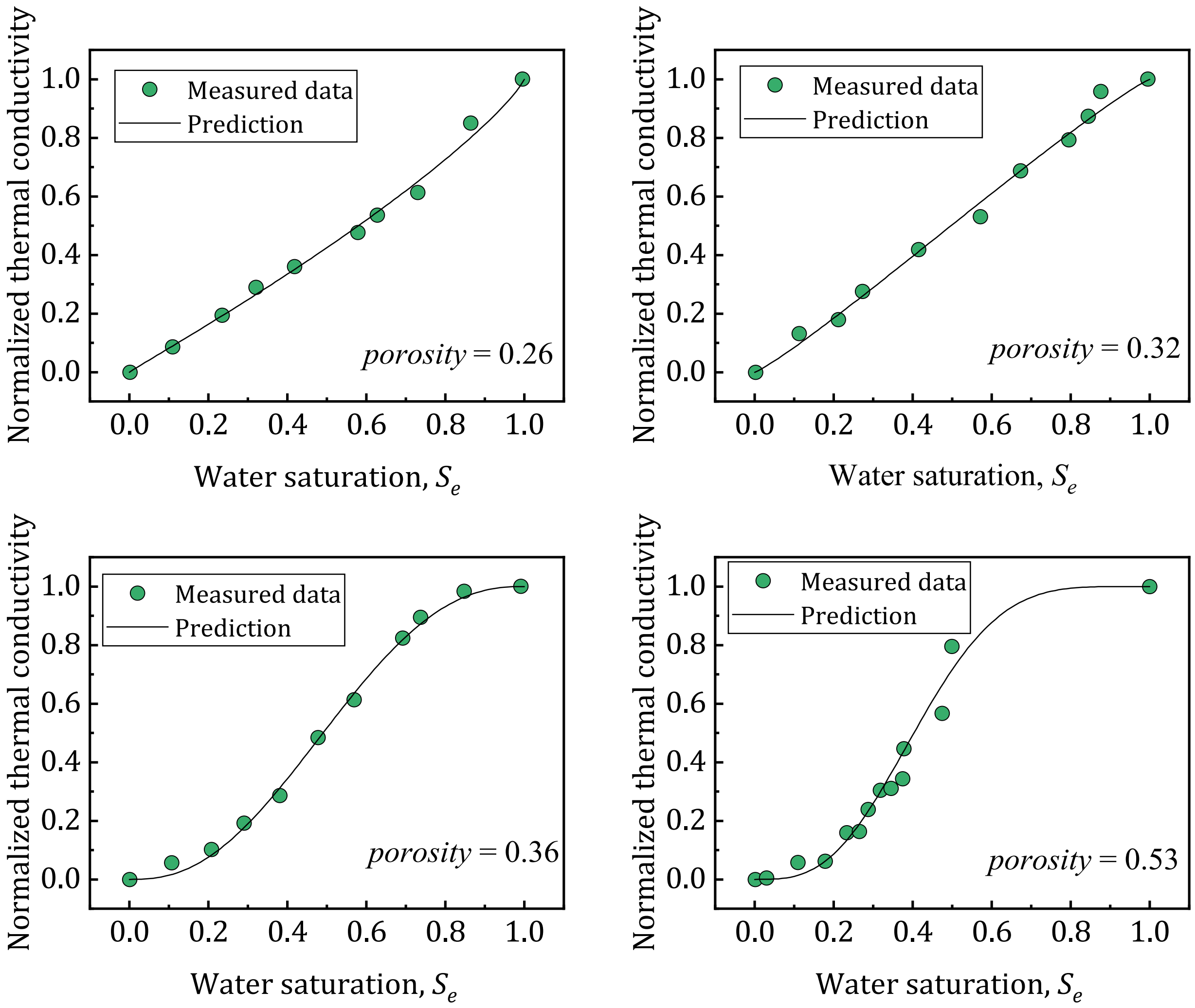

Fig. 2 Normalized thermal conductivity vs. water saturation for granite soils with different porosity

Parameter analysis

Fig. 3(a) illustrates the relationship between normalized thermal conductivity and water saturation for different values of the parameter n_1. As n_1 increases from 0.3 to 2.0, the shape of the curve changes significantly. Smaller values of n_1 (e.g., 0.3) lead to a gradual increase in thermal conductivity with water saturation, indicating a more uniform response across the saturation range. In contrast, larger values of n_1 (e.g., 2.0) produce a sharper rise in conductivity at higher saturation levels, reflecting greater sensitivity to changes in saturation near full saturation.

The parameter n_1 primarily controls the nonlinearity of the relationship, governing how quickly the thermal conductivity increases as saturation rises. Lower n_1 values emphasize early-stage sensitivity, while higher values delay the response until higher saturation is reached. This behavior can be interpreted as reflecting differences in pore structure or connectivity, with larger n_1 suggesting more abrupt transitions in thermal transport properties as the soil becomes increasingly saturated.

Fig. 3(b) presents the influence of η on normalized thermal conductivity across varying levels of water saturation. As η increases from 1 to 10, the curve becomes progressively flatter at lower saturation levels and steeper near full saturation, resulting in a more sigmoidal shape. Smaller values of η (e.g., 1) cause thermal conductivity to increase rapidly even at low saturation, whereas higher values of η delay the increase, indicating reduced sensitivity to initial water content. The parameter η thus controls the gradualness of the conductivity response, with higher values reflecting a more dispersed or delayed effect of water saturation on thermal conductivity, potentially corresponding to more heterogeneous pore structures.

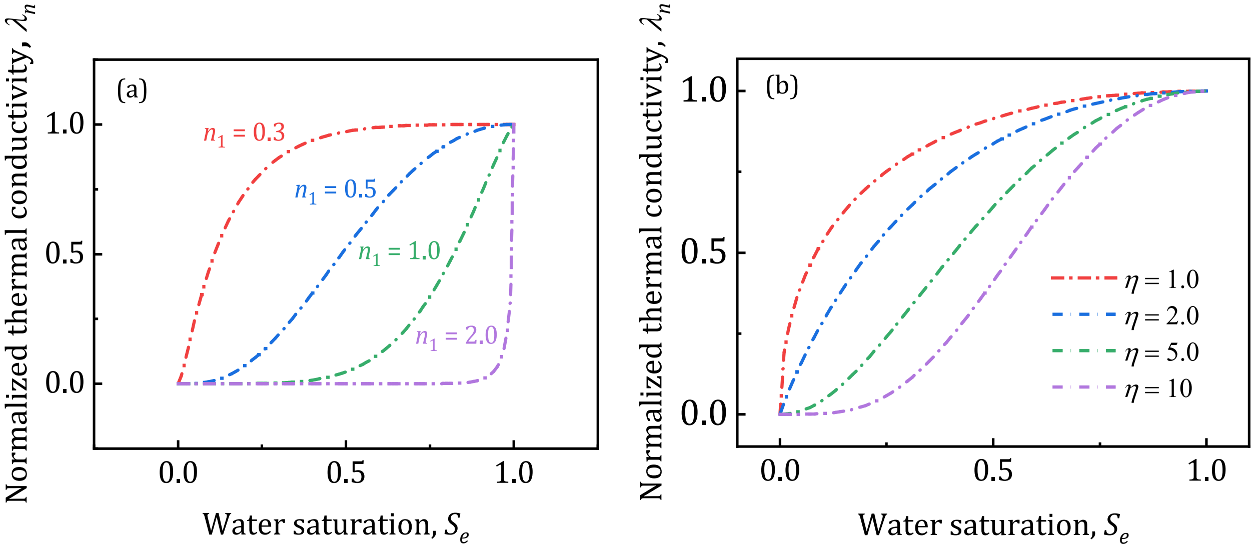

Fig. 3 Effect of two Parameters on the Normalized Thermal Conductivity: (a) n_1; (b) η

Conclusions

This study presents a new model for predicting the thermal conductivity of unsaturated soils by utilizing the Soil Water Characteristic Curve (SWCC). The model introduces two parameters, n_1 and η, which are both related to the soil's pore size distribution.

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The paper was published in the proceedings of the 4th Pan-American Conference on Unsaturated Soils (PanAm UNSAT 2025) and was edited by Mehdi Pouragha, Sai Vanapalli and Paul Simms. The conference was held from June 22nd to June 25th 2025 in Ottawa, Canada.