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Type of paper: full length article (Canadian Geotechnical Journal) 1 2 Date text written: Mar 2024 Number of words = 109363 Number of figures = 94 Number of tables = 35 6 7 _____ 8 9 Effective thermal conductivity of granular soils: a review of influencing factors and prediction models towards an investigation framework through multiscale characters 10 11 Author 1 Tairu Chen, ME, BE 12 13 Department of Infrastructure Engineering, The University of Melbourne, Parkville, Australia 14 ORCID: 0000-0003-4910-1980 15 Email: tairu.chen1@unimelb.edu.au 16 Author 2 17 18 Wenbin Fei[⊠], PhD, ME, BE ¹College of Civil Engineering, Hunan University, Changsha, Hunan 410082, PRC 19 ²Key Laboratory of Building Safety and Energy Efficiency of the Ministry of Education, Hunan 20 University, Changsha 410082, PRC 21 ³Department of Infrastructure Engineering, The University of Melbourne, Parkville, Australia 22 23 ORCID: 0000-0002-9275-8403 24 Email: wenbinfei@outlook.com 25 26 Author 3 Guillermo A. Narsilio, PhD, MSc (Math), MSc (CE), CEng 27 28 Department of Infrastructure Engineering, The University of Melbourne, Parkville, Australia ORCID: 0000-0003-1219-5661 29 Email: narsilio@unimelb.edu.au 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 Full contact details of corresponding author Wenbin Fei, Professor 46 A316, College of Civil Engineering, Hunan Univ., Changsha, Hunan 410082, PRC 47

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50 Abstract:

The effective thermal conductivity of soil is important to geo-engineering applications, and it 51 is controlled by factors across different length scales. Through a comprehensive review of these 52 factors, we found that while other more traditional factors have been well studied, there is still 53 54 a lack of characterisation of soil microscale and mesoscale structures and their influence on 55 effective thermal conductivity. In addition, after reviewing the models available in the literature 56 for soil effective thermal conductivity prediction, it was found that compared with empirical 57 and theoretical models, machine learning models can account for the influence of multi-scale 58 factors, however, research into them is scarce. To overcome the limitations of previous 59 research, we proposed a framework that can investigate the factors influencing soil effective thermal conductivity at multiple scale. It includes the impact of soil structural factors at micro 60 to mesoscale, and this impact is integrated with the influence from other factors for accurate 61 62 thermal conductivity prediction.

63 Keywords

64 Soil thermal conductivity; Influencing factors; Prediction models; Soil fabric; Microstructures

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1 Introduction

Heat transfer in geomaterials (soils and rocks) plays an essential role in the geotechnical and geologyengineering applications that contribute to a sustainable development, for example, hydrocarbon exploration (Schimmel et al. 2019), geothermal energy utilisation (Brandl 2006; Jia et al. 2019), thermal energy storage (Bauer et al. 2013), and carbon dioxide sequestration (Fei et al. 2015). Therefore, a clear and updated understanding of the heat transfer behaviour in geomaterials is of utmost importance to improve the reliability and productivity of associated engineering projects.

72 Soil is usually regarded as granular and composite material, and it mainly consists of solid particles and 73 voids. The solid particles are made up of minerals or organic matters; and the voids are usually filled 74 with water or air. Similarly, rocks can be thought as (mildly to highly) cemented granular materials, 75 this is particularly true for sedimentary rocks. Consequently, there are three mechanisms driving heat 76 transfer in soil: a) thermal conduction – heat is transferred from one solid particle to another if two 77 particles contact each other (or through the solid cementation between them); b) thermal convection -78 the heat transference happens in the voids that contain water or air; and c) thermal radiation – heat 79 transfer between different components and through electromagnetic waves at high temperature 80 (Asakuma et al. 2014). Thermal conductivity (λ) is the property that indicates materials ability to transfer heat, and the λ of different soil constituents varies. In particular, the λ of solid particles is of 81 82 different magnitude compared with that of water or air in the voids (Yun and Santamarina 2008). For example, $\lambda_{minerals} > 3$ W/(m·K), $\lambda_{water} = 0.56$ W/(m·K), $\lambda_{air} = 0.026$ W/(m·K) at room temperature 83 84 and atmospheric pressure. Considering the three heat transfer mechanisms in soil and the variation of λ 85 between different components, the *effective* thermal conductivity λ_{eff} is adopted to indicate the overall heat transfer ability. Therefore, studying and predicting λ_{eff} is crucial in understanding soil heat transfer 86 87 behaviour.

88 The soil λ_{eff} is controlled by soil structure, which can be quantified at different scales: macroscale, 89 mesoscale, and microscale. Macroscale structures are derived from regarding different phases in soil as 90 a corresponding whole unit, while ignoring, for example, the connection between solid particles and 91 particles shape and size. For instance, porosity is a macroscale parameter, and it is defined as the ratio 92 of the volume of voids to the total volume of soil. Porosity is mostly used to predict the λ_{eff} because it controls the contribution of different heat transfer mechanisms (e.g., heat conduction or heat convection) 93 94 to overall λ_{eff} (Yun and Santamarina 2008; Côté and Konrad 2005; Rizvi et al. 2020c). A number of 95 studies have investigated the soil λ_{eff} based on macroscale factors and corresponding models have been 96 proposed to predict the λ_{eff} (Zhang et al. 2017; Zhang and Wang 2017). Mesoscale structures involve 97 different particles in soil and characterise the connectivity between them and/or their interrelations with 98 the pore space. For example, particle connectivity, defined by network features based on complex 99 network theory (Fei et al. 2019b), indicates thermal conduction skeleton in soil. Microscale structures 100 focus on individual particles. They include information about particle size and shape, which control 101 inter-particle contact area and are defined through parameters like roundness and sphericity (Hryciw et 102 al. 2016; Lee et al. 2017; Fei et al. 2019a). Therefore, investigating the effect of factors at different scales on λ_{eff} is the key to comprehensive understanding of soil heat transfer behaviour. Nevertheless, 103 104 effects of multiscale (from micro to mesoscale) structural parameters on λ_{eff} have not been comprehensively reviewed and summarised. Furthermore, emerging models (e.g., machine learning 105 106 models) for soil λ_{eff} prediction have not been included in the previous review papers.

107 This article first reviews the relationship between soil λ_{eff} and various influencing factors at different 108 scales with comprehensive supporting data from the literature. The factors that have not been fully 109 researched yet are summarised. The soil λ_{eff} prediction models that involve different factors are 110 assessed and their potential limitations are identified. To conclude, a research framework is proposed 111 and demonstrated for investigating soil λ_{eff} through factors at multiple scales.

112 2 Influencing factors of effective thermal conductivity

For comprehensive review of all influencing factors, a detailed category including non-redundant factors is required, particularly when considering soil structure at different scales. A comparison between the categories in literature and the category adopted in this study is given. Based on the proposed category, the influence of each factor on λ_{eff} is then analysed.

117 2.1 Categories of influencing factors

118 2.1.1 Categories of influencing factors in literature

119 The factors influencing soil λ_{eff} have been categorised differently in the various studies. Table 1 120 summarises the methods in the literature to categorise those factors. The classification - compositional factors, environmental factors and other factors – was adopted in (Zhang and Wang 2017); however, 121 122 this classification could be clearer if compositional factors are further divided into components and 123 structures. Dong et al. (2015) divided the factors into soil constituent, soil type, water content and 124 particle contact; but these categories were redundant, because soil constituent and soil type are 125 correlated. Soil nature, soil structure and soil physical condition were three groups identified by Jin et 126 al. (2017), whereas these groups were not independent either. Abu-Hamdeh (2003) broadly classified 127 the factors influencing soil λ_{eff} into those inherent to soil itself and those can be managed or controlled; but this classification is too general to arrange all the specific influencing factors. 128

129 2.1.2 Categories of influencing factors in this study

130 To address the limitations of previous research in categorising the factors influencing soil λ_{eff} (Zhang and Wang 2017; Dong et al. 2015; Jin et al. 2017; Abu-Hamdeh 2003), this study classify those factors 131 132 into three types: components properties, structures and environmental conditions, as presented at the bottom of Table 1. The "components properties" consist of the thermal conductivity of the solid material 133 and that of the void typically filled with air or water. The "structures" are considered at three scale 134 135 levels: macro-level, meso-level and micro-level. Macroscale factors describe the material as a whole, 136 for example, porosity is regarded as a structural factor at macro-level. Mesoscale factors involve two or 137 more particles, for example, particle connectivity belongs to the meso-level. The microscale structural 138 factors, which are based on individual particles, comprise particle shape, particle size and interparticle 139 contact area. In addition, environmental conditions are composed of temperature, density, pressure, and 140 moisture content - these are all macroscale factors as well.

References	Categories	Factors	Limitations
Zhang and	Compositions	Mineral components;	Particle connectivity
Wang (2017)		gradation; particle size	and particle contact
		and shape;	area are not arranged
		interparticle physical	properly
		contact, e.g., the	
		number of contact	
		points; change of soil	
		structure during drying	
		and wetting cycle;	
	Environmental conditions	Water content and	
		movement; density;	
		temperature;	
	Other	Properties of soil;	
		ions, salts and	
		additives; hysteresis	
Dong et al.	Constituent	Particle thermal	The categories are
(2015)		conductivity;	correlated: the soil
		mineralogy	constituent differences
	Soil type	Mineral; gradation;	are due mainly to
		particle size and shape	different soil type
	Water content		
	Particle contact	Coordination number	
Jin et al. (2017)	Soil nature	Texture; mineralogy;	The categories are not
		particle shape and size	independent: soil
	Structural condition	Porosity; particle	particle size and shape
		arrangement	are classified into soil
	Physical condition	Water content;	nature, but they impact
		temperature; pressure	the soil structures
Abu-Hamdeh	Factors inherent to soil itself	Mineralogy;	The categories are too
(2003)		composition;	general to arrange all
	Factors manageable	Water content;	specific influencing
		density; porosity	factors
This study	Components properties	Particle / air / water	
		thermal conductivity;	
		materials' elastic	
		stiffness	
	Structures	Macro-level: porosity	
		Meso-level: particle	
		connectivity, e.g.,	
		coordination number	
		•••••••••••••••••••••••••••••••••••••••	
		quantified soil	
		quantified soil skeleton (Fei and	
		quantified soil skeleton (Fei and Narsilio 2020)	
		quantified soil skeleton (Fei and Narsilio 2020) Micro-level: particle	
		quantified soil skeleton (Fei and Narsilio 2020) Micro-level: particle size, particle shape,	
		quantified soil skeleton (Fei and Narsilio 2020) Micro-level: particle size, particle shape, particle contact area	
	Environmental conditions	quantified soil skeleton (Fei and Narsilio 2020) Micro-level: particle size, particle shape, particle contact area Temperature; pressure;	

141 Table 1 Categories of the factors influencing soil effective thermal conductivity

42 2.2 Soil components properties influencing the effective thermal conductivity

143 Heat conduction within particles is an important heat transfer process in geomaterials. Therefore, 144 particle thermal conductivity ($\lambda_{particle}$) influences the soil effective thermal conductivity (λ_{eff}) 145 (Tarnawski et al. 2009). In general, high soil λ_{eff} could be resulted from high $\lambda_{particle}$ (Côté and Konrad 2005; Zhang et al. 2015b; He et al. 2020). The $\lambda_{particle}$ is determined by the minerals that compose 146 147 particles, and it ranges from 1.8 to 8.8 W/(m·K) (He et al. 2020). Johansen (1977) summarised the 148 thermal conductivity of the minerals at common ambient temperatures around 25 °C, which shows 149 quartz has the highest thermal conductivity around 7.7 $W/(m\cdot K)$, while mica and feldspar have the lowest values, both of which are around 2 W/(m·K). Other minerals, e.g., pyroxene, amphibole, olivine, 150 151 and chlorite, possess a thermal conductivity ranging from 2 to 5.8 W/(m·K). Consequently, geomaterials 152 and soils that mainly consist of quartz show a higher λ_{eff} than those composed of other minerals. There 153 are many models considering $\lambda_{particle}$ for λ_{eff} prediction: series and parallel models by Wiener (1912), 154 uniform model by De Vries and Van Wijk (1963), geo-mean model by Johansen (1977) and Hashin and 155 Shtrikman boundary model (Hashin and Shtrikman 1962; Yun and Santamarina 2008). While ignoring 156 the influence of particle connection and contact on λ_{eff} , they could be used to show the relationship between λ_{eff} and $\lambda_{particle}$ to some extent. The equation based on geo-mean model (Johansen 1977) is 157 158 selected for the showcase considering the available data from He et al. (2020).

$$\lambda_{eff} = \lambda_{particle}^{1-n} \lambda_{water}^{S \times n} \lambda_{air}^{(1-S) \times n} \tag{1}$$

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$$n = \frac{V_{void}}{V_{total}} \tag{2}$$

160 where $\lambda_{particle}$ is the particle thermal conductivity; λ_{water} is the water thermal conductivity; λ_{air} is the 161 air thermal conductivity; *n* is porosity defined as the ratio of void volume V_{void} and total volume V_{total} ; 162 and *S* is degree of saturation (the ratio of water volume to void volume). Measured thermal conductivity 163 data from Birch and Clark (1940) shows that λ_{eff} prediction error using this model is within 20% 164 (Johansen 1977). Figure 1 exemplifies the influence of $\lambda_{particle}$ on soil λ_{eff} in dry conditions, assuming 165 $\lambda_{air} = 0.026$ W/(m·K). The figure shows the $\lambda_{particle}$ affects λ_{eff} to a larger extent in soil with low 166 porosity than in soil with relatively high porosity.



167

168 Figure 1 Influence of solid particle thermal conductivity $\lambda_{particle}$ on soil effective thermal conductivity λ_{eff} under 169 different porosity based on data from He et al. (2020)

170 In addition to the solid particle thermal conductivity, elastic stiffness is another component property 171 that affect the effective thermal conductivity (Morimoto et al. 2022). Morimoto et al. (2022) 172 investigated the relationship between the thermal conductivity and granular materials' Young's 173 modulus via the combination of DEM-generated granular samples and corresponding heat pipe network model. According to their findings, soil effective thermal conductivity may increase with its Young'smodulus.

176 2.3 Soil structures influencing the effective thermal conductivity

177 2.3.1 Structural feature at macroscale

Porosity n is one of soil properties at macro-level and it refers to the fraction of pore volume V_{void} of 178 total volume V_{total} as defined in Eq. (2) above. It is commonly used to describe the macro-structure of 179 180 granular and sandy soils (Ding et al. 2023) and selected as a key/sole structural feature when 181 establishing predictive models of thermal conductivity (Johansen 1977; Côté and Konrad 2005; Tong 182 et al. 2009; Rizvi et al. 2020a). The void usually contains water and air. Since the values of particle 183 thermal conductivity ($\lambda_{particle}$), water thermal conductivity (λ_{water}) and air thermal conductivity (λ_{air}) 184 have different magnitudes and they together determine the soil effective thermal conductivity (λ_{eff}) to 185 some extent, the porosity *n* influences the soil λ_{eff} remarkably.

Porosity is a result of soil texture and particle distribution. Sandy soil has a porosity range from 0.35 to 186 187 0.5, while finer soil porosity typically ranges from 0.4 to 0.6. Compacted soil possesses a porosity as low as 0.25 to 0.3 (Carter and Gregorich 2007). Overall, soil λ_{eff} decreases with the increase of porosity 188 (Côté and Konrad 2005). Figure 2(a) shows the change of dry soil λ_{eff} with porosity. The included data 189 190 are collected from Slusarchuk and Watson (1975); Johansen (1977); Côté and Konrad (2005); Yun and 191 Santamarina (2008); Narsilio et al. (2010); Fei et al. (2019b). Soil λ_{eff} in dry conditions ranges from 192 about 0.15 to 0.45 W/(m·K) while the porosity changes from about 0.25 to 0.55. Furthermore, Côté and 193 Konrad (2005) claimed that dry soil λ_{eff} is directly related to porosity and they proposed the following 194 exponential relationship between the two parameters:

$$\lambda_{eff,\,dry} = \chi \cdot 10^{-\eta n} \tag{3}$$

195 where $\lambda_{eff, dry}$ is the effective thermal conductivity of dry soil; χ and η are coefficients related to soil 196 particle shape. They applied the equation to various soils: χ and η are 0.75 W/(m·K) and 1.2 for natural 197 mineral sands, 1.7 W/(m·K) and 1.8 for crushed rocks, 0.3 W/(m·K) and 0.87 for organic fibrous soil. 198 Figure 2(b) shows the change of unsaturated and saturated soil λ_{eff} with porosity. The experimental 199 data for quartzite and granite are from Côté and Konrad (2005). It indicates that the porosity affects 190 λ_{eff} to a larger extent with high degree of saturation, *S*, than low degree of saturation.





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205 and *S* are 2 *W*/(*m*·*K*), 0.026 *W*/(*m*·*K*) and 0 for generating Eq. (1); (b) unsaturated / saturated soils predicted 206 values using Eq. (1) with $\lambda_{particle}=5$ *W*/(*m*·*K*), $\lambda_{water}=0.56$ *W*/(*m*·*K*), $\lambda_{air}=0.026$ *W*/(*m*·*K*); quartzite and granite 207 experimental data is from Côté and Konrad (2005)

208 2.3.2 Structural features at mesoscale

209 Particle connectivity indicates soil skeleton and thus relates to the pathways of heat conduction between 210 particles. Since heat conduction between particles dominates the heat transfer processes in soil, particle connectivity is important to soil effective thermal conductivity λ_{eff} (Dong et al. 2015). However, the 211 212 indices of soil particle connectivity have not been well studied. Cheng et al. (1999) described the particle 213 connectivity based on the results measured by Finney (1970), but only mono-sized spheres were 214 considered. Particle connectivity could also be obtained if employing Discrete Element Modelling 215 (DEM) for granular assemblies, since the contact between discrete particles and packing characteristics 216 of granular systems can be found within DEM. Although research has been conducted on heat transfer 217 using DEM, those work mainly focused on the computation of effective thermal conductivity and 218 structural characterisation was out of their scope (Vargas and McCarthy 2001; Feng et al. 2009). 219 Structural parameters such as packing fraction and macroscopic stress has been investigated by Peeketi 220 et al. (2019) but further quantification of particle connectivity change due to altered packing and stress 221 conditions is still missing. Many other studies used coordination number derived from DEM-generated 222 granular assembly to investigate thermal conductivities (Yun and Evans 2010; El Shamy et al. 2013). 223 Nonetheless, traditional coordination number alone cannot capture all information of complex granular 224 materials' structure. For example, traditional coordination number only considers the number of 225 contacts between particles but ignores the contact quality, which determine the thermal resistance between particles. Further description and quantification of particle connectivity cannot be achieved 226 227 without other theories and tools.

228 Fei and Narsilio (2020); Fei et al. (2020) used complex network theory to characterise soil particle 229 connectivity based on X-ray computed tomography (CT) images. To use complex network theory to 230 characterise soil particle connectivity, a network representing soil particles has to be built first based on 231 real soil CT images. This network's format is similar to that studied in (Feng et al. 2009; Yun and Evans 232 2010; El Shamy et al. 2013; Morimoto et al. 2022): soil is represented as a web composed of nodes and 233 edges; the nodes represent individual particles, and edges exist between contacted particles. Then, the 234 complex network theory can be applied to the built network to extract structural features. These 235 structural features provide more comprehensive indices for particle connectivity and soil structure 236 quantification, and these indices are classified into four types: centrality, network scale, cycles and 237 clustering, as listed in Table 2. These different types describe structures of a soil particle assembly via 238 different aspects (Newman 2003). The "centrality" type quantifies the importance of nodes (particles) 239 within a network (granular assembly) based on their position or the number of paths passing through 240 them. For example, the *degree* of a node in a network is the number of edges linked to this node, which 241 is equivalent to coordination number in soil mechanics and powder technology. Closeness centrality of 242 a node measures the how closely this node is related to other nodes, as exemplified in Figure 3 and 243 detailed in Table 2. Betweenness centrality measures how often a node appears on the shortest path between two other nodes. The "network scale" measures the network size and interactions between 244 245 nodes encompassed in a network. For example, network diameter is equal to the length of the longest 246 one among the shortest paths between any two nodes in a network, as illustrated in Figure 3. The "cycle" 247 type indicates the loop starting and ending at the same node and thus 3-cycles represent triangles. The "clustering" type measures the tendency of nodes to form tightly-knit groups or communities within a 248 249 larger network as detailed in Table 2 and Figure 3.

Furthermore, weighted networks are established by adding contact area or thermal conductance as the weight to network edges, resulting in new weighted sub-indices under each type. In an unweighted network, an edge only indicates two nodes are connected. Even though the edges in Figure 3 have different lengths, the lengths have not been considered as weight for the edges. For network representing granular soils, if the contact area between two particles in physical contact is used to weight the edge between two nodes that represent those two particles in a network, the length of this edge has a physical meaning of the contact area. This process of adding weights to edges in a network bring physical meanings to the network features, and consequently the network features account for not only the number of particles contacts but also the contact quality. The influence from contact area / thermal conductance-weighted network features on heat transfer is also included in Table 2.

260 In general, soil λ_{eff} correlates directly proportional to the degree (also known as coordination number 261 in soil mechanics and powder technology). For closeness centrality, soil λ_{eff} is related to the weighted 262 value directly proportional while the unweighted value inversely proportional. Besides, soil λ_{eff} decreases with the increase of the betweenness centrality. In terms of network scale indices, soil λ_{eff} is 263 264 inversely correlated to the average weighted shortest path. As for cycles and clustering, λ_{eff} increases with the number of 3-cycle in a network. Particularly, the weighted degree and weighted closeness 265 266 centrality are identified as the best predictors for soil λ_{eff} (Fei and Narsilio 2020). A quantitative relationship between soil λ_{eff} and network features is given below (Fei et al. 2020) : 267

$$\frac{\lambda_{eff}}{\lambda_{solid}} = -0.21 \left(\left[G^C \right]_{\kappa_w} \right)^2 + 0.67 \left[G^C \right]_{\kappa_w} + 0.25 \tag{4}$$

where λ_{solid} is the solid particle thermal conductivity; $[G^C]_{\kappa_w}$ is the *degree* weighted by the contact area between particles. Figure 4 illustrates the influence of *weighted degree* on soil λ_{eff} for different sands with data from Fei et al. (2021). The complex network methodology for soil structure quantification has not been extended to unsaturated soil, where water fills voids and bridges particles, and hence updated networks need to be proposed for studying heat transfer in unsaturated soil.

Table 2 Indices of soil particle connectivity at mesoscale based complex network theory and their relationship with soil effective thermal conductivity λ_{eff} (Fei and Narsilio 2020; Fei et al. 2020)

Туре	Sub-indices	Description	Correlation with λ_{eff}
Centrality	Degree*	The number of edges linked to a node	Directly proportional
	Closeness centrality*	Related to distance of a node to other nodes and defined as $[G]_{\mathcal{C}}(i) = \beta \left[\sum_{j=1}^{ \mathcal{V} -1} d(i,j) \right]^{-1};$	Directly proportional for weighted values but inversely proportional for unweighted values
		[G] _C (<i>i</i>) is closeness centrality of node <i>i</i> ; β is a normalisation term; <i>V</i> is a node-set including <i>i</i> and <i>j</i> ; d(i,j) is the shortest path length from <i>i</i> to <i>j</i> .	
	Betweenness centrality*	Related to the extent that a node or edge connects other nodes or edges: $[G]_B(i) = \beta \sum_{i \ k \in V} \frac{\sigma(j, k i)}{\sigma(i, k)};$	Inversely proportional
		[G] _B (i) is betweenness centrality of node i; β is a normalisation term; $\sigma(j, k)$ is the number of $d(j,k)$; $\sigma(j, k i)$ is number of $d(j,k)$ passing the node i.	
	Eigenvector centrality*	The contribution of a node to network connectivity	
Network scale	Network diameter	The longest one among the shortest length paths: $[G]_D = Max_{i,j\in V}[d(i,j)];$ $[G]_D$ is network diameter; <i>V</i> is the node set included in the network; d(i,j) is the shortest path length from node <i>i</i> to node <i>j</i> .	
	Average shortest path length*	The average of the shortest length paths from every node to other nodes.	Inversely proportional
	Network density	The ratio of actual edge number to potential edge number	
Cycles	Number of 3-cycle	Number of loops in a network that starts and ends at the same node and has 3 edges	Directly proportional
Clustering	Global clustering coefficient	Indicating how integrated or fractured the network is: $G_{GC} = 3 \frac{triangles'number}{connnected triples'number}$,	

Туре	Sub-indices	Description	Correlation with λ_{eff}
		G_{GC} is the global clustering coefficient;	
		a 'triangle' is a three nodes-set connected by three edges;	
		a 'triple' is a three nodes-set connected by three / two edges .	
	Local clustering coefficient*	$[G]_{LC}(i) = \frac{2T(i)}{\kappa(i)[\kappa(i) - 1]},$	
		$[G]_{LC}(i)$ is the local clustering coefficient of node <i>i</i> ;	
		T(i) is the number of triangles passing node <i>i</i> ;	
		$\kappa(i)$ is the degree of node <i>i</i> .	

275 * For the sub-indices calculated based on individual node or edge, the average value is adopted. The asterisk * indicates an average value.



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278



277 Figure 3 Network features illustration based on complex network theory from (Fei and Narsilio 2020)



279 Figure 4 Influence of contact area-weighted degree in complex network theory on soil effective thermal 280 conductivity λ_{eff} in with data from Fei et al. (2021)

281 2.3.3 Structural features at microscale

282 Soil particle shape and size control the contact area between particles, and the contact area governs the 283 heat conduction process in soil. Since heat conduction between particles dominates the heat transfer 284 processes in soil, particle shape and size are the key factors that influence soil effective thermal 285 conductivity λ_{eff} (Gan et al. 2017; Lee et al. 2017; Fei et al. 2019a). Many studies adopt coefficients rather than particle shape and size descriptors themselves to consider the effect (De Vries 1963; Côté 286 287 and Konrad 2005), where a quantitative relationship between λ_{eff} and particle shape and size is missing. To quantify the particle size and shape influence, this section firstly reviews the methods for particle 288 289 size and shape description.

290 Two-dimensional microscopic images-based descriptors for particle shape, such as circularity, 291 sphericity, roundness, etc., have been introduced in Cherkasova and Shan (2008); Cox and Budhu 292 (2008); Lee et al. (2017) and (Xiao et al. 2020); however, they have some limitations when 293 characterising irregular particles in natural soil, because the derived descriptor values may vary with 294 the directions of projections (Fei et al. 2019a). Three-dimensional sphericity is introduced and used in 295 Wadell (1932); Hamilton and Crosser (1962); Verma et al. (1991). Sphericity in these studies is defined Surface area of volume equivalent sphere . Nevertheless, elongated particles cannot be well described using 296 as 297 this definition. Lees (1964) described the angularity of particles using three main features: number of 298 corners, corners degree of projection, and corners degree of acuteness. Zhou et al. (2018) combined 299 roundness and sphericity to describe real sand particles with different shapes. Volume-based aspects 300 ratio was found to have a positive correlation to thermal conductivity of silver nanofluids 301 (Mirmohammadi et al. 2019). More recent works use sphericity in Eq. (5) and roundness in Eq. (6) for 302 particle shape representation (Fei et al. 2019a). These two descriptors can be computed using CT images 303 of real soil particles.

$$Sphericity = \frac{36\pi V^2}{(SA)^3}$$
(5)

$$Roundness = \frac{\sum_{n=1}^{r_i} N}{r_{\max,in}}$$
(6)

where *V* is particle volume and *SA* is particle surface area in Eq. (5); r_i is the radius of the *i*th particle corner, *N* is the number of particle corners and $r_{\max, in}$ is radius of the maximum inscribed sphere in Eq. (6). Figure 5 shows the soil λ_{eff} change with different particle shape. In general, soil composed of spherical and round particles has a higher λ_{eff} than that composed of elongated and angular particles.



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309 Figure 5 Influence of particle shape on soil effective thermal conductivity λ_{eff} (a) shape defined by surface areas 310 with dry glass experimental data from Verma et al. (1991); λ_{solid} is around 1 W/(m·K), λ_{air} is around 311 0.025 W/(m·K); (b) shape defined by Eq. (5) and Eq. (6) with data from Fei et al. (2019a); λ_{solid} 312 = 3 W/(m·K), $\lambda_{air} = 0.025$ W/(m·K), $\lambda_{water} = 0.591$ W/(m·K)

313 Parameters including 1) the fraction of relatively large particles in soil assembly and 2) particle mean 314 or median diameters are usually used to study the influence of particle size on soil λ_{eff} . In most cases, soil with a larger particle size shows a higher λ_{eff} than that with smaller particle size (Zhang et al. 315 316 2015a; Gan et al. 2017). Gan et al. (2017) argued that small particle size leads to less particle contact 317 area, and thus reduces the heat conduction between particles and lowers effective thermal conductivity 318 in dry condition. It should be noted that, however, for unsaturated soil, small particle size leads to high 319 soil λ_{eff} (Zhang et al. 2015b). This is because small particle size results in large surface area, and thus 320 water films and bridges are easily formed between particles, thereby reducing thermal resistance 321 considering that water has a greater ability for heat transfer than air. Furthermore, compared with the 322 λ_{eff} of soil with low particle thermal conductivity, the λ_{eff} of soil with high particle thermal 323 conductivity is more easily influenced by particle size (Zhou et al. 2010; Gan et al. 2017). Figure 6 324 presents general relationship between soil λ_{eff} and particle size. Mean particle diameters are used by 325 Midttomme and Roaldset (1998), where particles are derived from synthetic samples with relatively 326 uniform particle size. Median particle diameters are used by Fei et al. (2021), Lee et al. (2017) and Chen 327 (2008), where diameters are from sieve analysis. The λ_{eff} relates more closely with mean diameters 328 than median diameters.



331 Figure 6 Influence of particle size on soil effective thermal conductivity λ_{eff} with data from Midttomme and 332 Roaldset (1998); Chen (2008); Lee et al. (2017); Fei et al. (2021)

333 2.4 Environmental conditions influencing the effective thermal conductivity

334 2.4.1 Soil water content

335 The pores around solid particles in soil are typically filled with either air or water. Since water can reduce the thermal resistance between particles remarkably (Rao and Singh 1999), the water content, 336 337 or more precisely the degree of saturation S (the ratio of water volume to voids volume) and volumetric 338 moisture content θ (the ratio of water volume to soil volume) are considered as the prominent factors 339 that affect soil effective thermal conductivity λ_{eff} (Zhang and Wang 2017; Agrawal et al. 2019; Lu and 340 Dong 2015). Some studies report gravimetric moisture content w (the ratio of water mass to soil mass) 341 rather than S and θ . In general, soil λ_{eff} under unsaturated or fully saturated conditions is higher than 342 that under dry conditions (Johansen 1977; Chen 2008). Moreover, the soil λ_{eff} grows more rapidly at low S or θ compared with that at high S or θ (Zhang et al. 2015b; Dong et al. 2015). At low S or θ , 343 344 solid particle connections are established gradually by water bridges formed in the voids. Considering 345 thermal conductivity of water is greater than of air, these connections facilitate heat conduction in soil 346 thereby increasing the soil λ_{eff} . In contrast, at high S or θ moisture content, solid particles are almost fully connected by water bridges so the soil λ_{eff} grows slightly. Moreover, the influence of water 347 bridges depends on the void volume. Considering w is not as related to the void volume as S and θ , S 348 349 and θ could be indicators that truly and generally influence λ_{eff} . Lu and Dong (2015) further introduced 350 S_f and θ_f , at which the rate of change in thermal conductivity reaches maximum, for predicting soil λ_{eff} . Figure 7 shows the relationship between soil λ_{eff} and S with predicted values from De Vries 351 (1963), Johansen (1977), Côté and Konrad (2005), Lu et al. (2007), Chen (2008), and experimental data 352 353 from Zhang et al. (2015b).



Figure 7 Influence of degree of saturation on soil effective thermal conductivity λ_{eff} with data from De Vries (1963); Johansen (1977); Côté and Konrad (2005); Lu et al. (2007); Chen (2008); Zhang et al. (2015b)

357 2.4.2 Soil temperature

Soil temperature influences the thermal conductivity of soil components, i.e., soil particles, air and water (Kayaci and Demir 2018). Besides, temperature can result in components phase change in soil and thus change the soil effective thermal conductivity (Gori and Corasaniti 2002). For example, under temperature below freezing point, part of fluid water in soil changes into solid ice, whose thermal

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362 conductivity is different from that of fluid water. The effects of temperature ranging from 30 °C to 90 °C 363 are reviewed here. This temperature range is mostly encountered in shallow geothermal engineering, 364 disposal of radioactive waste and thermal remediation of contaminated soils. In general, soil λ_{eff} rises with temperature, and its value at 90 °C is three to five times of that at ambient temperature (Campbell 365 366 et al. 1994). This is attributed to latent heat transfer, caused by evaporation of water in soil voids, under 367 high temperature and pressures different from atmospheric pressure (Liu et al. 2011). Furthermore, soil 368 λ_{eff} increases more noticeably with temperature above 50 °C compared with that ranging from 30 to 50 369 °C (Smits et al. 2013), and temperature effect is negligible below 30 °C (Lu and Ren 2009). Besides, the 370 impact of temperature on λ_{eff} is greater in moist soil than in dry soil, and it is most obvious when the soil degree of saturation is between 22% to 50% (Sepaskhah and Boersma 1979). Figure 8 visualizes 371 372 the influence of temperature on soil λ_{eff} under different volumetric water content.



Figure 8 Influence of temperature on soil effective thermal conductivity λ_{eff} with experimental data selected from (a) quincy sand at different volumetric water content (Campbell et al. 1994) and (b) clay loam at different volumetric water content (Hiraiwa and Kasubuchi 2000)

2.4.3 Soil loading and gradation

379 Soil loading refers to the external forces acting on the soil beside self-weight. Soil loading induces 380 compression thus increases the particle contact area between particles, as well as reducing porosity. 381 Therefore, increasing loading increases the heat conduction process in soil and influences the soil 382 effective thermal conductivity λ_{eff} . The λ_{eff} variation should also be attributed to the stress 383 heterogeneity resulted from soil loading (Vargas and McCarthy 2001). Besides, soil structure (e.g., 384 porosity, density, and particle connectivity) changes under loading, and consequently the soil λ_{eff} 385 changes. In general, soil λ_{eff} is positively correlated to soil loading, and it almost increases linearly with the loadings (Vargas and McCarthy 2001; Weidenfeld et al. 2004). Weidenfeld et al. (2004) studied 386 387 the effective thermal conductivity of particle beds composed of glass/limestone/aluminium etc. and 388 found that λ_{eff} rises with different materials to different extents under compression. This finding should 389 also be applied to soil considering the similarity between the particle beds and soil packings. Moreover, 390 the influence of soil loading on λ_{eff} is negligible when the particle thermal conductivity is as low as 391 less than 1 W/(m·K) (Weidenfeld et al. 2004). Compared with soil with small particle size, the λ_{eff} of 392 that with large particle size is more easily influenced by the loading (Weidenfeld et al. 2004). 393 Furthermore, the dependence of soil λ_{eff} on loading increases with the irregularity of particles because 394 irregularity leads to more sensitive granular skeleton (Yun and Santamarina 2008). Cui et al. (2023) 395 conducted a series of thermal test for soil specimens under loading-unloading conditions and at various 396 degree of saturated. It was found that the change of thermal conductivity with loading-induced stress is 397 more obvious under unsaturated condition compared with that under dry conditions. This effect is 398 because that the addition of water improves soil suction and thus lowers soil compressibility. The

399 influence of stress on λ_{eff} also depends on soil initial compression state: more loose soil tends to be 400 more easily affected by stress. In addition, Xiao et al. (2018) studied the dependence of thermal 401 conductivity on soil gradation, and it was found that thermal conductivity increases with soil uniformity 402 coefficient.

Models for effective thermal conductivity prediction 3

404 After reviewing the influence of various factors on soil effective thermal conductivity λ_{eff} , models integrating those factors for λ_{eff} prediction are summarised in this section. Models for λ_{eff} prediction 406 are mainly classified into three types: theoretical models, empirical models, and machine learning 407 models.

408 Theoretical models are based on conceptual material geometry, and these models assume that different 409 components in soil, i.e., solid, air, and water, are uniformly distributed. Then, the mathematical 410 expressions for λ_{eff} are developed (Wiener 1912; De Vries and Van Wijk 1963; Gori 1983; Tong et al. 2009; Haigh 2012; Johansen 1977). Empirical models are proposed through comparing measured λ_{eff} 411 412 with the value of different influencing factors (e.g., particle thermal conductivity, porosity, moist 413 content). From this comparison, the key empirical coefficients that reveal the relationship between λ_{eff} 414 and various factors can be drawn (Kersten 1949; Johansen 1977; Donazzi et al. 1979; Rao and Singh 415 1999; Balland and Arp 2005; Côté and Konrad 2005; Lu et al. 2007; Chen 2008). Machine learning 416 models are based on trustable data and a learning process, which involve mathematic algorithms to 417 establish the relationship between inputs (influencing factors) and outputs (λ_{eff}) (Grabarczyk and Furmański 2013; Li et al. 2022a). Table 3 summarises the considered factors and features of each model. 418

3.1 Theoretical models 419

420 Wiener (1912) defined the lowest and highest value of λ_{eff} by assuming that different phases in soil are 421 ideally distributed. De Vries and Van Wijk (1963) model is a more complex one compared with Wiener 422 model. It accounts for particle shape effect on λ_{eff} but the related coefficient is not easy to obtain. 423 Johansen (1977) proposed a "geo-mean" model with a succinct mathematical expression. Gori (1983) 424 model focuses on the λ_{eff} under different water distribution regimes and it is complicated to implement. 425 Tong et al. (2009) model was developed from Wiener model. It is a comprehensive one because the 426 effects of pore structure, degree of saturation and temperature are considered. Haigh (2012) model 427 considers water film development (i.e., its width and thickness) when predicting λ_{eff} .

Empirical models 428 3.2

The λ_{eff} of soil with different temperatures, degree of saturation and mineral was measured by Kersten 429 430 (1949), and he proposed two prediction equations for silts (or clay) and sandy soil respectively. In 431 addition to the "geo-mean" model, Johansen (1977) also proposed "normalized thermal conductivity 432 λ_r ", which is expressed as:

$$\lambda_r = \frac{\lambda_{eff} - \lambda_{dry}}{\lambda_{sat} - \lambda_{dry}} \tag{7}$$

where λ_{dry} is thermal conductivity under dry conditions, and λ_{sat} is that under saturated conditions. 433 Johansen developed several relationships between λ_r and degree of saturation S. And λ_r can be used to 434 estimate λ_{eff} by interpolating λ_{sat} and λ_{dry} . This dimensionless coefficient has already involved many 435 436 factors (e.g., soil type, minerology) and thus simplifies the prediction and widens the application range 437 compared with the Kersten (1949) model. Balland and Arp (2005) model has an emphasis on the effect 438 of organic matters on λ_{eff} . Côté and Konrad (2005) updated the λ_r - S relationship by considering soil 439 type effect. Lu et al. (2007) claimed a linear correlation between λ_{eff} and porosity for dry soil. Chen

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440 (2008) model has a good accuracy when predicting λ_{eff} of soil with high quartz contents. Other 441 empirical models include Donazzi et al. (1979) model and Rao and Singh (1999) model.

442 3.3 Machine learning models

443 Machine learning models for λ_{eff} prediction are developed based on a large amount of trustable data 444 regarding influencing factors and λ_{eff} (Wei et al. 2018). Typically, their architecture includes three 445 layers: the input layer for influencing factors, the hidden layers for applying weights to the inputs, as 446 well as the output layers for λ_{eff} . They can provide fast and convenient predictions when validated by 447 trustable data.

448 Wei et al. (2018) used three methods: convolutional neural network (CNN), gaussian process regression 449 (GPR) and support vector regression (SVR), to train available data and develop machine learning 450 models. This work proves that machine learning models can provide accurate prediction. SVR and GPR are machine learning methods for non-linear regression analysis; and estimating porous media λ_{eff} from 451 various factors is a non-linear problem. CNN has been widely applied in face recognition and thus it is 452 453 able to capture the structure information in λ_{eff} prediction. Furthermore, six machine learning 454 algorithms for soil λ_{eff} prediction are investigated in Li et al. (2022b). These algorithms include SVR, 455 GPR, adaptive boosting method (AdaBoost), random forest (RF), decision tree (DT), and multivariance linear regression (MLR). The results show that AdaBoost provides good estimated values with the 456 457 lowest error. Seven algorithms, including GPR, RF, DT, MLR, gradient boosting decision tree (GBDT), 458 k-nearest neighbours (KNN), artificial neural network (ANN) were compared by Zhao et al. (2022) 459 using different databases from Li et al. (2022b). These studies conclude that GPR, DT, and MLR are 460 not the preferred algorithms for soil λ_{eff} prediction. Moreover, ANN was recommended by Zhao et al. 461 (2022). A screen ANN is used to offset the influence of soil database insufficiency, and it utilises back-462 propagation algorithm in the training stage (Zhang et al. 2020). In addition, in order to balance the 463 complexity with the accuracy of the prediction model, this study compares the model performances under different combinations of inputs. Rizvi et al. (2020a) developed an ANN model for unsaturated 464 soil λ_{eff} prediction. Different parameters, including porosity, degree of saturation and quartz content, 465 466 are used as inputs for the model; and the back-propagation algorithm is adopted for calculating the 467 weight values in the ANN hidden layer. The same author also used a ANN based on group method of 468 data handling (GMDH) to predict sand λ_{eff} (Rizvi et al. 2020b). Multilayer perceptron ANN is 469 considered as the optimal one for the prediction of sandstone λ_{eff} (Vaferi et al. 2014). Mesoscale and 470 microscale structures were firstly integrated into the inputs of ANN models in Fei et al. (2021). Inputs 471 in his model consist of particle thermal conductivity, porosity, coordination number, particle roundness 472 and sphericity. In general, machine learning models are able to account for more factors and can be 473 applied to a wide range.

Table 3 Summary of prediction models for soil effective thermal conductivity λ_{eff}

				Factors	involved	in each m	odel								
Model				λ, therm W/(m·K	al conduct	ivity,	ϕ , volum	e fraction		n, poro	sity		S, saturat	ion degree	;
category	Author	Expression	Comments	ρ , dry density, kg/m ³			<i>w</i> , gravimetric moisture			<i>T</i> , temperature, °C			<i>C</i> , coefficient		
				λ_{solid}	λ_{water}	λ_{air}	ϕ_{solid}	ϕ_{water}	ϕ_{air}	n	S	ρ	w	Т	С
Theoretical models	Wiener (1912)	$\lambda_{eff, lower} = \left[\sum_{\lambda_{\alpha}}^{\phi_{\alpha}} \right]^{-1}$ $\lambda_{eff, upper} = \sum \phi_{\alpha} \lambda_{\alpha}$ $\alpha \text{ indicates different phase}$	Determining the upper and lower boundary of λ_{eff} .	V	V	V	V	V							
	De Vries and Van Wijk (1963)	$\lambda_{eff} = \frac{\sum K_{\alpha} \phi_{\alpha} \lambda_{\alpha}}{\sum K_{\alpha} \phi_{\alpha}}$ K_{α} is the ratio of average thermal gradient of each constituent to that of continuous medium in soils	K_{α} is related to particle shape, and position, and it is difficult to be determined.						V						
	Johansen (1977)	$ \begin{aligned} \lambda_{eff} &= \\ \lambda_{solid}^{1-n} \lambda_{water}^{S} \lambda_{air}^{(1-S)n} \end{aligned} $	Developed from Wiener model (1912).	V	V	V				V					
	Gori (1983)	Recommend referring to the literature. This model considers: 1) soil absorbed water content, 2) soil permanent wilting point, 3) soil field capacity.	Uncertainties exist in parameters used in this model.												

Model				λ , therm W/(m·K	nal conduc	tivity,	ϕ , volum	ne fraction		n, poro	sity		<i>S</i> , satura	tion degre	æ
category	Author	Expression	Comments	ρ , dry d kg/m ³	lensity,	-	<i>w</i> , gravimetric moisture			<i>T</i> , temperature, °C			C, coefficient		
				λ_{solid}	λ_{water}	λ_{air}	ϕ_{solid}	ϕ_{water}	ϕ_{air}	n	S	ρ	W	T	
	Tong et al. (2009)	$\begin{split} \lambda_{eff} &= \\ \eta_1 (1-n) \lambda_{solid} + \\ (1-\eta_2) \\ & [1-\eta_1 (1-n)]^2 \\ & [\frac{(1-n)(1-\eta_1)}{\lambda_{solid}} + \frac{nS}{\lambda_{water}} + \\ & + \eta_2 \\ & [(1-n)(1-\eta_1) \lambda_{solid}] \end{split}$	Coefficients η_1 , η_2 relates to pore structure, saturation degree and temperature, which are difficult to be determined.	V	Ø	Ø				Ø	Ø			Ø	٤
	Haigh (2012)	 Recommend referring to the literature. 1) Based on 2D soil contact cell unit, 2) Water film formation is considered, 3) Applicable for <i>n</i> > 0.33. 	Involved coefficients are related to the thickness of water film, <i>S</i> and the width of water film, resulting in inconvenient implementation.	V	V	V					V				5
Empirical models	Kersten (1949)	$\lambda_{eff} = 0.144[0.9]$ log $w - 0.2]10^{1.6\rho}$, for silts or clay $\lambda_{eff} = 0.144[0.7]$ log $w + 0.4] \times 10^{1.6\rho}$, for sandy soils	The applicable range of <i>w</i> is limited.										V		

				Factors involved in each model											
Model				λ, therm W/(m·K	al conduct	tivity,	ϕ , volum	ne fraction		n, poro	sity		tion degree	e	
category	Author	Expression	Comments	ρ , dry density, kg/m ³			<i>w</i> , gravimetric moisture			<i>T</i> , temperature, °C			C, coefficient		
				λ_{solid}	λ_{water}	λ_{air}	$\phi_{\it solid}$	ϕ_{water}	ϕ_{air}	n	S	ρ	W	Т	С
	Johansen (1977)	$\lambda_{eff} = \lambda_r (\lambda_{sat} - \lambda_{dry}) + \lambda_{dry}$ $\lambda_r \text{ is the normalized thermal conductivity}$ $\lambda_{sat} \text{ is the saturated thermal conductivity}$ $\lambda_{dry} \text{ is the dry thermal conductivity}$	 Proposing the concept of λ_r, Obtaining λ_r by λ_r ~ S correlation, Obtaining λ_{dry}, λ_{dry} by his theoretical model. 	Ŋ	Ŋ					V	Ø	V			
	Donazzi et al. (1979)	$\lambda_{eff} = \lambda_{water}^{n} \lambda_{solid}^{1-n} \\ \exp\left[-3.08n(1-S)^{2}\right]$	Easy to implement with no coefficients.	V	V					V					
	Rao and Singh (1999)	$\lambda_{eff} = 10^{1.6\rho}$ (1.07log w + a) a is the coefficient	The coefficient is related to soils type. And $w \ge 10\%$ for clay and silts $w \ge 1\%$ for sands.									V	V		
	Balland and Arp (2005)	Recommend referring to the literature.	Predicting λ_{eff} through a proposed $\lambda_r \sim S$ relationship.	V		V					V				V

Model				Factors λ , therm $W/(m \cdot K)$	al conduct	in each n tivity,	ϕ , volum	ne fraction		n, poro	sity		<i>S</i> , satura	tion degre	e
category	Author	Expression	Comments	ρ , dry density, kg/m ³			<i>w</i> , gravimetric moisture			<i>T</i> , temperature, °C			C, coefficient		
				λ_{solid}	λ_{water}	λ_{air}	ϕ_{solid}	ϕ_{water}	ϕ_{air}	n	S	ρ	w	Т	С
	Côté and Konrad (2005)	$\lambda_{eff} = (\lambda_{water}^n \lambda_{solid}^{1-n} - a 10^{-bn})$ $\left[\frac{cS}{1+(c-1)S}\right] + a$ 10^{-bn} $a, b, c \text{ are empirical coefficients}$	Developing λ_r $\sim S$ correlation as $\lambda_r = \frac{cS}{1 + (c-1)S}$.	V	V					Ø	V				V
	Lu et al. (2007)	$\lambda_{eff} = \begin{bmatrix} \lambda_{water}^n \lambda_{solid}^{1-n} - (b - an) \\ \times \\ \exp \left[c(1 - S^{c-1.33}) \right] \\ + (b - an), a, b, c \\ \text{are coefficients} \end{bmatrix}$	The coefficients are related to the dry soil thermal conductivity and soil type.	V						Ŋ	V				
	Chen (2008)	$\lambda_{eff} = \lambda_{water}^{n} \lambda_{solid}^{1-n} \\ [(1-a)S + a]^{bn}, \\ a, b \text{ are coefficients}$	This model has high accuracy for high quartz content soil. The coefficients are related to soil type.	V	V					V	V				V
Machine	Rizvi et al. (2020a)	ANN algorithm	Only for unsaturated soil.							Ø	\checkmark				
learning models	Zhang et al. (2020)	ANN algorithm	Performances using different inputs are compared.								Ø	V			
				© The	Author(s)	or their In	stitution(s)	I							

				Factors involved in each model												
Model				λ , thermal conductivity, W/(m·K)		ϕ , volume fraction			n, poro	sity		<i>S</i> , saturation degree				
category	Author	Expression	Comments	ρ , dry d kg/m ³	ensity,		w, gravir	netric moi	sture	T, temp ℃	erature,	<i>C</i> , coeffic		coefficient		
				λ_{solid}	λ_{water}	λ_{air}	ϕ_{solid}	ϕ_{water}	ϕ_{air}	n	S	ρ	W	Т	С	
	Fei et al. (2021)	ANN algorithm	Mesoscale and microscale structure factors are considered.							V						
	Li et al. (2022b)	Six algorithms performance are compared	Adaptive boosting methods are recommended				Ø			V						
	Zhao et al. (2022)	Seven algorithms performance are compared	Neural networks are recommended							V						

476 **4** Research gaps and a methodological framework for futures studies 477 Based on the review regarding the factors influencing soil λ_{eff} and the models for the λ_{eff} prediction, 478 a holistic view of research gaps is given, followed by detailed explanations. Then, a methodological 479 framework for future studies is proposed.

480 In addition to the intrinsic properties of soil, its structure is an underlying factor that influences thermal 481 conductivity, as it determines the structure of heat transfer pathways. Other factors, such as water 482 content and gradation, also affect thermal conductivity by creating new structures for heat transfer 483 pathways. Previous research has investigated the impact of soil structure on thermal conductivity in dry 484 conditions; however, in unsaturated conditions, the addition of water connects soil particles, resulting 485 in a different soil structure. Lu and McCartney (2024) and Lu and Dong (2015) have linked the different 486 mechanisms of water retention to thermal conductivity. However, the altered heat transfer pathways 487 due to the addition of water, which are underlying reasons contributing to an increase in thermal 488 conductivity, remain an unexplored area of research. Furthermore, existing research on soil thermal 489 conductivity has effectively utilised complex network theory to quantify soil structure, establishing 490 correlations between network-derived features and thermal conductivity in dry conditions. This 491 innovative approach marks a significant advancement in understanding soil behaviour. However, 492 complex network theory alone may not fully capture the soil structure under unsaturated conditions 493 where the structure undergoes notable changes due to water addition. In this light, the potential of other 494 structural quantification methods should be explored. The alternative methods discussed below offer 495 diverse perspectives on soil structure quantification, yet their parameters have not been investigated in 496 relation to soil thermal conductivity.

Euler number is a topological invariant, and it is expressed as (Herring 2012; Herring et al. 2013;
Herring et al. 2019)

$$\chi = \beta_0 - \beta_1 + \beta_2 \tag{8}$$

499 where χ is the Euler number; β_0 is the zeroth Betti number, representing the number of discrete elements in the volume; β_1 is the first Betti number, indicating the number of redundant loops in the structure; 500 and β_2 is the second Betti number, referring to the number of cavities. Herring et al. (2013) used it to 501 502 quantify the connectivity of nonwetting phase in porous media. However, the connectivity of soil pores 503 that are based on Euler number has not been studied from the perspective of λ_{eff} . In addition, statistical approaches are also favourable to the description of soil structures. Minkowski functions are geometric 504 505 measurements that can quantify the soil structure statistically based on computed tomography images 506 of soil (Vogel et al. 2010). Specifically, the zeroth Minkowski function indicates total mass of the studied object (pore or solid); the first Minkowski function represents the interfacial area between pore 507 508 and solid; the second is the interface's mean curvature; the third measures the total curvature (Vogel et 509 al. 2010). The underlying theorem for using Minkowski functions to quantify the soil structure is 510 proposed by Hadwiger (2013); he claimed that any properties, related only to the object's form, can be 511 expressed by a combination of Minkowski functions. However, the relationship between Minkowski 512 functions and soil λ_{eff} has not been researched. Furthermore, the particle or pore connectivity does not 513 consider the local geometries (e.g., shape and size) of individual particles or pores; similarly, the local 514 geometries (e.g., shape and size) do not include global information (e.g., particle or pore connectivity). 515 But the soil λ_{eff} depends on both the global and local geometries. Persistent homology analysis can measure the global and local characteristic simultaneously (Herring et al. 2019). Therefore, parameters derived from persistent homology analysis could contribute to the comprehensive understanding of soil the λ_{eff} ; whereas they have not been studied from heat transfer aspect. A parameter describing the extent of the transition from disorder to order in a granular system is proposed by Dai et al. (2019), which could also be introduced to soil structures quantification.

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521 As previously pointed out, it is essential to quantify soil structure not only in dry conditions but also 522 under unsaturated conditions to better understand the relationship between structural quantification and 523 thermal conductivity. The goal of this endeavour is to include structural quantifications for thermal 524 conductivity prediction. However, it is crucial to recognise that soil thermal conductivity is also 525 influenced by other factors at various scales in addition to structural quantifications (Table 1). Therefore, a comprehensive framework that considers those additional factors presented in Table 1 is necessary 526 527 for accurate prediction of thermal conductivity. Current models for predicting soil thermal conductivity 528 fall short in this regard, as they do not fully account for all influencing factors, particularly the varied 529 structure of unsaturated soils. The application of machine learning presents a promising avenue for 530 developing a more integrative model (Fei et al. 2021). Current machine learning-based models in this 531 field, however, have not yet fully incorporated soil structure data from both dry and unsaturated 532 conditions as inputs. This limitation underscores the need for an updated machine learning framework 533 that is designed to process and learn from a comprehensive set of inputs. By integrating detailed 534 structural data from varying soil conditions along with other relevant factors at different scales, a 535 framework is proposed in Figure 9, which could advance our capability to predict soil thermal 536 conductivity with higher accuracy and relevance to real-world scenarios.





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Figure 9 Framework of investigation on unsaturated soil effective thermal conductivity through multiscale characters; tools for each stage could be: 1) computed tomography imaging equipment; 2) software including ImageJ, Simpleware ScanIP; 3) network approaches or statistical methods; 4) finite element modelling and experimental measurements and 5) Python.

542 Firstly, modern computed tomography devices are employed to scan real soil samples (dry/unsaturated) 543 and produce high resolution 3D image stacks. Afterwards, these images are used to reconstruct the 3D 544 samples digitally by image process tools. The reconstructed 3D models serve as the foundation for both 545 structural quantification and heat transfer processes modelling. The structural quantification relies on 551

network approaches or statistical methods. Meanwhile, Finite Element Modelling (FEM) is adopted to simulate heat transfer processes to compute λ_{eff} , which will be further validated by measurements. Machine learning techniques are employed to discern the relationship between thermal conductivity and a combination of structural parameters and other traditional factors at multiple scales, including but not limited to solid particle thermal conductivity, porosity, and degree of saturation.

5 Conclusion

552 In this review, we systematically examined the various factors influencing soil thermal conductivity. 553 Our findings highlight that soil structure impacts thermal conductivity significantly, but this area of 554 research remains relatively unexplored due to the lack of characterising particle connectivity. A 555 relationship between thermal conductivity and soil structure has been previously studied under dry 556 conditions through the application of complex network theory for structural quantification. However, 557 soil structure that undergoes notable changes due to the addition of water under unsaturated conditions 558 has not been well characterised. Given the increased complexity of soil structure in unsaturated 559 conditions compared to dry conditions, relying solely on complex network theory might be insufficient 560 to capture the complete structural information. Consequently, we have explored other potential methods 561 for a more comprehensive quantification of soil structure.

562 Furthermore, it is crucial to recognize that soil thermal conductivity is influenced not just by structural 563 factors but also by a range of other variables. Our investigation reveals that current models for predicting 564 soil thermal conductivity fall short of incorporating the full spectrum of influencing factors. To bridge 565 this gap, we proposed a new integrative framework that considers both structural parameters and other 566 relevant factors across different scales. This framework employs soil computed tomography (CT) 567 images. These images offer a robust physical basis for an accurate description of soil structures based 568 on quantification methods. Moreover, the framework integrates machine learning approaches, 569 capitalising on their ability to assimilate a multitude of factors as inputs when predicting effective 570 thermal conductivity. Machine learning's inherent strength in pattern recognition and data integration 571 makes it particularly suited for this task. By combining the detailed structural data with other relevant 572 factors, our framework aims to enhance the accuracy and applicability of predictive models, offering a 573 more holistic understanding of soil thermal conductivity.

574 CrediT authorship contribution statement

575 Tairu Chen: Conceptualization, Data curation, Methodology, Formal analysis, Writing – original draft;
576 Writing – review & editing., Wenbin Fei: Methodology, Writing – review & editing, Supervision.,
577 Guillermo A. Narsilio: Writing – review & editing, Supervision, Project administration, Funding
578 acquisition.

579 Declaration of Competing Interest

580 The authors declare that they have no known competing financial interests or personal relationships that 581 could have appeared to influence the work reported in this paper.

582 Acknowledgements

583 The authors acknowledge the funding provided by the Australian Research Council project 584 DP210100433 and China Scholarship Council (CSC)-University of Melbourne Scholarship provided 585 by the CSC and The University of Melbourne.

586 Data Availability

587 Data generated or analysed during this study are available from the corresponding author upon 588 reasonable request.

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