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How Can We Exploit DEM to Advance Understanding of Thermal Conduction in Granular Materials?

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ABSTRACT

Estimating the effective thermal conductivity (ETC) of granular materials is important in various engineering disciplines. The ETC of a granular material is not unique, rather it depends upon the material's packing characteristics, i.e. porosity and coordination number. Directly measuring the ETC of granular materials with a particular packing density and subjected to specific stress conditions is experimentally challenging. There is a need to develop reliable, indirect experimental methods to measure the ETC of granular materials. Here we explore the possibility of linking the ETC of granular materials to their elastic moduli. This study used a thermal pipe network model implemented in a Discrete Element Method (DEM) code to generate ETC data for ideal, virtual two-phase granular samples with stagnant pore fluid. Parametric studies considered the sensitivity of the ETC to the sample packing. Data from small deformation probes were used to explore links between the samples' elastic moduli and their ETCs. The results provide a theoretical background for the development of an indirect experimental method to predict the ETC or trends in the variation in the ETC by considering stiffness data which are relatively straightforward to acquire. The study

shows how DEM can be used as a sophisticated thought experiment to explore novel ideas for developing experimental procedures.

INTRODUCTION

Granular materials are encountered in a number of engineering fields and subjected to temperature changes in a variety of situations. Such temperature changes can be applied artificially, for example, to enhance chemical reactions of powders, process food grains, store thermal energy in packed beds, or exploit heat from soils for geothermal heat pumps. Chemical or nuclear reactions can lead to a change in the temperature of granular materials (e.g. hydration of cement; pebble bed reactors). Climate-induced temperature changes include the seasonal temperature changes experienced by food grains in silos. In all cases, understanding the effective thermal conductivity (ETC) of the granular materials considered is important to effectively run facilities and manage processes or to avoid significant failure of structures.

Both experimental and numerical studies have shown that the ETC of granular materials is affected by various factors. The experimental studies by Yun and Santamarina (2008) showed that the contact area and the particle stresses have a measurable effect on the ETC of granular materials. The ETC of a granular material is not always isotropic; for example, the experimental studies presented in Garrett and Ban (2011) demonstrated that the ETC can develop a significant directional dependency under anisotropic stress conditions. A numerical study by El Shamy et al. (2013) also suggested that the mean coordination number and the anisotropy of the contact normal orientations affect the ETC, however these parameters cannot easily be measured in experiments. Thus, in order to estimate the ETC of a granular material, all of these factors need to be accounted for. However none of the available theoretical models, which are summarised in van Antwerpen et al. (2010), can effectively include the effects of all of these factors.

On the other hand, the direct measurement of the ETC of granular materials is technically challenging, as it requires specific and often expensive temperature controlled devices. In particular, experimental systems that can measure accurately the response to changes in temperature while allowing control of the packing and stress state of granular materials remain very rare. This is due to the difficulties associated with the concurrent application of thermal and mechanical loads and also to the detrimental effects of changes in temperature on the accuracy of the equipment required

to measure the sample deformations.

Motivated by the observations presented above, this study explores the possibility of indirectly determining the ETC of granular materials by relating it to the small-strain elastic moduli of granular materials, which are also determined by the material packing characteristics and which can be more easily measured experimentally. This study employed both analytical and numerical models. The concept of using a network model to determine thermal conductivity underpins both models and so this is firstly outlined. In the analytical model Effective Medium Theory is used to express the elastic moduli of a granular material as a function of its basic packing characteristics (coordination number, contact radius, and void ratio). Then, a relationship between the ETC and the packing characteristics is formulated assuming a uniform temperature gradient within a granular medium. Comparing the expressions for the ETC and the Young's modulus of a granular medium, a relationship between these two properties is proposed. Complementary numerical analyses employed the Discrete Element Method (Cundall and Strack 1979) to create samples with differing void ratios, coordination numbers and contact normal anisotropies. Small deformation probes were simulated to measure the elastic moduli and heat pipe network simulations were conducted. These data confirmed the viability of the relationship developed analytically. Using the analytical model and the DEM results, a simple method to estimate the ETC of granular samples using the Young's modulus and the void ratio of a granular material is proposed and its predictive potential is demonstrated using the DEM-generated data.

PIPE-NETWORK MODEL TO SIMULATE HEAT TRANSFER

Heat Transfer Mechanisms within Granular Materials

As detailed in previous studies (e.g. Yagi and Kunii 1957; Yun and Santamarina 2008), various heat transfer mechanisms take place within a granular material. In this study, we focus on granular media with stagnant fluid under a moderate temperature (< 450 K), where heat transfer via radiation and convection is negligible. Referring to Fig. 1, under these conditions heat is transferred via conduction through the solid particles, conduction through the area of contact areas, and conduction through the gap fluid. Data presented in Cheng et al. (1999) demonstrated the importance of particle-

fluid-particle conduction; this accounts for approximately 50 % of the heat transfer even for a very high κ value of 1000, where $\kappa = \frac{k_s}{k_f}$, k_s is the thermal conductivity of the solid particles, and k_f is the thermal conductivity of the pore fluid. The "effective thermal conductivity" of a granular material is the macro-scale thermal conductivity of the material including the solid particles and the void space. Convective and radiative terms are not included in the effective thermal conductivity. The term is common in previous studies (e.g. Cheng et al. 1999; Dai et al. 2019).

Heat pipe network model

Heat conduction within an isotropic continuum material can be described by Fourier's law:

$$\mathbf{q} = -\mathbf{k}\nabla T \quad \text{or} \quad q_i = -k_{i1}\frac{\partial T}{\partial x_1} - k_{i2}\frac{\partial T}{\partial x_2} - k_{i3}\frac{\partial T}{\partial x_3} \equiv -k_{ij}\frac{\partial T}{\partial x_j} \tag{1}$$

where $\mathbf{q}$ is the heat flux vector through a unit area, $\mathbf{k}$ is the thermal conductivity matrix, and ∇T is the temperature gradient. Adopting the one-dimensional form of Eq. 1, the heat conduction through an element of a material with a cross-sectional area $A_{continuum}$ and a length $L_{continuum}$ can be described as:

$$\dot{Q} = qA_{continuum} = -kA_{continuum}\frac{\Delta T}{L_{continuum}} = C\Delta T \tag{2}$$

where $\dot{Q}$ is the amount of heat transferred per unit time, the thermal conductance, C, is equivalent to $kA_{continuum}/L_{continuum}$, and ΔT is the temperature difference across the element. When a granular material is considered within a continuum framework, k in Eq. 2 is the Effective Thermal Conductivity (ETC).

The prevailing approach in particle-scale simulations of heat transfer in granular materials is to apply Fourier's law using a heat pipe network model (Vargas and McCarthy 2001; Feng et al. 2009; Yun and Evans 2010). A schematic illustration of one element within a heat pipe network model is shown in Fig. 2. In this modelling approach, each particle is assumed to be isothermal, with a heat core whose temperature represents the particle's temperature. If two particles, $p1$ and $p2$, are in contact or sufficiently close to each other, a heat pipe is created between these particles. Then the amount of heat moving from particle $p1$ to particle $p2$ per unit time ($\dot{Q}_{p1p2}$) is calculated

following Eq. 2:

$$\dot{Q}_{p1p2} = -C^*_{p1p2}\left(T_{p1} - T_{p2}\right) \tag{3}$$

where C^*_{p1p2} is the effective thermal conductance of the heat pipe calculated from the thermal conductance of the particles $p1$ and $p2$ that define the heat pipe (C_{p1} and C_{p2}) and the thermal conductance of the contact region (C_c) as:

$$C^*_{p1p2} = \left(\frac{1}{C_{p1}} + \frac{1}{C_c} + \frac{1}{C_{p2}}\right)^{-1} \tag{4}$$

The amount of heat ($Q^{(\Delta t)}_{p1}$) received by a particle p during a time increment Δt is calculated as:

$$Q^{(\Delta t)}_{p1} = \sum_{p2=1}^{N_c^{(p1)}} \dot{Q}_{p1p2}\Delta t \tag{5}$$

where $N_c^{(p1)}$ is the number of the contacts involving particle $p1$. The increment in the temperature of particle $p1$ ($\Delta T^{(\Delta t)}_{p1}$) is then calculated as:

$$\Delta T^{(\Delta t)}_{p1} = \frac{Q_{p1}}{c_{p1}m_{p1}} \tag{6}$$

where c_{p1} and m_{p1} are the specific heat capacity and the mass of the particle $p1$, respectively.

Batchelor and O'Brien (BOB) model

An appropriate model for the effective thermal conductance of heat pipes (Eq. 4) needs to be selected to simulate heat transfer within a granular medium. As discussed above, consideration of particle-fluid-particle conduction is important. Batchelor and O'Brien (1977) conducted an analytical study of heat conduction through two particles considering the fluid in the gap between the two particles just adjacent to the contact point (Fig. 1). Referring to Fig. 3, they modelled the thermal conductance as a function of the contact radius, r_c, if the two particles are contacting, and as a function of the gap distance, h, if the two particles are separated. Kanuparthi et al. (2008) and Yun and Evans (2010) implemented this model in their heat pipe network models, and obtained

good agreement with experimental results. Dai et al. (2019) conducted particle-scale FEM analysis varying the thermal conductivity ratio, κ, and confirmed the excellent agreement between the FEM results and a modified version of the original Batchelor and O'Brien (BOB) model for a wide range of κ values (4 to 1000). In addition, Yun and Evans (2010) and Dai et al. (2019) demonstrated that a pipe-network model employing the BOB model agrees very well with experimental data for various solid-fluid combinations under different stress levels (glass-air, glass-water, sand-air, sand-water, and steel-air). A brief summary of the modified BOB model proposed in Dai et al. (2019) as implemented for the current study is provided in the Appendix II.

ANALYTICAL MODELLING

Use of Effective Medium Theory (EMT) to Determine Elastic Moduli

In granular physics/granular mechanics, a number of attempts have been made to predict the elastic moduli of granular materials theoretically. Chang and Liao (1994) calculated the elastic moduli of a granular medium from the material properties of the particles, the packing characteristics, and the stresses, assuming that a uniform strain field applies in a granular medium when the granular medium deforms (*kinematic assumption*). The packing characteristics can be expressed in terms of the void ratio (e), i.e. the ratio of the void volume (V_v) to the solid volume (V_s):

$$e = \frac{V_v}{V_s} \tag{7}$$

The mean coordination number ($\overline{Z}$) is a particle-scale measure to quantify the overall sample packing density. The coordination number (Z) of a single particle is the number of the contacts involving that particle:

$$\overline{Z} = \frac{2N_c}{N_p} \tag{8}$$

Where N_c is the number of contacts and N_p is the number of particles. Considering the case of an isotropic granular medium subject to an isotropic stress condition and a simplified Hertz-Mindlin contact model and applying a no-slip condition, Otsubo (2016) adopted the kinematic assumption proposed by Chang and Liao (1994) and expressed the Young's modulus of a granular material as

a function of e and $\overline{Z}$:

$$E = \frac{2\left(5-4\nu_p\right)}{5-3\nu_p}\left[\frac{\sqrt{3}}{\sqrt{2}\pi(1-\nu_p)}\right]^{2/3} G_p^{2/3}\left[\frac{\overline{Z}}{1+e}\right]^{2/3}\sigma_{iso}^{1/3} \equiv N_E\left[\frac{\overline{Z}}{1+e}\right]^{2/3}\sigma_{iso}^{1/3} \tag{9}$$

where the term N_E depends upon the material properties of the particles:

$$N_E \equiv \frac{2\left(5-4\nu_p\right)}{5-3\nu_p}\left[\frac{\sqrt{3}}{\sqrt{2}\pi(1-\nu_p)}\right]^{2/3} G_p^{2/3} \tag{10}$$

EMT predicts that the parameter m_σ should be $1/3$; however, experimental data have repeatedly shown that m_σ is higher than $1/3$ (Hoque and Tatsuoka 1998; Kuwano and Jardine 2002). The higher value of m_σ observed experimentally is attributed to the surface roughness and the shape of the particles (Goddard 1990; Yimsiri and Soga 2000; Otsubo and O'Sullivan 2018). Some studies (Makse et al. 1999; La Ragione and Magnanimo 2012; Khalili et al. 2017) showed that EMT over-predicts the moduli of granular media; however, La Ragione and Magnanimo (2012) showed that the EMT prediction of the ratio of a modulus to a reference modulus is reasonably accurate.

Here we discuss the method to calculate key contact parameters, namely the mean contact radius and the mean coordination number, from E and σ_{iso} exploiting EMT. Following Chang et al. (1989), an expression can be derived to relate an isotropic stress, σ_{iso}, to the ratio of the mean contact radius, $\overline{r_c}$ (calculated from Eq. A.6), to the particle radius, r:

$$\sigma_{iso} = \frac{2}{3\pi}\frac{G_p}{1-\nu_p}\frac{\overline{Z}}{1+e}\left(\frac{\overline{r_c}}{r}\right)^3 \equiv N_\sigma\frac{\overline{Z}}{1+e}\left(\frac{\overline{r_c}}{r}\right)^3 \tag{11}$$

Using Eq. 11, Eq. 9 can be rewritten in terms of $\frac{\overline{r_c}}{r}$ as:

$$E = \frac{2\left(5-4\nu_p\right)}{5-3\nu_p}\left[\frac{G_p}{\pi\left(1-\nu_p\right)}\right]\left[\frac{\overline{Z}}{1+e}\right]\left(\frac{\overline{r_c}}{r}\right) \equiv N'_E\left[\frac{\overline{Z}}{1+e}\right]\left(\frac{\overline{r_c}}{r}\right) \tag{12}$$

From Eq. 11 and Eq. 12, $\frac{\overline{r_c}}{r}$ and $\frac{\overline{Z}}{1+e}$ can be expressed in terms of σ_{iso} and E:

$$\frac{\overline{r_c}}{r} = \left(\frac{N'_E}{N_\sigma}\right)^{0.5} \left(\frac{\sigma_{iso}}{E}\right)^{0.5} \tag{13}$$

$$\frac{\overline{Z}}{1+e} = \frac{N_\sigma^{0.5}}{N'^{1.5}_E} \frac{E^{1.5}}{\sigma_{iso}^{0.5}} \tag{14}$$

Eq. 13 and Eq. 14 thus give expressions for the mean contact radius and the packing density ($\overline{Z}$ and e) in terms of the elastic moduli and the current stress level.

Relationship between the ETC and Packing Characteristics and Elastic Moduli

Itasca Consulting Group (2007) and El Shamy et al. (2013) calculated the effective thermal conductivity tensor (k^*_{ij}) of a granular sample from the effective thermal conductance of heat pipes in the sample assuming that the temperature gradient within the granular sample is uniform as:

$$k^*_{ij} = \frac{1}{V} \sum_{hp=1}^{N_{hp}} C^{*hp} \left[l^{hp}\right]^2 n_i^{hp} n_j^{hp} \tag{15}$$

where V is the sample volume, N_{hp} is the number of the heat pipes in the sample, and C^{*hp}, l^{hp}, and $\mathbf{n^{hp}}$ are the effective thermal conductance, the length, and the unit vector describing the orientation of heat pipe hp, respectively.

In a heat pipe network model that adopts the BOB model, there are two types of heat pipes (type 1 for contacting particles and type 2 for to separated particles), and so Eq. 15 can be rewritten as:

$$k^*_{ij} = \frac{1}{V} \sum_{c}^{N_c} C^{*(c)} \left[l^{(c)}\right]^2 n_i^{(c)} n_j^{(c)} + \frac{1}{V} \sum_{hp,s=1}^{N_{hp,s}} C^{*hp,s} \left[l^{hp,s}\right]^2 n_i^{hp,s} n_j^{hp,s} \equiv k_{ij}^{c*} + k_{ij}^{s*} \tag{16}$$

where hp, s is a heat pipe between two non-contacting (separated) particles, and the number of these heat pipes is $N_{hp,s}$. The unit vectors $\mathbf{n}^c$ and $\mathbf{n}^{hp,s}$ give the contact normal orientations and the orientation of the heat pipes between separated particles, respectively. As shown in Eq. 16, the number and the length of the heat pipes between the contacting particles are identical to the number of the contacts and the length of the branch vectors that join the centroids of contacting particles.

Assuming that the sample consists of monodisperse spheres and is isotropic:

$$k_{ij}^{c*} \approx \frac{4r^2\overline{C^{*(c)}}}{V}\sum_{c}^{N_c} n_i^{(c)} n_j^{(c)} = \frac{4r^2\overline{C^{*(c)}}}{V}\frac{\overline{Z}N_p}{2}\frac{1}{3}\delta_{ij} \tag{17}$$

where δ_{ij} is the Kronecker delta. The sample volume V can be expressed in terms of the void ratio e:

$$V = \frac{4}{3}\pi r^3 N_p (1+e) \tag{18}$$

Using the BOB model and substituting Eq. A.4 and Eq. A.10 into Eq. 4

$$\overline{C^{*(c)}} \approx \frac{\pi k_f r \chi^2 \kappa \left(\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right) + \ln\kappa^2\right)}{2\left(\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right) + \ln\kappa^2 + \frac{1}{2}\chi^2\kappa\right)} \tag{19}$$

where $\overline{C^{*(c)}}$ is assumed to be the $C^{*(c)}$ value for the mean $\beta\left(=\kappa\frac{r_c}{r}\right)$ value of all the contacts. Substituting Eq. 18 and Eq. 19 into Eq. 17,

$$k_{ij}^{c*} \approx \frac{1}{2}\frac{\overline{Z}}{1+e}\frac{k_f\chi^2\kappa\left(\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right) + \ln\kappa^2\right)}{2\left(\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right) + \ln\kappa^2 + \frac{1}{2}\chi^2\kappa\right)}\delta_{ij} \tag{20}$$

The magnitude of the combined term $\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right)$ depends on κ and $\overline{r_c}/r$. $\overline{r_c}/r$ can be calculated from Eq. 11, provided that $\overline{Z}$, e and σ_{iso}/N_σ are known. According to Song et al. (2008), $0.58 < e < 0.82$ and $4 < \overline{Z} < 6$ for monodisperse spheres. In the case of samples with $\kappa < 500$ and $\sigma_{iso}/N_\sigma < 1.29\times10^{-4}$, the combined term $\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right)$ is small compared to the term $\ln\kappa^2 + \frac{1}{2}\chi^2\kappa$ (at most 20%); thus, the combined term $\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right)$ in the denominator can be omitted from Eq. 20 to give:

$$k_{ij}^{c*} \approx \frac{1}{2}\frac{\overline{Z}}{1+e}\frac{k_f\chi^2\kappa\left(\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right)\right)}{2\left(\ln\kappa^2 + \frac{1}{2}\chi^2\kappa\right)}\delta_{ij} + \frac{1}{2}\frac{\overline{Z}}{1+e}\frac{k_f\chi^2\kappa\ln\kappa^2}{2\left(\ln\kappa^2 + \frac{1}{2}\chi^2\kappa\right)}\delta_{ij} \equiv k_{ij}^{\beta*} + k_{ij}^{(h=0)*} \tag{21}$$

The first term is the contribution to k_{ij}^* that depends on β (defined in Eq. A.5) and the second term

is denoted as $k_{ij}^{(h=0)*}$ because the term $\ln \kappa^2$ in the BOB model comes from the analytical result with a gap distance $h \to 0$.

When $\beta \ll 1$, the term $\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right)$ is proportional to β^2, which indicates:

$$k_{ij}^{\beta*} \propto \frac{\overline{Z}}{1+e}\left(\frac{\overline{r_c}}{r}\right)^2 \tag{22}$$

Referring to Eq. 13 and Eq. 14:

$$\frac{\overline{Z}}{1+e}\left(\frac{\overline{r_c}}{r}\right)^2 = \frac{1}{N'^{0.5}_E N^{0.5}_\sigma} E^{0.5}\sigma^{0.5}_{iso} \tag{23}$$

and so we can state that

$$k_{ij}^{\beta*} \propto E^{0.5}\sigma^{0.5}_{iso} \quad (\overline{\beta} \ll 1) \tag{24}$$

Using linear interpolation (see Eqns. A.7 and A.8 in Appendix. II) for $\beta > 1$:

$$\mathcal{H}_c\left(\beta\right) + \Delta\mathcal{H}_f\left(\beta\right) = 0.549\beta - 0.379 \tag{25}$$

When $0.549\overline{\beta}$ is sufficiently larger than 0.379, $k_{ij}^{\beta*}$ is proportional to $\overline{\beta}$; thus,

$$k_{ij}^{\beta*} \propto \frac{\overline{Z}}{1+e}\frac{\overline{r_c}}{r} \propto E \quad (0.549\overline{\beta} \gg 0.379) \tag{26}$$

and so the dependency on σ_{iso} is removed.

When $\mathcal{H}_c\left(\overline{\beta}\right) + \Delta\mathcal{H}_f\left(\overline{\beta}\right) \ll \ln\kappa^2 + \frac{1}{2}\chi^2\kappa$, the remaining terms k_{ij}^{s*} and $k_{ij}^{(h=0)*}$ are independent of the contact radius, and dependent on the distribution of h values for the sample. Thus, these components are denoted as:

$$k_{ij}^{s*} + k_{ij}^{(h=0)*} \equiv k_{ij}^{h*} \tag{27}$$

In denser systems, a larger number of small h values are expected. Thus, we predict that the term k_{ij}^{h*} has a correlation with e, which is explored using simulation results later.

To sum up with, the ETC of a granular medium (k^*_{ij}) can be divided in two components as

$$k^*_{ij} = k^{\beta*}_{ij} + k^{h*}_{ij} \tag{28}$$

with the EMT-based analysis presented here indicates that $k^{\beta*}_{ij}$ can be correlated with E and σ_{iso} and that k^{h*}_{ij} can be correlated with e.

There are a number of assumptions inherent to this proposition and so a numerical exploration of these correlations is needed to explore their applicability.

NUMERICAL MODELLING USING DEM

Sample Generation Using the Discrete Element Method (DEM)

Samples with various packing densities and confining stresses were created using the Discrete Element Method (DEM). A modified version of LAMMPS (Plimpton 1995), an open-source DEM software, was used. A simplified Hertz-Mindlin contact model was employed. The particle size distribution was relatively uniform, having a coefficient of uniformity D_{60}/D_{10} of 1.1 (60% of particles by volume have a particle diameter less than D_{60} and 10% of particles by volume have a particle diameter smaller than D_{10}). To apply constant temperature boundaries in the heat transfer simulations, the samples were enclosed by three pairs of smooth rigid walls; each pair of walls was orthogonal to one of the three Cartesian (x,y,z) axes. Detailed simulation parameters are presented in Table 1. In most cases the samples comprised 21,217 particles; a limited number of additional simulations were completed including 41,444 particles to confirm the results were independent of sample size.

Four sets of samples were produced as described below so that different levels of sample anisotropy could be considered. The anisotropy was quantified using the the second order fabric tensor (F_{ij}) based on the contact normals orientations, as follows:

$$F_{ij} = \frac{1}{N_c} \sum_{c}^{N_c} n_i^{(c)} n_j^{(c)} \tag{29}$$

where $\mathbf{n}^{(c)}$ is the unit vector of describing the contact normal orientation for contact c. The integral form of F_{ij} can be expressed using the distribution function of $\mathbf{n}$ ($E(\gamma, \theta)$):

$$F_{ij} = \int_0^{2\pi} \int_0^{\pi} n_i n_j E(\gamma, \theta) \sin\gamma d\gamma d\theta \tag{30}$$

For a cross-anisotropic case, Chang et al. (1989) expresses $E(\gamma, \theta)$ using Fourier series taking advantage of symmetry about the z-axis:

$$E(\gamma, \theta) = \frac{3(1 + a\cos 2\gamma)}{4\pi(3 - a)} \tag{31}$$

where a expresses the degree of anisotropy which is normally $-1 < a < 1$, with $a = 0$ corresponding to a perfectly isotropic distribution of the contact normals. A positive a indicates the sample has more contacts in the z-direction, with the opposite being true for negative a values. Based on Eq. 31, Yimsiri and Soga (2010) express the fabric tensor of a cross-anisotropic sample in terms of a only:

$$F_{ij} = \begin{bmatrix} \frac{3a-5}{5(a-3)} & 0 & 0 \\ 0 & \frac{3a-5}{5(a-3)} & 0 \\ 0 & 0 & \frac{-5-a}{5(a-3)} \end{bmatrix} = \frac{1}{3}\boldsymbol{I} + \begin{bmatrix} \frac{-4a}{15(3-a)} & 0 & 0 \\ 0 & \frac{-4a}{15(3-a)} & 0 \\ 0 & 0 & \frac{8a}{15(3-a)} \end{bmatrix} \tag{32}$$

where $\boldsymbol{I}$ is the second order identity tensor. In this study, the parameter a was used to quantify the anisotropy of the samples, which was determined by comparing the calculated contact normal based fabric tensor (Eq. 29) with that expressed in Eq. 32.

Isotropic compression samples (IC)

The particles were randomly generated within a region inside the rigid wall boundaries. Overlap was prohibited between particles and between particles and the boundary walls. The friction coefficient of the particles was varied ($\mu = 0.01, 0.05, 0.10, 0.20, 0.34$) to produce samples with a range of packing densities. Here, the packing density is quantified using the void ratio (e) (Eq. 7).

After the particles were generated, the six rigid walls were moved inward until an isotropic stress (σ_{iso}) of 1 kPa was achieved using a servo-control algorithm. Viscous damping with a damping coefficient of 0.1 was applied to minimize the kinetic energy of the particles. During compression the positions of the 6 rigid walls were adjusted using a servo-controlled algorithm until the isotropic stress reached a target value with the viscous damping on. The target isotropic stresses were 10, 100, and 1000 kPa. After the target isotropic stress was achieved, a vertical body force was applied to simulate gravity. Gravity was applied to avoid the presence of a large number of non-physical rattler particles that do not engage in any contacts, whose presence may affect the ETC of the sample because the BOB model includes heat conduction through separated particles. Gravity was introduced only after isotropic compression to achieve an ideal, isotropic packing. A typical sample after an isotropic compression is shown in Fig. 4. A total of 15 *IC* samples were considered.

Summary data on the packing characteristics of the *IC* samples after application of gravity are provided on Fig.5. Referring to Fig.5 (a), the $\overline{Z}$ values ranged between 4.07 and 5.92, while the e values were between 0.600 and 0.721. The magnitude of the anisotropy, $|a|$, was < 0.01, confirming isotropic samples were attained.

Samples formed by 1D compression (K_0)

For the K_0 samples the generation procedure initially followed the process used for the *IC* samples, i.e. random generation of particles and isotropic compression to $\sigma_{iso} = 1kPa$ while applying viscous damping. Once the assembly of particles was judged to be stable at $\sigma_{iso} = 1kPa$, the positions of the horizontal walls (i.e. the walls normal to the x and y axes) were fixed and the vertical walls (walls normal to the z-axis) were moved until a target vertical stress (σ_{zz}) of 10, 100, or 1000 kPa was achieved. As for the *IC* samples, various friction coefficients ($\mu = 0.01, 0.05, 0.10, 0.20, 0.34$) were considered. Also as before, after the target vertical stress was achieved, a vertical body force was applied to simulate gravity. Typically in soil mechanics one dimensional compression is referred to as K_0 compression, hence these samples are denoted K_0. A total of 15 K_0 samples were created.

Note that σ_{xx} and σ_{yy} were not controlled during the 1D compression while σ_{zz} was controlled.

The ratio of the horizontal stress to the vertical stress (SR) was calculated as:

$$SR = \frac{\sigma_h}{\sigma_v} \equiv \frac{\left(\sigma_{xx} + \sigma_{yy}\right)/2}{\sigma_{zz}} \tag{33}$$

In this study, the SR value varies from 0.654 to 0.946, and reduced with increasing μ and increasing σ_{zz}. Note that a lower SR value indicates a more anisotropic stress state. The aspect ratio of the sample, AR, was defined as:

$$AR = \frac{L_h}{L_v} \equiv \frac{\left(L_x + L_y\right)/2}{L_z} \tag{34}$$

The minimum AR value of the K_0 samples was 0.997, which indicates the shape of the K_0 samples was nearly cubic.

Summary data on the packing characteristics of the K_0 samples following compression are provided on Fig.5. Referring to Fig.5 (a), the $\overline{Z}$ and e values were very similar to those obtained for the *IC* samples. For these cases a range of anisotropy values were attained so that $0.01 < a < 0.07$. In general a tended to increase with increasing μ and increasing σ_{zz}, which is attributed to a higher difference between σ_v and σ_h.

Triaxial compression and unloading samples (TCUL)

In order to increase the level of fabric anisotropy of the samples, the "pre-shearing" approach described by Wei and Wang (2017) (modification of the approach proposed by Yimsiri and Soga (2010)) was conducted. The *IC* samples were used to produce these samples. All of the *IC* samples were subjected to triaxial compression, where ε_{zz} was increased at a constant rate while σ_{xx} and σ_{yy} were maintained effectively constant using the servo-controlled algorithm, until a target vertical strain (ε_{zz}) was achieved. The target ε_{zz} values considered were 1%, 3%, and 10%. After reaching the target value, ε_{zz} was then decreased while σ_{xx} and σ_{yy} were again maintained approximately constant using the servo-control system, until σ_{zz} reached the initial value. Throughout these procedures, the friction coefficient of the particles was set to be 0.35. 45 *TCUL* samples were created.

As a result of the generation process, in the *TCUL* samples more contacts are orientated in the

z-direction than in the x- and y-directions even though the stress state is isotropic. Referring to Fig.5a the *TCUL* samples attained a similar range of void ratios when compared with the *IC* and K_0 samples, but the range of $\overline{Z}$ values was significantly smaller ($4.64 < \overline{Z} < 5.15$). This confirms that there is not a unique relationship between e and $\overline{Z}$. The range of anisotropies attained was higher than in the K_0 cases, with $0.04 < a < 0.17$ (Fig.5b).

Triaxial extension and unloading samples (TEUL)

In this case the *IC* samples were also subjected to triaxial extension, where, in contrast to the *TCUL* samples, a negative vertical strain rate was applied to extend the sample. As a result, ε_{zz} decreased, becoming negative (note that the soil mechanics convention where compressive strains are positive is adopted), while the values of σ_{xx} and σ_{yy} were maintained constant. The triaxial extension was stopped when a target ε_{zz} value of -1%, -3%, or -10% was achieved. Then ε_{zz} was increased until σ_{zz} returned to its initial value. Throughout this deformation process σ_{xx} and σ_{yy} were maintained constant. 45 *TEUL* samples were created.

When compared with the *TCUL* samples, the *TEUL* samples have more contacts in the lateral (x and y) directions, explaining the negative a values observed in (Fig.5b), however the magnitudes of the anisotropies were similar with $0.07 < |a| < 0.21$. A similar range of e and $\overline{Z}$ were obtained for the *TEUL* samples when compared with the *TCUL* samples (Fig.5b), providing further evidence of the non-uniqueness of the e-$\overline{Z}$ relationship.

Small Deformation Probes to Determine Elastic Moduli

Overview of Elastic Moduli

Granular materials exhibit an elastic load-deformation response when subjected to deformations that result in small strains (Jardine 1992). Here we followed the process used in experimental soil mechanics where small increments of strain (termed probes) are applied to a sample, in order to determine the elastic moduli.

The samples prepared in this study should have transverse isotropy (i.e. they should be cross-anisotropic) so that, referring to Eq. 29, $F_{xx} = F_{yy}$. This anisotropy in the fabric tensor will be reflected in the cross-anisotropy of the sample's elastic moduli. In engineering, the relationships

between increments in the stress components and the resulting incremental strain components of a transversely isotropic elastic material can be written as:

$$\begin{bmatrix} \Delta\varepsilon_{xx} \\ \Delta\varepsilon_{yy} \\ \Delta\varepsilon_{zz} \\ \Delta\varepsilon_{yz} \\ \Delta\varepsilon_{zx} \\ \Delta\varepsilon_{xy} \end{bmatrix} = \begin{bmatrix} 1/E_x & -\nu_{yx}/E_x & -\nu_{zx}/E_z & 0 & 0 & 0 \\ -\nu_{xy}/E_x & 1/E_x & -\nu_{zx}/E_z & 0 & 0 & 0 \\ -\nu_{xz}/E_z & -\nu_{xz}/E_z & 1/E_z & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/G_{xz} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/G_{xz} & 0 \\ 0 & 0 & 0 & 0 & 0 & 2(1+\nu_{xy})/E_x \end{bmatrix} \begin{bmatrix} \Delta\sigma_{xx} \\ \Delta\sigma_{yy} \\ \Delta\sigma_{zz} \\ \Delta\sigma_{yz} \\ \Delta\sigma_{zx} \\ \Delta\sigma_{xy} \end{bmatrix} . \quad (35)$$

where E_i is the Young's modulus in direction i, and G_{ij} and ν_{ij} are the shear modulus and the Poisson's ratio corresponding to shearing within the ij plane, respectively. In experimental studies in soil mechanics, some or all of these components are conventionally obtained as a result of triaxial tests in which stress or strain probes are applied or/and bender element tests (Hoque and Tatsuoka 1998; Kuwano and Jardine 2002).

In DEM simulations using a periodic cell, it is easier to maintain accurately $\Delta\varepsilon_{ij} = 0$ than to maintain $\Delta\sigma_{ij} = 0$. Therefore, it is more convenient to re-write the constitutive equations in Eq. 35 as:

$$\begin{bmatrix} \Delta\sigma_{xx} \\ \Delta\sigma_{yy} \\ \Delta\sigma_{zz} \\ \Delta\sigma_{yz} \\ \Delta\sigma_{zx} \\ \Delta\sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} \Delta\varepsilon_{xx} \\ \Delta\varepsilon_{yy} \\ \Delta\varepsilon_{zz} \\ \Delta\varepsilon_{yz} \\ \Delta\varepsilon_{zx} \\ \Delta\varepsilon_{xy} \end{bmatrix} . \quad (36)$$

By comparing Eq. 36 and Eq. 35, the following relationships between the two sets of moduli can be obtained (Lubarda and Chen 2008):

$$E_z = C_{33} - \frac{2C_{13}^2}{C_{11} + C_{12}} \tag{37}$$

$$E_x = E_y = \frac{(C_{11} - C_{12})(C_{11}C_{33} + C_{12}C_{33} - 2C_{13}^2)}{C_{11}C_{33} - C_{13}^2} \tag{38}$$

C_{11}, C_{12}, and C_{13} can be measured by a small deformation probe where a small increment in $\Delta\varepsilon_{xx}$ is applied while maintaining $\Delta\varepsilon_{yy} = \Delta\varepsilon_{zz} = 0$. C_{11}, C_{12}, and C_{13} can be calculated using the changes in the three orthogonal stresses ($\Delta\sigma_{xx}$, $\Delta\sigma_{yy}$, and $\Delta\sigma_{zz}$) during this type of a small deformation probe as:

$$C_{11} = \frac{\Delta\sigma_{xx}}{\Delta\epsilon_{xx}} \tag{39}$$

$$C_{12} = \frac{\Delta\sigma_{yy}}{\Delta\epsilon_{xx}} \tag{40}$$

$$C_{13} = \frac{\Delta\sigma_{zz}}{\Delta\epsilon_{xx}} \tag{41}$$

C_{33} can be calculated from $\Delta\sigma_{zz}$ during a small deformation probe where a small value of $\Delta\varepsilon_{zz}$ is applied under $\Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = 0$:

$$C_{33} = \frac{\Delta\sigma_{zz}}{\Delta\epsilon_{zz}} \tag{42}$$

If the sample remains in the elastic regime during a strain probe, forward loading ($\Delta\epsilon < 0$) and unloading ($\Delta\epsilon > 0$) should give no difference in the moduli (Recchia et al. 2020). DEM simulation results by Recchia et al. (2020), comparing the moduli obtained from loading and unloading, suggest that such the elastic regime of monodisperse DEM spherical assemblies with $G_p = 29$ GPa and $\nu_p = 0.20$ should be within $|\Delta\varepsilon| < 1 \times 10^{-4}\%$.

Small strain probe simulations

The following four types of small deformation probes were applied to the samples in the current study:

- $\Delta\varepsilon_{xx} > 0, \Delta\varepsilon_{yy} = \Delta\varepsilon_{zz} = 0$ (*Probe 1*)
- $\Delta\varepsilon_{xx} < 0, \Delta\varepsilon_{yy} = \Delta\varepsilon_{zz} = 0$ (*Probe 2*)
- $\Delta\varepsilon_{zz} > 0, \Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = 0$ (*Probe 3*)
- $\Delta\varepsilon_{zz} < 0, \Delta\varepsilon_{xx} = \Delta\varepsilon_{yy} = 0$ (*Probe 4*)

Following Magnanimo et al. (2008), the interparticle friction value was increased to $\mu = 0.45$ while simulating the application of a strain increment. A constant strain rate of either 0.1 %/s or -0.1 %/s was applied until a maximum absolute strain of $< 5 \times 10^{-5}$% was achieved. The stress-strain responses from $|\varepsilon| = 0.2 \times 10^{-5}$% to $|\varepsilon| = 5.0 \times 10^{-5}$% were used to calculate C_{11}, C_{12}, C_{13}, and C_{33} following Eq. 39 - Eq. 42. The relationships between ε_{xx} and σ_{xx} during *Probes 1* and *2* and the relationships between ε_{zz} and σ_{zz} during *Probes 3* and *4* of a highly anisotropic *TCUL* sample ($e = 0.690$; $\overline{Z} = 4.74$; $a = 0.15$; $\sigma_{iso} = 100kPa$) are shown with linear fitting lines in Fig. 6. As shown in Fig. 6, the R^2 values are ≈ 1.0, which indicates that the stress-strain relationships during the probes are effectively linear. The values of C_{11}, C_{12}, C_{13}, and C_{33} were obtained from the loading and unloading simulatinos were compared and differences between the moduli were confirmed to be small, which is also shown in Fig. 6. In the study by Recchia et al. (2020), the maximum absolute difference between C_{33} and C_{11} in the elastic regime is approximately 10 % and that of C_{13} is around 30 %. In this study, a maximum absolute difference between C_{33}, C_{11}, C_{12} and C_{13} was 8.57%, which is comparable to those by Recchia et al. (2020). The averaged values of the moduli obtained from the loading and unloading simulations were used to calculate E_z and E_x following Eq. 37 and Eq. 38. The E_z and E_x values of the samples are shown in Fig. 7, where noticeable anisotropy in Young's modulus of *TEUL* samples can be seen.

A complementary study using a larger sample consisting of 41,444 particles was conducted to demonstrate that 21,217 particles are sufficient. An *IC* sample which has a similar e value to

one of the *IC* samples was produced using 41,444 particles. Sample properties ($\overline{Z}, a, E_{zz}, k^*_{zz}/k_f$) were measured and compared with an equivalent *IC* sample with 21,217 particles as Table 2. The difference between the two samples were very small.

Heat Transfer Simulatons

DEM model overview

To measure the ETC of the samples, a heat pipe network model which uses the modified BOB model (Dai et al. 2019) was implemented in LAMMPS. The implementation of the modified BOB model was validated by FEM models consisting of two hemispheres and gap fluid using ABAQUS (Dassault Systèmes 2019) following Dai et al. (2019). A schematic illustration of the system considered in this validation is shown in Fig. 8 (a). An axisymmetric condition was employed to reduce computational time. Three h/r values of 0.002, 0.02, and 0.2 were considered for cases where two hemispheres are separated while two r_c/r values of 0.002 and 0.02 were considered for cases where two hemispheres are in contact. Three κ values of 50, 100, and 500 were chosen. Steady state heat transfer simulations were conducted where the temperature difference between the upper and the lower boundaries (ΔT) was 1 K. Heat transferred through the upper or bottom boundaries (Q_{FEM}) was measured within a time increment of Δt. The temperature distribution predicted by a representative FEM model is shown in Fig. 8 (b).

The same system consisting of two spheres were created in LAMMPS. The difference in the initial temperatures of the two particles (ΔT) was set to be 1 K. Heat transferred between the particles (Q_{BOB}) was measured within a time increment of Δt.

Dai et al. (2019) defined normalised heat (denoted H^{norm} here) as Q normalised by Δt, ΔT, r, and k_s so that:

$$H^{norm} = \frac{Q}{\Delta t \Delta T r k_s} \tag{43}$$

Fig. 9 compares H^{norm} values obtained in FEM and DEM simulations, demonstrating a good agreement.

The heat pipe network model implemented in this study was further verified using heat pipe

network simulation data by Yun and Evans (2010). Samples equivalent to the samples used by Yun and Evans (2010) were created and the ETC of the samples were measured using a heat conduction model used by Yun and Evans (2010). The ETC values obtained from the implemented heat pipe network model agree well with those obtained by Yun and Evans (2010).

Heat transfer simulation procedure

During the heat transfer simulation, the positions of the particles were fixed. All the particles had an initial temperature of 273 K. To measure the ETC in a certain direction, i, the temperatures of opposite boundaries ($T_{\mathrm{i},0}$ and $T_{\mathrm{i},1}$) perpendicular to the i-axis were set to be 274 K and 273 K, respectively, and maintained constant during the heat transfer simulation. The simulation continued until a steady state was attained. The ETC of the sample (k^*_{ii}) in the i-direction was calculated using the rate of heat at the steady state ($\dot{Q}_{\mathrm{steady}}$):

$$k^*_{ii} = \dot{Q}_{\mathrm{steady}} \frac{L_i}{A_i (T_{\mathrm{i},0} - T_{\mathrm{i},1})} \ . \tag{44}$$

where A_i and L_i are the cross-sectional area and the length of the sample along the i-direction. The ratio of conductivities, κ, was varied in a parametric study considering κ = 10, 30, 50, 100, 150, 300, and 500 to represent various combinations of solid particles and pore fluid. The range of κ values considered by Dai et al. (2019) (κ = 10 to 1000), Cheng et al. (1999) (κ = 10 to 3000) and Yun and Evans (2010) (κ = 1.89 to 120) informed this choice of parameters. It is useful to consider typical κ values of soil as an example of granular materials with non-metalic solid particles. The κ value of a saturated soil ranges from 3.09 to 12.9 with k_s = 1.85 to 7.70 W/(m·K) (Horai 1971; Brigaud and Vasseur 1989) and k_f = 0.5984 W/(m·K) at 20 °C (Lide 2004). The κ value of a dry soil is between 70.6 and 294 with k_f = 0.0262 W/(m·K) at 27 °C (Lide 2004). κ may reach around 500 for Al_2O_3-air mixtures which are common in a packed bed energy storage (Anderson et al. 2015).

Note that the thermal expansion of the particles was not considered in this study because the effect of the thermal expansion of the particles on the ETC depends on the specific temperature

increment considered and the thermal expansion coefficient of the solid particles. In other words, to enable some general conclusions to be made it is best to isolate the system response from the effects of thermal expansion.

ETC values

The results of the heat transfer simulations are summarized in Fig. 10 in terms of the relationship between the void ratio and the ETC of the samples for (a) $\kappa = 10$, (b) $\kappa = 100$, and (c) $\kappa = 500$. The ETC values were normalised by k_f, the thermal conductivity of the pore fluid. One expects that $k^*_{ii}/k_f \rightarrow 1$ for $e \rightarrow \infty$ and $k^*_{ii}/k_f \rightarrow \kappa$ for $e \rightarrow 0$. For the lowest κ value considered ($\kappa = 10$), the void ratio and the ETC of appear to have a unique, almost linear relationship. However, for the larger κ values of 100 and 500, where an increase in contact areas between particles has a significant effect on the overall ETC, the data exhibit significant scatter. The best fit line obtained using regression is shown for $\kappa = 500$, and the data deviate from the line by up to ±22%, showing that a relatively simple relationship between e and kappa exists only when κ is very low (e.g. $\kappa = 10$).

EXPLORING THE LINK BETWEEN THE ETC AND PACKING CHARACTERISITCS, ELASTIC MODULI AND STRESS LEVEL

The analytical model presented in previous sections indicated a link between the ETC and E, σ_{iso} and e. The data generated in the DEM simulations allow an empirical exploration of this link.

Young's Modulus and ETC

Fig.11 presents plots of k^*_{zz}/k_f against E_z for the samples with (a) $\kappa = 10$, (b) $\kappa = 100$, and (c) $\kappa = 500$. The relationship between E_x and k^*_{xx} for $\kappa = 500$ is presented in Fig.11(d). The grayscales of the symbols on Fig. 11 give the values of e for the samples; a darker color indicates a denser sample (i.e. a lower e). The symbol shape indicates the sample type. In contrast to Fig. 10, for a given sample type, there appears to be a clearer correlation between E_z and k^*_{zz} or E_x and k^*_{xx}. This correlation is more evident for samples with a higher κ value, where the contribution of conduction through contact areas to the overall ETC is more important than in samples with a

lower κ value. These data support the hypothesis that predicting the ETC or the variation in ETC using Young's moduli data is possible, particularly for higher κ values. Fig. 11 also indicates that for similar values of E_i, a lower void ratio gives a higher k_{ii}^* value for various κ values.

To further explore the validity of the hypothesis proposed on the basis of the analytical model, for the *IC* samples the Young's moduli predicted by Eq.9 (E_{EMT}) data were determined using the e, $\overline{Z}$, G_p, ν_p and σ_{iso} values from the DEM simulations. These values of E_{EMT} are plotted against the Young's moduli measured in small deformation probes (E_{DEM}) in Fig.12(a). As previous studies have shown (Makse et al. 1999; Khalili et al. 2017), the E_{EMT} values are significantly larger than the E_{DEM} values. However, as shown on Fig.12(b), the ratio of E_{EMT} to a reference E_{EMT} (E_{EMTref}) reasonably agrees with the ratio of E_{DEM} to a reference E_{DEM} (E_{DEMref}) as La Ragione and Magnanimo (2012) suggested. Here the sample with the medium e value ($e = 0.6690$) and $\sigma_{iso} = 100kPa$ was chosen as the reference sample.

Effective Thermal Conductivity

Using the analytical model, we have shown that k_{ij}^* can be divided into two components, namely $k_{ij}^{\beta*}$ and k_{ij}^{h*}. The analytical k_{ij}^* adopting a uniform temperature gradient (Eq. 15) and the k_{ij}^* from the boundary heat rate (Eq. 44) differ by less than 10%. $k_{ij}^{\beta*}$ is dependent on the number of contacts and the contact radii in the sample and so it is related to the Young's modulus and the stresses within the sample as shown in Eq. 22 and Eq. 26. On the other hand, k_{ij}^{h*} is dependent on the distribution of h values for the sample, which can be correlated to e.

Fig.13 (a) is a plot of $k_{zz}^{\beta*}/k_f$ against E_z and it appears that, for a given value of σ_{zz} (indicated by the shape of the marker), E_z and $k_z^{\beta*}z$ have a nearly unique relationship (i.e. independent of the sample type). However, it is also clear from Fig. 13(a) that the effect of σ_{zz} on this relationship is substantial. As shown in Eq. 22, for a small σ_{zz}, which gives small contact radii, $k_{zz}^{\beta*}$ is proportional to $E_z^{0.5}\sigma_z^{0.5}$. The variation in $k_{zz}^{\beta*}/k_f$ with $E_z^{0.5}\sigma_z^{0.5}$ is shown in Fig. 13 (b). The relationship is unique for the data in this study.

Fig.13 (c) plots k_{zz}^{h*}/k_f against e and includes the best fit straight line. There is substantial scatter, though it is less evident than for the relationship between k_{zz}^* and e (Fig. 10 (c)), as shown

by the maximum deviations from the best-fit line.

Proposed Expression Relating the ETC to Young's Modulus and Void Ratio

Any method to indirectly predict the ETC or the variation in ETC should be based on parameters that can be measured in experiments. Experimental measurement of $\overline{Z}$ is only possible using sophisticated 3D image analysis of datasets obtained from micro computed tomography (e.g. Fonseca et al. 2013). Consequently, here we explore the potential to use the sample Young's moduli and void ratio values to estimate the corresponding ETC.

Informed by the analytical study and regression analyses of the DEM-generated data, the following equation gives a good fit to the ETC data for the DEM samples considered here:

$$\frac{k_{ii}^{*}}{k_{ref}^{*}} = \left(\frac{E_i}{E_{ref}}\right)^{m_E} \left(\frac{1+e}{1+e_{ref}}\right)^{m_e} \tag{45}$$

where k_{ref}^{*}, E_{ref}, and e_{ref} are the effective thermal conductivity, Young's modulus, and the void ratio of a reference sample and m_E and m_e are two empirical fitting parameters. The reference sample used here was the *IC* sample with $\sigma_{iso} = 100kPa$ and $\mu = 0.10$ during isotropic compression as this had a void ratio that was close to the mean void ratio for all the samples; however, we found that the reference sample chosen has little influence on the results. According to the analytical study, for small κ values, $k_{ii}^{\beta *}$ is expected to be very small, and so the effects of neglecting σ_{ii} in the expression are expected to be small.

To calibrate the empirical parameters, m_e and m_E, nonlinear least square regression was used employing MATLAB (MathWorks 2020). The resulting m_E and m_e values are given in Table 3. The R^2 values are higher than 0.9461 for all the κ values, which demonstrates a good applicability for a wide range of κ values. The best fit m_E value increased with increasing κ, which can be attributed to the larger effect of conductance through contact areas on the overall ETC for a higher κ. On the other hand, the best fit m_e value was less sensitive to the κ value than the best fit m_E value, with $2.2705 < m_e < 2.5586$. A comparison between the predicted and actual $\frac{k_{ii}^{*}}{k_{ref}^{*}}$ is presented in Fig.14 for κ = 10, 100, and 500. As shown in Table3 and Fig.14, reasonably accurate results were

obtained from the E and e. It should be noted that the k_{ii}^{*} values of all the samples (*IC*, K_0, *TCUL*, and *TEUL*) can be predicted only using the Young's modulus in the same direction, E_i, even though the analytical study considered only isotropic samples under an isotropic stress state.

Practically, k_{ref}, E_{ref} and e_{ref} can be obtained experimentally from the same sample using commonly used technique, specifically a thermal needle probe to measure k_{ref}, small strain probes or bender element tests to get E_{ref}, and measuring the weight and the volume of the sample to get e_{ref}. The accuracy of the model does not depend on the stress state, the fabric anisotropy, and the density of the samples, and so for example an oedometer with a thermal needle and bender elements installed can be used to get reference data.

CONCLUSIONS

This study has combined analytical modelling and analysis of DEM data to explore the relationships between the ETC and Young's modulus to establish a new approach to indirectly measure the ETC of granular media. Both studies adopt a heat pipe network model to apply Fourier's law for discrete elements. In order to model the effective heat conductance of discrete spheres and the gap fluid between them, the analytical model by Batchelor and O'Brien (1977) (BOB model) was employed for both analytical and DEM studies, and an excellent agreement with particle-scale FEM results was shown. The analytical study showed that the ETC of a granular medium can be related to its packing characteristics, namely e, $\overline{Z}$ and r_c/r, by assuming a uniform temperature gradient within the granular medium. Subsequently, the analytical study provided a relationship between the Young's modulus and the packing characteristics using Effective Medium Theory. Combining these two relationships, the analytical study demonstrated that a component of the ETC, $k_{ii}^{*\beta}$ can be correlated with the Young's modulus and the stress level. The analytical study also suggested that the other components of the ETC, k_{ii}^{*h}, can be linked to the e value of the medium.

The complementary DEM study was carried out to support the findings in the analytical study. The packing characteristics and the stress state of virtual DEM samples were varied by subjecting the samples to different stress paths (*IC*, K_0, *TCUL*, and *TEUL*). To obtain the small strain Young's moduli of the samples, small strain probes were conducted. The ETC values of the DEM samples

were measured using the heat pipe network model and the modified BOB model, which were implemented into LAMMPS and verified. These simulation results showed that for a small κ, the relationship between e and the ETC of the samples was nearly unique. Conversely, for a higher κ, the correlation between E_i and k_{ii}^* is more evident, which demonstrates that the consideration of E_i and e enhances the prediction of k_{ii}^*. The dependency of $k_{ii}^{*\beta}$ on E_i and σ_{ii} and the dependency of k_{ii}^{*h} on e, which were suggested in the analytical study, were shown by detailed analysis of the DEM data.

Based on the analytical study and the DEM study, this contribution has suggested a new method predicting the ratio of k_{ii}^* to the ETC of a reference sample, k_{ref}^*, using the ratios of the Young's modulus and the void ratio to those of the reference sample (E_i/E_{ref} and $(1+e)/(1+e_{ref})$). The parameters can be calibrated easily and the predictions showed excellent agreement with the DEM results. The indirect measurement method of the ETC proposed in this study may contribute to a variety of engineering fields by reducing the costs associated with the measurement of ETC of granular materials with a simple procedure that can achieve reasonable accuracy. Consideration of polydispersity, fluid flow, and three-phase granular materials remains for future work.

DATA AVAILABILITY STATEMENT

All data, models, or code that support the findings of this study are available from the corresponding author upon reasonable request.

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APPENDIX I. NOTATION

The following symbols are used in this paper:

$A_{continuum}$ = cross-sectional area of a continuum (m^2);

A_i = cross-sectional area along the i-direction (m^2);

AR = aspect ratio ($-$);

a = degree of anisotropy ($-$);

C = thermal conductance (W/K);

C_c = thermal conductance of contact region (W/K);

$C_c^{contact}$ = thermal conductance of a contact area and gap fluid between contacting two particles (W/K);

$C_c^{separated}$ = thermal conductance of gap fluid between separated two particles (W/K);

C_{ij} = elastic moduli (Pa);

C_p = thermal conductance of particle p (W/K);

C^*_{p1p2} = effective thermal conductance of a heat pipe (W/K);

c_p = specific heat capacity of particle p ($J/(g \times K)$);

d = distance between two contacting particles (m);

E_i = Young's modulus in direction i (Pa);

E_{ref} = Young's modulus of a reference sample (Pa);

e = void ratio ($-$);

e_{ref} = void ratio of a reference sample ($-$);

F_{ij} = fabric tensor ($-$);

G_{ij} = shear modulus corresponding to shearing within the ij plane (Pa);

G_p = shear modulus of particles (Pa);

$\mathcal{H}_c$ = term expressing an increase in a thermal conduction through a contact area ($-$);

$\Delta\mathcal{H}_f$ = term expressing a decrease in a thermal conduction through gap fluid ($-$);

H^{norm} = normalised heat ($-$);

h = gap distance between two particles (m);

$\boldsymbol{I}$ = second order unit tensor ($-$);

k_{ij} = thermal conductivity matrix ($W/(m \times K)$);

k^*_{ij} = effective thermal conductivity matrix ($W/(m \times K)$);

$k^{*(h=0)}_{ij}$ = component of effective thermal conductivity matrix defined in Eq. 21 ($W/(m \times K)$);

k^{*h}_{ij} = component of effective thermal conductivity matrix dependent on h ($W/(m \times K)$);

$k^{*\beta}_{ij}$ = component of effective thermal conductivity matrix dependent on β ($W/(m \times K)$);

k_f = thermal conductivity of fluid ($W/(m \times K)$);

k_N = incremental normal stiffness of a particle (N/m);

k_{ref} = thermal conductivity of a reference sample ($W/(m \times K)$);

k_s = thermal conductivity of solid particles ($W/(m \times K)$);

k_T = incremental tangential stiffness of a particle (N/m);

$L_{continuum}$ = length of a continuum (m);

L_h = horizontal length of a sample (m);

L_i = length of a sample along i-direction (m);

L_v = vertical length of a sample (m);

l = length (m);

m_E = empirical parameter in Eq. 45 ($-$);

m_p = mass of particle p (kg);

N_c = number of contacts in a granular sample ($-$);

N_{hp} = number of heat pipes in a granular sample ($-$);

N_{hp} = number of heat pipes between non-contacting particles in a granular sample ($-$);

N_E = material constant in Eq. 9 ($-$);

N'_E = material constant in Eq. 12 ($-$);

N_p = number of particles in a granular sample ($-$)

$N^{(p)}_c$ = number of contacts involving particle p ($-$);

N_σ = material constant in Eq. 11 ($-$);

n_i = unit vector ($-$);

$Q^{(\Delta t)}_p$ = amount of heat received by a particle p at a time increment Δt (J);

$\dot{Q}_{p1p2}$ = amount of heat moving from particle $p1$ to particle $p2$ per unit time (W);

$\dot{Q}_{steady}$ = rate of heat at a steady state (W);

$\mathbf{q}$ = heat flux vector through unit area (W/m^2);

R^2 = coefficient of determination ($-$);

r = radius (m);

r_c = contact radius (m);

r_p = radius of particle p (m);

r_{p1q2} = harmonic mean of the radii of particles $p1$ and $p2$ (m);

SR = stress ratio ($-$);

T_{i1} = temperature of a boundary 1 perpendicular to the i-axis (K);

T_{i2} = temperature of a boundary 2 perpendicular to the i-axis (K);

T_p = temperature of particle p (K);

$\Delta T_p^{(\Delta t)}$ = increment in the temperature of a particle p (K);

∇T = temperature gradient (K/m);

t = time (s);

V_s = solid volume (m^3);

V_v = void volume (m^3);

Z = coordination number ($-$);

β = dimensionless number as function of r_c ($-$);

ε_{ij} = strain tensor ($-$);

κ = ratio of k_s to k_f ($-$);

λ = dimensionless number as a function of h ($-$);

ν_{ij} = Poisson's ratio of a sample corresponding to shearing within the ij plane ($-$);

ν_p = Poisson's ratio of particles ($-$);

σ_h = horizontal stress (Pa);

σ_{ij} = stress tensor (Pa);

σ_{iso} = isotropic stress (Pa);

σ_v = vertical stress (Pa); and

χ = parameter used in BOB model ($-$).

APPENDIX II. BATCHELOR AND O'BRIEN MODEL

A brief description of BOB model is provided here. If two particles are separated, the conductance ($C_c^{separated}$) through the gap fluid is based on a dimensionless number λ whcih depends on h:

$$\lambda = \kappa^2 \frac{h}{r_{p1p2}} \tag{A.1}$$

where r_{p1p2} is is the harmonic mean of the radii of particles $p1$ and $p2$ (r_{p1} and r_{p2}, respectively):

$$r_{p1p2} = \frac{2 r_{p1} r_{p2}}{r_{p1} + r_{p2}} \tag{A.2}$$

Dai et al. (2019) found that the following expressions for $C_c^{separated}$ agree well with their FEM simulation results where particles are not contacting:

$$C_c^{separated} = \begin{cases} \pi k_f r_{p1p2} \ln \kappa^2 & (\lambda < 0.01) \\ \pi k_f r_{p1p2} \ln \left[1 + r_{p1p2}/h\right] & (\lambda > 100) \\ \text{Minimum value of the above two} & (\text{otherwise}) \end{cases} \tag{A.3}$$

Where there is contact between particles $p1$ and $p2$, the $C_c^{contact}$ proposed by Dai et al. (2019) is given as:

$$C_c^{contact} = \pi k_f r_{p1p2} \left(\mathcal{H}_c(\beta) + \Delta \mathcal{H}_f(\beta) + \ln \kappa^2 \right) \tag{A.4}$$

where β is a dimensionless number defined by Batchelor and O'Brien (1977) as a function of r_c/r_{p1p2}:

$$\beta = \kappa \frac{r_c}{r_{p1p2}} \tag{A.5}$$

and r_c is calculated based on Hertzian contact theory as:

$$r_c = \sqrt{\frac{r_{p1p2}(r_{p1} + r_{p2} - d)}{2}} \tag{A.6}$$

where d is the distance between the centroids of the two contacting particles.

Dai et al. (2019) proposed the following expressions for $\mathcal{H}_c(\beta)$ and $\Delta\mathcal{H}_f(\beta)$:

$$\mathcal{H}_c(\beta) = \begin{cases} 0.22\beta^2 & (\beta < 1) \\ 2\beta/\pi & (\beta > 100) \\ \text{Linear interpolation between the above two} & (\text{otherwise}) \end{cases} \tag{A.7}$$

$$\Delta\mathcal{H}_f(\beta) = \begin{cases} -0.05\beta^2 & (\beta < 1) \\ -\ln\beta^2 & (\beta > 100) \\ \text{Linear interpolation between the above two} & (\text{otherwise}) \end{cases} \tag{A.8}$$

Substituting Eqns. A.7 and A.8 into Eq. A.4, for a given contact, the combined thermal conductance through the contact area and the gap fluid is written as:

$$C_c^{contact} = \begin{cases} \pi k_f r_{p1p2}\left(0.17\beta^2 + \ln\kappa^2\right) & (\beta < 1) \\ \pi k_f r_{p1p2}\left(2\beta/\pi - \ln\beta^2 + \ln\kappa^2\right) & (\beta > 100) \\ \text{Linear interpolation between the above two} & (\text{otherwise}) \end{cases} \tag{A.9}$$

Dai et al. (2019) modeled each particle as a cylinder to determine its thermal conductance of (Fig. 2) so that the conductance of each of the contacting particles $p1$ and $p2$ is given by:

$$C_{p1\,or\,p2} = \frac{\pi\left(\chi \min\left[r_{p1}, r_{p2}\right]\right)^2 k_s}{r_{p1\,or\,p2}} \tag{A.10}$$

where the parameter χ is a function of κ (Dai et al. 2019):

$$\chi = 1.3121\kappa^{-0.19} \tag{A.11}$$

Thus expressions for each term in Eq. 4 are given so that the effective conductance of each pipe in the heat network model can be determined.

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TABLE 1. Simulation parameters

Parameters	Values
Number of particles	21,217, 41,444 (A complementary study)
D_{50}	1.0 mm
C_u	1.1
Contact model	Simplified Hertz-Mindlin model
G_p and G_{wall}	29.2 GPa
ν_p and ν_{wall}	0.20
ρ_p	2600 kg/m^3
μ_p (During *IC* and K_0)	0.01, 0.05, 0.10, 0.20, 0.34
μ_p (During *TCUL* and TEUL)	0.35
μ_p (During small deformation probes)	0.40 - 0.45
μ_{wall}	0.00
k_s and k_{wall}	1.0 W/m·K
$\kappa = k_s/k_f$	10, 30, 50, 100, 150, 300, 500

∗ D_{50} . . . the median particle diameter

∗ C_u . . . the coefficient of uniformity

∗ G_p and G_{wall} . . . the shear moduli of the particles and the walls, respectively

∗ ν_p and ν_{wall} . . . the Poisson's ratios of the particles and the walls, respectively

∗ ρ_p . . . the density of the particles

∗ μ_p and μ_{wall} . . . the friction coefficients of the particles and the walls, respectively

∗ k_s and k_{wall} . . . the thermal conductivity of the particles and the walls, respectively

TABLE 2. Sample size effect

Sample properties	$N_p = 21,217$	$N_p = 41,444$
σ_{iso} [kPa]	100	100
e	0.669	0.666
$\overline{Z}$	5.10	5.08
a	0.00	0.00
E_{zz} [MPa]	334	333
k^*_{zz}/k_f ($\kappa = 100$)	12.0	12.0

TABLE 3. m_E, m_e and R^2

κ	Best fit m_E	Best fit m_e	R^2
10	-0.0010	2.5177	0.9967
30	0.0077	2.5556	0.9708
50	0.0154	2.5586	0.9563
100	0.0331	2.5117	0.9461
150	0.0474	2.4655	0.9473
300	0.0802	2.3718	0.9570
500	0.1154	2.2705	0.9664

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