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A hybrid approach for predicting the effective thermal conductivity of sintered porous materials

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ABSTRACT

Estimating the effective conductivity of porous media has been widely based on homogenisation techniques with a limited number of discrete analyses. Though bulk estimates may be sufficient within prescribed bounds and applications, localised properties are not readily available. This work employs resistive network analytics in conjunction with 2D and 3D porous media modelling, to estimate the effective conductivity through local interrogation of porous sintered bronze disks. The resulting hybrid method uses rigid body simulations to generate the porous network and analytical mathematics to evaluate the effective conductivity. The analytics are herein verified and validated for both 2D and 3D cases. The 2D analysis used printed circuit boards to validate the analytics and produced an experimental mean and standard error of $308.7 \pm 12.6\,\mu\Omega$ for networks having resistors ranging from 10 to 1000 Ω. A 3D analysis of sintered porous bronze disks was performed for both electrical and thermal conductivities. A set of simulated samples consistent with the physical specimens were generated using an open source 3D creation software and tested in manners consistent with experiments. The electrical tests across the diameter of the bronze samples yielded equivalent experimental and theoretical resistances of $1.93 \pm 0.42\,m\Omega$ and $2.03 \pm 0.17\,m\Omega$ respectively. A Xenon flash analysis across the thickness of the samples produced an experimental and theoretical Effective Thermal Conductivity (ETC) of 21.9 ± 3.4 W/mK and 18.1 ± 0.3 W/mK respectively. This method was able to successfully estimate the ETC within 17% of the measured mean, while traditional contact-based empirical correlations were found to underpredict the ETC by as much as 58%. The models align well with both experimental studies in both thickness and diametric analysis. Extension of the models to samples of differing particle sizes revealed the ETC to increase with particle size.

1. Introduction

The conductive properties of porous media are important to a range of engineering applications such as thermal management [1], biomaterials [2], fuel cells [3], composites [4], and pebble bed reactors [5] among others. How heat migrates through porous media is dictated by the complexity of the network and the interplay of heat transfer modes. This work is focused on the analysis of porous networks to estimate the Effective Thermal Conductivity (ETC) of sintered porous bronze, how it may be measured experimentally, and its relation to models and analytics.

The conductive properties of porous media have been estimated using variety of techniques including but not limited to volume averaging (based on the constituent thermal conductivities), network connectivity and contact resistances [6]. Although versatile, homogenisation techniques are not well suited to the development of engineered porous media. Rather, discrete approaches are sought to capture the local properties otherwise ignored in traditional ETC methods. Discrete approaches like FEM and FEA allow for the capture of local thermal properties for a given network architecture. Though robust, such methods can be computationally expensive due to meshing and iterative convergence, thereby making them potentially unsuitable for statistical or parametric analysis.

Early porous media models characterised the upper and lower bounds of equivalent networks using resistance networks based on their respective series and parallel circuits [7]. These two cases clearly demonstrate the importance of the formed network as they have the same porosity through a 90° rotation, yet define the upper and lower ETC bounds. The parallel circuit model was enhanced by Liang et al. [8] and bridged the two limits using calibrated coefficients. Alternatively, a hybrid mapping approach was developed by Wang et al. [9] to analyse

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Nomenclature

Latin

A	Area [m^2]
d	Sample diameter [m]
D	Particle diameter [m]
h	Sample height [m]
i	Summand index
k	Thermal conductivity [W/mK]
m	Sample mass [kg]
n	Particle count
R	Resistance [K/W or Ω]
V	Volume [m^3]

Subscripts

eq	Equivalent
exp	Exposed

Greek

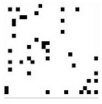
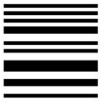
α	Reference node
β	Reference node
λ	Eigenvalue
π	Mathematical Const
ρ	Material density [kg/m^3]
ϕ	Porosity
ψ	Eigenvector

random porous media samples as their equivalent structured networks. In contrast to the one-to-one mapping approach, bulk based approaches were developed to describe the ETC of randomly structured samples, namely Effective Medium Theory (EMT) and Maxwell-Eucken. These models consider stochastic networks of multi-component mixtures and account for percolation effects [7]. Such simplified network models are well suited to investigating materials such as carbon fibre reinforced polymers [4], patterned structures [10] and burn char residues [11]. The resistive network limits and interstitial models are graphically illustrated in Table 1, and more extensively described in Refs. [7,11].

The EMT and Maxwell-Eucken models can capture shifts in bulk conductivity due to changes in the network, however they are principally focused on the global properties rather than local. To address this, researchers looked to the Discrete Element Method (DEM) to replicate the discrete nature of the individual particles of porous media. The foundations of DEM are based on soil and rock mechanics which was extended to porous media analysis as they share packing structures, formed networks, interfacial junctions and surface contacts [9,12–17]. Such assemblies are common to a range of problems including bio aggregates [2], soils [18], and pebble bed reactors [5] among others.

Yun et al. [19] used DEM to simulate 3D particulate assemblies of Ottawa 20–30 sand with variable external forces. Changes in the applied forces were found to affect the network and contact areas through which heat was conducted [19]. Each sample simulated was found to have different conductance networks and corresponding thermal properties while maintaining the same porosity. Similarly, Zhang et al. [12] simulated granular assemblies using DEM with imposed isothermal contact resistances on each particle to make computations tractable. The simulation time was noted to take seconds while FEM took several hours. Of the simulated samples, the ETC was found to increase with compaction, particle size and solid volume fraction. These finding suggest that the thermal performance of porous materials is, at least in part, driven by the formed network and may be a weak function of porosity if at all.

Table 1
Range of ETC models for heat loads travelling from top to bottom.

Parallel	Maxwell-Eucken	EMT	Maxwell-Eucken	Series
				

Given the importance of the formed network, detailed studies of physical specimens are critical for validation. Grandjean et al. [20] analysed physical tin oxide porous structures using a scanning electron microscope and converted them into 2D mesh structures for use in finite element analysis. The simulation results were accurate for close packing arrangements but deviated for pore volume fractions greater than 40%. Similarly, Roussel et al. [3] used GeoDict software to discretize the sample slices into voxels and create a three-dimensional structure. The minimum voxel ratio per particle results in an increase in computations as a multiple of the particle count. This approach was noted to take several minutes of computational time depending on the voxel resolution yet proved inferior when compared to resistor-based approaches for small contact resistances [3].

Depending on how porous media is formed, it is liable to impact the overall thermal performance of the material. Though porous media may take many different physical forms, this work is focused on packed bed forms with the particles being spherical in nature. For such cases, simple porous media structures can be described as a variation of the circle packing problem. Fortunately, the circle packing problem has been widely studied for both mono- and unequally-sized circles. A brief introduction is provided here as it applies to sintered bronze; additional material can be found in Refs. [21,22].

In the case of two-dimensional packing problems, Huang et al. [23] developed deterministic algorithms to pack a prescribed rectangle with a predefined set of unequal circles. Alternatively, George et al. [24] used a heuristic approach to pack the space with the greatest number of circles, using *a priori* knowledge of the circle set to selectively place the circles for the greatest packing density. While this achieves maximal packing structures, the packs were noted to be geometrically stable but physically unstable [24]. The method used to mimic porous media manufacturing must be given some consideration as to its suitability to problem. A form more consistent with manufactured porous media was developed by Visscher and Bolsterli [25] who used Monte Carlo simulations to fill a rectangular domain subject to gravity and domain shaking to promote settling. The packing density for 2D assemblies was limited by the lack of interstitial passages for smaller circles.

The Visscher and Bolsterli [25] study included 3D simulations using mono-sized particles. In the more general case of irregularly shaped particles, Gan et al. [13] investigated the ETC of ellipsoid particles in a packed bed. The particles were noted to arrange themselves such that the major axis was normal to gravity as one might expect. The resulting packed beds produced a higher ETC than spherical packed beds, which was attributed to the change in coordination number and contact area [13]. Further investigation demonstrated that the interplay between the conduction network and the fluid network changed the ETC, while particle size had no significant effect for similar packing arrangements.

With the formed samples, comes a need for local analytical interrogation of the samples. Of the methods utilised in prior works, point-to-point resistance methods show promise regarding accuracy and speed. Numerous point-to-point resistance calculation methods have been studied as summarised by Vos [26]. Many are limited to networks that are small, symmetric or infinite. While there have been advancements made for infinite lattices [27], they provided no tractable means of solving large finite networks like those of porous media. This gap was addressed by Wu [27], who developed a closed form analytical approach to calculating the two-point resistance for finite networks. The network is represented as a weighted, undirected graph with the nodes and edges all encapsulated in a weighted Laplace matrix. The derivation yielded a single expression, Eq. (1), which was verified for regular (structured)