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The permeability of virtual macroporous structures generated by sphere packing models: Comparison with analytical models

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ABSTRACT

Realistic porous structures typical of those made by replication of packed beds of spherical particles have been produced by a novel modelling method. Fluid dynamics simulation of the permeability of these structures agrees well with experimental measurements and similar modelling of structures derived from X-ray tomographic images. By varying the model structures the "bottleneck" flow concept proposed by analytical models in the literature was substantiated, confirming the high dependence of permeability on the size of the windows connecting the pores but also highlighting the need for accurate determination of the connectivity of the pores for these models to be accurate.

Porous metals are commonly used as structures that interact with a fluid in processes such as heat exchange and storage, filtration and separation. Pivotal to the performance of these structures is the resistance to fluid flow that is provided by the porous body, usually described by the pressure drop per unit length developed across the structure as a function of the flow rate (or velocity) of the fluid through it. For laminar flow conditions in a given fluid, the permeability of the porous structure, which is affected by the porosity, pore size, shape and connectivity, relates flow rate and pressure gradient through Darcy's law.

Porous metals made by the infiltration of liquid metal into a bed of sacrificial particles offer a convenient fabrication method with the potential to vary the porosity and pore size independently, thereby giving a good level of control over the structure and hence the fluid flow behaviour [1–3]. Fig. 1 shows the typical structure of porous metals made by replication of packed beds of near-spherical NaCl beads [4]. Important structural features to note include the size of the pores (dictated by the size of the porogen) the fraction of pores (dictated by the packing behaviour of the porogen - in this case affected by tapping in a mould) and the number and size of the windows connecting the pores (dictated by the ability of the infiltrating molten aluminium to penetrate the small spaces at the contact points between salt beads and the number of particle-particle contacts).

Simple permeability models for laminar flow have been developed [5,6] which could assist with the design of these porous metal structures to meet the requirements for specific applications. Both approaches use the same premise, considering the window between the pores to be a "bottleneck" to the flow through the structure. The models consider different particle contact cases (loose packing [6] and packing enhanced through compaction [5]) with different approaches to including contributions from the window size and coordination number. The model to predict the permeability according to [6] is presented in Eq. (1) where ϕ is the porosity, N_c the coordination number, r_w the window radius and r_p the radius of the pore. The coordination number and window radius are defined in separate equations, the coordination number as a function of the packing fraction (also shown in Eq. (1), and the window radius in terms of the infiltration pressure and particle (pore) size. The model in [5] reduces to the same expression for permeability for the case of dense random particle packing if $N_c = 6$ (which is not atypical of this packing condition [7,8])

$$K = N_c \frac{\varnothing r_w^3}{6\pi r_p} \quad \text{where} \quad N_c = \frac{4-\varnothing+\sqrt{2+7\varnothing+\varnothing^2}}{2(1-\varnothing)} \tag{1}$$

Reasonable correlation between experimental measurements of permeability and the models was observed in both cases, with deviations attributed, in part, to the non-spherical nature of some of the salt particles used. Thus a strong dependence upon the size of the windows connecting the pores and the permeability is apparent and controlling the window size, through varying the infiltration pressure [6] has the capacity (for a given pore size) to vary the permeability by more than a factor of 10 and would be more convenient way to vary the permeability rather than by altering the packing (porosity) through additional and potentially costly processing steps.

This paper aims to further test the "bottleneck" flow assumption and the accuracy of these models by simulation of fluid flow through virtual 3D structures that are accurate reproductions of real porous metals made by the infiltration route, but in which the structural characteristics can be controlled precisely, as demanded by the analytical models. The

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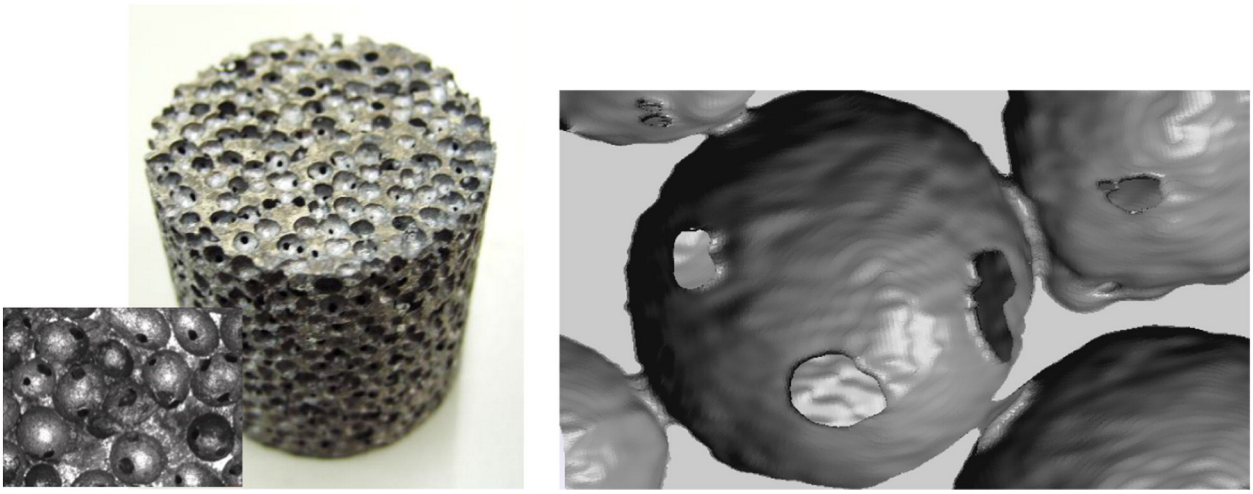

Fig. 1. Optical micrographs, left of a porous sample made by vacuum casting using near-spherical NaCl beads [4] and right, an X-ray CT image showing the typical pore connectivity.

novel approach to generating these virtual structures, which could be further exploited to predict the permeability in more complex porous structures, is detailed.

A prior study by this group [4] demonstrated that the discrete element method (DEM) can be used to accurately model the packing of spherical NaCl particles (both monosized and in binary mixtures) and from this the structures of porous metals made by the infiltration thereof. Coupled with simple mathematical processing of the spatial data for the packed spheres and development of the conditions for contacting of neighbouring beads, the number of windows linking neighbouring pores, and their size, was also accurately predicted, enabling useful insights into the connectivity of these structures.

This study has adopted this same DEM method and has created packed beds of monosized spheres, controlling the packing fraction by altering the coefficient of friction between the particles, giving packing conditions varying from loose to dense random packing (in the range of packing fraction from 0.59 to 0.64). Simple code written in MATLAB was used to process x, y, z particle coordinates and radius data from the DEM simulation, applying a criterion to determine whether particles are connected. This method is detailed in [4] but in brief, two particles are assumed to be connected if the gap separating them cannot be filled by the infiltrating liquid. This ability to fill the gap is controlled by the capillary radius, r_c, determined from the Laplace equation. For the Al-NaCl system [9,10] an infiltration pressure of 1 bar leads to a capillary radius of approximately 20 μm and hence particles separated by <40 μm are deemed "contacting" for this infiltration condition. An extension to this previous study is the graphical representation of this connection through calculation of the radius of the zone that is excluded from infiltration by the liquid (using a simple geometrical model also presented in [4]) and adding the position of the centre of the contact and the radius to the data set. The Matlab code then draws a series of 2D sliced (binary) images of the particles and contacts and exports them as tiff files (in this case at a resolution of 300 dpi).

A representative model was created by converting the 2D slices into a 3D volume within the ScanIP package of Simpleware™, a 3D image processing, analysis and model generation software package. The binary images were thresholded and then a smoothing function was applied to minimise facets created by the slicing process. A smart mask process (with 10 iterations) was preferred to a recursive Gaussian smoothing operation as this more accurately preserved the imported geometry, in particular the geometry of the windows. A cubic representative volume element (RVE) that was 6 times the particle or pore radius was extracted from the centre of the samples, the size of which was determined by shrinking a volume until the porosity differed by 2% from the initial (bulk) value. Porosity and pore radius measurements were made within Scan IP to ensure that the sphere dimensions and packing characteristics were a close representation of the DEM data.

Fig. 2 shows images of the structures generated through DEM and that they closely replicate "real" structures as presented in the CT images in Fig. 1. The key features are replicated viz. the typical number, size and geometry of contacts. It is also clear from these images (taken from the same location) how increasing the capillary radius not only increases the size of the inter-particle contacts (window radius) but also the number of particle contacts (coordination number). It is also apparent that for identical distributions (and packing fractions) of spheres, the porosity of the porous metal will increase (albeit slightly) with

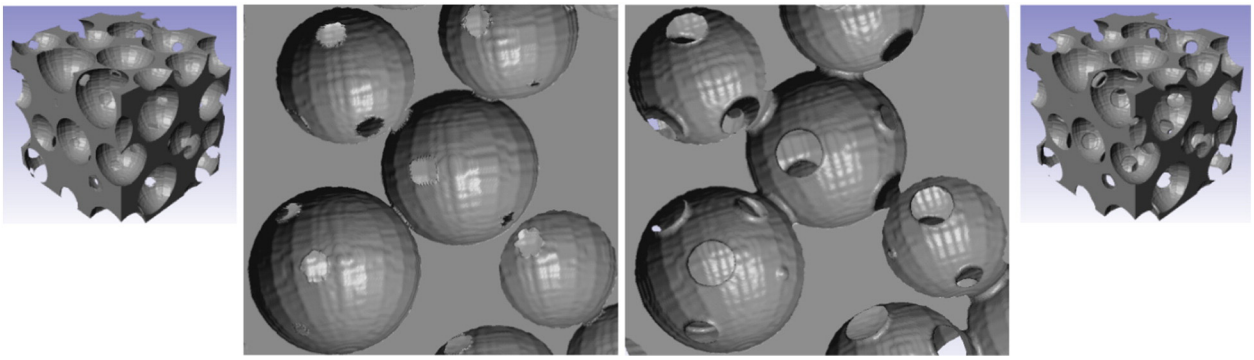

Fig. 2. Images of DEM structures and RVE for different capillary radii (left) 10 μm and (right) 80 μm.