Impact of pore scale parameters on the thermal conductivity of porous building blocks

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Abstract. Increasingly stringent energy requirements push for better performing building blocks with reduced thermal conductivity. A numerical framework to predict the heat transfer through porous materials is employed to investigate the effect of several microscale parameters on the macroscale thermal conductivity. Two different algorithms are used to generate a range of different cellular materials. Simulation results highlight the effect of the porosity, pore size distribution, matrix structure and matrix conductivity on the total thermal conductivity.

1 Introduction

Cellular porous building blocks are frequently applied in the building industry because of their good thermal and structural properties. Examples include aerated concrete, cellular glass and materials based on upcycled waste products. Their low effective thermal conductivity (ETC) can indeed play a key role in the reduction of energy demands from dwellings. However, better performing materials are still needed to cope with increasingly stringent energy regulations. To this end, several studies have already indicated the strong relation between the ETC and the microstructural parameters like porosity, pore volume distribution, matrix tortuosity etc. A correct understanding of the quantitative impact of selected parameters is still lacking though, impeding the optimization of new and existing porous building blocks.

Experimentally quantifying the impact of the pore structure is very cumbersome and makes it very hard to study one parameter at a time. Analytical-theoretical studies on the other hand are usually based on physical or geometrical simplifications and only include selected parameters. Numerical modelling strategies, finally, show great promise for detailed investigation of the influence of the pore structure on the ETC [1-2]. So far, they have been mainly applied on extremely high-porosity foams and less on porous building blocks.

This study employs a recently developed framework to study the heat transfer at the microscale of a set of virtually generated cellular porous materials. The paper starts with a short revisit of the framework before explaining two virtual generation strategies used to produce a range of cellular samples with different pore structures and pore size distributions. The ETC of each sample is calculated using the model framework and is related to the pore size distribution, average pore size and matrix conductivity.

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2 Model framework

For reasons of clarity, a brief overview of the model framework is presented here. The workflow consists of three main parts: (1) obtaining a geometrical representation of the microstructure of the material, (2) creating a finite element mesh and (3) simulating the conductive and radiative heat transport at the pore scale. All three steps are illustrated in Fig. 1. More details can be found in [4]. Thermal radiation is taken into account through an adapted version of Loeb's method: a radiative conductivity is calculated in every pore based on its size, shape and wall emissivity [5]. As such, radiation is modelled as a surface-to-surface process in every pore and is incorporated locally during the simulation. The assumption of radiation being absorbed at the cell wall surface is justified by the relatively thick cell walls studied in this paper together with the fact that opacifiers are often added to the material to suppress the transparency of the cell walls.

The model framework has been validated using a sintered glass filter sample of 36 % porosity and a Reapor block of 89 % porosity with a mixed cellular-granular pore structure. For both materials, good agreement was achieved between numerical and experimental results, with deviations below 10 % [4].

Fig. 1 The model workflow: acquiring the geometry (a&b), meshing (c) and simulation (d).

3 Simulations setup

The model framework is employed to study the impact of the cellular pore structure and the matrix conductivity on the resulting ETC. To this end, a range of porous samples with different characteristics are virtually generated using two different techniques. The first is a bubble-insertion technique, creating a structure of spherical pores, while the second one is a Voronoi-based technique, mimicking more a foam-like structure of cell struts and cell walls. The techniques are explained in the next section, followed by an overview of all parameters varied and studied in this paper.

3.1 Sample generation techniques

A random bubble insertion (RBI) algorithm is implemented based on the one proposed by Wei et al. [2]. It starts with generating a list of pore diameters according to a specified statistical distribution (i.e. lognormal). A random location in the cubic sample is assigned to every pore in the list, ensuring that the overlap with previously located pores does not exceed a previously set threshold. If no location is found for the concerning pore, the algorithm skips this pore and continues with the next pore in the list. A 3D voxel image is finally generated based on the list of successfully inserted pores.

At porosities above 60 %, the algorithm is extended with a second pore generation sequence to overcome the increasingly time-consuming procedure of random localization at such high sphere packing densities. In this second generation sequence, pore diameters are again generated randomly according to the specified distribution and are immediately attempted to be inserted. Using the distance transform of the 3D voxel image, suited locations are retrieved easily. Pores that don't fit anymore in the sample are skipped, hence favouring the generation of smaller pores filling up the remaining space. Fig. 2a-b shows an example of a sample generated using the RBI algorithm with a lognormal distribution.

Fig. 2 Slice through (a/d) and 3D view of (b/e) a generated sample combined with pore size distributions around 10 μm (c/f) for RBI/Voronoi samples.

The other virtual generation algorithm is a Voronoi-based technique implemented according to the method described by Randrianalisoa et al. [6]. A number of seeds are located in the 3D voxel image on a body-centred cubic lattice and subsequently displaced in a random direction with a magnitude dependent on a specified perturbation factor. The Voronoi technique will subsequently divide the image in separate pores by creating cell walls between the seeding points. The thickness of the cell walls is gradually increased to decrease the porosity to a desired value. The algorithm is extended with a strut-rounding algorithm based on spherical dilation and erosion to obtain more rounded struts depending on a rounding factor. As discussed by Randrianalisoa, obtained samples usually have a monomodal pore size distribution, with a width depending on the perturbation factor [6]. An example of a virtually generated sample using the Voronoi algorithm with a perturbation factor of 0.3 and rounding factor of 0.2 is shown in Fig. 2d-e.

3.2 Simulation parameters

Both the RBI and Voronoi algorithm are employed to generate sets of samples with different porosities between 60 % and 90 %. A lognormal distribution is chosen for the RBI algorithm with a mean of 100 μm and a variance of 800 μm^2 . For the Voronoi-based technique, 341 seeds are inserted on a BCC lattice and displaced with a perturbation factor of 0.3. A rounding factor of 0.2 is used to round the sharp edges of the obtained pores. 600^3

voxels are used in the 3D voxel image of each sample. Each generated sample is rescaled 3 times to obtain a pore size distribution in the order of 10 μm , 100 μm and 1000 μm . The thermal conductivity of the solid matrix is set to 0.25 W/mK or 1 W/mK. The gaseous conductivity is kept at 0.0257 W/mK. The temperature difference is set to 1 K with an average sample temperature of 293.15 K, the emissivity of the cell walls is set to 0.9.

4 Results & Discussion

4.1 Sample characteristics

The RBI generated samples have a porosity varying between 65 % and 81 %. The pore size distribution of each sample is determined based on the list of the inserted pores' diameters. The resulting distribution curves are shown in Fig. 2c for the samples with pore sizes around 10 μm , displaying the relative amount of pores at every pore diameter. The colour highlights the porosity of the respective sample. For lower porosities, the distribution curves follow the specified lognormal distribution. At increasing porosity, the distribution curves tend to have a more bimodal character, due to the second step of the generation algorithm filling up the free space between the pores with smaller pores. The porosity of the Voronoi-based samples varies between 59 % and 89 %. Since the pore shapes are non-spherical in this case, the pore size distribution is determined by calculating for every pore the diameter of the equivalent sphere having the same pore volume. Fig. 2f shows the resulting distribution curves for the samples with pore sizes around 10 μm . The curves have a normal type of distribution, as was predicted by Randrianalisoa et al. [6]. The samples' porosity has only a negligible effect on the pore size distribution, contrary to the case for the RBI samples.

4.2 Simulation results

First, the simulation results are discussed for the samples with a pore size distribution around 10 μm . At these small pore sizes, thermal radiation will have a negligible influence (< 1 % contribution), so the effects of the parameters on the conduction can be studied separately [7,8]. Subsequently, the effect of an increasing average pore size is discussed.

4.2.1 Results at 10 μm pore size

The effective thermal conductivity calculated with the model framework for samples with a pore size distribution around 10 μm is summarized in Fig. 3a. Colours highlight the generation technique (RBI or Voronoi), while the symbols depict the different used matrix conductivities. Fig. 3b zooms on the resulting ETC for the RBI-generated samples: colours correspond to the colours in Fig. 2c to facilitate assessing the effect of the pore size distribution.

Results show an expected decrease of the ETC with increasing porosity. Furthermore, the samples with a solid matrix conductivity of 0.25 W/mK have a significantly lower ETC than the ones with 1 W/mK. The absolute difference between both decreases though with increasing porosity due to the decreasing importance of solid matrix conduction. Fig. 3b indicates that the effect, if any, of the pore size distribution is far less important than the effect of the sample's porosity.

Fig. 3 Simulated effective thermal conductivity for Voronoi- and RBI-generated samples (a); Results for RBI-generated samples highlighting effect of porosity and effect of distribution curve (b). (for samples with pore size distributions around 10 μm).

Lastly, it seems that samples generated with the RBI technique have a (significantly) lower ETC compared to samples generated with the Voronoi-based technique (at a similar porosity). The effect is even more pronounced for the high-conductivity material based samples, suggesting that it is indeed due to their different matrix structure. A possible explanation could be the different ratio of solid material located in the struts versus solid material located in the cell walls. Indeed, Glicksmann & Torpey [9] already predicted that material located in cell walls is more favourable to conduct heat compared to material located in struts. This effect was also confirmed with numerical simulations for high-porosity foams by Coquard & Baillis [10]. The RBI-generated samples will intrinsically have a higher concentration of material in the cell struts compared to the Voronoi-based samples, possibly explaining their better performance. On the other hand, an explanation might still be found in the strongly differing pore size distributions. The studied RBI samples have a wider pore size distribution compared to the Voronoi-based samples, which might lead to a more effective blockage of the heat flow through the solid material. Further research is needed to clearly pinpoint the exact cause.

4.2.2 Results at increasing pore size

Rescaling the pore size distribution will theoretically have no effect on the pure conduction through the material. However, at increasing pore size, the effect of thermal radiation inside the pore space becomes more relevant, increasing the resulting ETC. The ETC of the RBI-generated samples is shown for all pore sizes in Figure 4a as function of porosity, the relative contribution of thermal radiation to the total ETC in Figure 4b as a function of the samples' pore size order of magnitude.

The simulation results clearly indicate an increasing ETC at increasing pore size due to the contribution of thermal radiation. Furthermore, the effect becomes more important at increasing porosity and decreasing matrix conductivity. For the Voronoi-based samples, similar results are obtained (not shown here). The contribution of the thermal radiation is slightly higher for the RBI samples due to their lognormal pore size distribution including some larger pores compared to the Voronoi-based samples. Furthermore, as shown before, the total ETC due to conduction is higher for the Voronoi-based samples, which also reduces the relative importance of thermal radiation.

Figure 4: Effect of increasing average pore size on the ETC (a) and on the relative contribution of thermal radiation (b) for RBI generated samples.

5 Conclusions

A numerical framework is employed to study the heat transfer through cellular porous building blocks, aiming to assess the impact of the pore structure on their effective thermal conductivity. Two generation techniques are used in this paper to generate a set of porous samples with varying porosity and pore size distribution. Samples generated with the RBI technique tend to have a lower ETC than Voronoi-based samples at equal porosity, the difference becoming more pronounced at increasing matrix conductivity. This could either be due to the higher concentration of material in the cell walls for the Voronoi-based samples, or due to the wider pore size distribution of the RBI generated samples. Lastly, the relative contribution of thermal radiation inside the pore space is demonstrated to increase significantly with increasing pore size, increasing porosity and decreasing matrix conductivity. Simulation results obtained in this paper can assist optimization efforts to reduce the thermal conductivity of existing and novel porous building blocks.

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