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Implementation and validation of a 3D image-based prediction model for the thermal conductivity of cellular and granular porous building blocks

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Highlights

- A framework to predict the thermal conductivity of porous materials is introduced
- It allows performing pore-scale thermal simulations on 3D images of microstructures
- The verification with analytical reference solutions shows very good performance
- The experimental validation demonstrates the accuracy of the prediction framework

Abstract

Porous building blocks are increasingly being used in the building sector, as they offer a relatively high thermal resistance because of their porous microstructure. A clear understanding of the relation between the material's microstructural properties and effective thermal conductivity is still lacking though, impeding a correct analysis and design of existing and new porous building blocks. Therefore, this paper presents a 3D model framework to study the heat transfer through both cellular and granular porous building blocks, performing simulations directly at the pore scale. A 3D voxel-grid representation of the pore structure is adopted, allowing to study both virtually generated materials and actually available materials. The accuracy and the impact of the grid parameters is verified on a set of elementary microstructures, demonstrating a good performance when using adequate settings. The thermal conductivity simulation framework is validated against experimental measurements on two highly different porous materials: a low-porosity granular sintered glass filter and a highly-porous cellular-granular acoustic absorber. Comparison of simulation outcomes with experimental results confirms the good performance of the model, indicating its potential to evaluate and optimize the thermal conductivity of porous building blocks.

Keywords

Thermal conductivity; Thermal insulation; Porous building materials; Prediction model; Pore-scale simulations; Image-based; Micro-CT scanning; Virtual materials; Sintered glass filter; Reapor

Nomenclature

Roman

T Temperature (K)

d Distance between opposing pore cell walls

q	Heat flux (W/m ²)
V	Volume (m ³)
L	Length of cube side (m)
f_v	Pore volume distribution

Abbreviations

ETC	Effective thermal conductivity (W/mK)
SC	Simple cubic
BCC	Body-centered cubic
FCC	Face-centered cubic
Cel.	Cellular
Gran.	Granular
MIP	Mercury intrusion porosimetry
Exp. Meas.	Experimental measurements
CT	Computed tomography

Greek

λ	Thermal conductivity (W/mK)
ϵ	Emissivity (-)
σ	Stefan-Boltzmann constant $\left(5.67 * 10^{-8} \frac{W}{m^2 K^4}\right)$
γ	Pore shape factor (-)

Subscripts

rad	Radiative
max	Maximum

44

45 1. Introduction

46 1.1. Background

47 Heat transfer through opaque building components constitutes an important part of the total energy
 48 consumed by residential buildings. Insulation materials like mineral wool or several types of plastic
 49 foams are therefore often used to improve the thermal resistance. Their highly-porous nature
 50 effectuates indeed very low thermal conductivities, but on the other hand also relatively poor
 51 mechanical properties. Hence, they require to be used in combination with load-carrying elements
 52 like solid bricks or concrete slabs. Porous building blocks, on the other hand, aim to combine both

load-carrying and thermal insulation capacities [1–3]. Well-known commercial variants are cellular glass or cellular concrete. Typically, these blocks come as large brick-like elements, usually available in different thicknesses, sizes and densities. Hence, they provide alternative design options and easy on-site construction while reducing the heating and cooling energy requirements [4–6]. Furthermore, porous building blocks show great potential for upcycling secondary materials: several studies illustrate the production of porous building blocks including or based on e.g. slags or recycled ceramics [1,7–9]. Such valorization provides increasing economic return while reducing industry-generated waste streams. However, due to increasingly stringent energy requirements, a further reduction of the heat flow through these materials is needed to improve their performance and boost their application [10].

The heat transfer through porous materials is often described at the macroscale using Fourier’s heat conduction law making use of the material’s effective thermal conductivity (ETC). However, as illustrated in Figure 1, the total heat flow through the material originates from the complex interaction of several heat transfer mechanisms occurring at the microscale: thermal conduction through the solid matrix and the gas-filled pores, natural convection in the gas-filled pores, and radiation between the pore walls. Microstructural properties like the porosity and the matrix connectivity majorly affect each of these microscopic heat transfer mechanisms and accordingly also the macroscale effective thermal conductivity. Research on modelling and understanding this close relation is hence crucial in the development of improved building blocks.

Figure 1: Overview of heat transfer mechanisms at the pore scale: (a) matrix conduction, (b) gaseous conduction, (c) natural convection and (d) thermal radiation.

1.2. Literature and state-of-the-art

Several techniques have already been employed to characterize the impact of the microstructural properties on the ETC. These can roughly be classified in three categories: experimental, analytical and numerical studies. A non-exhaustive overview is discussed in this section.

Experimental studies, firstly, allow for a direct and reasonably accurate characterization of the thermal and microstructural properties of a porous material. Examples are the studies of Benoit-Ali et al. [11], Coquard et al. [12] and Smith et al. [13], who investigated a set of porous ceramics and metal foams with varying porosities, pore size distributions and matrix constitutions. Via detailed measurements of their macroscopic ETC, they studied the impact of, for example, the matrix conductivity or the spatial distribution of pores in the matrix. A similar study was performed by Goual et al. [14] on insulating clayey aerated concrete samples, while Aurangzeb et al. [15] conducted measurements on a set of limestone samples. Their results again clearly show the considerable effect of porosity and matrix conductivity on the ETC. While such experimental investigations provide interesting insights in the combined impact of these microstructural properties, a detailed study of the isolated influence of specific parameters is very difficult. Furthermore, the experimental preparation and measurement of porous samples is often expensive in time and cost. The inherent limitation to already-existing materials finally yields insufficient versatility to study and design new porous materials.

A second class of studies investigate the thermal behaviour of porous materials by developing analytical relations linking the ETC to a number of microstructural parameters. Excellent overviews of some analytical models can be found in Progelhof [16], Collishaw et al. [17] and a chapter by Singh [18]. The proposed relations are usually acquired through either theoretical considerations of the geometry and heat flow, or through the extrapolation of experimental measurements. Two well-known examples of the theoretical type are the series and parallel models attributed to Wiener, giving the absolute upper and lower bounds for the ETC. In this case, the analytical prediction formulas are

derived using a simplified serial or parallel organization of the matrix and gas phase. Similarly, other often-cited analytical-theoretical models like the models of Maxwell [19], Bruggeman [20] and Landauer [21] are usually deduced using some sort of simplification of the pore structure geometry or the present heat transfer mechanisms. Hence, although being very fast, their thermal conductivity prediction ability is rather indicative and lacks accuracy. The empirical type of analytical models provides increased accuracies by including an empirical factor that should be derived through experimental measurements. Well-known examples are the model of Asaad [22], Pande-Chaudhary [23] or Kunii-Smith [24]. Obtaining this empirical factor is cumbersome though and limits the applicability of the model to a certain class of existing materials.

Numerical models finally show great potential for a more thorough understanding of the material's thermal properties [25,26]. Simulating the heat transfer directly on the pore scale, they allow to obtain an effective thermal conductivity taking into account the material's true microstructural properties. Studied pore structures are usually obtained in one of three ways. A first strategy is employed by the unit-cell-based models [27–29]. The approach allows studying specific microstructural properties like pore size or matrix connectivity. Adopting a repetitive geometry furthermore maintains a relatively low complexity and computational cost. The number of possible unit cells is limited though and results are often not directly applicable to real materials because of their geometric simplicity. Hence, a second strategy comprises stochastically generating virtual microstructures to approximate the irregular nature of real materials. Wei et al. [30], Randrianalisoa et al. [31,32], Nait-Ali et al. [11] and Gaiselmann et al. [33] generated cellular structures representing foamed concrete, insulation foams, ceramic foams etc. Chen et al. [34] and Zang et al. [35] employed such generation algorithms to generate granular structures studying asphalt concrete and random particle distributions. These techniques hence facilitate the investigation of a broad range of material types and structures, and moreover to design new pore structures. Parameters needed to generate realistic microstructures are however difficult to define, impeding a thorough validation of the obtained results with experimental outcomes. Hence, a third strategy is adopted by a growing number of numerical investigations,

modelling the heat transfer in microstructures obtained through several imaging techniques. Coquard & Baillis [36], Mendes et al. [37] and Petrasch et al. [38] for example used micro-CT scanning to acquire a detailed representation of the microstructure of highly-porous plastic and ceramic foams. This enabled them to study the heat transfer taking into account the material's true microstructural parameters, like the porosity and pore connectivity. Furthermore, simulation results can be directly compared with experimental measurements performed at the macroscale like the ETC and the porosity. The thorough validation of this strategy is at present lacking though, clouding its merit for profound application on a broad range of materials.

Concluding, numerical modelling seems very promising for studying the micro- and macroscopic heat transfer through porous materials, with different pore structure representation strategies showing different advantages. However, validation and application on the broad range of porosities and microstructures encountered in typical porous building blocks still remains a daunting task. Furthermore, it still lacks of a unified approach integrating the different pore structure representation strategies and taking into account all relevant heat transfer mechanisms. A comprehensive and reliable framework could profoundly advance the study and design of new porous building blocks with improved thermal properties.

1.3. Paper scope & outline

In this paper, a numerical framework performing pore-scale simulations to quantify the heat transfer in porous building blocks is implemented and validated. Emphasis is placed on granular and (nearly-)closed-cell cellular types of porous microstructures. Both types are often encountered in porous building blocks due to their interesting mechanical and thermal properties. Indeed, cellular materials on the one hand, consisting of gas-filled cavities enclosed in a solid matrix, combine a relatively low thermal conductivity with excellent structural properties up to very high porosities [39]. Granular materials on the other hand, consisting of closely packed or partially overlapping particles, provide an improved thermal resistance in the low-porosity range compared to cellular materials [40,41].

Furthermore, both types of building blocks show great application value for the upcycling of secondary materials. Currently, the model framework does not target fibrous materials (like mineral wool) or highly reticulated materials consisting mainly of struts and very open-porous cells. Recent numerical work on these types of materials can i.e. be found in [42,43] (fibrous) and [44,45] (open-porous).

The paper starts with the implementation of a 3D image-based model framework, allowing to study the heat transfer for a wide range of porous materials, both virtually generated or scanned through micro-CT scanning. Subsequently, the model is verified numerically using a set of well-known regular pore structures. Finally, the model is applied and validated on two real materials. First, a sintered glass filter having a granular pore structure is studied, characterizing the microstructural and thermal properties experimentally and numerically. Subsequently, the same procedure is repeated for an acoustic absorber, having a two-scale cellular-granular pore structure. Hence, the model is validated for both cellular and granular materials with different thermal and microstructural properties.

2. Model framework

To quantify the effective thermal conductivity of cellular and granular porous materials, a novel numerical model framework performing pore-scale heat transfer simulations is implemented. The framework consists of three main steps, as shown in Figure 2: (1) obtaining the geometric representation of the microstructure, (2) creating a finite element mesh based on the microstructural image and (3) performing the thermal simulation of the microstructure. The entire framework is controlled via a set of MATLAB routines allowing an easy automatization and parametrization. All three steps are discussed in more detail below.

Figure 2: Overview of the model workflow: (a) micro-CT image as input; (b) virtually generated image as input; (c) finite element mesh; (d) temperature profile after simulation.

2.1. Geometry input

A correct representation of the material's microstructure is primordial to accurately capture the influence of the microstructural features – like the material porosity, matrix connectivity, ... – on the effective thermal conductivity. A 3D volumetric voxel image is adopted here since it provides easy and versatile modelling of both virtually generated and image-based structures. Besides, it alleviates the known underestimation encountered in 2D simulations models [46,47]. Similarly to 2D pixel images, voxel images consist of cubical elements organized in a regular 3D grid. The intensity value of each voxel depicts the material phase located at that specific position. The total amount of voxels and the side length of one voxel is called respectively the **image size** and the voxel size. These 3D images are generally acquired in one of 2 ways: through microscale scanning techniques for real materials, or through microstructure generation algorithms for virtual materials.

2.1.1. Real materials

Performing simulations on real materials enables a direct comparison of the model with experimental measurements of the thermal conductivity and microstructural features. Micro-CT scanning is a commonly used technique to characterize the microstructure of porous materials: the X-ray penetration of the sample is measured at incrementing sample rotation angles after which the obtained 2D projections are reconstructed into a 3D voxel image [48,49]. Typically, the smallest voxel size attainable with these systems is about 1 μm , while the maximum **image size** is around 1000^3 voxels. Major advancements throughout the past decennia have furthermore significantly reduced the amount of scanning inaccuracies and artefacts, allowing an adequate and detailed characterization of the microstructure. The resulting voxel image of a scanned cellular concrete is shown in Figure 2a.

2.1.2. *Virtual materials*

Performing simulations on virtual materials facilitates the study of specific microscale features and the evaluation of newly designed microstructures. The voxel image format is also adopted here, allowing a deterministic or stochastic generation of pore structures. Examples of deterministic generation are unit-cell-type materials like honeycomb structures or spheres organized on a regular lattice. Stochastic generation algorithms on the other hand can be used to generate a wide variation of microstructures, mimicking the typically stochastic nature of the microstructure of porous materials. Recent examples can be found in [30–33,50]. An example of a generated cellular material is shown in Figure 2b.

2.2. *Meshing of volumetric image*

A tetrahedral finite element mesh is constructed directly on the 3D voxel image using the Delaunay triangulation technique implemented in the open source MATLAB toolbox Iso2mesh and the CGAL C++ library [51,52]. The meshing algorithm allows a fast generation of a qualitative mesh of the complex pore structure, inherently smoothing out the jagged interfaces caused by the voxel representation. The mesh density in every material phase is controlled mainly through specifying the maximum radius of the Delaunay balls circumscribing the tetrahedral and triangular mesh elements. To ensure the conformity of the meshed interfaces with the 3D voxel image, the maximum distance between the center of the triangles and the original interface is usually set to half of the voxel size. Furthermore, an edge point insertion algorithm is added to the existing code to improve the approximation of the straight edges of the cubic sample. Finally, a quadratic shape function is used in every mesh element. An example of a finite element mesh is shown in Figure 2c.

2.3. *Thermal simulation*

Steady-state heat transfer is simulated by applying a temperature difference across the sample and setting adiabatic boundary conditions on the other sides. Conduction is modelled by specifying the thermal conductivity of the matrix and pore space elements. Values for these material properties are

commonly found in existing literature. Natural thermal convection is not modelled here since the characteristic dimensions of the pores in most porous building materials are below 2-4 millimeters, meaning that the contribution of convection to the total heat flow is negligible [53–56]. Thermal radiation between the pore cell walls, finally, is often neglected due to its modelling complexity. Detailed modelling strategies using view factor or ray-tracing algorithms indeed quickly become computationally exhaustive for irregular pore structures with large surface area. The contribution to the total ETC is, on the other hand, known to be strongly case-dependent, with increasing importance for open-celled materials, at elevated porosities and at high sample temperatures [26,53,57]. Since temperatures typically encountered in porous building blocks remain relatively low, a simplified approach for (nearly-)closed-cell materials is adopted in this paper, preserving the simplicity of the whole framework. An equivalent radiative thermal conductivity is defined for every pore according to the method described by Loeb [58]. This radiative conductivity ($\lambda_{rad,pore}$) is calculated as a function of the pore's characteristics using Equation (1). Apart from the emissivity ϵ of the pore walls, the Stefan-Boltzmann constant σ and the temperature T , the radiative conductivity depends linearly on the diameter $d_{max,pore}$ of the pore and a shape factor γ . This factor was calculated by Loeb to be 2/3 for spherical pores and was later corrected by Bakker to 0.45 [59].

$$\lambda_{rad,pore} = 4 * \epsilon * \sigma * d_{max,pore} * \gamma * T^3 \quad (1)$$

A set of algorithms is implemented in MATLAB to perform the calculation of the radiative conductivity for every pore, comprising 4 main steps. First, the whole pore space is subdivided into several pore clusters using a watershed-based separation-and-rejoin procedure similar to the algorithm used in Morpho+ [60]. Indeed, porous materials often consist of larger pore bodies interconnected via smaller pore throats. If the opening area of the throat is relatively small compared to the size of the connected pore bodies, the thermal radiation travelling from one pore body to another is effectively negligible. Hence the two pore bodies are split and a different radiative conductivity for both bodies is calculated. Subsequently, for every pore body the maximum internal distance $d_{max,pore}$ parallel to the direction

of the general heat flow is calculated. Thereafter, the radiative conductivity is calculated for every pore body using Equation (1). Although pores in real materials are commonly neither spherical nor ellipsoid, the shape factor of 0.45 proposed by Bakker for spherical pores is still adopted in this study for all the pores. Current work focuses on obtaining a more detailed calculation procedure for the shape factor per pore body. Finally the computed radiative conductivity is added for every pore body to the gaseous conductivity of the respective cluster. Inherently, this approach is limited to cellular-like materials with optically thick cell walls, since the methodology assumes no transmission through the cell walls. More complex strategies taking transmission into account can be found in a chapter by Baillis & Coquard [61]. Nonetheless, the methodology allows a computationally straightforward modelling of the radiative heat transfer at the pore scale, taking into account the pore's geometrical characteristics.

Thermal simulations have been performed in two numerical packages, COMSOL Multiphysics and Elmer [62], both leading to the same results. An example of a resulting temperature profile is shown in Figure 2d. After the simulation, the effective thermal conductivity of the sample can be calculated using Fourier's heat conduction law, rewritten for cubic samples in Equation (2) [34], where q_x is the heat flow in every element in the general heat transfer direction, V_{cube} the volume of the simulated sample, T_{hot} and T_{cold} the applied boundary temperatures and L_{sample} the width of the cubic sample.

$$ETC = \frac{\int_{V_{cube}} q_x * dV}{(T_{hot} - T_{cold}) * (L_{sample})^2} \quad (2)$$

3. Numerical verification

A thorough analysis of the impact of different microstructural properties requires an adequate framework performance over a wide range of possible pore structures. The model's accuracy is therefore assessed for three unit cell reference microstructures with varying porosities and composition. Numerical outcomes are verified with available reference results from literature. Subsequently, the influence of the voxel size and mesh size settings on the predicted thermal

conductivity is tested using the same reference structures, further investigating the model's numerical performance.

3.1. Verification of accuracy

The model's accuracy is verified using 3 different virtual periodic microstructures, consisting of equal-sized spherical inclusions organized in a continuous phase: the simple cubic (SC), the body-centered cubic (BCC) and the face-centered cubic (FCC) structure. The SC system contains a spherical inclusion on every corner of a cubic unit cell, while the BCC and FCC structure extend the SC system with a spherical inclusion in the middle of the cube or in the middle of every face of the cube, respectively. The cubic elemental lattice of all 3 systems is shown in Figure 3 for the case where the spheres touch. Both cellular and granular materials can be represented using these structures, considering the spheres as a gaseous phase embedded in a solid matrix (cellular) or as solid particles with gas around them (granular). The sample porosity, defined as the volume ratio of the low-conducting phase to the high-conducting phase, is varied from 10 to 90 % by adapting the sphere's diameter, yielding both structures with overlapping and non-overlapping spherical inclusions. Although this means that at high porosities granular materials lose their structural integrity, results are shown to widen the conclusions.

Figure 3: Unit cell examples of the three studied elementary arrangements of spheres in a regular lattice. Simple cubic (a), body-centered cubic (b) and face-centered cubic (c). The spheres are either designated as the high-conducting phase (granular configuration) or as the low-conducting phase (cellular configuration).

The model framework introduced in section 2 is applied to calculate the ETC of the different virtual microstructure systems. The voxel images are generated using a voxel size of $1/200^{\text{th}}$ of the sphere diameter, while setting the mesh size parameter to $1/50^{\text{th}}$ of the sphere diameter. The thermal conductivities of the conducting and insulating phase are set to respectively 1 W/mK and 0.01 W/mK, resulting in a conductivity ratio of 100. The spheres and the continuous matrix are consecutively designated as the conducting phase or insulating phase, simulating the heat transfer through granular

and cellular materials. Thermal radiation is not included to allow comparison with the conduction-only reference solutions explained below. Results are shown in Figure 4a-c for all three packing types as a function of the porosity. As expected, the thermal conductivity decreases with increasing porosity for both cellular and granular materials. For the granular case, the conductivity exhibits a steep drop until the packing porosity of the respective structure is reached. At higher porosities, the spheres become non-touching, meaning no direct heat flow path exists anymore through the high-conducting phase. For the cellular material, the continuous conducting phase is never fully interrupted, hence no such steep drops can be observed.

Figure 4: Simulation results and relative errors for the cellular and granular SC (a), BCC (b) and FCC (c) configuration. Graph (d) shows the relative errors for all three arrangements as a function of the sphere-matrix conductivity ratio. Results for the SC and FCC configuration are shown at a slightly different conductivity ratio for clarity.

The obtained conductivities are compared with analytical reference solutions for conductive heat flow found in literature [63,64]. Since these reference models are not defined for the whole porosity range, they are extended with numerical simulations performed in COMSOL using the software's proprietary geometry and meshing functionalities instead of the image-based approach implemented in the framework. The numerical reference results show very good agreement with the analytical solutions in their applicable porosity range. The relative error between the model framework and the reference solutions is calculated and depicted on the right axis of the graphs in Figure 4a-c. For the granular configuration, the largest deviations are observed around the packing porosity of the respective structure, where the spheres are just (not) overlapping. This can be explained by the voxel-based representation of the geometry, inherently resulting in a discretization error. In small, high-conducting regions, this effect becomes more articulated due to the absolute nature of this discretization error. This is indeed particularly the case at the packing porosity where an infinitely small contact surface is formed between the spheres. For the cellular configuration, deviations are generally increasing with increasing porosity. Again, at higher porosities the continuous conducting phase becomes relatively smaller, hence leading to increasingly relevant discretization errors. An appropriate voxel resolution should therefore be chosen considering the relative size of the conducting phase, as will be further elaborated in section 3.2.

The influence of the ratio of both material phases' thermal conductivity on the model's performance is studied by repeating the same simulations and changing the insulating phase's thermal conductivity from 0.01 W/mK to 0.1 W/mK. This results in a conductivity ratio of 10 instead of 100. The relative errors with the reference model are presented for all porosities in Figure 4d as a function of the sphere-matrix thermal conductivity ratio. As expected, the deviations decrease when the conductivity ratio approaches 1, since the effect of the geometrical discretization error diminishes.

3.2. Grid and mesh sensitivity

The numerical performance of the model is mainly affected by the 2 discretization parameters: the spatial resolution or voxel size of the 3D image, and the mesh size of the finite element mesh. Indeed, a fine resolution is needed to correctly represent the microstructural geometry, while an adequate mesh size ensures a satisfactory structural conformity of the microstructure and a reasonable approximation of the temperature and heat flow distribution. The influence of both parameters on the accuracy of the predicted ETC is investigated using the 3 regular lattice structures mentioned previously. 4 different voxel sizes, varying from $1/25^{\text{th}}$ to $1/200^{\text{th}}$ of the sphere diameter, are tested to build the 3D images. For the mesh size, the radius of the surface faces Delaunay balls and the tetrahedra circumscribing balls is varied from $1/10^{\text{th}}$ to $1/50^{\text{th}}$ of the sphere diameter. The thermal conductivity ratio is set to 100 and 0.01 to obtain cellular and granular arrangements respectively. The deviations between the numerical reference model and the model framework simulations are shown in Figure 5.

As expected, a finer voxel size (or improved resolution) and a smaller mesh size (or higher mesh density) generally lead to increased accuracies. For cellular materials, the error generally increases with increasing porosity, meaning a finer voxel grid and mesh size should be used to obtain accurate results for high-porosity samples. As already stated in the previous section, this is due to the discretization error of the conducting matrix induced by the voxel-based representation, which becomes more pronounced for thin microstructural features. For the granular materials, the error increases till the packing porosity where the conducting particles just overlap, after which the error generally decreases with increasing porosity. This is again explained by the discretization error in the representation of the microstructures, since the contact zones between the particles become gradually smaller at increasing porosity till the packing porosity. In conclusion, the attained accuracy varies appreciably with the type of structure (cellular or granular), the configuration of the matrix (SC, BCC and FCC), and the concerning porosity, making it difficult to formulate universal guidelines for choosing optimal discretization parameters. Cellular materials with high porosities or granular

355 materials with small contact surfaces between the particles demand a finer discretization to obtain a
356 certain accuracy. However, the selection of the discretization settings should be performed with
357 caution and a convergence analysis should be performed if possible. Finally, as indicated in Figure 4d,
358 it is expected that these effects depend on the phases' thermal conductivity ratios as well, mostly
359 requiring less fine voxel and mesh sizes with decreasing matrix-fluid conductivity ratios. Indeed, the
360 geometrical discretization errors induced by the voxel-based representation become less pronounced
361 at lower thermal conductivity ratios.

Figure 5: Influence of discretization parameters on the accuracy of the model framework for three regular structures as a function of the porosity. A thermal conductivity ratio of 100 is employed.

4. Experimental validation on glass filter

The previous section discussed the well-functioning of the model framework for repetitive configurations of the pores and matrix. However, real materials have much more irregular pore structures implicating a more complex heat flow pattern. Therefore, this section validates the model's performance for studying a real granular material, in casu a sintered glass filter. Pore-scale simulations performed on micro-CT scans are compared with experimental results. Measurements and simulations are performed on both air-dry and water-saturated samples: this enlarges the validation set and the resulting conclusions.

4.1. Material

A commercial ROBU P100 sintered glass filter is used as a first validation material. The material has a granular type of microstructure, produced by sintering together finely milled borosilicate 3.3 glass particles. Typically applied to filter liquids, the material has an open pore structure with a reasonably well controlled porosity and narrow pore volume distribution, making it a very suitable first validation material.

4.2. Experimental characterization

The material's thermal conductivity is measured experimentally to allow for validation with the numerical simulations in the following paragraph. Subsequently, the pore structure of the sintered glass filter is characterized and visualized using different techniques.

4.2.1. Thermal conductivity

The thermal conductivity of the sintered glass filter is measured using a Heat Flow Meter apparatus designed for the measurement of small samples. The setup is calibrated using a known reference sample and has an estimated error below 5 %. Six samples of $10 \times 10 \times 3.33 \text{ cm}^3$ are used for these thermal conductivity experiments. All measurements are performed at an average temperature of 20 °C and a temperature difference of 10 K between the hot and cold plate. The air-dry thermal conductivity is obtained after oven-drying the samples for several days until no meaningful change of

mass could be observed. For the water-saturated thermal conductivity, samples are first saturated using the vacuum saturation setup and subsequently carefully packed in plastic foil. Measurement of the mass before and after the thermal conductivity measurement revealed no loss of water content. The air-dry and water-saturated thermal conductivity results are shown in Table 1.

Table 1: Results of experimental characterization of the sintered glass filter.

Measured property	Average	Standard deviation
Bulk density	1431.8 kg/m ³	4.9 kg/m ³
Open porosity	35.8 %	0.2 %
Dry ETC @ 20 °C	0.376 W/mK	0.008 W/mK
Saturated ETC @ 20 °C	0.889 W/mK	0.01 W/mK

4.2.2. Porosity

The open porosities of the same six samples of the sintered glass filter are determined using a vacuum saturation setup [65], yielding an average open porosity of 35.8 %, conform with the manufacturer's technical data, see Table 1. Furthermore, the total porosity (calculated by comparing the dry bulk density with the glass particle density) corresponds almost perfectly with the open porosity, indicating the absence of closed porosity in the samples.

4.2.3. Pore volume distribution

The pore volume distribution is characterized using the mercury intrusion porosimetry technique [66] on an oven-dried sample of 2 x 1 x 1 cm³. The resulting pore volume distribution is shown in Figure 6a. It can be noted that the material has a relatively narrow pore volume distribution, ranging from 20 µm to 100 µm, meaning all pores are properly visualizable in one X-ray scan.

4.2.4. Micro-CT scanning

A detailed 3D image of the pore structure is obtained using micro-CT scanning. A total of 5 cylindrical samples are extracted from the sintered glass filter samples, with diameters varying around 4 mm. 3 samples were scanned using the GE Nanotom with a voxel size of 2.5 µm. Two other samples were

scanned using a Skyscan 1172 machine, with a voxel size of 1.9 μm and 2.9 μm respectively. Sample details are specified in Table 2.

Table 2: details of the samples used in the Micro-CT scanning process.

Sample	Machine	Voxel size [μm]	Scanning location	Porosity after segmentation [%]
A	GE Nanotom	2.5	Bottom/middle/top	30.9/32.8/32.5
B	GE Nanotom	2.5	Bottom/middle/top	34.7/35.2/32.4
C	GE Nanotom	2.5	Middle	36.6
D	Skyscan 1172	1.9	Middle	36.6
E	Skyscan 1172	2.9	Middle	36.6

After reconstruction of the scans, a dual threshold segmentation algorithm is applied on all obtained 3D grayscale images, differentiating matrix and pore space voxels [67]. The total porosity of each scanned sample can subsequently be derived from the 3D voxel image, see Table 2. The results for sample C, D and E correspond very well to the measured porosity shown in Table 1, while parts of sample A and B show larger deviations probably due to local inhomogeneities. A slice result of sample C is shown in Figure 6b.

Figure 6: (a) measured pore volume distribution of the sintered glass filter; (b) a slice of the glass filter Micro-CT scan; (c) a render of the temperature profile after the simulation.

4.3. Numerical simulation

The model framework is applied to numerically predict the thermal conductivity of the sintered glass filter. Four subsamples are extracted from each of the segmented 3D images. The simulated image size of the subsamples from samples A, B, C, sample D and sample E is set to respectively 500^3 , 600^3 and 400^3 , yielding each time a simulated cubic volume with a side length above 1 mm. The tetrahedral and triangular mesh size parameter is set to 10 μm , the edge points insertion size and the surface

approximation size are set to half of the voxel size. Mesh refinement analysis shows no further improvement. The thermal conductivity of the solid glass particles is set to 1.13 W/mK, according to the manufacturer's datasheet [68]. The thermal conductivity of the pores was set to 0.026 W/mK for the air-dry case [69] and 0.598 W/mK for the water-saturated case [70]. Thermal radiation is expected to be negligible for the low porosity and small average pore size involved [53]. This was confirmed by a simulation on 1 subsample of sample C, revealing an increase of only 0.1% in the ETC when including thermal radiation. It is therefore not taken into account in the other simulations. The resulting temperature profile of one of the air-dry simulation samples is shown in Figure 6c.

4.4. Results and discussion

The experimental and numerical results are shown in Figure 7a and c for the air-dry respectively water-saturated case, together with the results predicted by 5 known analytical models. A least-squares power-law trendline is fitted through all the numerical results, showing an expected decrease of the ETC with increasing porosity for both cases. To allow for a reliable assessment of the model's accuracy, a zoom is shown for the region around the experimentally measured results in Figure 7b and d; the analytical models are not repeated in the zoom for clarity.

Figure 7: Comparison of experimental and simulation results for the sintered glass filter together with a zoom on the region around the experimental results in air-dry (a,b) and water-saturated (c,d) condition. Analytical models are not repeated in the zoom for clarity.

Starting with the air-dry case, the results agree relatively well with the average measured ETC, showing a similar trend with porosity as the analytical models but with a highly improved accuracy. For sample C and the bottom and middle of sample B, all scanned with a voxel size of 2.5 μm and showing porosities close to the experimental, average deviations vary between 4.1 % and 11 %, differences occurring due to local inhomogeneities. The average results of sample D and E on the other hand, scanned at 1.9 μm and 2.9 μm , perform respectively very well and slightly worse. This is probably explained by the differing voxel sizes of the scans. Indeed, as revealed by the verification study in the previous section, simulations on granular materials are relatively sensitive to the voxel size used in the geometric representation of the material's microstructure. This effect is also clearly visible here in Figure 7b, showing an increasing accuracy with decreasing voxel size at approximately equal sample porosity. Lastly, the simulations on sample A and the top side of sample B agree less with the

experimentally measured thermal conductivity, due to the larger discrepancy between their porosity and the macroscale porosity. On the other hand, they clearly indicate the logical variation of the sample's ETC with changing porosity, similar to the analytical models. Samples with microstructural properties close to the average macroscale properties should hence be selected when trying to obtain a simulated thermal conductivity close to the material's macroscale ETC.

For the water-saturated case shown in Figure 7c and d, both the simulations and the analytical models give very similar results. The relative deviations with the experimental measurements are below 5 %, which is generally smaller compared with the air-dry case. Furthermore, results are less scattered around the trendline fitted through the simulations. This can be explained by the lower solid-fluid thermal conductivity ratio: the relative impact of the microstructural properties like porosity, connectivity etc. is hence less important.

Concluding, both the air-dry and water-saturated simulation results agree relatively well with the experimental outcomes. The framework clearly outperforms common analytical models for high matrix-fluid conductivity ratios. This demonstrates the importance of taking into account the true microstructural properties of the porous material when studying its ETC. However, samples with porosities close to the macroscale porosity should be selected to obtain results similar to the macroscale thermal conductivity. Furthermore, the applied voxel size plays an important role, indicating an increasing accuracy with decreasing voxel size. With proper settings, the model shows the capability to reliably study the thermal conductivity of granular porous materials and obtain results with deviations below 10 %.

5. Experimental validation on acoustic absorber Reapor

A second validation study is performed on a commercial acoustic absorber Reapor, having a relatively high porosity and a mixed cellular-granular type of microstructure. The microstructural and thermal properties are again characterized experimentally and are compared with the simulation results

obtained using the model framework. A hierarchical approach is used to overcome the multiscale nature of the material.

5.1. Material

Reapor is a highly-porous material mainly applied for acoustic absorption. The production process is based on recycled glass and consists of sintering together expanded granules, hence leading to a pore structure with a two-scale type of pore volume distribution: a cellular structure inside the granules and a granular structure overall, both open-celled to maximize the acoustic absorptivity. A photograph of the material's pore structure is shown in Figure 8a.

5.2. Experimental characterization

Similarly to the study on the sintered glass filter, the pore structure is characterized experimentally to interpret obtained results. The thermal conductivity is again measured in air-dry and water-saturated condition.

5.2.1. Thermal conductivity

The thermal conductivity of five Reapor samples of $10 \times 10 \times 2 \text{ cm}^3$ is measured using the Heat Flow Meter apparatus. Since the datasheet [71] mentions a thermal conductivity of 0.08 W/mK at $10 \text{ }^\circ\text{C}$, all measurements are performed at an average temperature of $10 \text{ }^\circ\text{C}$ to permit a comparison. The temperature difference between the hot and cold plate is kept at 10 K . The air-dry thermal conductivity is obtained after oven-drying the samples for several days until no meaningful change of mass could be observed. For the water-saturated thermal conductivity, samples are first saturated using the vacuum saturation setup and are subsequently inserted into a water-filled container made of PUR insulation, which can be brought into the heat flow meter setup. The air-dry and water-saturated thermal conductivity results are shown in Table 3.

Table 3: Results of the experimental characterization of the acoustic absorber Reapor.

Measured property	Average	Standard deviation
Bulk density	262.8 kg/m ³	2.5 kg/m ³
Open porosity	88.5 %	0.2 %
Dry ETC @ 10 °C	0.084 W/mK	0.002 W/mK
Saturated ETC @ 10 °C	0.617 W/mK	0.014 W/mK

5.2.2. Porosity

The open porosity of the Reapor material is determined for the same five samples using a vacuum saturation setup, yielding an average open porosity of 88.5 %, see Table 3. Again, the total porosity, calculated by comparing the dry bulk density of 270 kg/m³ stated by the manufacturer [71] with an average glass matrix density of 2500 kg/m³, corresponds almost perfectly with the open porosity, confirming the interconnected nature of the pore space.

5.2.3. Pore volume distribution

The pore volume distribution is characterized using the mercury intrusion porosimetry technique on an oven-dried sample of 2 x 1 x 1 cm³. The resulting pore volume distribution is shown in Figure 8b. It can be noted that the material has two pore classes: the first is indicated by the peak around the pore diameter of 15 µm, representing the pore throats given access to the cellular pores inside the granules. Part of the second pore class is indicated by the peak starting above 100 µm, corresponding to the pore space in between the sintered granules with pore diameters in the millimeter range. Although these large pores cannot be characterized in more detail using the MIP setup, visual inspection of the sample clearly shows the existence of these pores.

5.2.4. Micro-CT scanning

To obtain a detailed visualization of both classes of pore diameters, micro-CT scans are made at both discussed scales. At the intragranular scale, two scans are made on some extracted granules, with a voxel size of 1.5 µm and 1.6 µm. At the intergranular scale, a scan is made on a cylinder of about 2.5 cm diameter at a voxel size of 16 µm, characterizing the granular structure of the material. Pores that are still visible inside the granules are artificially solidified since these were already visualized in the

intragranular scan. All scans are performed using the GE Nanotom machine. After reconstruction, the same dual threshold algorithm is applied on all obtained 3D grayscale images for segmentation [67]. A slice is shown in Figure 8c and d for the intra- and intergranular scanning results together with a reconstructed and segmented 3D image of both scans (e-f).

Figure 8: (a) photograph of sample pore structure with the bimodal pore volume distribution clearly visible; (b) measured pore volume distribution of the Reapor material; (c-d) Micro-CT slice scan result of the intra- and intergranular scale; (e-f) segmented 3D image of intra- and intergranular scale scans.

5.3. Numerical simulations

The model framework is applied to predict the thermal conductivity of the Reapor material. As there is a clear separation between the intra- and intergranular pore structures, a hierarchical approach is adopted to overcome the two-scale nature of the material: simulation results obtained on the intragranular level are averaged and used in the simulations performed on the intergranular scale. All simulations are performed at a mean sample temperature of 10 °C to allow for a correct comparison with the experimental measurements and the technical datasheet.

5.3.1. Intragranular scale

A total of 7 subsamples is extracted from both scans made at the intragranular scale. A simulated image size of 300^3 is employed to ensure that every sample fits completely inside the granules. The tetrahedral and triangular mesh size parameter is set to $4.8\text{ }\mu\text{m}$, the edge points insertion size and the surface approximation size are set to half of the voxel size. Mesh refinement analysis again shows no further improvement. Based on the chemical composition mentioned in the technical datasheet [71], the glass matrix thermal conductivity is determined to be 1.06 W/mK according to the formula of Choudhary [72]. The thermal conductivity of the pores is set to 0.025 W/mK for the air-dry case [69] and 0.578 W/mK for the water-saturated case for $10\text{ }^\circ\text{C}$ mean temperature [70]. Thermal radiation is taken into account in the air-dry case using the previously described method of Loeb, setting the emissivity of the glass pore walls to 0.9 [73]. Thermal radiation is not taken into account in the water-saturated case: the relatively large absorption coefficient of water at room temperature eliminates almost all radiative heat exchange between opposing pore cell walls [74].

5.3.2. Intergranular scale

Five subsamples are extracted from the scan made at a voxel size of $16\text{ }\mu\text{m}$, each having a simulated image size of 400^3 and hence a side length of 6.4 mm . The tetrahedral and triangular mesh size parameter is set to $48\text{ }\mu\text{m}$, the edge points insertion size and the surface approximation size are set to half of the voxel size. Mesh refinement analysis again shows no further improvement. The thermal conductivity of the (now considered completely solid) granules is set to the value corresponding to the average porosity encountered at the intragranular scale. Obviously, the thermal conductivity of the air or water inside the pores remains the same as in the lower-scale simulations. Thermal radiation is again taken into account using an emissivity of 0.9 for the glass pore walls [73].

5.4. Results and discussion

5.4.1. Intragranular scale

The simulation results of the 7 subsamples extracted from sample 1 and 2 are shown in Figure 9 for the air-dry and water-saturated case. A least-squares power-law trendline is fitted through the results, showing an expected decrease of the thermal conductivity with increasing porosity for both cases. The rather large variation between the different samples is due to the small size of the simulated volumes, limited to fit inside the granules. The average porosity encountered in the simulated samples is 81.2 %, which results according to the trendline in an average thermal conductivity of 0.129 W/mK and 0.655 W/mK for the granules in the air-dry and water-saturated case respectively. Thermal radiation accounts only for about 2 % of the calculated ETC for the air-dry case, due to the small pore sizes inside the granules and the relatively low average sample temperature (10 °C).

Figure 9: Simulation results on the intragranular scale in the air-dry case (a) and the water-saturated case (b).

5.4.2. Intergranular scale

The experimental and numerical results for the whole material are shown together with a zoom in Figure 10a and b for the air-dry case and Figure 10c and d for the water-saturated case. Results predicted by the analytical models and the value retrieved in the manufacturer's technical datasheet [71] are also shown. A least-squares power-law trendline is fitted through the numerical results. For the calculation of the porosity of the simulation samples, the calculated average porosity of 81.2 % is

assumed inside all the granules, leading to overall porosities very close to the experimentally measured values.

Figure 10: Comparison of experimental and simulation results for the Reapor material together with a zoom on the region around the experimental results in air-dry (a,b) and water-saturated (c,d) condition. The technical data is also shown for the air-dry case. Analytical models are not repeated in the zoom for clarity.

The simulated air-dry thermal conductivities are relatively close to the experimental results, showing a decrease with porosity similar to the analytical models. On average, a relative deviation of about 5 % is achieved, indicating the good performance of the model framework and validating its application for two-scale hierarchical simulations. The framework performs furthermore much more accurate than the results predicted by the analytical models. For the air-dry case, thermal radiation accounts for about 3 % of the total ETC. This rather low influence is explained by the small pore size inside the granules, the low macro-porosity between the granules and the low average sample temperature (10 °C). For the water-saturated case, simulations agree almost perfectly with the measurements, achieving deviations around 1 %. Similarly as in the sintered glass filter case, the model shows a better

performance relative to the air-dry case because of the lower solid-fluid thermal conductivity ratio. The results of the analytical models also agree very well with the experiments, for the same reason. Concluding, the model framework allows to accurately predict the thermal conductivity of the Reapor material both in air-dry and water-saturated conditions, indicating its capability to study the thermal conductivity of highly porous building blocks with a cellular, granular or even mixed pore structure. Furthermore, the possibility to apply the model in a hierarchical approach to study materials with a multiscale pore network is demonstrated to give good results, widening its applicability to a broad range of materials.

6. Conclusion

In this paper, a numerical framework is presented to study and predict the effective thermal conductivity of porous building blocks. The model is based on a voxel-grid representation of the material's microstructure, allowing to perform 3D heat transfer simulations on both real and virtual materials. Both conductive and radiative heat transfer is taken into account directly at the pore scale. Verification of the framework against 3 regular lattices showed a very good performance for porosities varying from 10 to 90 %, for cellular and granular compositions. A grid sensitivity study highlighted the importance of using an appropriate voxel size to represent the microstructure, demanding a finer grid for high-porosity cellular materials and for granular materials with small contact zones between the conducting particles. The framework is validated against measurements on two different materials: a low-porosity granular sintered glass filter, and a high-porosity cellular-granular acoustic absorber with a two-scale microstructure. Simulations were performed on images of the materials obtained through micro-CT scanning and were compared with the experimental thermal conductivities. For the Reapor material, a hierarchical approach was used to overcome the multiscale nature of the material. When using appropriate settings and samples with a porosity close to the macroscale porosity, simulations showed deviations below 10 % for both materials in dry condition, hence outperforming commonly used analytical prediction models. For the water-saturated case, deviations below 5 % were obtained,

which can be attributed to the lower solid-fluid thermal conductivity ratio. Concluding, the numerical framework shows the capability to reliably study and predict the effective thermal conductivity of porous building blocks over a wide range of porosities and for both cellular and granular types of pore structures. Hence, it provides a promising tool to investigate the impact of several microstructural properties on the total heat flow through the material, allowing to design and optimize new porous building blocks.

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