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Investigation of the relationship between morphology and permeability for open-cell foams using virtual materials testing

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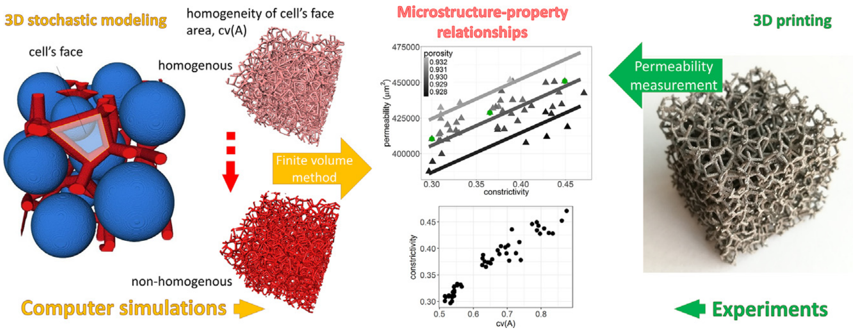
HIGHLIGHTS

- A stochastic 3D microstructure model is used to generate open-cell foam structures with varying distribution of face sizes.
- The coefficient of variation of face sizes strongly influences constrictivity, a measure for bottleneck effects
- Permeability of the virtual, but realistic microstructures with different values of constrictivity is simulated.
- An experimental validation is performed by 3D printing of some structures and experimental measurement of pressure drop.
- A linear relationship between constrictivity and permeability is found, where other structural properties are kept fixed.

GRAPHICAL ABSTRACT



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ABSTRACT

The effect of the morphology of open-cell foam structures on their functional properties is investigated. A stochastic microstructure model is used to generate representative 3D open-cell foam structures, where morphological properties are systematically varied. Subsequently, permeability of these virtual, but realistic microstructures is determined using the finite volume method. This procedure, which is called virtual materials testing, has recently been employed to investigate the effect of the variation of cell sizes on permeability. In the present paper, we introduce a stochastic microstructure model that can be used to generate structures with varying distribution of (open) face sizes between cells. It turns out that this characteristic strongly influences the so-called constrictivity, a measure for bottleneck effects which, in turn, has a strong impact on the resulting permeability. Moreover, we show how the virtual materials testing approach can be applied to derive empirical formulas between descriptors of 3D morphology and functionality. Additionally, an experimental validation of the simulation results is performed by printing three of the virtual structures using selective laser melting and subsequent experimental measurement of pressure drop, which allows calculation of the permeability using Darcy's law.

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1. Introduction

Open-cell foams offer a wide range of possible applications, e.g. as filters [1], as materials for heat exchangers [2], or as catalyst supports [3]. For an overview, we refer to [4]. Depending on the application, different functional properties are desirable and the identification of foam structures that optimize functionality is an important goal. It is known that the microstructure of open-cell foams has a strong influence on their functional properties, see, e.g., [5]. There are many experimental studies which investigate this relationship, see, e.g. [6–8] for the effect of porosities and pore densities on pressure drop in open-cell alumina foams. However, laboratory experiments require huge efforts, which involve manufacturing, tomographic imaging, quantification of structural characteristics and analysis of functional properties.

A way to facilitate the materials design process is to use modeling and simulation. An early approach to express functional properties in a formula by geometric parameters can be found in [9]. There, permeability is considered as a functional property, which is expressed as a function of geometric parameters under certain assumptions of the underlying geometry. To be more precise, the flow phase is assumed to consist of non-intersecting tubes canted at a given angle. It is shown that the function correctly predicts the order of magnitude of permeability also for more complex systems, however, the exact value is misjudged already by a factor of 2 for random lattice networks. Extensions of this work are presented in [10] and [11], where sound absorption properties are related to morphological characteristics. Still, an idealized structure is considered, i.e., a so called unit-cell. This approach neglects more refined morphological properties. An overview on further modeling approaches for thermal conductivity and hydraulic properties in open-cell foams can be found in [12] and [13].

In the present paper, in contrast to analytical models and models for idealized structures, we propose a different approach, which is purely data-driven, where data is gained from simulated, realistic 3D microstructures. The idea is to generate a wide spectrum of virtual, but realistic microstructures, and to analyze functional properties using, e.g., the finite volume method (FVM) or finite element method (FEM), see, e.g., [14]. As, in many materials, different regions in the same piece of material can have slightly different microstructures, which are, however, similar in a statistical sense, stochastic microstructure models are used for generating 3D microstructures as input information for the simulation of functional properties. These models capture the local heterogeneity of the material, but reflect its overall statistical properties, see, e.g., [15,16]. The whole procedure, which is called virtual materials testing, can then be used to derive relationships between morphological and functional properties, which finally allows one to identify structures with preferable functional properties. This has, e.g., successfully been done in [17] for predicting effective conductivity in materials dedicated to fuel cell applications. While the resulting formulas are not directly deduced by arguments from theoretical physics, the procedure has two main advantages. On the one hand, instead of idealized unit cells, realistic 3D structures are considered, where the stochastic modeling approach ensures that the local randomness of the structure within materials is captured. On the other hand, the formulas that are derived typically lead to a high prediction accuracy [17].

Thus, if a tool is on hand that systematically generates virtual open-cell foam microstructures with varying morphological properties on the computer, numerical simulations can be used to predict the permeability of these virtual materials. A stochastic model based on Laguerre tessellations induced by a random packing of non-overlapping spheres is widely used in literature [18,19]. A Laguerre tessellation divides the region of interest into a system of convex polytopes. Each polytope is interpreted as a cell of the foam structure, and the edges of each cell are considered as a model of the strut system of open-cell foams. The edges are either dilated to tubes [18] or dilated by spheres with locally varying size to account for the fact that in real microstructures struts are thicker near the junctions than in their middle parts [20]. A great advantage of the approach via Laguerre tessellations is that it allows for a systematic variation of the cell volume distribution, see e.g. [21]. This allows (in combination with FVM) an investigation of the influence of variations of cell volumes on pressure drop, see [22]. However, it is well known that the performance of functional materials is typically influenced by several morphological characteristics, see, e.g., [17]. The goal of the present paper is to investigate the influence of the coefficient of variation of (open) face sizes (where a ‘face’ is the surface between two cells). For open-cell foams, the faces play an important role, as the transport paths are passing through them. Note that in [10], the effect of the so-called ‘throat size’, which is related to the face size, has been investigated based on a single, idealized cell. Here, we consider a realistic 3D system of cells with random variation of cell and face sizes, as they occur in real materials. This allows us to not only investigate the effect of one deterministic face size for all cells in the system, but the variation of face sizes within each structure.

In order to investigate the influence of the distribution of face sizes, a modeling approach for open-cell foams that allows a systematic variation of the face size distribution, while keeping other properties fixed, is needed. The modeling approach via random Laguerre tessellations based on non-overlapping spheres can be extended to systems of overlapping spheres, as the tessellation can be defined in the same manner. This generalization of the modeling approach enlarges the set of possibly generated structures, giving the option to systematically vary other morphological characteristics. In particular, with increasing overlap of spheres, the distribution of face sizes can be modified. Moreover, the stochastic model renders it possible to keep the coefficient of variation of cell volumes almost constant, while varying the coefficient of variation of face sizes. This finally enables us to investigate the influence of the face size distribution on permeability independently of the influence of the cell volume distribution. It turns out that the coefficient of variation of the face sizes is strongly correlated with the so-called constrictivity, a morphological parameter describing bottleneck effects [23]. Subsequently, an analysis of permeability of the simulated structures is performed using FVM. The results indicate that with increasing coefficient of variation of face sizes, the constrictivity increases, which ultimately leads to an increase in permeability.

An experimental validation of our findings is performed by 3D printing of three of the virtual structures generated by the stochastic model using selective laser melting (SLM) [24] and subsequent experimental analysis of pressure drop. Permeability is then calculated using Darcy's law [25].

The outline of this paper is as follows. In Section 2, the applied methods are introduced. In particular, the stochastic microstructure model is described in detail in Section 2.1, its usage to generate structures with different morphological properties is discussed in Section 2.2, fluid flow simulations via FVM are described in Section 2.3, SLM for printing virtual structures is explained in Section 2.4, and the experimental measurement of pressure drop is described in Section 2.5. In Section 3, an experimental validation of our approach is presented. Then, in Section 4 the results of our investigations are presented and discussed. A comparison to structures with a different morphology of the struts is shown in Section 5. Conclusions are given in Section 6.

2. Methods

2.1. Stochastic microstructure model

As already mentioned above, random Laguerre tessellations based on systems of overlapping spheres are used for the stochastic