Abstract

A stochastic microstructure model based on a random Laguerre tessellation is used to simulate virtual open cell foam structures. Both, circular cylindric and concave triangular strut cross section shapes are considered. Additional geometry modifications are introduced by relaxation of the tessellation cells using the Surface Evolver and by closing a certain percentage of the foam windows. The effect of these modifications on the foams’ permeabilities is investigated. In particular, permeability anisotropies resulting from anisotropic closing of the windows are taken into account. The dimensionless permeability (Darcy number) in the different directions is well explained by regression models using porosity, tortuosity, and constrictivity as explanatory variables.

Keywords: Laguerre tessellation, anisotropy, porous medium, virtual material design, stochastic microstructure model, computational fluid dynamics

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1 Introduction

Foam structures are used in a wide range of application areas such as filtration [31], separation science [9, 16], solid-phase extraction [24], or chromatography [8]. The design of foam structures for these applications requires a characterization of the flow through the foam’s pore space. It is well known that flow characteristics such as permeability or equipollent pressure drop highly depend on geometric microstructure characteristics such as the porosity, the specific surface area, or the tortuosity. Additionally, the flow properties in different directions may differ depending on the degree of anisotropy of the pore space. An understanding of relations between geometric microstructure characteristics and the foam’s performance is crucial for finding an optimal design for a specific application.

Modern methods of material synthesis such as 3D printing enable the production of a wide range of microstructure geometries [32 40]. Simple foam structures for 3D printing can be obtained by dilating the edge system of a deterministic tessellation such as the Kelvin foam [36]. In practice, a certain amount of randomness of the cell structure may be beneficial. This suggests the use of random tessellation models like Voronoi or Laguerre tessellations for the generation of the cell systems. By choosing the system of generators of the tessellation appropriately, the distributions of size and shape of the tessellation cells can be varied [30]. Additional geometry modifications can be introduced by changing the cross section shape of the struts [6] and by closing some of the foam’s windows [35, 19]. As these modifications increase the specific surface area of the foam, they are of particular interest for applications where particles or cells should be captured on the foam surface.

Motivated by these applications, we will investigate the influence of several geometry modifications on the permeability of (partly) open foam structures. The permeability is an important criterion for characterising flow through a porous medium. It quantifies the pressure loss due to the flow through the structure. Therefore, it is an indicator of the energy consumption during usage. Permeability can be interpreted as a function of different geometric characteristics of the foam. It is obvious that the permeability
will decrease with increasing cell density and decreasing porosity, see e.g. [27]. The influence of further cell characteristics such as the variation of cell or facet sizes, the cell shape, or the cross section shape of the struts is less obvious. To systematically analyze correlations between these characteristics and the permeability of an open-cell foam, virtual foam structures can be simulated from a stochastic geometry model whose geometric features can be controlled by a number of parameters. With the help of flow simulations and the subsequent computation of permeability in foam structures with different parameters, the influence of different geometric characteristics on permeability can be investigated. Ambrosio et al. [1] investigated the influence of the strut cross section shape on the pressure drop in a deterministic foam model based on the Kelvin cell. Strut cross sections could be varied from convex triangular to highly concave using a given shape parameter. In comparison, minimal pressure drop was observed for convex cross section shape. Mills et al. [26] simulated air flow through wet Kelvin cells. Their results suggest that, for fixed cell size, permeability is governed by the area of the tessellation facets which form the windows between the foam cells. The Weaire-Phelan foam [38] is another well-known deterministic foam model. For high porosities, the pressure drop computed in this model was shown to be similar to that of the Kelvin foam [11].

Models that allow for a stochastic variation of the cell geometry are the Voronoi and the Laguerre tessellation. In [32], the effect of cell size variation was studied. Lower pressure drop was obtained for more inhomogeneous cell sizes. Homogeneity of the cell size distribution was measured by using the coefficient of variation (CV) of the cell volume distribution, i.e. the ratio of the standard deviation over the mean. As the windows between the foam cells are bottlenecks for the flow, the facet size distribution is another parameter influencing the permeability of a foam. In [10], an increasing CV of the facet area distribution was shown to result in a higher permeability. In the same work, it was shown that a locally varying strut thickness with reduced thickness in the center also increases the permeability. In [6], the difference between a circular and a triangular cross section shape in a Voronoi model was investigated. For otherwise equal cell systems, the triangular cross section resulted in a 15-20 % increase of pressure drop compared to a
circular strut cross section.

Depending on the production process, real foams may not be completely open but contain a certain fraction of closed windows. As outlined above, adding closed windows may also be of interest in synthetic foams to increase their surface area. Since this changes possible flow paths through the pore space, closed windows affect the permeability. Hoang and Perrot [35] studied the influence of the fraction of closed windows in a Kelvin foam on the (acoustic) transport properties of the material. Langlois et al. [23] considered partly closed windows, i.e. windows closed up to a circular aperture, in a Kelvin foam and derived a power law relating permeability to the aperture size. Additionally, the influence of the fraction of closed windows in Kelvin foams was investigated when using completely closed windows. In [31], anisotropy of the permeability tensor due to a preference of certain directions in the system of closed windows was reported but not systematically analysed, see also [19].

In this paper, realizations of random Laguerre tessellations are used to investigate the permeability of open-cell foam structures. The effect of several modifications in the microstructure geometry is investigated. In the first step, completely open foams with two different cross section shapes (circular and concave triangular) are considered. To simulate partially closed foams, a certain percentage of the tessellation facets are randomly selected to represent closed windows in the foam. Two different selection procedures are implemented: isotropic selection and selection of facets with a given normal direction. Finally, the foams are relaxed by using the Surface Evolver software which results in more realistic cell shapes [37]. For all cases, the permeability is computed from flow simulations in microstructure realizations discretized as voxel images.

Additionally, regression models predicting the permeabilities from established characteristics for porous media, the porosity, the specific surface area, the tortuosity, and the constrictivity, are analyzed. We describe the effect of the different geometry modifications on these explanatory variables and, hence, the permeability. In particular, we investigate the ability of the regression models to predict the anisotropy of the permeability tensor due to an anisotropic direction distribution of the closed windows. To the best of our
knowledge, this has not been studied so far.

2 Stochastic models

To allow for a certain variation in cell sizes and shapes, we model the cell systems of the foams by random Laguerre tessellations. Let $\Phi$ be a locally finite system of spheres in $\mathbb{R}^3$, i.e. each bounded domain $\Omega \subset \mathbb{R}^3$ is intersected by finitely many spheres. We will identify a sphere in $\mathbb{R}^3$ with a pair $(x, r)$ where $x \in \mathbb{R}^3$ is the center and $r > 0$ the radius of the sphere.

The Laguerre tessellation $L_\Phi$ generated by $\Phi$ is the collection of cells $C_L$ such that

$$C_L((x, r), \Phi) = \{y \in \mathbb{R}^3 : ||y - x||^2 - r^2 \leq ||y - x'||^2 - r'^2 \text{ for all } (x', r') \in \Phi\}$$

where $(x, r) \in \Phi$ and $||\cdot||$ denotes the Euclidean distance [28]. If all spheres have the same radius, the Laguerre tessellation equals the Voronoi tessellation of the sphere centers. For computing the Laguerre tessellations, we follow the algorithm stated in [34]. The required convex hull is computed using qhull [3].

As suggested in [30], we choose $\Phi$ as a dense packing of non-overlapping spheres. This choice will generate regular cell shapes as they are observed in real foams. Additionally, the cell size distribution can be controlled by varying the size distribution of the spheres. For simulating the sphere packings, the force-biased algorithm [5] is used.

For our simulations, the volume fraction of the sphere system is fixed to $V_v = 0.6$. Additional parameters are the mean number of spheres per unit volume $N_v$, and the distribution of the sphere volumes. The volume distribution is chosen as a lognormal distribution with parameters $\mu_v$ and $\sigma_v$. The mean sphere volume is given by $\bar{v} = V_v/N_v$, leaving the coefficient of variation $cv(v) = sd(v)/\bar{v}$, with $sd(v)$ denoting the standard deviation of the sphere volumes, as free parameter. These parameters are related to the parameters of the lognormal distribution via

$$\bar{v} = \exp\left(\mu_v + \frac{\sigma_v^2}{2}\right) \quad sd(v) = \exp\left(\mu_v + \frac{\sigma_v^2}{2}\right) \sqrt{e^{\sigma_v^2} - 1}.$$
For flow simulation, the foam geometry is discretized as 3D voxel image. The edges of the tessellation form the skeleton of the foam struts. Both, cylindric struts with a circular cross section and struts with a concave triangular cross section are generated. Figure 1 illustrates these two strut shapes. Cylindric struts are generated by a spherical dilation of the foam skeleton. The radius is chosen such that the desired volume fraction is reached. The triangular struts are constructed by using the wet foam simulation offered by the Surface Evolver software package \cite{7}. Again, strut thickness can be varied such that a given volume fraction is obtained.

![Figure 1: Foam struts with different cross section shape. Left: cylindric, right: concave triangular.](image)

Additionally, we study the effect of closing some of the windows in the foams. In the following, we present two mechanisms for selecting the closed windows in our models. As a first case, we use an isotropic closing procedure: windows are closed independently of each other and irrespective of their size, position, and orientation with a fixed probability $0 < p_1 < 1$. As a second option, we apply an anisotropic selection procedure: Only windows orthogonal to the $z$-axis (the desired flow direction) are considered for closure. Let $n$ be the window (facet) unit normal vector and $z = (0, 0, 1)^T$ be the $z$-axis. For a selected threshold $c$, we only consider windows such that

$$\langle n, z \rangle > c.$$  

In the following, we use $c = 0.92$. The thus selected windows are closed independently
of each other and irrespective of their size, position, and orientation with a probability $0 < p_2 < 1$. The value of $p_2$ is chosen such that the total fraction of closed windows in the foam is equal in the isotropic and in the anisotropic case.

To process the voxel data, i.e. closing the windows as well as calculating porosity and specific surface area (both Section 5), we use MAVI [13] and ToolIP [14].

3 Flow and permeability computation

The flow computations are performed in a representative elementary volume (REV) (or representative volume element (RVE)), namely a box $\Omega = [0, \ell_x] \times [0, \ell_y] \times [0, \ell_z] \subset \mathbb{R}^3$. It can be decomposed into two subsets $\Omega = \Omega_p \cup \Omega_s$, where $\Omega_p$ is the pore space and $\Omega_s$ is the solid component (foam geometry). The surface of $\Omega_s$ is denoted by $\Gamma_s$ and the faces of the box as $\Gamma$.

3.1 Flow computation

The basic equations for the flow computation are the Navier-Stokes equations. Since we assume an incompressible, stationary, slow, and laminar flow, it is sufficient to use a simplified version, the Stokes equations (see e.g. [41]). The equations read

\[
\mu \Delta u - \nabla p + f = 0, \quad x \in \Omega_p, \quad (1)
\]

\[
\nabla \cdot u = 0, \quad x \in \Omega_p, \quad (2)
\]

\[
u = 0, \quad x \in \Gamma_s, \quad (3)
\]

\[
u, p \text{ periodic}, \quad x \in \Gamma. \quad (4)
\]

Here $u$ denotes the fluid velocity field and $p$ the pressure distribution. The vector $f$ denotes different forces and $\mu$ is the dynamic viscosity of the fluid.

Below we show that it is sufficient to consider the Stokes equations for our case. The equations are discretized by using the finite volume method (FVM) on a regular voxel grid.
The above equations are used in the resolved microstructure describing the geometrical details. In general, a microstructure can also be seen as an unresolved porous medium and effective properties can be assigned. In this case, the flow through a porous medium can be modelled by the Darcy equation

\[ u_{\text{avg}} = -\frac{K}{\mu} \nabla p. \] (5)

Here, \( u_{\text{avg}} \) is the averaged velocity (or from the macroscopic point of view the superficial velocity also called Darcy velocity) and \( K \) denotes the permeability tensor which measures the resistance of the microstructure to the flow [4]. The tensor can be represented by a matrix, where the diagonal terms measure the permeability in the coordinate directions and the off-diagonal terms describe the lateral directions. For an isotropic medium, the permeability tensor can be replaced by a single value. In this case, the Darcy equation basically claims that the average fluid velocity is proportional to the pressure gradient where the proportionality constant is given by the ratio of permeability and viscosity. Note that the permeability is an intrinsic property of the microstructure and its morphology, see, e.g., [21, 12].

The flow through a porous medium can be classified in different regimes. They range from pre-Darcy to turbulent flows (e.g. [2, 22]). As we assume a slow flow, we can stick to the Darcy regime and do not use an additional viscous term as in the Forchheimer equation (see e.g. [20]). To verify this assumption, we compared the results of the Stokes equations to those of the Navier-Stokes equations with viscous term. For one structure, we fixed the pressure difference \( \Delta p \) and computed the resulting velocity. The results are shown in Figure 2 on the left hand side for the complete considered velocity range and on the right hand side only for the small velocities. For them, the results of Stokes and Navier-Stokes are approximately the same. If the velocity is raised, the influence of the inertia term increases and the solutions start to deviate. The results from the Stokes equations follow the linear Darcy regime and can therefore be used to compute the permeability.
3.2 Permeability computation

In this subsection, we describe how the (effective) permeability can be computed from a flow simulation at the microscale. We stick to the approach implemented in the software GeoDict [15]. To calculate the full permeability tensor, three computations are required. Assume that the velocity field $u$ and the pressure distribution $p$ are obtained from a flow simulation on the resolved scale. Since the flow simulation in GeoDict is performed aligned to the coordinate axes, a pressure difference in each coordinate direction is computed.

Let us assume that the flow was computed in $z$-direction. Then the pressure drop in this direction can be considered as a force $f$

$$f = \frac{\Delta p}{\ell_z} = \frac{p(\ell_z) - p(0)}{\ell_z},$$

where $\ell_z$ is the thickness of the medium in $z$-direction. In principle, this corresponds to a linearization of the pressure drop

$$p(z) = p(0) + \frac{\Delta p}{\ell_z} z$$

with $\nabla p = f$ in this case.
Following the dissertation of Linden [25], the entries of the permeability tensor can be obtained in the following way: Use the axis-aligned pressure drop as force and compute the mean velocity $\overline{u_z}$ in $z$-direction as described below. Using this procedure, equation (5) can be written as

$$\mu \overline{u_z} = -\begin{pmatrix} K_{xx} & K_{yx} & K_{zx} \\ K_{xy} & K_{yy} & K_{zy} \\ K_{xz} & K_{yz} & K_{zz} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ -f \end{pmatrix}. \quad (8)$$

Thus, we can write

$$\begin{pmatrix} K_{xx} \\ K_{zy} \\ K_{zz} \end{pmatrix} = \frac{\mu}{f} \overline{u_z} = -\mu \frac{\ell_z}{\Delta p} \overline{u_z}. \quad (9)$$

The mean velocity $\overline{u_z}$ is computed by averaging over all velocity values of the single components of the velocity, i.e. in the already discretized form,

$$\overline{u_z} = \sum_{i=1}^{N_{vox}} \frac{u_z|_i}{N_{vox}}, \quad (10)$$

where $N_{vox}$ is the number of voxels of the entire domain $\Omega$ and $u_z|_i$ is the velocity in $z$-direction evaluated at the center of voxel $i$. Note that also solid voxels are counted here, even though the velocity is zero there.

The same procedure is applied for the other coordinate directions. In general, one is interested in the diagonal elements of the permeability tensor since these three components represent the flow resistance in the corresponding directions.

### 3.3 Dimensionless formulation

In practice, the physical dimensions of a real foam or the scale of a model realization may vary. To ease the analysis of the problem and to simplify the comparison of the solutions, the equations can be converted to a nondimensional or dimensionless form. The variables are transformed using a characteristic length scale $L$ and a characteristic speed $U$ (see
e.g. [39]). The following new variables are introduced:

\[ x^* = \frac{x}{L}, \quad \nabla^* = \frac{L}{\nabla}, \quad u^* = \frac{u}{U}, \quad p^* = \frac{pL}{\mu U} \]

If for example \( L = \ell_x = \ell_y = \ell_z \), the problem is transformed to the unit cube. Neglecting the force term \( f \), the dimensionless Stokes equations read

\[
\Delta^* u^* - \nabla^* p^* = 0, \quad x^* \in \Omega^*_p \tag{11}
\]
\[
\nabla^* \cdot u^* = 0, \quad x^* \in \Omega^*_p \tag{12}
\]
\[
u^* = 0, \quad x^* \in \Gamma^*_s \tag{13}
\]
\[
u^*, p^* \text{ periodic }, \quad x^* \in \Gamma^*. \tag{14}
\]

Using the same procedure for the Darcy equation [5], the dimensionless formulation reads

\[ u^*_\text{avg} = -K^* \nabla^* p^*, \tag{15} \]

where \( K^* \) is the dimensionless permeability. In the isotropic case, the dimensionless scalar permeability is also called Darcy number \( Da \). As a generalized notation, we introduce the dimensionless tensor \( Da \) as

\[ Da = K^* = \frac{K}{L^2}. \tag{16} \]

4 Simulation results

We start by simulating the random tessellation models in the unit cube. We use a Laguerre tessellation model with the following parameters: \( V_V = 0.6, \ N_V = 500 \) and a log-normal distribution of the sphere volumes with \( cv(v) = 0.2 \). Struts are dilated with either circular or triangular cross section shape. For computing the permeability, the geometries are discretized as voxel images.
4.1 Evaluation of flow simulation results

To take possible anisotropies of the foam structure into account, we compute the complete permeability tensor $D_a$. The permeability tensor is always symmetric and positive-definite. Thus, it can be diagonalized and the eigenvalues represent the principal permeabilities and the eigenvectors the principal directions of the flow [29]. In our case, the off-diagonal values of the tensor are much smaller than the diagonal values, and the eigenvalues of the tensor are approximately equal to the diagonal values. Therefore, we only investigate the diagonal values of the permeability tensor:

$$D_a \approx \begin{pmatrix} K_{xx}^* & 0 & 0 \\ 0 & K_{yy}^* & 0 \\ 0 & 0 & K_{zz}^* \end{pmatrix} = \begin{pmatrix} D_{ax} & 0 & 0 \\ 0 & D_{ay} & 0 \\ 0 & 0 & D_{az} \end{pmatrix} \quad (17)$$

In other words, the open-cell foam is considered as orthotropic.

4.2 Resolution of discretization

As a first step, we study the dependence of the computed permeability on the resolution of the voxel grid. In [27], it is recommended to use geometries with at least 10 cells in flow direction. Initially, we follow this recommendation by choosing a volume consisting of 500 cells. According to stereological results for random tessellations [10, p. 443], this will result in on average roughly 11.5 cells intersecting a unit length line segment. Five realizations of the Laguerre tessellation model are generated, dilated by using cylindric and triangular cross section shapes, and discretized at six different resolution levels. Porosities studied in the literature range from 70 to 95 %, see [27, 32]. In our study, the porosity is fixed at approximately 95 % as this implies relatively thin struts which is the most challenging case regarding resolution. The foam structure is discretized in voxel images consisting of $500^3$, $1000^3$, $1500^3$, $2000^3$, $2500^3$, and $3000^3$ voxels. Boxplots of the resulting Darcy numbers in the three coordinate directions are shown in Figure 3. The results for the cylindric struts are more stable when changing resolution than
those for the triangular struts. We consider an image size of $1500^3$ sufficient for further investigations.

Figure 3: Boxplots for the Darcy numbers computed with different resolutions of the voxel grid. 500 cells. Left: cylindric struts, right: triangular struts.

4.3 Representative volume

In the next step, we investigate the size of the representative volume element. Based on the previous results, we fix the image size at $1500^3$ voxels for a volume consisting of 500 cells. Additionally, volumes containing 100, 250, 750, and 1000 cells are simulated at the same resolution. This corresponds to image sizes of $877^3$, $1191^3$, $1717^3$, and $1890^3$ voxels. For each case, 20 realizations of the Laguerre tessellations are simulated. Boxplots of the resulting Darcy numbers are shown in Figure 4.

Figure 4: Boxplots for the Darcy numbers of different volume element sizes. Image resolution corresponds to $1500^3$ voxels for 500 cells. Left: cylindric struts, right: triangular struts.

For both cylindric and triangular struts the Darcy numbers stabilize for 500 cells.
Hence, for the following analysis, systems of 500 cells are discretized in images of size 1500\(^3\) voxels.

5 Influence of selected geometry parameters

5.1 Cross section shape and fraction of closed windows

First, the influence of the strut cross section shape and the fraction of closed windows on the magnitude and the anisotropy of permeability is investigated. To this end, ten realizations of the microstructure model described above are simulated. According to the representative volume study, systems of 500 cells are discretized into images of 1500\(^3\) voxels. Both, cylindric and concave triangular struts are considered. The porosity of the open foams is fixed to 95%. Furthermore, foam structures with 5, 10, and 15% of closed windows are generated by using both the isotropic and the anisotropic mechanism described in Section 2. The strut systems of the closed foams coincide with the open foams. Hence, closing windows decreases the porosity of the foams, see Table 1. However, the change in porosity by closing the windows is quite small. As porosity is well known to have a high impact on permeability, a second series of open foams is generated matching the porosity of the partially closed foams with the highest fraction of closed windows (15%). They are labelled as ‘0: porosity as 15%’ in the following.

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Table 1: Porosities for the open and partially closed foams. Mean and standard deviation (in brackets) of ten realisations.

Boxplots of the resulting Darcy numbers in the three coordinate directions for these
samples are shown in Figure 5. A significant decrease of the Darcy numbers is observed when increasing the percentage of closed windows. In foams using the isotropic closing mechanism, the Darcy numbers also show an isotropic behaviour. In the anisotropic foams, the Darcy numbers in z-direction decrease drastically. However, also the Darcy numbers in x- and y-direction are slightly reduced compared to the completely open case. Comparing the results for the open foam with reduced porosity to the partially closed foams shows that the reduction in permeability in the latter cannot solely be explained by porosity. In both cases, the permeability is comparable to the structures with 5% closed windows. The results reported by Westhoff et al. [40] for slightly smaller porosities correspond to a mean Darcy number of 0.00035 which is in a similar range as our data.

Figure 5: Boxplots for the Darcy numbers of closed foams with cylindric and triangular struts. Left: cylindric struts, right: triangular struts. The plots labelled '0: porosity as 15%' refer to completely open foams matching the porosity of the partially closed foams with the highest fraction of closed windows (15%).

5.2 Relaxation

In [37], it was shown that Laguerre tessellation models as used in this study contain significantly more short edges than most real foams. As a consequence, facet shapes also tend to be more irregular which can have an impact on the permeability. This may be fixed by relaxing the foams by using the Surface Evolver software [7]. As an effect of relaxation, also the facet area distribution becomes more homogeneous. The empirical coefficient of variation of facet areas is \( cv(A) = 0.530 \) before relaxation. In the relaxed foams, it reduces to \( cv(A) = 0.388 \). The study in [40] showed that a reduction of \( cv(A) \)
decreases the permeability of the foam. Repeating the simulation study described in the previous section on relaxed foam skeletons, we observe the same trend. Compared to the non-relaxed case, a slight reduction (4-5 % for cylindric struts, 3.5-4 % for triangular struts) of the Darcy numbers is observed for the relaxed structures, see Figure 6.

Figure 6: Boxplots for the Darcy numbers of closed relaxed foams with cylindric and triangular struts. Left: cylindric struts, right: triangular struts.

6 Predicting permeability

Several geometric characteristics of a microstructure have been suggested as predictors for permeability. Clearly, permeability is correlated with the porosity of the filter medium. As porosity is nearly constant in our study, we will additionally characterize the foam structures by the tortuosity and constrictivity of their pore space.

Tortuosity is a measure for the complexity of paths through the pore space. For two points $x_1$ and $x_2$ in the pore space, let $d_g(x_1, x_2)$ denote the geodesic distance between $x_1$ and $x_2$, i.e., the length of the shortest path within the pore space connecting these points. Additionally, we consider the Euclidean distance $d_e(x_1, x_2)$ between $x_1$ and $x_2$. The geometric tortuosity is defined as the ratio

$$\tau_{x_1,x_2} = \frac{d_g(x_1, x_2)}{d_e(x_1, x_2)} \geq 1.$$ 

For a porous medium, the average tortuosity $\tau$ is defined as the mean of $\tau_{x_1,x_2}$ for all pore points $x_1$ located on the inlet plane, e.g., the coordinate plane $z = 0$, and pore points $x_2$. 

16
located on the outlet plane at the opposite side of the material. Inlet points that are not
connected to the outlet plane are ignored. In the foam models considered here, this only
happens rarely due to edge effects.

In [17], constrictivity was introduced as a measure for bottlenecks in porous structures.
It is defined as follows: Let \( r_{\text{max}} \) denote the maximal radius such that 50\% of the pore
volume can be covered by spheres of radius \( r_{\text{max}} \). Spheres are allowed to overlap, but may
not intersect the solid component. By \( r_{\text{min}} \) we denote the maximal radius such that 50\% of
the pore volume can be covered by spheres of radius \( r_{\text{min}} \) that are passing through the
pore structure from a fixed direction. Constrictivity is defined as

\[
\beta = \frac{r_{\text{min}}^2}{r_{\text{max}}^2} \in [0, 1].
\]

The smaller the constrictivity, the stronger the bottlenecks in the structures.

In [40], the permeability in open foam structures is described by a linear regression
model using constrictivity and porosity as explanatory variables. In our setting, con-
strictivity is rather constant for both isotropic and anisotropic foams and all considered
fractions of closed windows, see Figure[7]. However, there are two clusters for the different
cross sections shapes. Hence, constrictivity alone is not sufficient to explain differences in
the Darcy numbers. In contrast, a linear dependence between tortuosity and the Darcy
numbers can be observed in the plots in Figure[7] if the two cross section shapes are
treated separately. The same models can be used for all coordinate directions. Hence,
\( Da_\bullet (K_\bullet) \) below refers to \( Da_x, Da_y \) or \( Da_z (K_{xx}, K_{yy} \) or \( K_{zz} \)) depending on which direc-
tion is considered. Due to the isotropy of the models in the \( xy \)-plane, only the \( x \)-direction
and the \( z \)-direction are used for fitting the models. A least squares fit of a regression line
results in the model

\[
Da_\bullet = -6.5639 \cdot 10^{-3} \tau + 6.9748 \cdot 10^{-3} \quad \text{Adjusted R-squared: 0.9435}
\]
for the cylindric struts, while the fit for the triangular struts yields

\[ Da_\bullet = -4.9864 \cdot 10^{-3} \tau + 5.3170 \cdot 10^{-3} \quad \text{Adjusted R-squared: 0.8982.} \]

As all characteristics involved in this model are dimensionless, the parameters do not carry any unit. Including \( \beta \) or the porosity \( \phi \) in the model does not improve the goodness-of-fit.

On the other hand, using the constrictivity \( \beta \) as an additional explanatory variable allows to fit a joint model for both cross section shapes, namely

\[ Da_\bullet = -6.020 \cdot 10^{-3} \tau + 7.671 \cdot 10^{-4} \beta + 6.180 \cdot 10^{-3} \quad \text{Adjusted R-squared: 0.9288.} \]

Additionally including the porosity \( \phi \) in the model further increases the goodness-of-fit. Here, we get

\[ Da_\bullet = -4.210 \cdot 10^{-3} \tau + 9.891 \cdot 10^{-4} \beta + 4.527 \cdot 10^{-3} \phi \quad (18) \]

with an adjusted R-squared of 0.9966.

Note that the intercept is removed from the model. This may be due to the nearly constant porosity in our data. A model including an intercept yields an adjusted R-squared of 0.9292 which is only slightly better than the model using only \( \tau \) and \( \beta \).

Further note that the models are able to predict the Darcy numbers for all three coordinate directions and for both the isotropic and the anisotropic closing mechanism. According to relation (16), a regression model for the permeability \( K_\bullet \) is obtained by multiplying the model for the Darcy numbers by \( L^2 \).

All regression models listed above were fitted by using only the data for the non-relaxed structures. If the relaxed data are included, the model (18) changes to

\[ Da_\bullet = -4.199 \cdot 10^{-3} \tau + 9.457 \cdot 10^{-4} \beta + 4.522 \cdot 10^{-3} \phi \quad (19) \]

with an adjusted R-squared of 0.9954.

When predicting the Darcy numbers for the relaxed structures using the model (18),
they are overestimated by 6% on average. Overestimation is more pronounced for completely open structures and reduces with increasing amount of closed windows. This means that the reduction of permeability due to relaxation reported in Section 5.2 is not captured by the model fitted to unrelaxed Laguerre tessellations. A comparison of the characteristics of relaxed and unrelaxed foams and the resulting residuals are shown in Figure 8.

As an alternative approach for modelling the permeability $K_\bullet$, we tried regression models with explanatory variables containing the factors $1/S_N^2$ where $S_N$ is the specific surface area, that is

$$K_\bullet = a \cdot \frac{\tau}{S_N^2} + b \cdot \frac{\beta}{S_N^2} + c \cdot \frac{\phi}{S_N^2} + d \cdot \frac{1}{S_N^2}.$$ 

The model is chosen such that the regression parameters are dimensionless as the unit of permeability ($m^2$) is equal to the unit of the explanatory variables. The least squares fit yields $a = -0.182783$, $b = -0.027500$, $c = -0.45041$, and $d = 0.627690$ with an adjusted R-squared of 0.9967. Again, the model is able to explain all considered structures.

7 Conclusion

In this paper, the effect of various modifications of the microstructure geometry of (partly) open foams on their permeability has been investigated. A similar study by Westhoff et al. [40] predicts permeability by a linear regression model depending on porosity and constrictivity. Our results indicate that for partially closed foams, tortuosity should be included as a further parameter. It is remarkable that the same model could be used for all directions, closing mechanisms (isotropic or anisotropic, different percentage of closed windows), and strut cross section shapes considered in our study. Due to its formulation in dimensionless form, the formulas are not restricted to a specific length scale. An alternative model including the specific surface area performed equally well. Note that porosity and constrictivity values in our study are restricted to a very small range. Hence, the validity of the regression models should be investigated before applying them to foams with very different values of these quantities. In particular, a larger variation of porosity
Figure 7: Dependence of the Darcy numbers on tortuosity (top left) and constrictivity (top right) for the non-relaxed foams. Purple refers to the $x$-direction and blue to the $z$-direction. Symbols with black frame are for isotropic foams, symbols without frame are for the anisotropic foams. The shape of the symbols represents the cross section shape (circular, triangular). The brightness indicates the percentage of closed windows. The darker the color the more windows are closed.

may require adding an intercept to the model in (18). As shown in [37], the relaxed structures considered in Section 5.2 may be closer to real foams regarding cell shape and edge length distributions. When using the regression model fitted to the foams based on non-relaxed Laguerre tessellations, permeabilities of the relaxed structures were overpredicted. This should be kept in mind when deriving regression models for real foams based on parametric tessellation models. A detailed analysis of this effect may be subject to future research.
Figure 8: Top: Tortuosity, constrictivity, porosity, and specific surface area of the relaxed (violet) and unrelaxed (blue) foams. Bottom: Residuals of prediction of the Darcy number \[ D \] for relaxed and unrelaxed foams. Symbols with black frame are for isotropic foams, symbols without frame are for the anisotropic foams. The shape of the symbols represents the cross section shape (circular, triangular). The brightness indicates the percentage of closed windows. The darker the color the more windows are closed.
When generating random foam samples, the distribution of cell shape and size, the
cross section shape and thickness of the struts, and the amount and orientation of closed
windows can be modified.

The porosity is mainly controlled by the dilation radius of the struts. Adding closed
walls decreases the porosity. For fixed dilation radius, porosity is also influenced by the
regularity of the cell and facet shapes. Irregular shapes form acute angles between the
struts. This results in a strong overlap of struts in the nodes which reduces the volume
fraction, thus increases the porosity, compared to foams with more regular cell shapes.
This effect explains the slightly higher porosity of the original foams compared to the
regular relaxed structures, see Table 1.

As shown in Figure 7, tortuosity is influenced by the cross section shape and the pres-
ence of closed windows. Constrictivity, finally, is determined by the cross section shape of
the struts which influences the size of the windows between the foam cells. Additionally,
it depends on the facet shapes of the tessellations. For instance, the relaxed structures
considered here have more regular shapes which can be more easily be penetrated by a
sphere. This results in an increase of constrictivity compared to the original Laguerre
models.

The above discussion shows how different geometric characteristics and the perme-
ability are influenced by different modifications of the foam. These insights can be used
to optimize the foam properties and to predict them for real (relaxed) foams, too.

Acknowledgements

This work was supported by the German Federal Ministry of Education and Research
(BMBF) under grant 05M16 (AMSCHA).

References

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