**Open-cell foams modeling: workflows for geometry generation and CFD simulations for**

**pressure drops and mass transport**

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**1.Introduction**

The interest of the process industry towards ceramic and metallic open-cell foams has greatly increased over the last twenty years. The reasons reside in the unique properties of these porous materials such as mechanical resistance, very high porosity, which results in lower pressure drops compared to other packing media, large specific surface area and high thermal conductivity, which are important factors for mass and heat transfer. Notable uses of these solid foams are filters, monolithic catalyst supports, column packing for packed bed reactors and heat exchangers.

Despite the great advancements in the scientific research and in the production technique during the last 30 years, correlations that links the key geometric parameters (porosity, specific surface) to the performances of these materials are still hard to find. The main parameters used to characterize commercially available open-cell foams are porosity *ε* and the *pore per inch* (PPI); which indicate the average pore diameter. However, these physical properties do not give any clue regarding specific surface *SV*, which is important for the design of industrial devices and estimation of the pressure drops *ΔP/L* and heat and mass transfer coefficients, such as *h* and *kc*. For all these reasons the optimization of such structures remains an open problem.

A first approach to model the geometric structure of open-cell foams, used by many authors, relies on the *Kelvin’s Cell* structure, an ideal periodic polyhedron, called *Tetrakaidecahedron*, representing a single pore. The advantages of such an approach come from the limited computational effort required and the possibility of conceiving analytical correlations for the estimation of geometrical properties (*SV*, *ε*), pressure drop *ΔP/L* and transfer coefficients. However, because of the random nature of open-cell foams, the necessity for more complex and realistic geometrical models has arisen in order to explain the key factor influencing transport phenomena occurring at the micro-scale. In literature there is evidence that random *Voronoi* or *Voronoi-Laguerre* tessellations can be effective in representing the cellular random nature of solid foams. The advantage of these algorithms, that subdivide a confined space into distinct regions, is that they allow the creation and the study of many more structures and configurations that would experimentally be viable.

The objective of this abstract is to introduce the digital workflows we have developed, tested and validated to reproduce a great variety of structures, exploring large parameter ranges, in order to be able to optimize the geometric structure according to the different application areas.

**2. Methods**

The first tool [1] relies only on the open-source computer graphics code Blender and on Python programming language code to calculate and create the final geometry. This workflow is able to create both ordered lattice geometries, such as the *Kelvin’s Cell*, and random models such as those originated from *Voronoi-like* tessellations, by providing the coordinates of the nodes and edges of the structures.

In the first case, the coordinates are well known, whereas in the case of the random tessellations they must be generated starting from an initial set of points in space. The initial set of random points, called *seeds*, is achieved by using the centers of spheres randomly packed (either mono- or poly-dispersed), following an already validated workflow proposed by [2], then the tessellation is calculated and the position of the edges and nodes of the tessellation is retrieved. Finally, Blender creates cylinders and sphere at the supplied coordinates to generate the foam structure. An example of a polydisperse foam geometry generated by the workflow is reported in Fig. 1.

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**Figure 1.** An example of an open-cell foam structure, obtained with a periodic Laguerre-Voronoi algorithm, overlapped to its generating sphere packing (which will be removed in the actual CFD simulation).

The resulting geometry is used to build a computational mesh and run CFD simulations in the OpenFOAM environment. First, the flow field is calculated by solving Navier-Stokes equations, to estimate the pressure drop and from them the hydraulic permeability *k* of the generated geometries, using Darcy’s Law equation. Then, micro-scale mass transfer simulations are carried out to explore the transport of colloidal particles through these porous media, in the particular case of fast surface deposition occurring during clean-bed filtration[5].

In this situation the phenomena at the surface are driven by Brownian motion and steric interception mechanisms. Following the model and methodology proposed by [3] the results of the scalar transport simulations are used to calculate an effective macroscopic particle deposition rate coefficient *Kd*, which is used to estimate a macroscopic measure of the efficiency of clean-bed filtration for the open-cell foams in exam, estimated by means of the Damköhler number Da.

The geometrical model explored with the first workflow are: the Kelvin’s Cell model, one mono-dispersed and two poly-dispersed structures originated from random tessellation, respectively from Voronoi and Laguerre-Voronoi tessellations. In the case of mono-disperse foam the originating sphere packings have grains with constant diameter, whereas for poly-disperse foams the packings have grains with normally distributed diameters around a mean value µ. Two different instances have been generated with same mean sphere diameter and different coefficient of variation CV = σ / µ, namely 0.2 and 0.35.

The second tool was developed with the aim of creating realistic foam structures, with geometric features comparable to real foams. To achieve this result the new workflow is based on the creation and morphological modification of three-dimensional binary volumes, composed of regular grids of voxels. The advantages of working on voxelized volumes instead of on surfaces, like in Blender, is the much greater flexibility and potentials. These operations were carried out using the free software PlugIm! (<https://www.plugim.fr/>), which offers a great variety of plugins not only to create and modify voxelized volumes but also to create sphere packings. The overall process is very similar to the previous developed tool: spheres are packed in a cubic volume, then the centroids are retrieved and used as seed for the Voronoi algorithm, which creates the skeleton of the foam structure. Then, cylinders and spheres are placed according to the edges and nodes of the tessellation, creating a so called *balls and sticks* model of the foam. Finally, morphological operations, such as closing, opening, dilation and erosion, are carried out on the structure in order to achieve the desired values of porosity and specific surface. The additional novelty lies in the way spheres are packed: instead of using a *hard spheres* model, like in the previous tool, this new workflow relies on the sphere aggregation model proposed by [4], which allows to modify the compactness of the spheres aggregates as well as the repulsion between spheres. This results in the possibility of creating a huge variety of foam structures with similar macroscopic characteristics (ε, *SV*, τ) originated from spheres aggregates with different compacity. Fig. 2 report an example of comparison between a Nickel-Chrome metallic foam and its digital replica and Tab. 1 report the geometrical data.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Porosity ε (%) | Specific surface *SV* (m2/m3) | Tortuosity τ ( - ) |
| Experimental | 92 | 1000 | - |
| Tomography | 91.9 | 1054 | 1.26 |
| Digital replica | 92.5 | 995.5 | 1.22 |

**Table 1.** A comparison between the values of the macroscopic geometrical descriptors for the Nickel-Chrome 14 PPI metallic foam, calculated with experimental technics, using digital reconstruction from tomographic images and from the digital replica

A close-up of a puzzle

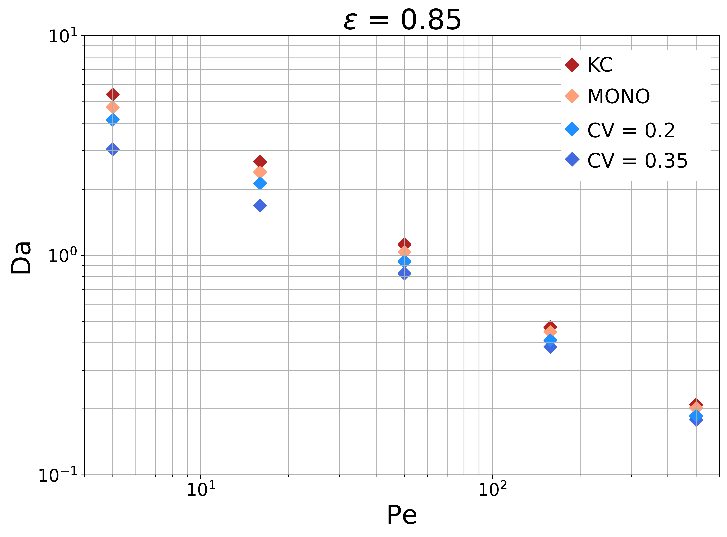
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**Figure 2.** (a) metallic 14 PPI Nickel-Chrome foam geometry obtained from digital reconstruction of x-ray tomography, (b) Digital replica with the same target geometric parameters (ε, *SV*, τ) obtained using the PlugIm! software. The error on porosity, specific surface and tortuosity of the digital model with respect to the real foam is inferior to 5%.

**3. Results and discussion**

For each type of geometry, four values of pore per inch (PPI) have been considered, namely 10, 20, 30 and 45, and five values of porosity ε, ranging between 77% and 95%, for a total of 20 different foams. The flow field simulations were carried out in steady state conditions, considering water as fluid, at constant atmospheric conditions, under laminar flow regime (Re ≈ 1 · 10−3).

The obtained flow fields are then used in mass transport simulations, for five different values of colloidal particles dimensions, ranging from 1· 10−9 and 1· 10−6 m, with resulting Péclet number ranging between 5 and 500, for a total of 100 cases.



**Figure 3.** Particle deposition efficiency, as Da at constant porosity (ε = 0.85) for the four different geometries showing a power-law relationship between the Damköhler number and the Péclet number.

Fig. 2 shows the relationship between the advective Damköhler number Da and the Péclet number, for all the values of PPI and porosity ε = 0.85, for the four geometrical models (Kelvin’s Cell, mono-disperse, poly-disperse with CV = 0.2 and CV = 0.35). At constant Pe values and geometry model, the Da values for different PPI collapse to the same point because the Damköhler number normalizes the deposition rate with respect to the operating conditions and dimension of the computational domain. Globally, at increasing Pe number, the quantity of colloids impacting on the solid surface of the foam decreases following a power law, as reported by previous studies [5] on Brownian clean-bed filtration. The results were first interpreted using well known constitutive equations ([6],[7]), and then several different power law functions, depending on *SV*, ε and tortuosity τ and their combinations. This was done to verify if these relationships could be used to exactly predict the impact of the macroscopic parameters on the filtration efficiency of the foams. However, this strategy didn’t bring out any significant correlation, since the global relative error, calculated as the sum of the mean squared relative errors of the data with respect to the fitting at each Pe value, showed values well over 100%. Therefore, the results show how this kind of (usually employed) macroscopic geometric features are insufficient in explaining the variations in filtration performance, highlighting the need for more detailed explorations of the pore-scale phenomena over a wider range of geometrical parameters.

To validate the second workflow, an experimental campaign was carried out to measure pressure drops on four open-cell foams: two Nickel-Chrome metallic foams (14 and 30 PPI) and two Alumina ceramic foams (20 and 40 PPI). Moreover, a three-dimensional digital reconstruction of these foam was obtained using images of the foam structure extracted using X-ray tomography. Pressure drop from experiments were compared to the results obtained from CFD simulations carried out both on the reconstructed foam models and the digitally generated models. The experiments were carried out on a column 60 cm long and 4.4 cm wide packed with foam pellets of the same size. Several different operating conditions were considered, with flow rate ranging between 12.5 and 1000 L/hr, resulting in Reynolds numbers ranging from 10 to 700.

An example of the results obtained is shown in Fig.4 which report the results for a Nickel-Chrome 14 PPI foam. Along with experimental and CFD results, two very commonly used literature correlations ([8],[9]) for the estimate of the pressure drops in open-cell foams are also reported for comparison. The results of the CFD are in good agreement with both the experimental data and the literature correlations. Moreover, the pressure drops estimated from the digital replica, created with PlugIm!, are in very good agreement with the other CFD results.

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**Figure 4.** A comparison for a Nickel-Chrome 14 PPI metallic foam between experimental pressure drop measurements and CFD simulation results for the real foam structure and its digital replica. The plot report also two empirical correlations found in literature as a reference. The CFD results for both models are consistent with both experimental and literature data.

**4. Conclusions**

The results obtained in the first work highlight how the macroscopic parameters, such as porosity, specific surface, or tortuosity alone are not enough to derive macroscopic relations to describe the particle deposition during early filtration; neither by using available analytical correlations, nor by developing new simple ones based on these geometrical parameters. Thus, while we consider the value of the first workflow to lie in the capacity for users to create numerical analysis campaigns at a limited cost, decreasing the overhead of the foam modeling, the study of the different geometrical models and their performance in terms of colloidal particles deposition is conceived as just an example of the exploration capabilities. The second workflow has proved to be able to correctly describe foam structures and reproduce their performances in terms of pressure drops, at limited computational cost, while still being able to produce a wide range of digital foam structures at very low cost. Future perspectives on this topic are then to further improve the understanding of the transport phenomena occurring inside these foams, by exploring in-silico a wider number of cases and especially by better discerning the geometrical peculiarities of each - beyond simple, and oft-used, descriptors like porosity or tortuosity.

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