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A systematic procedure for the virtual reconstruction of open-cell foams

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HIGHLIGHTS

- Structure accounting for variable strut diameter and solid clustering at nodes.
- Geometry based on Voronoi tessellation computed from a random set of points.
- Good agreement between geometrical properties of reconstructed and real foams.
- Complex flow field in real foams effectively reproduced in reconstructed foams.

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ABSTRACT

Open-cell foams are considered a potential candidate as an innovative catalyst support in many processes of the chemical industry. In this respect, a deeper understanding of the transport phenomena in such structures can promote their extensive application. In this contribution, we propose a general procedure to recover a representative open-cell structure starting from some easily obtained information. In particular, we adopt a realistic description of the foam geometry by considering clusters of solid material at nodes and different strut-cross sectional shapes depending on the void fraction. The methodology avoids time-consuming and expensive measuring techniques, such as micro-computed tomography (μCT) or magnetic resonance imaging (MRI). Computational Fluid Dynamics (CFD) could be a powerful instrument to enable accurate analyses of the complex flow field and of the gas-to-solid heat and mass transport. The reconstructed geometry can be easily exploited to generate a suitable computational domain allowing for the detailed investigation of the transport properties on a realistic foam structure by means of CFD simulations. Moreover, the proposed methodology easily allows for parametric sensitivity analysis of the foam performances, thus being an instrument for the advanced design of these structures. The geometrical properties of the reconstructed foams are in good agreement with experimental measurements. The flow field established in complex tridimensional geometries reproduces the real foam behavior as proved by the comparison between numerical simulations and experiments.

1. Introduction

Open-cell foams are cellular materials made of interconnected solid struts that enclose void regions, named cells, which communicate by means of pores, thus enabling fluids to flow across the structure. The open-cell geometry determines high void fractions resulting in low pressure drops even with high flow velocities. The complex flow field established inside the random and tridimensional geometry increases both the local mixing and the gas-to-solid transport properties, since foam ligaments may result in boundary layer disruption and enhanced mixing [1–3]. Moreover, the typically large specific surface areas allow for high mass transfer rates in the case of catalytically active structures. By considering highly conductive foams, the continuous solid matrix guarantees high axial and radial thermal conductivity, making thermal conduction the dominant heat transport mechanism inside these structures, in particular for systems operating with low conductive fluids and/or low flow rates [4–6]. These features make foams attractive as novel catalyst supports: a great potential is expected, in particular, where heat and mass transport are key factors in the design and operation of the catalytic reactors [7]. Several applications have been investigated in the open literature mainly regarding NOx removal from exhaust gas and catalytic partial oxidation (CPO) of methane to syngas [8–10]. Moreover, foams might be a suitable solution also in highly endothermic, e.g. steam reforming [11], and exothermic systems, e.g. selective oxidation [12,13], methanation and Fischer-Tropsch reactions [14], methanol synthesis [15,16], hydrocarbon hydrogenation reactions [17].

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Notation

Latin letters

d_c	cell diameter [mm]
d_p	pore diameter [mm]
t_s	strut diameter [mm]
t_n	node diameter [mm]
S_v	specific surface area [m^{-1}]
L	sample length [mm]
W	sample width [mm]

Greek symbols

ε	void fraction [–]
ρ	fluid density [kg/m^3]
μ	dynamic viscosity [Pa·s]

Dimensionless numbers

$Re_{d_p} = \frac{\rho d_p u}{\mu}$ Reynolds number based on the pore diameter [–]

Subscripts

rec	evaluated on reconstructed foam
μCT	evaluated with μCT/MRI techniques

Many correlations have been proposed in the open literature to describe the complex geometrical features of open-cell foams and the pressure drop due to flow across such structures. Edouard et al. [18] extensively reviewed the available correlations for prediction of the pressure drop and investigated the performances of the correlations against an extensive set of experimental data covering a wide range of different foams. They stated that the standard deviation between predicted and experimental values might be up to 100%. The description of the transport properties of foams is even more complex resulting in a poor understanding of those phenomena. Despite the considerable potential, this scenario is hampering a wide application of open-cell foams as catalyst supports. Hence, a fundamental analysis of open-cell foams is needed to investigate their properties and behavior. Computational Fluid Dynamics (CFD) is a valuable tool to improve the understanding of open-cell foams, being able to take into account their random tridimensional geometry and to grant deep insights in the complex flow field, enabling detailed analysis of the gas-to-solid transport phenomena. CFD, however, requires the accurate description of the foam microstructural geometry in order to generate the computational domain for CFD simulations. The generation of suitable structures for CFD simulations, with the capability of reproducing both the geometrical properties and the experimental behavior of open-cell foam, is a challenging and crucial task.

Currently, this task has been addressed through two different approaches in the open literature. The first exploits microcomputer tomography (μCT) or magnetic resonance imaging (MRI) techniques to obtain CAD data closely resembling the microstructure of real foams, which can be used to produce the computational domain needed for the CFD simulations [19–22]. The geometries recovered with this method are unique for each sample and might be not representative, in particular, when investigating small foam pieces. Moreover, this approach requires many steps for both the preparation of the sample and the post-processing of the data, resulting in an expensive and time-consuming methodology. The second approach relies on the generation of a virtual microstructure that resembles the real foam structure in terms of geometrical properties. Commonly, this is obtained by the description of a repetitive unit cell consisting of polyhedrons of a well-defined geometry. Lord Kelvin proposed the first deterministic model consisting of tetrakaidecahedrons, i.e. polyhedrons with six square faces and eight hexagonal faces, solving the problem of recovering the space-filling arrangement of cells of equal volume, which minimizes the surface area [23,24]. Several authors have investigated this structure [25–29]. Weaire and Phelan [30] have proposed an improved model consisting of eight cells, six tetrakaidecahedrons and two pentagonal dodecahedrons, which shows a reduction of the surface area of 0.3%. The simulations of pressure drop across these repetitive and ordered structures usually underestimate the experimental values by 30% [31]. Other unit cell models can be found in the open literature, such as the ordered cubic structure [1] or the dodecahedral unit cell model [32]. These structures have been exploited to derive correlations for the geometrical features and transport properties, whereas no application in the field of CFD simulation of real open-cell foams is reported in the available literature. Deterministic ensembles of unit cells do not account for the stochastic nature of the real foam structure, resulting in deviations between numerical and experimental behaviors mainly due to the preferential flow pattern established in the regular geometry. Therefore, it is necessary to take into account the characteristic randomness of real foams. Habisreuther et al. [33] and Lucci et al. [34] proposed to randomize the perfectly ordered Kelvin structure by means of a stochastic displacement of nodes. These methods allow for a good description of the specific surface area, but show significant deviations in the prediction of the transport properties. On the other hand, Gibson and Ashby [35] proposed the Voronoi tessellation as a candidate method to generate the foam structure, since it satisfies the topological requirement on edge and face connectivity [36]. Moreover, Roberts and Garboczi [37] analyzed different stochastic approaches, such as sphere overlapping, Voronoi tessellation, Gaussian random fields, ellipsoid overlapping. They stated that the Voronoi tessellation shows a microstructure similar to the open-cell foam geometry. Along these lines, Randrianalisoa et al. [38] exploited the Laguerre-Voronoi tessellation to generate open-cell structures and analyzed the pure heat conduction phenomena assuming a circular cross-sectional shape with promising results. Wehinger et al. [39] proposed a methodology to reconstruct foams using the Voronoi tessellation, assuming the pore diameter as the characteristic length. A good agreement with experimental geometrical data for foams with a porosity up to 0.85 was claimed, but a very poor description of the fine ligaments structure was adopted. The strut cross-sectional shape, circular and trapezoidal, respectively, was kept constant without taking into account any variation with the void fraction. Moreover, the material clustering at the nodes was neglected by assuming a constant strut diameter.

In structures as open-cell foams, the transport properties strongly depend on the peculiar morphology and on the local modifications of the microstructure. Hutter et al. [39] showed that strut thickness and shape influence the mixing properties of the foam structure. Kanaun and Tkachenko [40] elucidated the effect of the variations of the strut size on the effective solid thermal conductivity. Hence, the accurate description of these properties, i.e. strut cross-sectional shape, constrictions, solid clustering at nodes, is an essential aspect for an accurate reproduction of real foams behavior.

In this work, we establish a systematic methodology for the digital reconstruction of a realistic foam structure. The reconstructed foams show the same topology, e.g. number of faces per cell, and geometrical properties, e.g. different strut cross-sectional shapes,