Micro-computed tomography for the development of virtual models of open-cell foams

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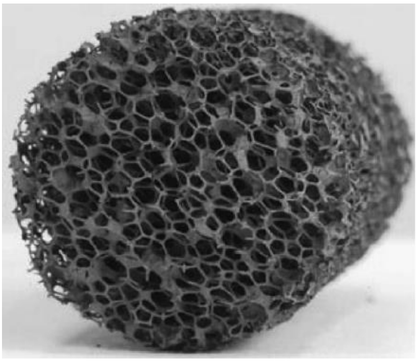
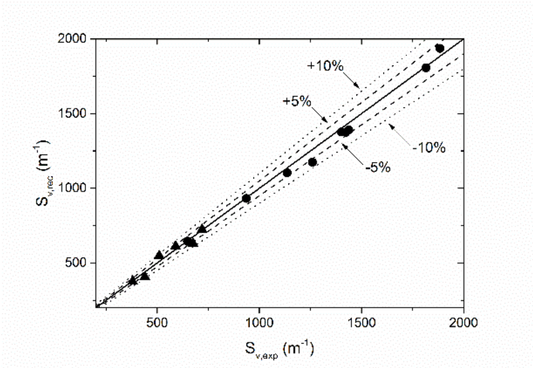
Structured reactors are widely acknowledged to be at the hearth of process intensification, one of the most challenging and trending topic in chemical engineering [1]. In this view, honeycomb monoliths, periodic open cellular structures (POCs), open-cell foams are candidate for next generation packing in fixed bed reactors. Open cell foams – cellular materials made of interconnected solid struts which enclose void regions, see Figure 1a – are recently receiving growing attention as innovative catalyst supports, particularly for processes strongly limited by mass and heat transfer. The description of the geometrical and transport properties in such structures is not trivial due to their complex tridimensional structure, resulting in a poor description of those features by means of the current engineering correlations. Hence, a fundamental analysis of open-cell foams is needed to investigate their properties. In this respect, Computational Fluid Dynamics (CFD) is a valuable tool to improve the understanding of open cell foams, being able to offer a deep insight in the complex flow field within the random tridimensional foam matrix. A CFD analysis requires however the accurate description of the foam microstructural geometry. Currently, digital reconstruction of the foam geometry is carried out by means of micro-computed tomography (µCT) or magnetic resonance imaging (MRI).



(a)



(b)

Figure 1. Open-cell foam sample (a) and comparison between the specific surface area [1] evaluated on the tomographic and Voronoi-based reconstruction

Those methodologies generate a faithful reproduction of the microstructure enabling further analysis of the geometrical and transport properties. However, these techniques are expensive and time-consuming preventing large scale screening and µCT-aided design of these structures. To overcome this limitation, we have proposed a Voronoi-based methodology for the virtual reconstruction of these structures based on a few pieces of geometrical information [2]. In this respect, tomographic reconstructions of real foams played a key role in the development of the model. The deep insight in the structure helped to define both the topological requirements of the virtual reconstruction and the meaningful geometrical parameters adopted as input of the procedure. The geometrical features predicted by means of the Voronoi-based reconstruction have been validated against the results of the tomographic reconstruction, as shown in Figure 1b, resulting in an accurate reproduction of the topology and specific surface area. The transport properties evaluated through CFD simulations on both the virtual and tomographic reconstruction showed the capability of our procedure in properly modeling the interaction between the fluid flow and the structure. In particular, a good agreement with experimental pressure drops ensures the capability of the reconstructed sample to reproduce the real foams behavior.
Micro-computed tomography has been a valuable tool for the development of a virtual methodology able to faithfully reconstruct the complex structure of open-cell foams by allowing a deep investigation of the real foam geometry and by enabling the validation of the reconstructed by the comparison with tomographic measurements.

References

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[2] M. Bracconi et al., Chem. Eng. Journal (2017) 315 608-620