Effective thermal conductivity in open cellular structures: a fundamental analysis of the effect of the geometrical properties and a comparison of the performances

Mauro Bracconi[1], Matteo Ambrosetti[1], Matteo Maestri[1], Gianpiero Groppi[1], Enrico Tronconi[1]*

1 Laboratory of Catalysis and Catalytic Processes, Dipartimento di Energia, Politecnico di Milano, via La Masa 34, Milano, Italy

**Corresponding author: enrico.tronconi@polimi.it*

Highlights

- Systematic investigation of effective thermal conductivity in open cell foams and POCS
- CFD simulations of heat conduction in the solid matrix
- Selection of the most appropriate configuration with respect to the solid fraction

1. Introduction

Heat management and thermal control are key aspects in the design and operability of several catalytic processes enabling a safe operation and increasing process selectivity and yield. Common fixed bed reactors are usually loaded with catalytic pellets; this reactor configuration enables high catalyst inventory but suffers from a poor radial heat transfer. Heat transfer in this configuration relies on the contribution of the convection and diffusion in the gas phase, in this solution high flow velocity implies long catalytic reactors and high pressure drops. To overcome this problem, structured catalysts have been proposed as a suitable solution for the efficient management of strongly exo- and endothermic processes. In this view, open-cell foams and periodic open cellular structures (POCS) are considered among the most promising candidates as catalyst supports. They are random and ordered reticulated interconnected solid structures, whose repeated open cells are composed by solid struts and permeable open windows. The totally interconnected solid matrix promotes high heat transfer rates, being the conduction in the solid matrix the main contribution to the heat transport. This is crucial in view of process intensification in exothermic and endothermic processes preserving the catalyst and boosting the performances of the system. The analysis of the heat conduction mechanism is crucial to enable the rational design of these structures. We analyzed the heat transfer in the solid matrix in both structures by exploiting CFD simulations carried out on virtually reconstructed structures, aiming at deriving engineering correlations for the effective thermal conductivity.

2. Methods

We generated the computational domain for the CFD simulations by exploiting accurate reconstructions of the geometries. Random open-cell foams are generated according a previously proposed methodology [1]. This procedure is based on the generation of the foam skeleton by means of the Voronoi tessellation, while the effective solid distribution is calculated with a theoretical geometrical model [2]. This methodology has already proven to be representative of the geometry of open cell foams [1]. The generation of the computational domain for POCS is carried out starting from the CAD files generated by repeating in the space the basic unit cell, i.e. cubic, diamond, tetrakaidekahedral. The simulations of heat conduction in the solid matrix are carried out by imposing a temperature difference between two opposite faces and by imposing null heat flux boundary conditions at the remaining patches. The heat flux across the solid matrix is calculate and used for the evaluation of the effective thermal conductivity. The *laplacianFoam* solver, part of the OpenFOAM framework, has been employed being able to accurately solve the Laplace equation.

3. Results and discussion

In Figure 1, the results obtained with the proposed procedure, when systematically changing the void fraction and the cell size of the open cell foam is performed, are reported, along with experimental results [3] and simulations on tomographically reconstructed samples [4]. Our results show that the main parameter controlling the heat conduction is the solid volumetric fraction, whereas a negligible effect of the cell size is observed. Increasing the solid fraction, the effective thermal conductivity increases more than linearly. A good agreement has been obtained for porosities higher than 0.85, while widely scattered experimental data are observed at lower porosity.

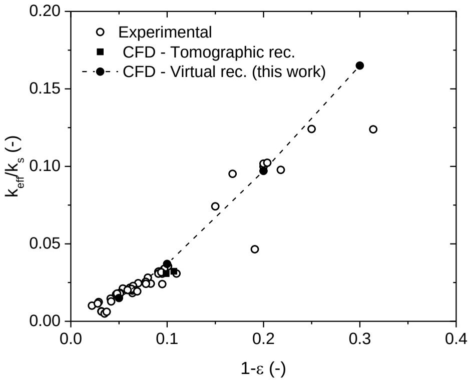

Figure 1. Effective thermal conductivity evaluated for open-cell foams by means of CFD simulations on virtual reconstruction (full circle) compared with experimental data (empty circle) and simulation on tomographically reconstructed samples from the literature

We explain this trend by the very complex topological structure of foam at such low porosities. In these structures, struts and nodes may merge together determining very large solid elements, whose presence is compensated by very thin ligaments which limits the heat conduction. The reconstructed foams employ a parabolic profile for the variation of the strut diameter along the axis, which results in characteristic distribution of the solid material between struts and node, which might not correspond to the real one in the low porosity range. We investigated the effect of the solid distribution on the effective thermal conductivity by varying the ratio of the node to the strut size. As expected, an increase of the ratio reduces the overall performances due to the higher resistance to the heat flow through the reduced strut cross-section. Accordingly, the most convenient geometry is represented by a ratio between node and strut close to one. Foam structures with a uniform strut and node diameter can be obtained by addictive manufacturing techniques whose direct application to random structure is still challenging. Thus, a comparison with the performances of POCS has been carried out to quantify the different behavior of ordered and random structure and to analyze the effect of different unit cells.

4. Conclusions

Our analysis enabled to accurately describe the effect of the geometrical properties in open-cell foams and periodic open cellular structures. The void fraction is the performance controlling parameter for both structures. Moreover, the ratio between the strut and node diameters is a crucial parameter whose value should be as close to one as possible. A relationship between the effective thermal conductivity and the solid fraction has been derived for several structures enabling a rational choice of the most adequate geometry.

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Keywords
open-cell foams; periodic open cellular structures; heat conduction, effective thermal conductivity