

Assessing virtually reconstructed structures for the CFD simulation of multiphase flows in open-cell foams

Mauro Bracconi^{1,2}, Matteo Maestri¹, Gianpiero Groppi¹, Enrico Tronconi¹, Claudio Fonte², Xiaolei Fan^{2*}

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

2 School of Chemical Engineering and Analytical Science, University of Manchester, Manchester, United Kingdom

*xialoei.fan@manchester.co.uk

Highlights

- VOF simulation of multiphase flow in open-cell foams
- Investigation of static hold-up in open-cell foams by means of CFD
- Analysis of liquid spreading in upper part of the packing

1. Introduction

Structured packings have been proposed as innovative catalyst supports in the context of multiphase reactors, such as trickle bed reactors. In particular, open-cell foams have been proposed to overcome the transfer limitations of conventional packed beds [1]. The high degree of isotropy of these structures is crucial for achieving a homogeneous phase distribution increasing both the gas-liquid and the liquid-catalyst contacts. Moreover, the high void fraction enables low pressure drops without compromising throughputs. Depending on the gas and liquid flowrate, the flow regime of the multiphase flow can be adjusted to realize either a low or a high interaction regime. The low interaction regime is also known as trickle flow, whereas the high interaction regime comprises pulse, spray, and bubble flow [2]. The analysis of multiphase flow in open-cell foam from an experimental standpoint is extremely demanding. Complex experimental set-ups which usually involve *in-situ* micro-computed tomography are needed to accurately investigate the complex phenomena. In this context, Computational Fluid Dynamics (CFD) might be a valuable tool to obtain insights into the interaction between gas, liquid and the solid structure. The application of CFD to these structures faces several challenges. Among all, the generation a suitable and representative computational domain is crucial to extract the gas-liquid-solid interactions. We have previously proposed a virtual reconstruction methodology [3] which is able to generate open-cell foams fully retaining the geometrical properties of real structures. The evaluation of the static hold-up has been carried out by means of CFD simulations on the reconstructed foam to assess the capability of the virtual structure to reproduce the complex interaction between the fluids and the solid matrix. Then, a preliminary simulation of a lab scale trickle bed reactor has been carried out.

2. Methods

A reliable structural model representing cellular foams is crucial for accurate CFD simulations. Thus, we generate the computational domains according to the methodology proposed in [3]. This procedure is based on the generation of the foam skeleton by means of the Voronoi tessellation, while the effective solid distribution between nodes and struts is evaluated with a theoretical geometrical model [4] and is used as initial guess for the virtual reconstruction. The reconstructed foams predict with very good agreement the specific surface area and the pressure drops in single phase flow [3]. Thus, they are a reliable reproduction of real foams which can be explore in the CFD simulation of multi-phase flows. We carried out CFD simulations using the Volume of Fluid (VOF) method and the OpenFOAM solver *interFoam*, enabling the accurately track of the interface evolution between the phases. We analyzed the static hold-up by carrying out simulation on single or stacks of foam disks of 26.8 mm of diameter and 20 mm length. Then, we

analyzed the liquid spreading in the upper portion of the packing in a column of 80 mm of diameter using a single input of 9 mm and exploiting the symmetry of the system simulating a quarter of the reactor.

3. Results and discussion

Two different aspects of a multiphase flow in open-cell foams have been addressed. First, the static hold-up, defined as the liquid in the foam which does not drain from the packing when the liquid supply to the column is discontinued, has been evaluated as a function of the geometrical properties. The static hold up is pivotal indicator of the capillary effects which are strongly correlated to the liquid properties and, above all, to the geometrical properties of the packing. We achieve a good agreement between the CFD simulation and literature correlation [2] derived from experimental data, as shown in Figure 1(a). An overestimation of the liquid content is experienced for low Eötvös number due to the relative short length of the packing [5].

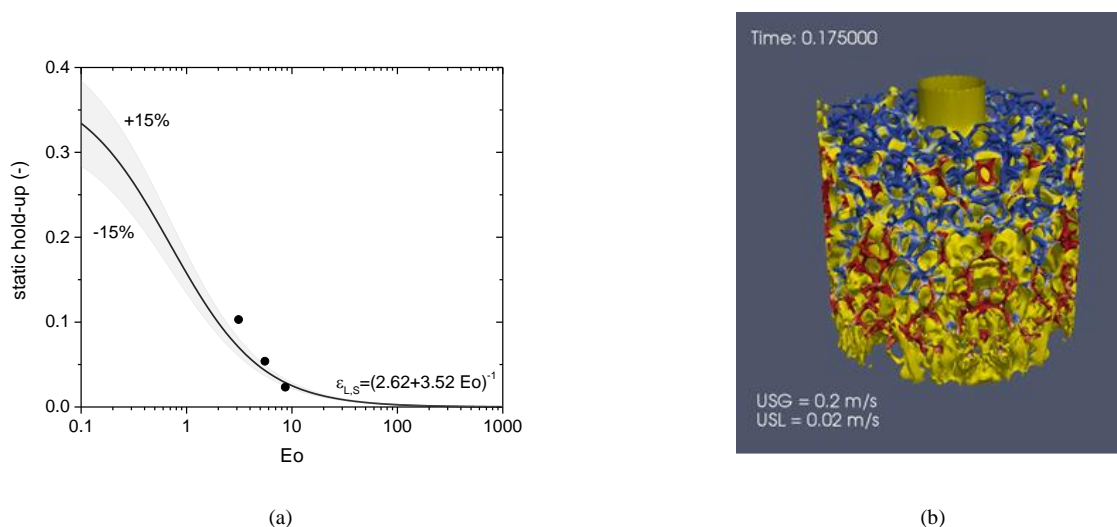


Figure 1. Static hold-up evaluated by means of CFD (symbols) and a literature correlation [2] (a); liquid distribution in open-cell foams (b)

Then, we described the behavior of a laboratory scale packing to assess the effect of the foam in reducing the liquid maldistribution. We adopted the same reactor configuration used in literature [2] and compared the liquid spreading in the upper part of the packing obtaining a good qualitative agreement in the distribution, as show in Figure 1(b).

4. Conclusions

In this contribution, we have assessed the capability of virtually generated foam models to represent the complex multiphase behaviors in real foams. We demonstrate that with this approach the interaction between the complex and tridimensional structure and the multiphase flow can be described using CFD, paving the way for a more fundamental investigation of transport phenomena in structured foams.

References

- [1] Mohammed, T. Bauer, M. Schubert, R. Lange, Chem. Eng. Sci. 108 (2014) 223–232.
- [2] J. Zalucky, M. Wagner, M. Schubert, R. Lange, U. Hampel, Chem. Eng. Sci. 168 (2017) 480–494.
- [3] M. Bracconi, M. Ambrosetti, M. Maestri, G. Groppi, E. Tronconi, Chem. Eng. J. 315 (2017) 608–620.
- [4] M. Ambrosetti, M. Bracconi, G. Groppi, E. Tronconi, Chem. Ing. Tech. 89 (2017) 915–925.
- [5] J. Grosse, M. Kind, Ind. Eng. Chem. Res. 50 (2011) 4631–4640

Keywords

open-cell foams; pressure drops, 3D print