Doctoral Dissertation
Doctoral Program in Chemical Engineering ($35^{th}$cycle)

# Fluid dynamics and mass transfer in porous media

## Modelling fluid flow and filtration inside open-cell foams

By

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# Abstract

Open-cell foams are a class of porous materials which have seen an increase in interest and usage over the last twenty/thirty years, because of their peculiar characteristics: they are characterized by an open cellular structure, with porosity ranging between 75 and 95 % and a very high bulk specific surface.

The combination of these factors results in the features for which they became appreciated: lower pressure drops compared to classic reactor packings, such as granular beds, and improved radial heat and mass transfer due to reduced channeling effects. Because of the increasing potential applications of these porous media the modeling and characterization of open-cell foams is of great importance but remains a challenging issue.

The work reported in this manuscript aims to propose possible methodologies for the modeling of the geometric structure of these materials, using in-silico tools for their generation and Computational Fluid Dynamics (CFD) numerical simulations for the investigation of the transport phenomena of a fluid flowing within the porous medium. Moreover, the performances of solid foams for the filtration of colloidal and fine particles are investigated with CFD and analyzed by means of classic clean-bed filtration models, commonly employed for the evaluation of the deposition efficiency.

The first Chapter introduces open-cell foams and their principal geometric and morphological features as well as giving an outline of the state of the art in the literature for such porous media, focusing on the use of CFD and other computational methods for the generation of the geometry and the transport phenomena investigation.

Different methods are reviewed, such as the well-known ideal periodic polyhedron known as the Kelvin's Cell, as well as more complex methods based on the use of random tessellations, such as the Voronoi tessellation, an algorithm that generate a cellular structure similar to the basic skeleton of open-cell foams. This latter method is able to describe with higher accuracy the randomness and complexity of real

ceramic and metallic foams. Finally, a brief review on the use of computational methods and numerical simulation to investigate and model transport phenomena in open-cell foams is proposed.

The second Chapter provides a synthesis of the equations governing the simulated systems and the framework used for the analysis of the filtration phenomena. Furthermore, the theoretical background of the main algorithm used for the generation of foam digital geometries is reported, with particular focus on the ideal Kelvin's Cell model, the random Voronoi tessellations and the processing of binary images.

Chapter 3 introduces an open-source workflow able to reproduce a great variety of geometries at different levels of complexity, developed using the open-source software `Blender` and `Python` programming language code. This workflow is then tested by performing numerical simulations to explore the flow field on the created geometries and investigate the mass transfer phenomena occurring during the filtration of colloidal particles. The simulations are carried out with the open-source software `OpenFOAM`, and the data obtained are used to calculate an effective deposition rate coefficient $K_d$. The results are interpreted using well-known constitutive equations of classical clean-bed filtration models, Yao et al. (1971), and other functional forms of the main geometric descriptors. However, they are found insufficient in explaining the variations in filtration performances, highlighting the need for both more detailed exploration and modelling.

This last issue is tackled in Chapter 4, where an updated and improved geometry generation workflow is proposed and validated. Pressure drops measurements across a column packed with ceramic or metallic foam cylindrical pellets, with different geometrical properties, are obtained both via experiments and through CFD simulations, carried out with `Ansys Fluent`, using geometries reconstructed from tomography images. The workflow is tested by generating replicas of the examined foams: a geometric comparison shows that the in-silico workflow is able to generate, in-silico, structures whose macro-descriptors, porosity, specific surface and tortuosity, commonly employed in the field of porous media, lie within a 5-6 % range of error, compared to the original foams. Also, from the fluid dynamic point of view the results of the CFD simulations using the replicas are in good agreement with both experiments and simulations on the digitally reconstructed real foams. The novel in-silico tool proves to be accurate in reproducing the behavior of porous media as well as effective, because of the low computational costs required to generate a digital sample. This part of the work has been carried out in collaboration with French research institute IFP – Energies Nouvelles.

Chapter 5 focuses on a practical problem affecting the refinery industry, the separation of fine particles from hydrocarbon streams ahead of catalytic reactions. The system is simulated coupling CFD for the solution of the flow field and Lagrangian simulations, carried out with `Ansys Fluent`, for the calculation of the particles trajectories. The model is first validated by comparing the results obtained for a granular bed configuration with the deposition model proposed by Yao et al. (1971). Then, the same methodology is employed to three ceramic foams geometries, with the aim of identifying which characteristic lengths can be used to describe the deposition phenomena interpreted according to the filtration model of Yao. The results highlight how the complex structure of the materials in exam cannot be described by a single geometric parameter and stress the need of further detailed investigation on the topic. This work as well has been carried out in collaboration with IFP – Energies Nouvelles.

Finally, Chapter 6 concludes the manuscript, focusing on the objectives of the different subjects tackled, the model proposed and the workflows developed. The main results are delineated as well as the issues arisen from the research that requires further investigations. Possible future perspectives and developments of the proposed workflows are addressed as well as where their use could lead to an improvement and an optimization of the employment of open-cell foams in the field of process industry.