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# Combined CFD and experimental and investigation of mass transfer in open-cell foams

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***Highlights***

- External mass transfer characterization of open-cell foams
- CFD simulations and experiments to investigate the effect of morphological parameters
- Derivation of a new engineering correlation for the mass transfer coefficients

## 1. Introduction

Open-cell foams are potential innovative structured catalyst supports particularly promising for industrial applications limited by gas/solid heat and mass transfer. They are cellular materials made of interconnected solid struts which enclose void regions communicating through open pores. The remarkable combination of beneficial properties, such as high specific surface area, low density and high permeability to the fluid flow, makes these structures very attractive as enhanced catalyst carriers especially for exhausts aftertreatment applications. In this respect, a deeper understanding of the transport phenomena in such structures can promote their extensive application. Computational Fluid Dynamics (CFD) is a powerful instrument to enable accurate analyses of the complex flow field and of gas-to-solid transport, also driving dedicated experimental activities. The application of a hierarchical approach [1] makes CFD a valid tool for the derivation of lumped parameters which can be easily plugged in conventional reactor models. Selected experimental tests are however needed in order to provide a cross-validation of the CFD results. In this contribution, we propose a systematic CFD + experimental investigation of the effects of the geometrical properties of open-cell foams on mass transfer coefficients, aimed at increasing our understanding of the complex transport phenomena in open-cell foams. Moreover, we derive an engineering correlation for the description of gas/solid mass transport able to account for the effect of the foam morphological features in different flow regimes over the widest range of Re numbers investigated so far.

## 2. Methods

The numerical analysis of the effect of the morphological parameters requires the accurate reconstruction of the foam geometry. In this view, we proposed a virtual reconstruction procedure able to generate synthetic open-cell foams fully retaining the geometrical and fluid dynamic properties of the real structures [2]. The reconstruction procedure is based on the generation of the foam skeleton by means of the Voronoi tessellation. The accurate description of struts and nodes is carried out with a dedicated model accounting for solid distribution and different cross-sectional shapes. The reconstructed foams are then exploited to investigate the gas-to-solid mass transfer properties. The CFD simulations are carried out using catalyticFOAM [3], a numerical framework coupling the solution of the Navier-Stokes equations with the description of the surface reactivity. Experimental evaluation of mass transfer was based on CO oxidation runs on Pd/CeO2 in a tubular reactor in a fully diffusional regime. The numerical and experimental results are interpreted by means of a fully-theoretically based geometrical model [4].

## 3. Results and discussion

The CFD simulations of mass transfer are carried out on virtually-generated structures enabling a parametric analysis of the effect of each geometrical feature. The adequacy of the reconstructed foams to represent the mass transfer in real structures is assessed by reproducing experimental results. In the CFD simulations we adopt the same operating conditions of the experiments and we compare the predicted conversion to the experimental data.

A very good agreement is experienced confirming the adequacy of the reconstructed geometry in reproducing external transport phenomena. We then investigate the influence of the porosity, the cell size and the strut cross-sectional shape. A broad range of flowrates are exploited to cover conditions of industrial relevance. The parametric analysis of the effect of the geometrical features reveals that the porosity strongly affects the mass transfer coefficients. This effect has been quantified as a dependence on the inverse of the square of the void fraction. The cell sizes and the different strut cross-sectional shapes have a negligible influence on the mass transfer. Moreover, two distinct contributions can be identified in these structures according to the flow regime: a viscous creeping flow contribution at low Reynolds numbers, and a term related to the instabilities formed in the wake behind the struts and nodes at higher flowrates. These results have been validated and confirmed by dedicated experimental measurements. We selected as characteristic length the average strut size, i.e. the strut diameter and the strut side for the circular and triangular cross-section, respectively. This quantity reconciles the data for both triangular and circular struts in a unique correlation. Moreover, the transition between the Darcy to the post-Forchheimer flow in open-cell foams occurs close to the values reported in literature for circular and triangular cylinders in cross-flow. Therefore, the average strut size seems a physically sound characteristic length most appropriate to describe the flow phenomena in such structures. An engineering correlation able to well describe the mass transfer in open-cell foams has been developed. Deviations between measured/simulated and predicted values are typically below 15 %, as shown in Figure 1.

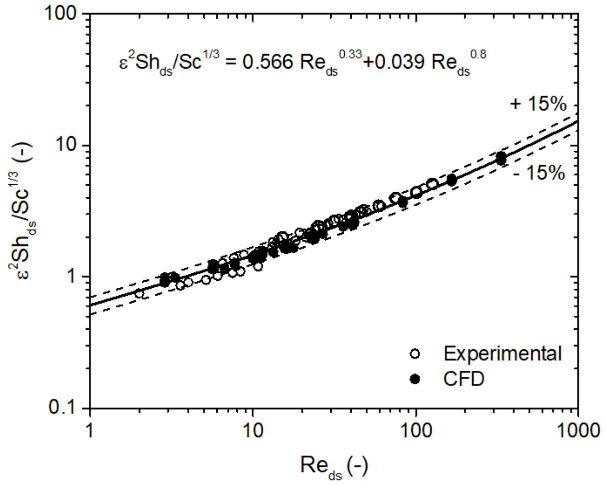

**Figure 1.** Mass transfer results from both simulation (full symbol) and experiments (empty symbol)

## 4. Conclusions

We propose a systematic investigation of the external mass transfer phenomena in open-cell foams by means of a coupled experimental and numerical approach. The effects of geometrical parameters have been elucidated. A dependence on the inverse of the square of the void fraction is experienced, whereas negligible effects of the cell size and strut cross-sectional shape have been observed. An engineering correlation accurately describing the mass transfer coefficients as a function of the flow conditions and of the complex geometrical properties of the foams has been derived over a wide range of Re numbers.

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***Keywords***
open-cell foams; computational fluid dynamics; experimental test, mass transfer