Intensified POCS structured supports with optimized cell and streamlined strut shape for mass-transfer limited catalytic applications

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

1 Laboratory of Catalysis and Catalytic Processes, Department of Energy, Politecnico di Milano, Via La Masa 34, 20156 Milano, Italy

**enrico.tronconi@polimi.it*

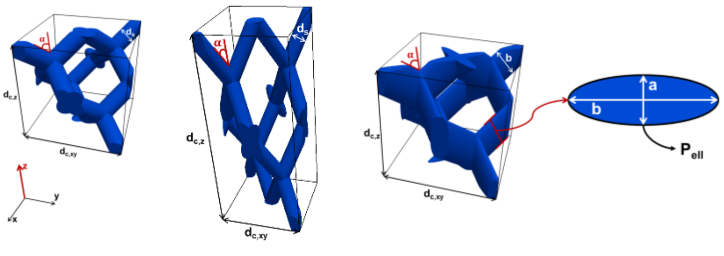
Highlights

- Strut orientation and shape of POCS are modified to fine-tune the fluid-solid interaction
- POCS are optimized to intensify the trade-off between mass transfer and pressure drop
- POCS provide higher mass transfer coefficient than honeycomb supports with same pressure drop

1. Introduction

Periodic Open Cellular Structures (POCS - Figure 1) are innovative structured catalytic supports for Process Intensification thanks to their enhanced heat and mass transfer rates inside catalytic reactive systems [1-3]. They are produced by means of additive manufacturing, which allows for high freedom in design thus enabling to optimize POCS geometrical features to tailor them for specific process needs, e.g., to improve the flow distribution inside chemical reactors [1,2]. POCS are envisioned as a possible alternative to state-of-the-art structured supports for processes dominated by a trade-off between gas-solid mass transfer and pressure drop [4], such as in many environmental catalysis applications rooting their success on honeycomb monoliths. Despite conventional POCS shapes (Figure 1 (a)) offer worse overall performances than the state-of-the-art structured support, we have previously demonstrated [3] that modification to the cell geometry, e.g., modifying the orientation of the struts of the unit cell to the flow direction (Figure 1 (b)), results in lower pressure drop without a significant penalization of the mass transport properties, obtaining better performances than honeycomb monoliths.

Herein, we propose an evolution of the geometry by considering streamlined elliptical struts aligned to the flow direction (Figure 1 (c)), which enables a further boost of the POCS performances.



(a) (b) (c)

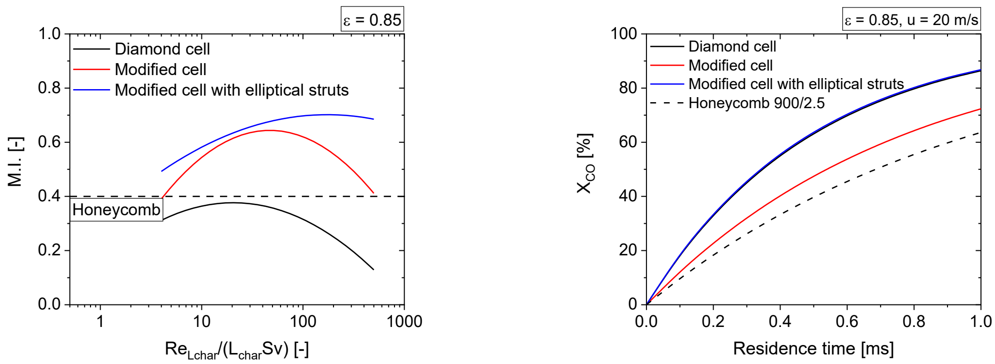
Figure 1. (a) Regular diamond lattice with circular struts, (b) modified design with circular struts [3], (c) modified design with elliptical struts.

2. Methods

In this work, we adopt a numerical approach rooted on reactive Computational Fluid Dynamics (CFD) simulations to evaluate the transport properties and pressure drop of POCS. A detailed description of the approach is reported in [3] and is hereby briefly summarized. Detailed CFD simulations are employed to fundamentally investigate the properties of POCS. To do so, computational domains consisting of one unit cell are generated, which was identified as Representative Elementary Volume [3] of the POCS. Periodic boundary conditions are set at the domain side boundary, thus obtaining asymptotic fluid flow and concentration profiles inside the system. These conditions are achieved when the size of the equipment is orders of magnitudes greater than the unit cell itself (i.e., 10^0 m vs. 10^{-3} m).

3. Results and discussion

The regular POCS unit cell (a) was previously modified by changing the angle α between the struts and the fluid flow direction z, obtaining a stretched unit cell along z (Figure 1 (b)) [3]. Herein, the geometry is further manipulated by introducing elliptical struts lined up to the flow direction (Figure 1 (c)) while keeping constant the solid volume fraction. This enables higher specific surface areas for catalyst deposition, hence larger volumetric mass transport coefficients, with a concomitant reduction of the pressure drop thanks to the lower drag given by the streamlined struts. The effect of these two combined features is reported in Figure 2 (a). The Merit Index (M.I.), a dimensionless group representative of the ratio between mass transfer and pressure drop performances, is shown for the optimized cell with elliptical struts and compared against the previous shapes and a reference honeycomb (HC) monolith 900/2.5. The POCS share the same porosity ε with the HC, i.e., 0.85. The original Diamond cell always provides poorer performances than the HC, conversely, the modified cell provides up to 1.5-fold higher trade-off index. A further enhancement of the M.I. is obtained by using streamlined elliptical struts with a concomitant extension of the range of Re where the new structure overcomes state-of-the-art supports. This is a crucial result for the adoption of this structures in automotive applications where significant load variations occur during the driving cycle. This is beneficial at high exhaust gas velocity, e.g., u = 20 m/s, as shown in Figure 2 (b), where CO oxidation at 300°C is considered as a mass transfer limited reaction occurring in an abatement system. POCS with a strut size of around 340 μm have been considered, corresponding to a $Re \cdot (L_{char} S_V)^{-1} = 250$. The simple Diamond cell provides up to 20% higher mass transfer limited CO conversion (X_{CO}) than the HC, however, a 5-fold higher pressure drop is obtained preventing its possible application. The modified cell provides the same pressure drop as the HC, and 10% higher X_{CO}. Finally, the structure with elliptical struts grants the same conversion as the standard shape, along with same pressure drop as the HC, hence resulting in a significant enhancement of the abatement efficiency without any additional penalty.



(a) (b)

Figure 2 (a) Trade-off index between mass transfer and pressure drop evaluated through the Merit Index (M.I.). (b) Mass transfer limited CO conversion X_{CO} versus residence time.

4. Conclusions

This work reveals that optimized POCS with finely-tuned geometrical features offer high potential as intensified structured supports, paving the way for a new generation of intensified catalytic reactors.

References

[1] Do G. et al., Chem. Eng. Process 148 (2020) 107786
[2] Lämmermann M. et al., Chem. Eng. Process. 126 (2018) 178-189
[3] Ferroni C. et al. Chem. Eng. Process. 195 (2024) 10961
[4] Giani L. et al., Ind. Eng. Chem. Res. 44 (2005) 4993-5002

Keywords

Process Intensification, Structured Catalytic Supports, Heat and Mass Transfer, Lattice Materials