

# Enhanced heat management in 3D printed catalyst structures: from CFD modelling to experimental demonstration

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# Enhanced heat management in 3D printed catalyst structures: from CFD modelling to experimental demonstration

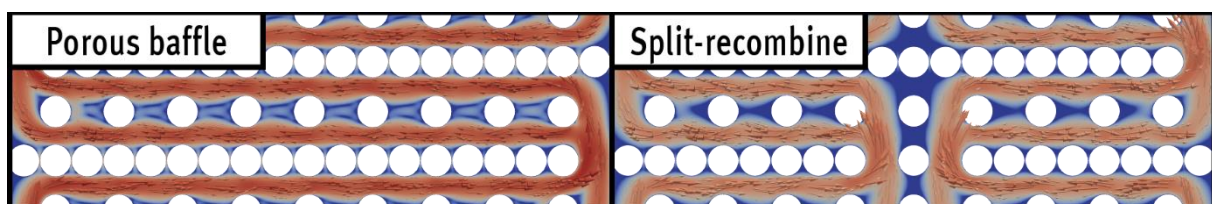
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## Introduction

Heat management is key in chemical reactor design, as deviations from the intended operating temperature may lead to decreased product yield and catalyst degradation. Conventional packed catalyst beds exhibit a relatively low effective radial thermal conductivity and this necessitates costly multi-tubular reactor configurations with low diameter tubes for adequate temperature control. Structured catalytic reactor internals enable higher wall-to-bed heat transfer thanks to catalyst supports with a high thermal conductivity, but the washcoat configuration limits the catalyst holdup. As an alternative, 3D printed baffled logpile structures are proposed in this work, relying on a cross-flow regime with radial convection for enhanced heat management. A visual representation of such structures is shown in Figure 1. By 3D printing of baffles out of cylinders (spaced in the order of tens to hundreds of microns), the high pressure drop and stagnant volume of conventional baffles can be overcome. The properties of these porous baffles can be further tuned to provide an optimal trade-off between pressure drop and heat transfer properties at relatively high catalyst holdups.



*Figure 1, 2D representation of two baffled logpile configurations. White circles represent printed catalyst and shaded area represents the fluid phase with colors indicating the velocity magnitude with scaling from blue to red (low to high). Direction of flow is upwards.*

## Selected results and conclusions

The heat transfer performance and pressure drop of pseudo-2D geometries with varying configuration, baffle fraction and spacing were investigated using OpenFOAM CFD simulations. Figure 2 shows these two performance indicators as a function of

the cylinder spacing, relative to a conventional, non-porous baffle. It can be seen that the heat transfer may be slightly lower for the baffled logpile structure, but with a much lower pressure drop. This clearly illustrates the potential for process intensification exploiting these structures.

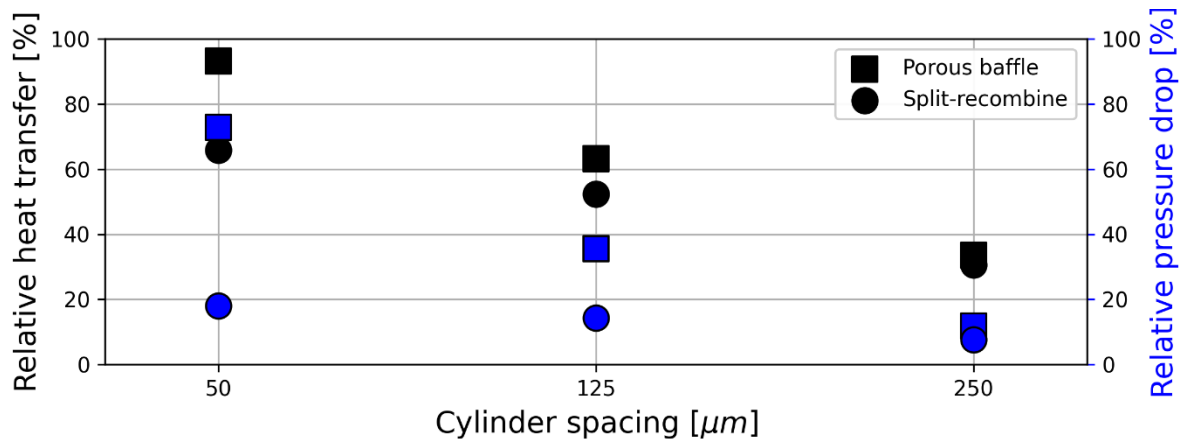


Figure 2, Comparison of the relative heat transfer (in black) and pressure drop (in blue) of two exemplary structures as a function of cylinder spacing.

Motivated by these findings, first polymer-based structures were produced, because of their large (and particularly fast) possibilities in geometrical design and good mechanical stability. For different baffle configurations the pressure drop and heat transfer characteristics were measured and the experimental findings were compared with CFD modelling results to determine the optimal design of these baffled logpile structures. Finally, catalyst was structured in similar geometries through Direct Ink Writing to experimentally quantify the heat transfer, pressure drop and catalytic performance and demonstrate the potential of these structures.

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