Detailed Numerical Investigation of the Effective Radial Thermal Conductivity of Cellular Catalyst Support Structures

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Aiming at safe, sustainable and efficient chemical processes, the structuring of reactor internals is a main strategy for process intensification. The geometry of internals significantly dictates a reactor's performance due to the direct influence on the underlying transport processes of momentum, heat and mass. Up to this day, the research on cellular support structures for heterogeneous catalysts is a still growing field to overcome inherent limitations of randomly packed beds with catalyst particles. State-of-the-art structures are monolithic honeycombs; novel approaches include open cell foam structures (OCFS) and periodic open cellular structures (POCS) as promising options. Characteristic for all types of these structures are the continuous solid matrix and a high porosity, resulting in a low pressure drop yet a high effective thermal conductivity. In contrast to monolithic honeycombs, OCFS and POCS allow for cross-mixing of the fluid. The unique feature of POCS is the high degree of freedom in design and their potential for tailored reactor optimization, thanks to fabrication by additive manufacturing [1]. Nonetheless, in order to design optimized reactor internals, knowledge about all transport characteristics and scaling correlations are required. Recently, a study on the tubular application of POCS revealed a hyperbolic dependency of the effective radial thermal conductivity $k_{eff,r}$ on the ratio of tube diameter-to-cell size (number of cells per tube diameter, CPD_t), yet this study was performed on a limited data basis [2]. With our current contribution, we provide further insights and confirm the hypothesis that this phenomenon applies to cellular structures in general. For this, spatially resolved numerical simulations of heat conduction in several structures were carried out, applying a steady-state radial temperature gradient of 20 K. Special focus was set on different unit cell types of POCS and a varying porosity. To save computational effort, only a section of the structure with symmetry boundary condition was used, see Figure 1. Contrary to expectations and to the case of mono-directional heat conduction in Cartesian coordinates, in tubular applications with cylindrical coordinates the type of the unit cell has an impact on the effective radial

thermal conductivity $k_{eff,r}$. An additional effect is observed on the asymptotic threshold value of $k_{eff,r}$ for high CPD_t with increasing solid fractions of the structures.

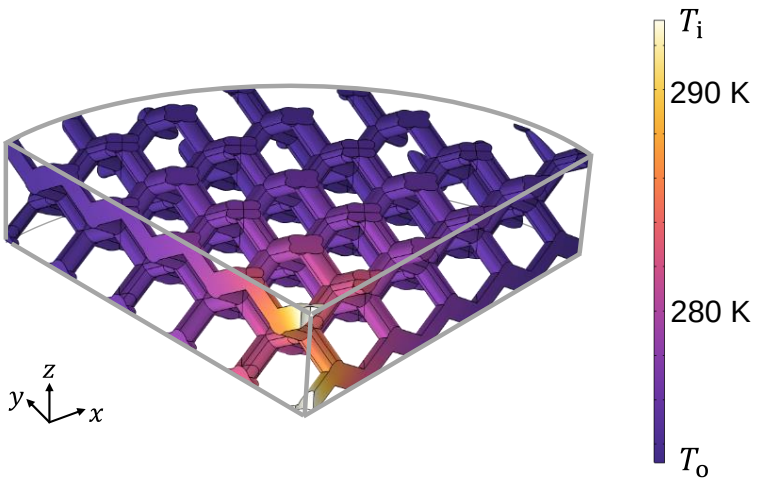

Figure 1: Graphical simulation result for a cutout of a diamond cell POCS with CPD_t = 10 and an applied radial temperature gradient of 20 K.

References

[1] Eckendörfer, L., Rudolf, D., Brix, A., Börnhorst, M., & Freund, H., Periodic Open Cellular Structures in Chemical Engineering: Application in Catalysis and Separation Processes, *Annu. Rev. Chem. Biomol. Eng.,* 2024, 15:163–186

[2] Rudolf, D., Fink, A., Körner, C., & Freund, H., Thermo-Mechanical Study on Auxetic Shape Memory Periodic Open Cellular Structures—Part I: Characterization of Reentrant Geometry and Effective Heat Conductivity, *Adv. Eng. Mater.,* 2024, 26, 2401717