Intelligent Design of Structured Catalysts for Flexible, Safe and Efficient Reactor Operation

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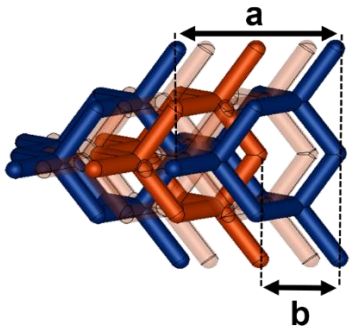
- **Structured catalyst supports with optimized and tailor-made properties**
- **Additive manufacturing as enabling technology for unlocking a new degree of freedom in design**
- **Combination of improved reactor performance with operational flexibility**

An intelligent matching of reaction and transport processes is key to the design and operation of optimal catalytic reactors. For the realization of optimal reaction and process conditions, the system specific requirements regarding heat and mass transport characteristics demand for suitable catalyst support materials and reactor geometries. In this regard, additive manufacturing (AM) techniques have emerged as enabling technology, which unlocks a new degree of freedom in the design of structured reactors with tailored properties. AM allows for the fabrication of open cellular structures of nearly arbitrary geometrical complexity, and this in a well-defined and highly reproducible manner.

In our work, we study periodic open cellular structures (POCS) that were manufactured using different AM techniques such as FDM or SLA for polymers and L-PBF or EB-PBF for metals. POCS are promising novel catalyst supports as they offer clear advantages over conventional randomly packed fixed-bed reactors in terms of pressure drop [1-4] and heat management [5-9, 16-17] as well as liquid distribution in multiphase applications [3, 10-11, 15]. In fact, POCS combine the advantages of randomly packed beds (radial mixing, tortuosity of the flow) and honeycombs (high geometric specific surface area, low pressure drop) owing to their high porosities and their characteristic 3D cellular architecture.

Based on extensive experimental investigations as well as modeling and simulation, correlations for specific surface area, pressure drop and heat transport for POCS were developed. These models enable the design and optimization of POCS that are tailor-made according to the needs of the reaction system. In our work, such tailor-made POCS were manufactured, functionalized by catalytic coating, and then applied in different catalytic reaction systems with focus on the optimization of heat transport (for highly exothermic gas phase reactions) and gas-liquid distribution and mass transfer (in trickle-bed reactors), respectively.



$$\text{shift } \% = \frac{a-b}{a} * 100\%$$

Figure 1. Scheme of the diamond unit cell interPOCS. Blue: fixed structure, Orange: movable structure

To achieve even more flexibility with regard to transport characteristics, we have recently proposed several novel variants of POCS with unconventional unit cell design. One of them is a new type of interpenetrating POCS (interPOCS) which are formed by inserting a diamond unit cell based structure in the cavities of a second diamond cell structure (see Figure 1). These interPOCS allow for in operando flow field and mass transport adjustments by shifting the (relative) position of the movable structure [4]. With detailed computational fluid dynamics (CFD) simulations and an additional in-house particle-tracking algorithm implementation [12] we systematically investigated the flow field and mass transport characteristics within the interPOCS in dependency of the relative positioning of the movable structure [13]. The highly adjustable structure allows for a broad variation of mass transport characteristics in a catalytic reactor without changing the system's periphery. This functionality enables mass transport optimization for a given system and represents a completely new application of additively manufactured catalyst support structures for highly flexible in operando tuning of flow field and mass transport characteristics.

Further novel intelligent designs include the novel DiaKel hybrid unit cell for improved liquid distribution in trickle bed applications [10]. To enhance gas-solid mass transfer stretched unit cells resulting in anisotropic POCS were proposed [14], while for improving gas-liquid mass transfer a specially designed unit cell that enforces meandering flow was developed [15]. To address the challenge of realizing a perfect wall contact between structure and wall in tubular reactors, yet with the possibility to exchange the structured catalyst when deactivated, auxetic POCS made of shape memory alloy were designed, manufactured and evaluated to enable a reversible wall contact [16-17].

These novel support structures allow combining improved performance with higher flexibility in their application, which is an important next step for industrial implementation in catalysis and separation processes [18].

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