Particle-resolved CFD simulations of metal foams used as structured catalyst support

Gregor D. Wehinger[1*], Stan T. Kolaczkowski[2],

Didier Beton[3], Robin Kolvenbach[3], and Lars Torkuhl[3]

1 Chemical and Electrochemical Process Engineering, Clausthal University of Technology; 2 Chemical Engineering, University of Bath, 3 Alantum Europe GmbH

**Corresponding author: wehinger@icvt.tu-clausthal.de*

Highlights

- Local transport phenomena are captured by detailed CFD simulations.
- CFD model is validated by experiments.
- Different foam-pellet shapes are explored by this model.
- Metal foams pellets show promising characteristics.

1. Introduction

Typically, ceramic pellets are used as catalyst support in fixed-bed reactors. Those pellets can have different shapes, like spheres, one- or multi-hole rings, trilobes, etc. During the last two decades, a certain interest has arisen to apply open-cell solid foams as structured catalyst support [1-3]. They are characterized by a high porosity (>80%), good mechanical and structural properties, and remarkable global thermal conductivity. For exothermic reactions, like catalytic converters, monolith structures show interesting results. However, for endothermic reactions, e.g., steam reforming of methane, heat needs to be transferred from the tube wall into the center of the bed. Recently, Kolaczkowski et al. [4] compared pellets made from metal foams with monolith structures in terms of pressure drop and heat transfer performance. The foam pellets showed advantages, especially due to their mixing behavior.

The most detailed description of transport phenomena is captured by so called particle-resolved CFD simulations [5,6]. Every single pellet of the fixed bed is resolved geometrically. Then, transport of momentum, heat, and mass, as well as heterogeneous reactions can be calculated on a high spatial resolution.

In order to explore the influence of different pellet shapes, the particle-resolved CFD approach is applied to metal foams used as structured catalyst support. First, the synthetic generation of fixed beds of foam pellets is validated against experimental data. Second, pressure drop and heat transfer are compared between experiments and CFD simulations. Finally, the influence of the foam-pellet shape is explored with the developed model.

2. Methods

Pressure drop and heat transfer characteristics were investigated in a recently developed apparatus [4]. A reactor tube with an inner diameter of 71.4 mm and a height of 500 mm was filled with different foam pellets and heated with an electric furnace. The inlet temperature was varied in the range of 300-700 °C. The resulting radial outlet-temperature profiles were recorded with thermocouples inserted into a ceramic monolith.

The bed structures for the CFD simulations were generated synthetically with DEM simulations, see [7] for the detailed description of the applied methodology. The resulting geometry was meshed using polyhedral cells in the bulk and prism cells in near-wall regions. The foam pellets were described with the porous media model with an effective thermal conductivity and a pressure-drop description based on [8]. The model includes surface-to-surface radiation. Boundary conditions were used in accordance with the experiments. All simulations were realized with the CFD software STAR-CCM+ version 12.04 from Siemens PLM Software.

3. Results and discussion

As a starting point, Figure 1 (A) shows a photograph of a bed of 10 mm foam cubes from the top. In (B) the synthetically generated bed can be seen, where the observed global porosity is in line with the experiment. In (C) heat transfer from the wall into the a bed of 15 mm cubes is illustrated. The mixing behavior, and likewise the radial heat transport, differs significantly from foam monoliths, which fill the entire tube.

With the validated CFD model, not shown, different foam-pellet shapes are explored and characterized in terms of pressure drop, residence time distribution, and heat transfer performance.

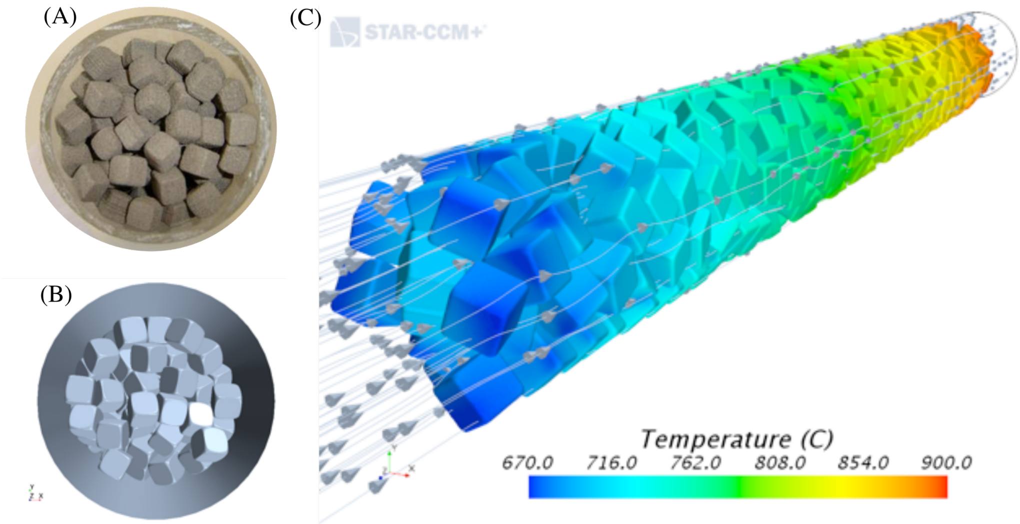

Figure 1. (A) Photograph and (B) synthetically generated bed of 10 mm cubes. (C) Temperature distribution inside a bed of 15 mm foam cubes (CFD results). Wall temperature 900 °C.

4. Conclusions and outlook

This work, continuously supported by experiments, shows the application of particle-resolved CFD simulations for the description of fixed-bed reactors made of foam pellets. Bed morphology, pressure drop and heat transfer characteristics agree reasonably well with experimental data. This model allows for a virtual design exploration of the influence of different foam-pellet shapes towards transport phenomena. Ongoing simulations with different pellet geometries and intrinsic foam properties suggest that pressure drop, mixing behavior and likewise convective radial heat transport can be controlled and improved. Consequently, this model is a valuable tool for research and development of this novel type of structured catalyst support.

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Keywords
Metal foams; fixed-bed reactor; CFD; heat transfer