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Numerical simulations of fluid dynamics in carrier structures for catalysis: characterization and need for optimization

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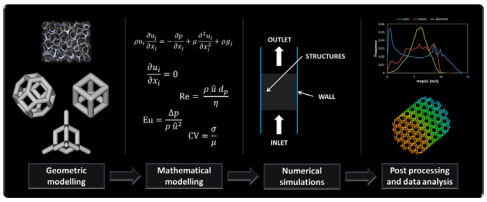
HIGHLIGHTS

- Numerical simulations of open cell foams as carrier structures for catalysis.
- Three different structures: cubic lattice, Kelvin cell, diamond structure.
- Characterization due to pressure and velocity fields with dimensionless numbers.
- Optimization of reactor design due to the underlying chemical reaction.

GRAPHICAL ABSTRACT



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ABSTRACT

3D fluid dynamic numerical simulations of different structured open-cell foams are presented: a cubic lattice, the tetrakaidecahedron geometry (Kelvin cell geometry), and the diamond structure. The simulations are done with the open-source software OpenFOAM. Beneath the pressure drops of the different structures, which are compared using dimensionless numbers such as Reynolds number and Euler number, also the development of velocity and its frequency distribution, as an important parameter for chemical reactions, are evaluated. As a main result, the diamond structure provides good conditions with respect to dwell time distributions for the underlying chemical reaction. All the results give a deep knowledge in terms of the underlying principles and optimization approaches.

1. Introduction

Chemical engineering science widely applies porous media as carriers for catalytic reactions. In addition to chemical properties, process parameters and geometric structures of catalytic fixed-bed reactors, including the porous media, play a crucial role in the course of chemical reactions. This holds not only for the quantity but also for the selectivity of catalytic reactions. To achieve stable and robust operation of the reactors under industrial conditions, it is necessary to be able to control the thermo-fluid dynamic phenomena in the reactor.

The operation regime of catalytic reactions regarding the chemical reaction (e.g. exothermal/endothermal) or their applicative field defines characteristic requirements and limitations of the reactors. Some of these quantities are geometric size, throughput, heat transfer, homogeneity, residence time distributions, pressure loss, and selectivity.

It is indispensable for a stable and stressed process under industrial conditions to handle the thermo-fluid dynamic processes in a very controlled way. Numerical simulations offer a method to characterize catalytic fixed-bed reactors for their planned application and to optimize them when aimed at a special use.

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Packed-bed reactors with their relatively high pressure drop are often used in cleaning polluted air (Mendes et al., 2011). In addition, other reactors, structured reactors, are becoming more and more important. Here, the expression "structured reactors" means reactors with fixed porous media, and not a random packing of spheres or other particles with different sizes. A well-known example is from the field of automotive applications, more precisely the catalytic converter (Shuai and Wang, 2004). Porous media are also used in other fields of engineering, in waste water treatment as a filter (Janzen et al., 2009), in bacteria transport in connection with groundwater decontamination (Walczak et al., 2011) and in the food industry (Braeken et al., 2004).

They are also used without a chemical reaction, e.g. for the cooling of electronic components with special interest in the heat-transfer characteristics (Hsieh et al., 2004).

Nowadays, with increasing size and capacity of computers, the ability of numerical simulations to mirror wider and wider ranges of problems is also increasing. The simulations are often used to analyse the fluid dynamic phenomena in porous media, and packed-bed and structured reactors, and to provide locally resolved information. The flow through a packed-bed reactor has been simulated with the lattice Boltzmann method and the results were validated with experimental values (Freund et al., 2003). A different simulation approach with a packed-bed bio-reactor was reported (Esterl et al., 2003), in which the Navier–Stokes equations were discretized with a Finite Volume method in combination with the Chimera approach, which uses several grids to solve the equations. The substrate transport and conversion were also studied there.

In addition to packed-bed reactors, structured reactors with a foam-like structure are treated more and more numerically. The case of conjugate heat transfer through an open-cell foam has been studied (Kopanidis et al., 2010). Even special representatives for foams have been used, e.g. a Weaire–Phelan periodic cellular unit (Boomsma et al., 2003). The obtained underestimated pressure drop regarding the experimental data was explained as being due to missing surface effects, and the influence of these effects was shown using numerical modelling. Other publications deal with the simulation of only a part of a reactor (Bai and Chung, 2011) or a part of a tetrakaidecahedron cell (Kelvin cell) (Xu et al., 2008). Mills (2005) used different flow directions to simulate the velocity and the pressure field in prismatic volumes, including representative parts of a Kelvin cell. Habisreuther et al. (2008) built a well-ordered Kelvin cell and a geometric randomized version of this structure to calculate pressure drop and tortuosity. In a recent study (Horneber et al., 2012), a part of a reactor a single Kelvin cell was observed, followed by extraction of information on the simulation of the whole reactor. With simulation of a single cell, the influence of surface roughness could be shown. By comparison of the single cell and the whole reactor, contributions of entrance and exit effects to the pressure loss were demonstrated.

This paper does not deal with single cells but only with whole reactors. It addresses to a detailed and precise extent the characterization and optimization of fluid-dynamic phenomena in whole catalytic fixed-bed reactors with the aid of numerical simulations. The characterization includes fluid-dynamic and procedural indicators important for the course of chemical reactions. Different types of fixed-bed reactors are considered. The range covers a wide field from very simple rectangular lattices through structured representatives for foams, such as Kelvin cells, to diamond structures.

2. Geometric and mathematical modelling

2.1. Geometries: cubic lattice, Kelvin cell, diamond structure

Three different geometries are used as representatives for open-cell foam structures. The first is a simple cubic lattice built with the left unit cell in Fig. 1. A more foam-like geometry is the Kelvin cell structure; the unit cell is shown in the middle of Fig. 1. This structure is often used as a representative for open-cell foam structures (Bai and Chung, 2011; Xu et al., 2008; Mills, 2005; Inayat et al., 2011a, 2011b). The third geometry, a diamond structure (Fig. 1, right), is similar in open porosity to the Kelvin cells, but without narrow pores in the flow direction, which may be blocked due to bubble formation in a gas-releasing chemical reaction.

The values given in Table 1 are the average diameter d_w of the pores, the length of the struts l_s, the porosity ε and the volumetric specific surface area of the struts S_s. The strut diameter is the same for all structures: $d_s = 0.5$ mm. Every structure has three pore sizes: small (porosity $\varepsilon = 0.85$), medium ($\varepsilon = 0.9$), and large ($\varepsilon = 0.95$). These values characterize the complete geometry. The constant value of the strut diameter and the same porosity of the different structures with small, medium, and large pore sizes allows the comparison of the structures. The sizes l_s and d_s are sufficient to define all other geometric values. Here the porosity is the open porosity, calculated by

$$\varepsilon = \frac{V_{\text{empty}}}{V_{\text{total}}}, \tag{1}$$

where V_{empty} is the empty volume and V_{total} is the total volume.

The value S_s is calculated by

$$S_s = \frac{S_a}{V_{\text{total}}}, \tag{2}$$

where S_a is the surface area of the struts.

2.1.1. Cubic lattice

The cubic lattice consists of orthogonal, in all three directions, crossing, cylindrical struts. The strut length l_s for every pore size is

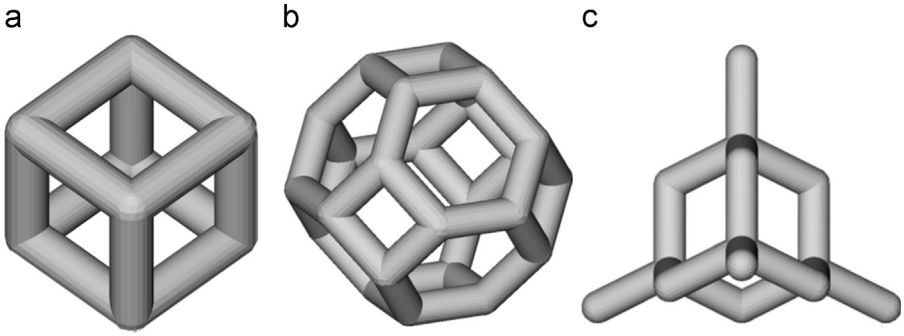

Fig. 1. Unit cells of the different geometries. (a) cubic lattice, (b) Kelvin cell and (c) diamond structure.