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Modeling Fixed-Bed Reactors using Particle-Resolved Computational Fluid Dynamics (CFD)

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Highlights

- Latest advances of detailed modeling of fixed-bed reactors are summarized
- Current challenges are described: packing generation, meshing, and solving
- Applications and best practice are discussed
- Future research fields for particle-resolved CFD simulations are identified

1. Introduction

Fixed-bed reactors are a commonly used type of reactor in the chemical and process industry. Many applications lead to a reactor arrangement with a small tube-to-particle diameter ratio ($D/d_p = N$). For fixed beds with a small N conventional approaches like pseudo-homogeneous or heterogeneous models are not well suited, since they do not take into account local flow effects. They can have a dramatic influence on fluid dynamics, as well as heat and mass transfer. For that reason, starting in the late 1990's, a considerable growing number of researchers developed methods to investigate the physical phenomena that occur in fixed-bed reactors by applying CFD for three-dimensional particle-resolved simulations. This modeling approach takes into account the actual geometric structure in beds consisting of pellets. That means, the transport of momentum, heat and species mass is resolved in the interstitial region of the pellets.

2. Methods

This work summarizes the advances that have been made within the last decade in the field of fixed-bed reactor modeling. Earlier development was reviewed comprehensively by Dixon et al. [1]. We present and discuss recent results, new and improved modeling approaches and limitations that still exist. Challenges are highlighted during a typical workflow that needs to be tackled for a successful CFD simulation. Finally, recent applications of particle-resolved CFD simulations are discussed.

3. Results and discussion

As an example for the application of particle-resolved simulations, radial porosity and specific velocity profiles are compared between experiments from [2] and simulations [3], see Figure 1. As can be seen, the morphology of the bed consisting of cylinders is in line with the experimental data. There is also a high agreement between the specific velocity profile from the experiments and the simulation. Further results will be discussed with a focus on residence time distribution, heat transfer, and fixed beds with surface reactions.

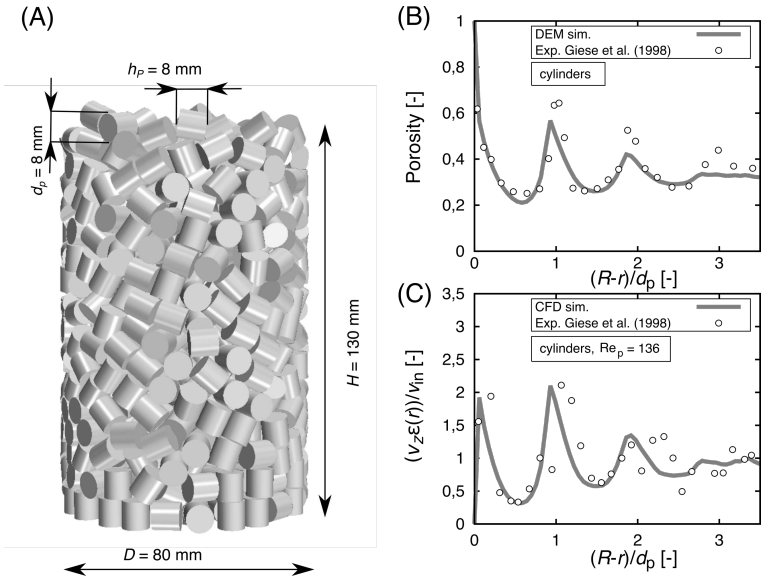

Figure 1. (A) Synthetically generated fixed bed of cylinders. (B) Radial porosity and (C) specific velocity as function of radial coordinate. Comparison between experiments from [2] and simulations [3].

4. Conclusions

CFD simulations, where the actual pellet shapes are geometrically resolved, have become the accepted most detailed modeling approach for fixed-bed reactors. In the last decade this method was further developed and many of the current issues are investigated by different research groups. This work summarizes the latest advances, describes the current challenges and shows best practice examples. Furthermore, emerging research-fields for particle-resolved CFD simulations are identified.

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Publications in peer-reviewed journals

1. G. D. Wehinger, M. Kraume (2017) CFD als Designtool für Festbettreaktoren mit kleinem D-zu-d_p-Verhältnis: Heute oder in Zukunft? *Chemie Ingenieur Technik, 89 (4),* 447-453
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Selection of scientific talks

1. G. D. Wehinger, M. Kraume (2016) Ist die CFD bereit als Design-Tool für Festbettreaktoren eingesetzt zu werden? *ProcessNet-Jahrestreffen Reaktionstechnik 2016*, Würzburg
2. G. D. Wehinger, M. Kraume, V. Berg, K. Mette, M. Behrens, R. Schlögl, O. Korup, R. Horn (2015) Dry Reforming of Methane on Ni in a Fixed-Bed Reactor: Spatial Reactor Profiles and Detailed CFD Simulations, *AIChE Annual Meeting 2015*, Salt Lake City, USA elected as ***Best Presentation***.
3. G. D. Wehinger, M. Kraume (2015) Interstitial-Scale Modeling of Catalytic Foam Reactors: Partial Oxidation of Methane, *AIChE Annual Meeting 2015*, Salt Lake City, USA
4. G. D. Wehinger (2015) Particle-resolved CFD simulations of heterogeneous catalytic reactors: Dry reforming of methane, invited talk at *Air Products*, Allentown, PA, USA
5. G. D. Wehinger, T. Eppinger, M. Kraume (2014) Spatially Resolved Simulations of Heterogeneous Dry Reforming of Methane in Fixed-bed Reactors, *AIChE Spring Meeting 2014*, New Orleans, USA elected as ***Best Presentation***.

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