CFD Calculations of Flow, Dispersion and Chemical Reactions in Fixed Bed Tubular Reactors Using the Lattice Boltzmann Method

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Abstract. Detailed 3-D simulations are required to correctly predict the coupled behaviour of flow and mass transport in chemical reactors with \(\Theta\)-asymmetry. These simulations can be of great technical and economical interest as the reactor performance and safety during operation are significantly influenced by the local flow behaviour. One particular interesting example are randomly filled tubular fixed bed reactors with small tube-to-particle diameter ratios. New numerical methods such as the lattice Boltzmann approach together with the increasing computational power can provide detailed insight into the flow and transport processes in complex geometries. The present paper demonstrates the applicability of this approach by investigating complex flows and showing first results of the inhomogeneities in the 3-D flow of reacting species in a tubular fixed bed reactor.

1 Introduction

In contrast to other industrial sectors, CFD methods are not yet widely used in chemical engineering. The typical approach in this field is still to set up an experiment, to measure, to extract some empirical correlations and finally use them in semi-empirical equations which are in most cases of lowdimensional order. The reasons for this approach are quite easy to understand: The geometries typically used are complex. They cannot be described analytically and CAD data are, in contrast to applications in the automobile industry, often not available. A second point is, that the relevant phenomena are strongly non-linear and highly coupled. The geometrical structure determines the flow field. Both, the flow field and also the geometrical structure influence the mass transport. Therefore, the effective coefficients of the mass transport (e.g. dispersion coefficients) are not material properties but strongly depend on the actual set-up. Chemical reactions, especially in the case of heterogeneous surface-catalytic reactions, depend on the interaction

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of all mentioned phenomena. If energy conversion and transport are relevant, it is becoming even more complicated than bulk transport, because the boundary layers and the conduction inside the solid have to be considered in addition. For simplicity, energy was not taken into account in the calculations presented here.

As a first conclusion, we can summarize: complex and coupled phenomena are typical for the field of chemical engineering. If we want to apply CFD methods in this area, they must be able to deal with these complex flows.

As has been shown in the last decade, lattice Boltzmann (LB) methods are an efficient numerical simulation approach especially in the case of complex geometrical structures such as porous media. The extension of the LB method to the needs of chemical engineering therefore seems to be very promising.

In Sect. 2, we define one particular example, tubular fixed bed reactors with small tube-to-particle diameter ratios, which clearly show the requirement of detailed simulations. The basic ideas of the lattice Boltzmann method are briefly summarized in Sect. 3. With some rather simple test-cases, the method and its implementation are quantitatively validated in Sect. 4. In Sect. 5, we discuss details of the flow field and its consequences on the mass transport and the surface reaction in a tubular fixed bed reactor. High-performance computing aspects are given in Sect. 6. Finally, the main points are summarized in the conclusions (Sect. 7).

2 Requirement for Detailed Simulations in Chemical Engineering: Tubular Fixed Bed Reactors with Small Tube-to-Particle Diameter Ratios

Tubular fixed bed reactors are of particular significance in the chemical process industries. They are, among others, used as catalytic reactors, adsorption columns and separation towers. Therefore, they are perhaps even the most widely used type of reactor at all. The typical structure consists of two major parts: a confining tube which is filled with particles either randomly or strongly ordered. In the simplest but often used case, the particles are monodisperse spheres. For some applications, e.g. in the case of strongly exothermic or endothermic reactions, very thin tubes must be used to remove or provide the heat. In order to nevertheless achieve the required throughput, up to several thousand tubes are arranged in parallel. In the calculations shown later, we focus on one single tube with the detailed particle structure inside.

The typically applied modelling approaches used in chemical engineering are based on empirical correlations derived from local averaging. The averaging can be performed on different levels, ranging from 0-D models with "plug-flow" assumption (i.e. homogeneous voidage distribution all over the packing, resulting in a constant axial velocity and no radial velocity at all) to sophisticated 2-D "non-parallel flow" models. The latter only assume symmetry in the circumferential (\(\Theta\)) direction. The averaged velocity can vary in