# Pore-Scale Simulation of Transport Processes in Fixed-Beds: Combining a Lattice Boltzmann CFD Method and a Particle Tracking Method

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## Introduction and definition of the problem

Modeling and simulation of fixed-bed reactors is usually based on classical pseudo-homogeneous modeling approaches that rely on simplifying assumptions and the use of semiempirical effective parameters, which have been adopted to results obtained from a certain experimental setup. This inevitably leads to problems when trying to perform reliable simulations for a priori predictions and optimization purposes. This applies especially to packed beds of low tube-to-particle diameter ratios, which are used in many applications (e.g. strong exothermic reactions). Here the wall effects are relevant over the entire cross section of the bed and local phenomena dominate. In order to account for the local inhomogeneities, the complete 3D structure of the packing has to be considered and a simulation of the transport processes on a pore-scale level has to be performed.

## Aim

The aim of the work presented here is to provide suitable numerical methods for the detailed numerical simulation of the fluid flow and mass transport in fixed-beds. The modular simulation steps include the generation of the packing geometry, the simulation of the isothermal fluid flow and the mass transport, respectively.

## Numerical Methods

For the detailed simulation of the local flow field in complex geometries, we use a lattice Boltzmann approach, which requires only physical properties as input data (i.e. no semiempirical parameters are used) and a 3D pore-scale image of the void space. Instead of using advanced (but also costly) experimental imaging techniques, we apply a Monte-Carlo process for the numerical generation of the 3D packing geometry of spherical particles on a 3D equidistant Cartesian lattice with proper resolutions as basis for the subsequent CFD calculations [1]. While the packing generation and the fluid flow simulation have been discussed in detail previously [1,2], the present study focuses on the combination of these numerical schemes with a tool for the simulation of the mass transport in fixed-beds [3]. Using the results of the 3D flow field simulation, a Lagrangian particle tracking of a tracer in the interparticle void space is performed. First, a few aspects concerning the implementation and the validation of the particle tracking tool will be addressed. Then, the results of the mass transport simulation will be discussed, demonstrating the great potential of the combined simulation procedure.

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## Results

The implemented numerical tools for the packing generation (Monte Carlo packing generation, *MCPackGen*) and the lattice Boltzmann flow simulation (Boltzmann equation solving tool, *BEST*) have been validated extensively and the results of the simulations are discussed elsewhere [1,2].
The implemented particle tracking tool (*ParTrack*) presented in this work shows an excellent agreement with analytical solutions of simple test cases that were chosen for validation purposes. Since it is based on a Lagrangian method, no numerical grid is required and therefore, at high Peclet numbers numerical dispersion does not cause convergence or stability problems. Thus – in contrast to Eulerian methods that are often used for mass transport simulations – the range of high Peclet numbers (which is of importance in several technical applications) is also accessible. The pore-scale simulation of the tracer displacement demonstrates the interaction of convective and dispersive transport processes and allows for the examination and evaluation of the mass transport characteristics of different packing geometries on a local scale by comparing e.g. a structured and a random packing [3]. In addition to this improved physical insight into the local transport processes, the detailed results on the pore-scale level can also be condensed to global characteristics, e.g. to axial and radial dispersion coefficients, using the simulations as "numerical experiments" and establishing cross-links to classical pseudo-homogeneous modeling approaches. Finally, in contrast to most conventional experimental techniques, with this simulation tool it is possible to examine in detail the local residence time behavior (e.g. for different radial segments of a random packing). As an instructive result the simulations reveal that the mean residence time of a single circle can differ remarkably from the overall mean residence time of the fixed-bed. This will also influence the overall reactor performance, since the residence time distribution has a strong impact on the course and the progress of the reaction in a fixed-bed reactor and is thus an important characteristic of the reactor configuration.

## Conclusion

The presented numerical tools – and especially their combined application – have been proven to be powerful tools for the simulation of local transport processes in fixed-beds. The detailed information provided is superior to classical experimental approaches and – in terms of resolution and accuracy – comparable to the results of recent experimental techniques, which in turn require high (financial) efforts.

## References

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