Modeling of processes at the microscale

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The macroscopic models are often unable to produce conclusive evidence for a given mechanism in systems with the complexity characterizing almost all chemical and biochemical processes. By contrast, particle-based mesoscale methods possess the unique ability to model relatively large physical systems, and, at the same time, effectively capture the essential features of the micro- and nanoscale structure, architecture, and relevant interactions. Multiscale modeling combines existing and emerging methods from diverse scientific disciplines to bridge the wide range of time and length scales that are inherent in a number of essential phenomena and processes in materials science and engineering. Multiscale modeling may help to design and optimize microsystems technology for chemical and biochemical processes from a microscopic point of view.
In this work, the microscale process development is presented in combination with modeling-based optimization. Theoretical description of transport phenomena and the kinetics at the micro scale is discussed and illustrated on the cases of a lattice Boltzmann simulations for flow distribution in the packed bed microreactor and the biocatalytic enzyme surface reaction. The model verification and on-line validation is presented in few cases followed by the multiscale modeling concept.

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Research Interest: Microreactor Engineering