

# Multiscale modelling of chemical and biochemical processes in microfluidic devices

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Flow devices used in chemistry and chemical manufacturing, that have at least one dimension smaller than a millimeter, may be characterized as microfluidic devices. Among characteristics that arise from this property are: high area-to-volume ratio, better efficiency, improved process control, improved heat and mass transport, and due to their small volume, reduced solvent use. Chemical engineers use modelling to gain better understanding of a process, as a tool in process scaling and optimization, and even for process control. In our field we traditionally use continuum-based models to describe processes. These models inherently neglect the particle composition of matter. It is due to microfluidic devices' small characteristic size that the continuum assumption may not be valid when modelling them. The lattice Boltzmann method has a lot of potential for modelling of microfluidic devices as with its statistical-mechanics background it does not fully neglect the particle composition of matter, and it may be used to model fluid mechanics, and transport phenomena even in complex geometries. Due to it not being computationally very cheap it is desired to use the lattice Boltzmann method in a multiscale model setup, where it serves to solve transport phenomena in complex geometries, and the rest of the microfluidic device is modelled with a simpler macroscopic method. In this dissertation we present our work with the lattice Boltzmann method. First we use it to model mass transport in a packed-bed microbioreactor with randomly packed spherical particles. This is followed up by a study in which we compare different lattice Boltzmann collision models, and a study where we theoretically design a membrane-free microseparator by simulating the flow of a binary mixture of immiscible fluids. Finally, we expand the lattice Boltzmann method to a multiscale model of dry-reforming of methane in a catalytic reactor.

**Keywords:** modelling, multiscale modelling, lattice Boltzmann method, microfluidic devices, microreactors