

Computational study of multi-step catalysis in fibrous membranes

Multi-step (cascade) catalytic reactions with incompatible catalysts are notoriously difficult to realize in technical settings. The major challenge is to achieve efficient flux of the intermediate products from the first catalytic site to the second, third etc. while at the same time preventing physical contact and thus annihilation of the incompatible catalysts. Fibrous membranes fulfill both requirements since they combine (i) the ability to precisely locate different catalysts in compartments spatially separated from each other with (ii) a high porosity required for efficient mass transport.

The goal of the PhD project is to develop a computational model for cascade reactions in fibrous membranes in close collaboration with experiments by our partners in the group of Seema Agarwal (Bayreuth). For this, a computational procedure based on the Lattice-Boltzmann method will be developed which can accurately compute the time-dependent concentration profiles throughout the reactor. After validating the results by corresponding experiments, the simulations will be able to answer important questions such as the reaction efficiency as function of pore size in heterogeneous media etc. which are not available from the experiment.

The required supercomputer resources will be provided by the local computing cluster available at the University of Bayreuth as well as by projects on national supercomputing system such as SuperMUC (Garching) and JURECA (Jülich).

The successful candidate should be interested in writing and using computer codes (C/C++). A background in fluid mechanics or biology is not explicitly required. For PhD/PostDoc candidates we offer competitive salary, funded by the SFB 840. Research will be conducted in the Biofluid Simulation and Modelling group at the University of Bayreuth, Germany. Bayreuth is a medium-sized town with a fairly large student population and is situated in a beautiful natural setting between the mountains of the "Fränkische Schweiz" and "Fichtelgebirge".

For applications or further information please contact: Stephan Gekle, stephan.gekle@uni-bayreuth.de or see our website biofluid.physik.uni-bayreuth.de

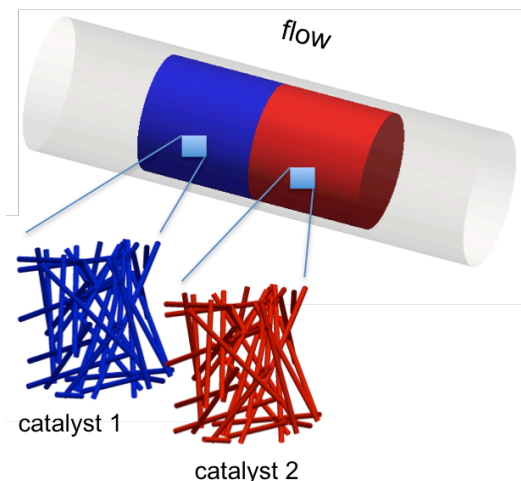


Fig. 1: Example of a flow-through reactor for a two-step catalytic reaction.

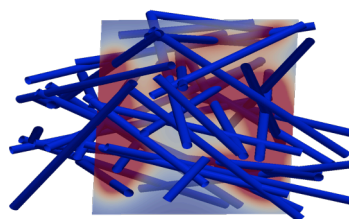


Fig. 2: Concentration profile of a reacting species in a fibrous membrane.