127th MSS-Seminar
Thursday, August 1st, 15:00 hrs,
Seminarraum (00.156),
Cauerstraße 3, Erlangen.

Multiscale modeling of heterogeneous catalysis in porous metal foam structures using particle-based simulation methods

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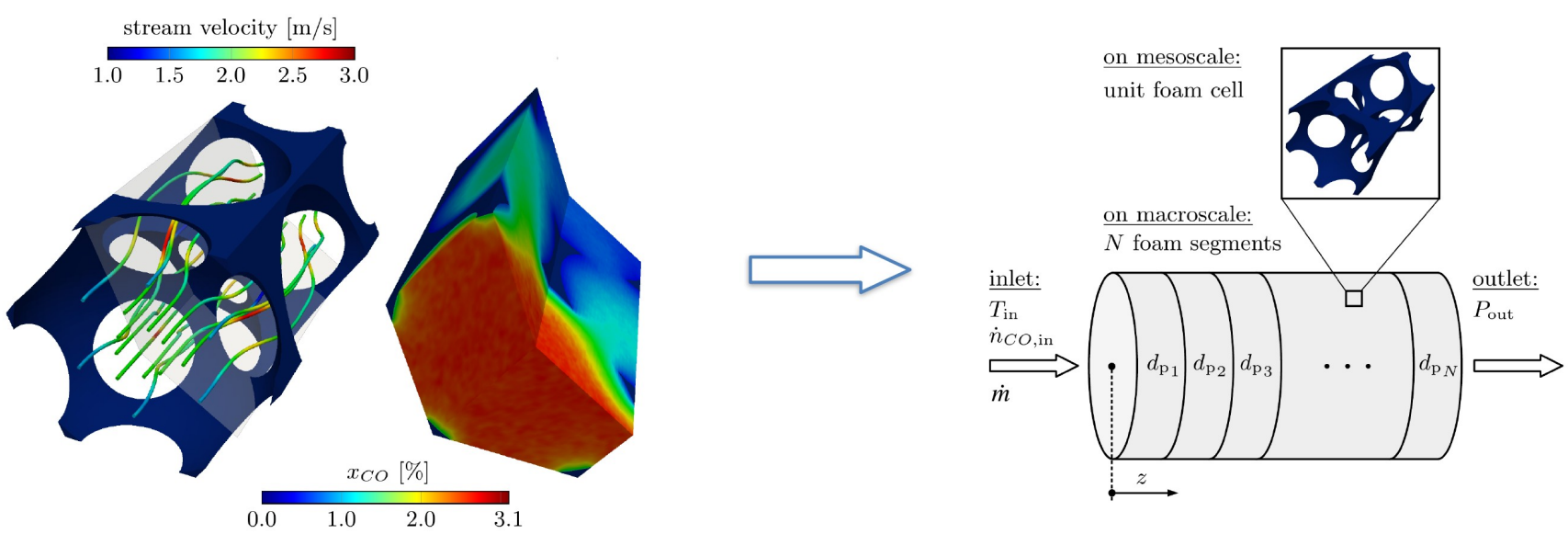

The multiscale approach links the macroscale model for catalytic converters to mesoscale simulations results.

Heterogeneous catalysis is omnipresent in the chemical industry. Hence, in this work, we investigate and optimize heterogeneous catalysis in porous metal foams, which are extremely promising as support structures in this context. First, we consider the gas dynamics together with the reaction and diffusion processes in individual foam pores on the mesoscale. Second, we condense the detailed simulation results on the mesoscale to relations between few, dimensionless numbers. Based on these relations, we follow a multiscale approach to derive an efficient, one-dimensional, macroscale model for metal foam filled catalytic converters. Due to its industrial importance, we focus on the mass transfer limited regime. Finally, we develop a simple recipe to determine optimum pore size configurations. For realistic heat release values, the heat transfer out of the catalytic converter is critical. We show that, in order to keep temperature fluctuations small, the optimum configuration consists of several, stacked foam segments with decreasing pore size along the main flow direction. For typical parameters, we observe that, compared to foam with constant pore size, the tradeoff between chemical conversion and flow resistance can be increased significantly, while the required reactive surface area, i.e., the amount of catalytic material, is reduced substantially.