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Multiphysics design optimization of continuous flow microreactors

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Abstract

The miniaturization of chemical reactors has many fundamental and practical advantages, especially when operating under continuous flow conditions. And, although there are now many industrial and academic applications of continuously operated microfluidics, the predicted theoretical efficiencies can usually not be attained in practice. One of the prominent reasons is the non-uniformity of the flow distribution in the reactor.

The internal geometry of a continuous flow chemical reactor determines to a high degree the performance of the chemical processes inside. The layout defines the flow distribution and therefore where reactants are gathered or separated; it can induce mixing and it determines the residence time distribution. However, up until now, most microreactor designs are based on rather simple, suboptimal combinations of long, folded microchannels on a microfluidic chip. At the same time, modern manufacturing capabilities allow for a huge design freedom, which is still mainly left unused.

To optimize the reactor geometry, we apply an approach inspired by density-based topology optimization techniques. The reactor geometry is determined by the channel height distribution in the planar microfluidic chip. The local flow resistance is directly related to the local channel height and does not require any artificial penalization. After solving the 2D flow distribution, the transport phenomena are simulated, and used to determine performance. Based on adjoint sensitivity analysis the reactor layout is then iteratively optimized using the Method of Moving Asymptotes.

The advantage of design optimization is that it can handle the highly coupled physics of the system to exploit synergies and to tune the design to the optimal balance. In the considered numerical examples, we generated novel reactor designs and their efficiencies approach the theoretical efficiencies of reactors that are not attainable using the classical microchannel designs.