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DESIGN OPTIMIZATION FOR ISOTHERMAL MICROREACTORS

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Introduction The miniaturization of chemical reactors and operating these under continuous flow conditions has many fundamental and practical advantages for the process industry. The increased the area-to-volume ratio improves mass and heat transfer, it allows for more control and reduced use of resources[1]. Although, there are now many industrial and academic applications of continuously operated microfluidics, the predicted theoretical efficiencies can usually not be attained in practice[2]. One of the prominent reasons is the non-uniformity of the attained flow distribution inside the reactor. However, up until now, most microreactor designs are based on simple combinations of long, folded microchannels on a microfluidic chip that are not well suited to obtain a uniform flow distribution. In this work, we apply Topology Optimization techniques to microfluidic reactors, to create new designs that take advantage of the complete design space.

Methodology To optimize the reactor geometry, we apply a density-type topology optimization method. The reactor geometry is defined by the channel height distribution in the planar microfluidic chip, and by applying the lubrication approximation, the local flow resistance is directly related to the local channel height and does not require any artificial penalization. After solving the flow distribution, the transport phenomena are simulated, and used to determine performance and perform an adjoint sensitivity analysis. This is then iteratively optimized using the Method of Moving Asymptotes[3] until the performance requirements are satisfied.

Results To demonstrate the applicability of the method, it was used it to design a microreactor for a elementary $A \longrightarrow B \longrightarrow C$ reaction, where B is the product of interest. The goal is to produce as much B from A as possible at the maximum attainable selectivity, for a specified pressure drop between the ports. Unfortunately, in this particular

chemical process, the reaction rate is in favor of C, such that the rate from B to C occurs at twice the rate of A to B. Theoretically, in this situation, an ideal plug flow reactor will perform the best and will lead to a maximum selectivity of 25% [4]. A typical optimized reactor design can be found in Fig 1., where it shows in (d) that the reactor is able to approach the theoretical limit upto 24.7% B at the outlet (right circle). The final design has very wide channels compared to classical microreactors and therefore should allow for higher throughput rates.

Conclusions and outlook Using the proposed procedure, it becomes possible to generate effective designs, for user chosen process parameters, without any a priori design information. Work in the near future is focused on experimental verification and application to other, more complex reactions. We are also investigating non-isothermal reactors and the inclusion of porous catalysts.

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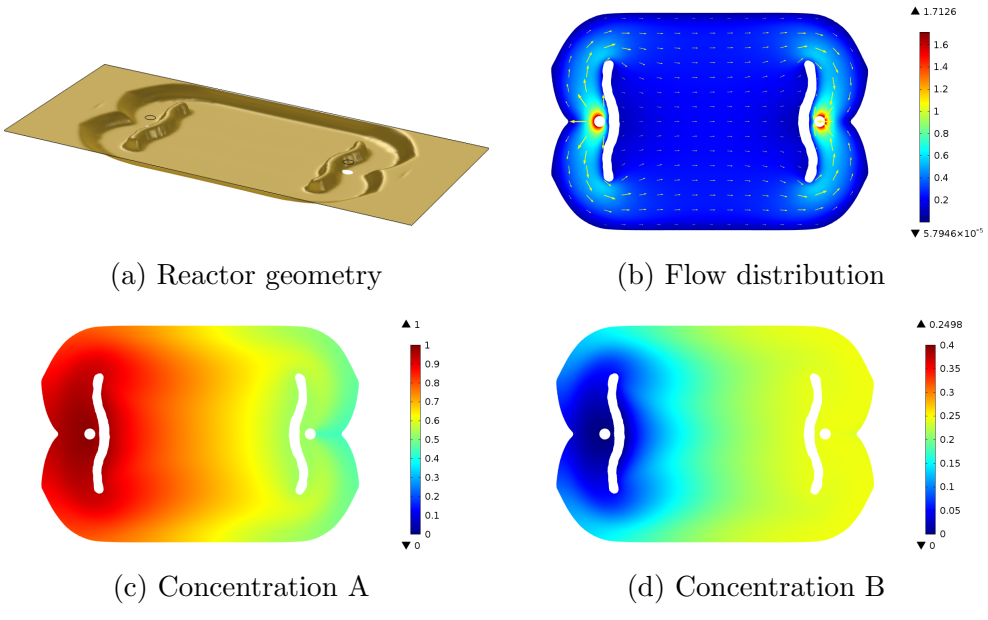

(a) Reactor geometry (b) Flow distribution

(c) Concentration A (d) Concentration B

Figure 1: Example of an optimized microreactor. (a) shows the local channel height, with black circles indicating the inlet (left) and outlet (right). (b) shows the z-average fluid flux distribution and the flow direction using arrows. The concentrations of species A and B are displayed in (c) and (d) respectively. All values are non-dimensionalized.