Effect of geometrical parameters on the performance of a micro-reactor

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Micro-reactors, i.e. devices with characteristic dimensions in the submillimeter range, offer significant advantages over conventional reactors, such as increased safety and reliability, as well as better process control and scalability. Since the flow is usually laminar due to the small conduit dimensions, the extent of the chemical reactions that take place in the reactor is governed by the slow diffusive mass transfer, which in turn is controlled by the extent of mixing. Thus, an enhancement of the mixing efficiency leads to higher reaction rates. In recent years, experimental and computational studies(Baier et al., 2005) were performed to determine the rate of mixing in various types of micro-mixers and micro-reactors operating at low Re.

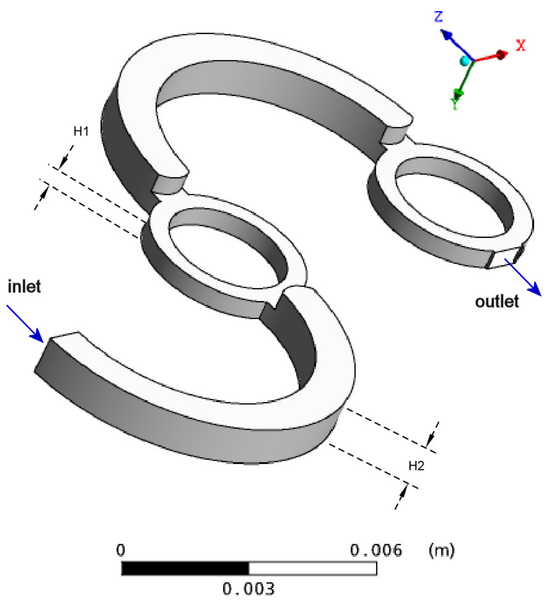

Figure 1. A module of the micro-mixer.

For this study, a micro-reactor consisting of a micro-channel (i.d.=1mm) with consecutive curves is considered. This micro-reactor comprises several features, i.e. curved conduits, split and recombine structures as well as backward and forward facing steps that are known(Mouza et al., 2008) to influence the mixing performance of the device. A simple reaction between two reactant fluids is employed inside the channel and the extent of conversion is steadily monitored. A *CFD* code (i.e., ANSYS CFX) is used to simulate the micro-reactor behaviour and to obtain results regarding the flow pattern and the reaction efficiency along the micro-channels. A parallel computing cluster is employed for the simulations.

The scope of the work is to investigate the effect of the curvature of the conduit and of *Reynolds* number on the efficiency of the micro-reactor. As it is known diffusive mixing can be optimised by maximising the interfacial surface area. For a given micro-device module an increase of *Re*, improves the mixing efficiency, regardless of the shorter residence time, because in this case mixing is predominantly induced by *Dean* flows. On the other hand, for a given *Re*, mixing efficiency is improved by increasing the curvature of the conduit segments, in other words the degree of complexity of the flow per length unit. This is inevitably accompanied by an increase of pressure drop and it must be always considered whether the excess pressure drop is counterbalanced by the improvement of mixing, and consequently the reaction efficiency

A quadratic model(Box and Behnken, 1960) that predicts the length where reactant conversion is 80% has been also formulated :

$$\eta = a_0 + a_1 D_1 + a_2 D_2 + a_3 Re + a_{11} D_1^2 + a_{22} D_2^2 + a_{33} Re^2 + a_{12} D_1 D_2 + a_{13} D_1 Re + a_{23} D_2 Re$$

The coefficients of the model were calculated using the results of the *CFD* simulation. The correlation is in good agreement compared with *CFD* data. The optimal solution, i.e. the parameter values that give the better mixing performance, were also calculated using a polynomial-based *Response Surface Method* (*RSM*). For the present case the optimal values of the design parameters, i.e. the values that result to a higher product concentration at the exit of the device, are given in ***Table 1***.

Table 1: Optimal values of the design parameters.

D_1, *mm*	5.5
D_2, *mm*	8.0
Re	135

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