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Effect of flow regimes on reaction yield in a T-shaped micro-reactor.

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Highlights

- Simulations carried out using both NEK5000 and Ansys Fluent computer codes.
- Reaction yield depends on both Reynolds number, *Re,* and Damköler number, *Da*.
- When Da>>1, reaction yield equals the degree of mixing and depends only on *Re*.
- When Da<1 and Re>200, time periodic mixing patterns strongly increase reaction yield.

1. Introduction

Micro-reactors, constituted by channels with typical dimensions < 1 mm, are receiving an increasing attention in the pharmaceutical and fine-chemistry industries as they can provide a continuous operation with enhanced heat transfer (due to the high surface-to-volume ratio) and well controlled residence time. This may lead to higher reaction yields (and thus lower material and energy consumption, as well as environmental impact) with respect to conventional batch processes, the latter often demanding for high dilution levels for safety reasons, i.e. to avoid reaction runaways.

Since the tiny dimensions, the flow is laminar so that special techniques should be adopted to promote the mixing of reactants. Among them, the interest is towards passive micro-reactors that are able to mix efficiently reactants without any external force and just through a special design of the micro-device, able to ensure a break of the flow symmetries and, thus, to enhance mixing through convection.

Experiments in micro-reactors are difficult to be carried out because the small dimensions so that Computational Fluid Dynamics appears well suited to address the problem, and provide a full characterization of the flow and concentration fields. Numerous CFD investigations have recently analyzed micro-mixers, showing the presence of different flow regimes depending on the Reynolds number.

For instance, some studies on T-shaped micro-reactors have even pointed out the presence of unsteady time-periodic regimes than can improve strongly mixing [1].

However, most of the available investigations have been performed in absence of any chemical reaction, thus focusing only on the mixing process.

The present work intends to study the dependence of reaction yields on flow regimes in a T-shaped micro-reactor.

2. Methods

In this study, Direct Numerical Simulations are performed using both the open-source spectral-element code for fluid dynamics NEK5000 and the commercial code ANSYS Fluent. Different cases are addressed by varying the Damköhler number, hence to span from small (chemical controlled regime) to large reaction rates (mixing controlled regime).

A preliminary analysis is devoted at understanding the required numerical resolution (both in time and in space). In case of too fast reactions, the underlying differential equations can in fact become too stiff in order to be solved with standard methods, them requiring too small time-steps; instead, the assumption of an infinite fast reaction may be applied. As for the spatial resolution, this should be able to resolve the mixing of reactants; mesh adaption techniques on the concentration gradients are proposed to address this issue.

3. Results and discussion

We find that, for large Peclet numbers, $Pe = UL/D >> 1$ (*U* is the mean fluid velocity at the entrance region, *L* the hydraulic radius and *D* the molecular diffusivity), the reaction yield depends on the Reynolds number *Re* and the Damköhler number, $Da = kL/U$ (*k* is the reaction rate), the latter representing the ratio between the convection-driven mixing time, *L/U*, and the reaction time, *1/k*. When $Da>>1$, reaction is fast and takes place as soon as the two entrance streams mix together; therefore, the results are very similar to those concerning the degree of mixing that we have presented elsewhere as depending on *Re*. However, when $Da<1$, results strongly depend on the interplay between reaction and mixing patterns. In particular, when Re > 200, we see that the fluid in the mixing channel starts to oscillate, with a characteristic time periodic behavior that can be described in terms of a characteristic Strouhal number [2] . Therefore, when the reaction rate is equal to the characteristic time frequency, i.e., when the Damköhler number is equal to the Strouhal number, the reaction yield is very large, thus providing important indications on different strategies of process optimization.

4. Conclusions

We have studied the effect of flow regimes on the reaction yield in a T-shaped micro-device, assuming that the Peclet number is large, so that mixing is a convection-driven process. In general, the reaction yield depends on the Reynolds number *Re* and the Damköhler number, *Da*. We saw that, when reaction is fast, so that we are in a mixing controlled regime, predictably the reaction yield is identical to the Reynolds-depending degree of mixing, which has been presented elsewhere. On the other hand, when reaction is not fast, i.e. when the Damköhler number is not large, results are very interesting and different regimes can be observed. In particular, when the flow pattern is periodic, the reaction yield can increase dramatically.

References

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