Numerical Analysis of Mass Transfer Rate in Droplet Flow at Microscopic Scales

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Introduction: Droplet flow at microscopic scale is often used to enhance many (bio)chemical processes (i.e. liquid–liquid extraction, nanoparticle synthesis, slow reactions in microfluidic devices, etc.). [1,2]

Objectives: The present work numerically analyzes the mass transfer rates during the two phase flow of droplets generated by a micro-nozzle (tip-radius smaller than *25 μm*), which protrudes/extends inside a circular microchannel with a radius *100-300 μm (fig 1)*.

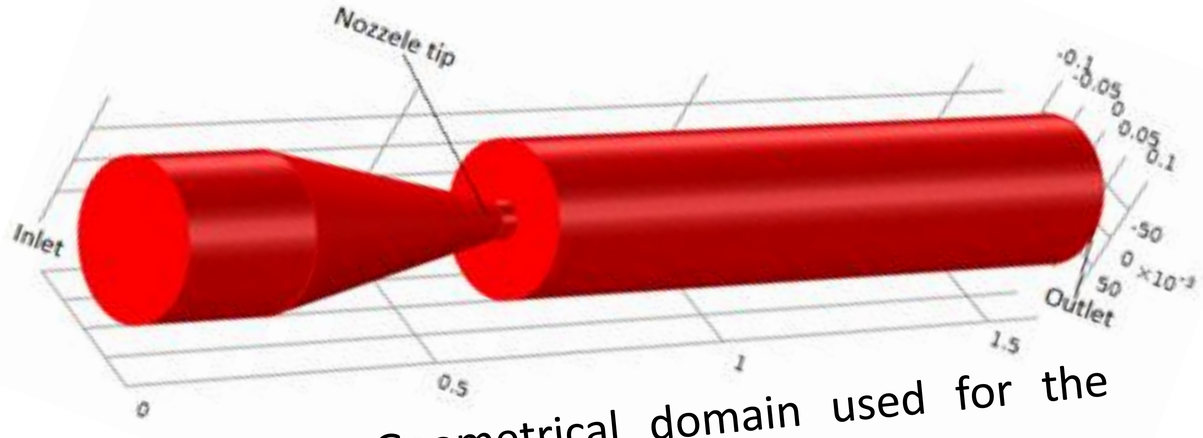

Figure 1: Geometrical domain used for the simulations

Computational Methods: We performed simulations using the Laminar Two-Phase Flow interface of the commercial code COMSOL Multiphysics® and solved numerically the governing momentum (including surface tension) and mass transfer equations.[3]

Results: The reactant is diluted from fluid 1 (from micro-nozzle) into fluid 2 (circular channel) at a mass transfer rate proportional to the diffusive and convective forces acting inside and outside of the drop.

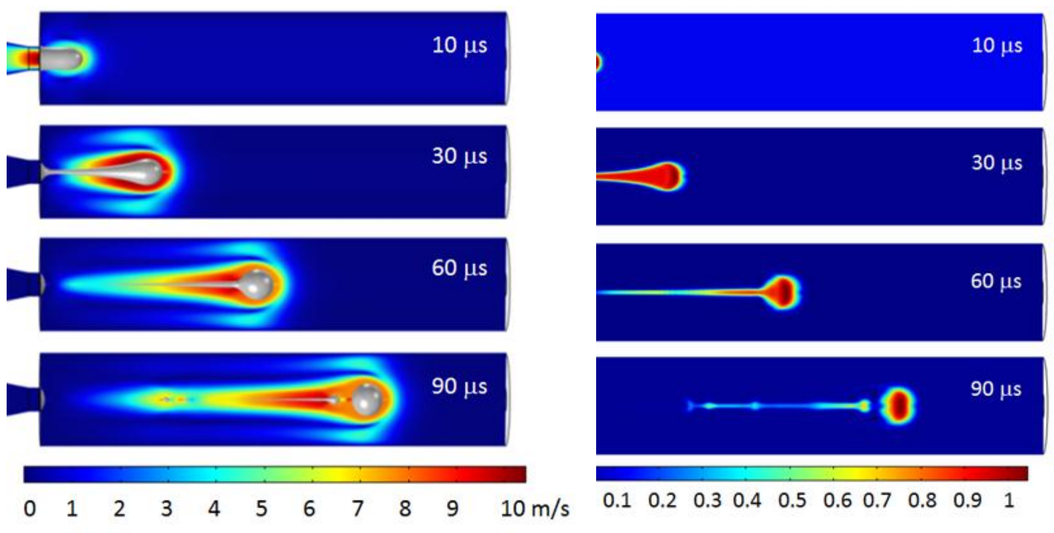

Figure 2: *Contour of velocity (left) and concentration field (right). Two recirculations are located around the drop*

The flow field around the drop showed to have two recirculations that enhance the average mass transfer rates (fig 2).

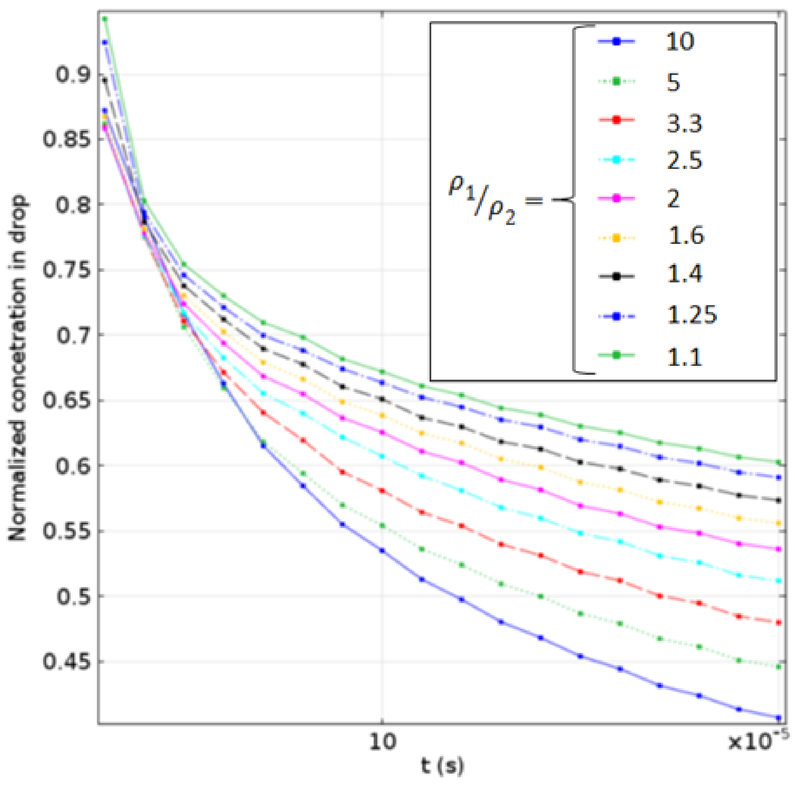

Figure 3 : Average decay of concentration with time

Increasing the density ratio, between the two fluids, the rate at which the reactant is diluted, from the drop to the surrounding fluid, increase consistently (fig 3).

Conclusion: These results can be used for rational design of chemical devices that deal with, for instance, liquid–liquid extraction, nanoparticle synthesis and slow reactions.

References:

1. Choi, et al. *Journal of Chromatography. A*, *1217*(24), 3723–8. (2010).
2. Olsson et al. *Journal of Computational Physics*, *225*(1), 785–807. 2007).
3. Xu, et al. *Chemical Engineering Journal*, *141*(1-3), 242–249. (2008).

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