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

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## Abstract

Droplet flow at microscopic scale is often used to enhance many pharmaceuticals processes (i.e. liquid-liquid micro-extraction, nanoparticle synthesis, slow reactions in microfluidic devices, etc.) [1,2]. In all these processes, the mass transfer rate, at the interface between the droplets and the surrounding fluid of diluted reactants plays a key role [2]. The purpose of this work is to analyze numerically the mass transfer rates generated by the two phase flow of droplets generated by a micro-nozzle (with tip-radius smaller than 25 µm), which is connected to a circular microchannels with internal radius between 100 and 300 µm (Figure 1). To carry out this numerical analysis we performed simulations of the two phase flow by solving numerically the governing momentum equations (including surface tension) and mass transfer equations using the finite element commercial code COMSOL Multiphysics®. Specifically, we adopted the Laminar Two-Phase Flow, Level Set physics interface of COMSOL Multiphysics® which implements a reinitialized conservative level set method to describe and predict the fluid-fluid interface. In this method a level set function φ is introduced which equals 1 in fluid-1 and 0 in fluid-2. The 0.5 value of the level set function φ defines the interface and in the transition layer close to the interface, φ goes smoothly from 0 to 1. With this approach, the interface moves with the fluid velocity near the interface [3]. The differential equation of our model are solved imposing parabolic velocity and constant reactant concentration at inlet (Vmax=3-5 m/s), constant pressure and zero diffusion flux of the reactant at outlet and non-slip condition at walls. All simulations are initialized assuming that the space between the inlet and the nozzle is filled with fluid-1 which contains a reactant with constant concentration, while the microchannel is filled with fluid-2. Afterward, fluid-1 is injected through the inlet during a period of 10 µs, consequently a drop of fluid-1 flows out of the nozzle and it crosses the entire microchannel after approximately 100-200 µs (Figure 2). During this time lapse the reactant is diluted from fluid-1 into fluid-2 at a mass transfer rate proportional to the diffusive and convective forces acting inside and outside of the drop (Figure 3 and 4). The flow field around the drop showed to have two recirculations that enhance the average mass transfer rates. From this study we are able to quantify the effect of the velocity inlet, of the density and viscosity ratio between fluid-1 and fluid-2 and of the channel and nozzle geometry on the time evolution of the averaged mass transfer rates. Specifically, in the plot of figure 4 we can see that 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. These results can be used to make a rational design of pharmaceutical devices that deal with liquid-liquid micro-extraction, nanoparticle synthesis and slow reactions.

## Reference

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2. Olsson, E., Kreiss, G., & Zahedi, S. A conservative level set method for two phase flow II. Journal of Computational Physics, 225(1), 785–807. (2007)
3. Xu, J. H., Tan, J., Li, S. W., & Luo, G. S. Enhancement of mass transfer performance of liquid –liquid system by droplet flow in microchannels. Chemical Engineering Journal, 141(1-3), 242 –249. (2008).

## Figures used in the abstract

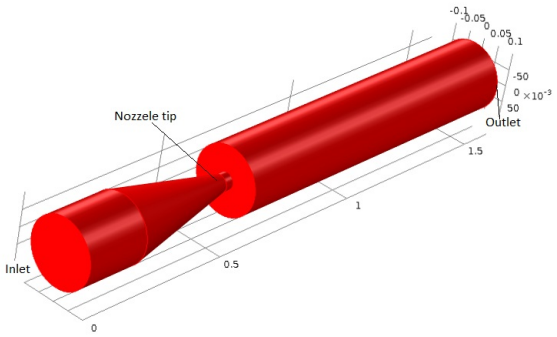


**Figure 1**: Schematic of the geometrical domain used for the simulations. the scale of the axis is given in mm.

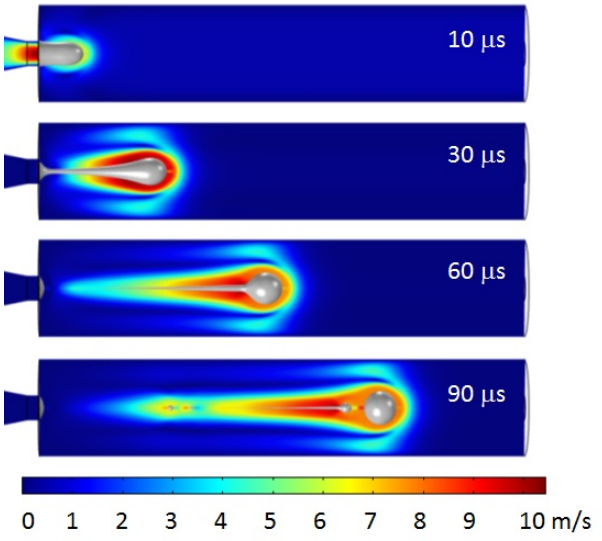


**Figure 2**: Contour of the velocity field around the drop formed at nozzle tip at different times.

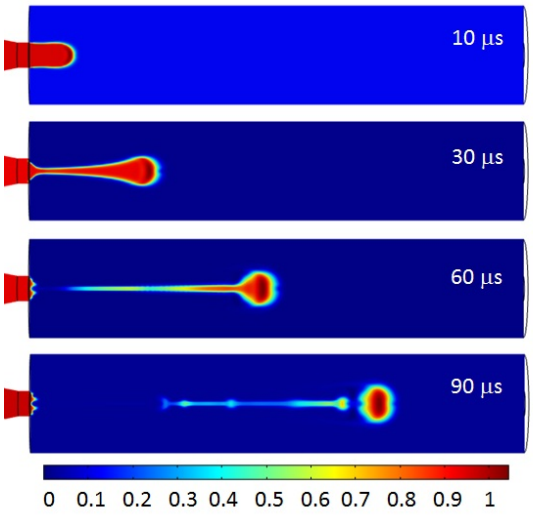


**Figure 3**: Contour of the reactant concentration field at different times.

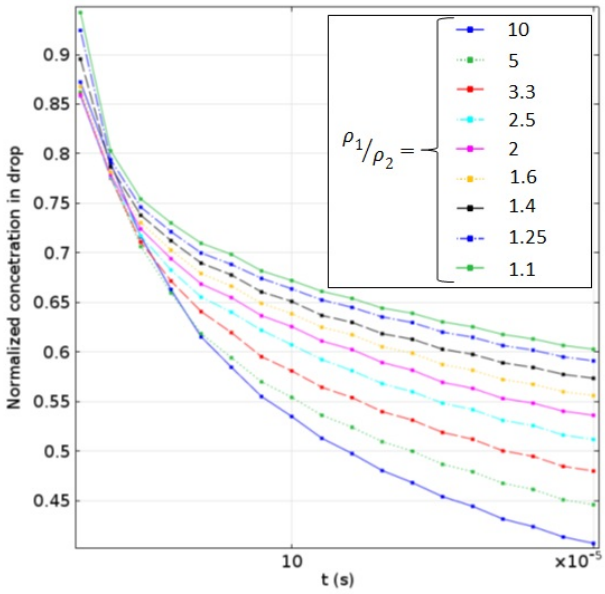


**Figure 4**: Plot of average decay of normalized concentration in drop versus time for different value of density ratios.