Chemical Reactions at Interfaces During Droplet Formation in Microchannels

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Abstract

Emulsions, small liquid droplets of oil in water or water in oil, find wide application in, pharmaceutical products, fine chemicals, analytical chemistry. Microfluidic devices allow creation of uniform droplets with a tight distribution.

The COMSOL Multiphysics® software model presented here is an extension of the tutorial "Droplet Breakup in a T- junction". In this tutorial uniform droplets are created in an microchannel T-junction using the Two-Phase Flow, Laminar, Level Set physics interface. The fluid, organic phase, to be dispersed into small droplets enters through the vertical channel. The other fluid, continuous aqueous phase flows from the right to left through the horizontal channel. The size of the droplets formed depends on the viscosities and the velocities of the two phases, but also on the surface tension between them.

The calculation of the droplet size was obtained by solving, the momentum transport equation the continuity equation (for the velocity field) and a level set equation where the fluid interface (between organic and aqueous phases) was defined by the 0.5 contour of the level set function. This function for the organic phase is 1 and for the aqueous phase is 0.
In our model, in addition to the previous equations we solve the convection diffusion equation, in the two phases. In the inlet of aqueous phase and we suppose a concentration A and in the inlet of the organic phase a concentration B. At the interface the reaction between A and C (A + Bà⌅ C) produces C that can diffuse only into the organic phase.

Experimentally, the reactive liq-liq extraction, through droplet formation in microchannels, due to the high contact area, is much more efficient compared to those of a continuous interface.

The reactive liq-liq extraction, in the case of droplet formation, can be simulated using COMSOL Multiphysics. Such a simulation allows sizing of reactors used in microfluidics.

Figures used in the abstract

Figure 1

Figure 2

Figure 3

Figure 4