Mass transfer modelling between supercritical carbon dioxide and an ionic liquid in a micro- two-phase flow

Nayane Macedo Portela da Silva, Hugo Helouvry, Jean-jacques Letourneau, Fabien Baillon, Fabienne Espitalier

Mass transfer modelling between supercritical carbon dioxide and an ionic liquid in a micro- two-phase flow

N. Macedo Portela da Silva [a], H. Helouvry [a], J.-J. Letourneau [a*], F. Baillon [a], F. Espitalier [a]
[a] Université de Toulouse, Mines Albi, CNRS UMR 5302, Centre RAPSODEE, Campus Jarlard, 81013 ALBI Cedex 9
*Jean-Jacques.Letourneau@mines-albi.fr

Microreactors and supercritical fluids have great potential to intensify chemical processes, making them safer, cleaner and more efficient. An additional advantage of the small length scale is the potential for high-pressure applications due to lower mechanical stress in the microreactor material. The hydrodynamic and the mass transfer of two-phase flow under high pressure in a micro-capillary have been modeled. The model can take advantage of the 2D axisymmetry due to the cylindrical geometry of the capillary. This model allows an indirect estimation of binaries physicochemical properties such as mass transfer coefficient – estimations which are based on the geometrical values characterizing the two-phase flow such as velocities, frequency, sizes and volumes. To obtain these values, an accurate image processing is done on the high-speed camera images, which take advantages of the micro-reactor's transparency[1,2]. The binary mixture $[BMIm^+][PF_6^-]$ / supercritical carbon dioxide (SC-CO_2) have been chosen as the model system. Under pressure, the unidirectional transfer of CO_2 in $[BMIm^+][PF_6^-]$ induces significant changes in physico-chemical properties of continuous phase: viscosity decreases (divided by ten) and density increases (1.5 fold). Due to the wide variations of the continuous phase properties along the capillary, size and shape of the dispersed phase bubbles are simultaneously modified. In the generation region, the bubbles of SC-CO_2 are squeezed and look like bullet-shaped bubbles moving quickly through the capillary and between them the gap of continuous phase is almost saturated. Internal circulations arise within the bubbles. This Taylor flow region is surround by a thick film of viscous $[BMIm^+][PF_6^-]$ pressed against the capillary's inner surface. This film is not stagnant because slugs exert considerable shear stress on it, which keeps the film moving at a low velocity. Furthermore, a significant slip velocity has been identified located between these two regions. As the CO_2 diffuses in this wall-film its viscosity decreases by one order of magnitude and its thickness decreases until it disappears further down the capillary. The droplet's size decreases too and its shape evolves to become spherical. The mean velocity decreases and the flow behavior evolves in a Poiseuille flow. The aim of this study is to further develop a microsystem able to do screening of ionic liquids with solute under pressure of fluidizing CO_2. For this kind of system the prediction of the hydrodynamic behavior, mass transfer and physic-chemical properties (which drastically vary in a few centimeters) is a key to develop applications in which ionic liquids are involved as a solvent [3].

References

[1] N. Macedo Portela Da Silva, Doctoral Dissertation Mines Albi – INP Toulouse 28 Mars 2014.

[2] N. Macedo Portela da Silva, J-J. Letourneau, F. Espitalier, L. Prat, *Chem. Eng. Technol.* 2014, *37,* 1929.

[3] J. Resende, Doctoral Dissertation Mines Albi – INP Toulouse 25 Mars 2014.