Numerical simulation of nanoparticle formation in a co-flow capillary device

R. Othman[a,b]*, G.T. Vladisavljević[a]*, H.C.H. Bandulasena[a], Z.K. Nagy[a,c]

[a]Department of Chemical Engineering, Loughborough University, Loughborough, LE11 3TU, UK, [b]School of Bioprocess Engineering, Universiti Malaysia Perlis, Malaysia, [c]School of Chemical Engineering, Purdue University, IN 47907-2100, USA
***Corresponding authors: G.vladisavljevic@lboro.ac.uk, R.Othman@lboro.ac.uk**

The purpose of this study was to simulate the flow and concentration fields in a co-flow glass capillary device during formation of poly-ε-caprolactone (PCL) and polylactide (PLA) nanoparticles by nanoprecipitation ("diffusion-stranding" process). A numerical simulation using computational fluid dynamics (CFD) has been done by coupling Navier-Stokes and convection-diffusion equations for laminar flow. The organic phase (0.1 % (w/w) polymer in tetrahydrofuran (THF)) was injected through the inner capillary tube with a tapered cross section culminated in a circular orifice. The water phase was delivered co-currently through the outer square capillary. The inner diameter of the orifice was 60 μm and the water phase flow rate was 5 ml h^{-1}. The flow rate ratio of the water to organic phase was varied from 1.5 to 10 by varying the organic phase flow rate between 0.5 and 3.3 ml h^{-1}. Both THF and the polymer diffused to the water phase causing a decrease in the concentration of THF and the polymer downstream from the orifice in both the longitudinal and perpendicular direction. Nanoprecipitation of PCL and PLA occurred when the mass fraction of THF decreased to 0.82 and 0.66, respectively. The mixing time was found to reduce from 1.26 to 0.29 s when the aqueous-to-organic-phase flow rate ratio increased from 1.5 to 10. We observed a vortex formation in the vicinity of the orifice as a result of the high shear rate at the interface between the organic and water phase. The maximum vortex was formed at the organic phase flow rate of 3.3 ml h^{-1}, creating a shear rate between the two phases at the orifice of 1.8×10^4 s^{-1}. Due to local vortex formation, the polymer was mainly transferred by convection near the orifice and by molecular diffusion farther downstream.