Numerical simulation of multiphase dynamics in droplet-based microfluidics

Candidate: Mesuli Bonani Mbanjwa **Degree:** Doctor of Philosophy

Supervisor: Prof I.M.A. Gledhill

Co-supervisor: Prof K. Harding

Abstract

This work aimed to investigate dynamics involving mass transport in droplet flowing in microchannels system using numerical modelling and simulation. Droplet-based microfluidics or droplet microfluidics is a branch of microfluidics that deals with generation, manipulation and control of droplets in microchannels. Droplets flowing in microfluidic channels are effective self-contained micro-reactors for use in biological and chemical applications. The ability to generate multitudes of droplets with narrow size distribution and to control reagent volumes within individual droplets, allows for parallelisation of chemical processes in microfluidic channels. Droplet microfluidics is, thus, an exceptional tool for manufacturing and analysis in biological, chemical and nanotechnology applications.

Mixing processes in droplet microfluidics often involve three-way coupled physics of two-phase flow and mass transport (convection and diffusion) of chemical species, governed by a set of partial differential equations which require simultaneous solution. For two-phase flow, the equations for the movement and evolution of the interface are coupled to the Navier-Stokes of flow. In the case of transport of chemical species, the scalar mass transport equation is coupled to two-phase flow. The effects experienced in these systems are both multiscale and multiphase. Finite Element and Level Set simulations have been investigated and validated for modelling mass transport in droplet microfluidics systems. A set of benchmark cases has been developed for the purpose. Using Finite Element and Level Set simulations, a 2D two-phase moving-frame-of-reference modelling approach has been introduced and has been demonstrated to be an appropriate technique for investigation of mixing within droplets travelling in straight microchannels. This approach had not been previously demonstrated for the problem of mixing in droplet microfluidics, and requires less computational resources compared to the fixed frame-of-reference approach. Key conclusions of this work are:

- A limitation of the method exists for flow conditions where the droplet mobility approaches unity due to the moving wall boundary condition which results in an untenable solution under those conditions.

- As the size of the plug increases ($L_d >> w_d$), the efficiency of the mixing is reduced.
- The initial orientation of the droplet influences the mixing and the transverse orientation provides better mixing performance than the axial orientation.
- The recirculation inside the droplet depends on the superficial velocity and the viscosity ratio.