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Numerical simulation of microdroplet dynamics in microfluidics using finite element and level set methods

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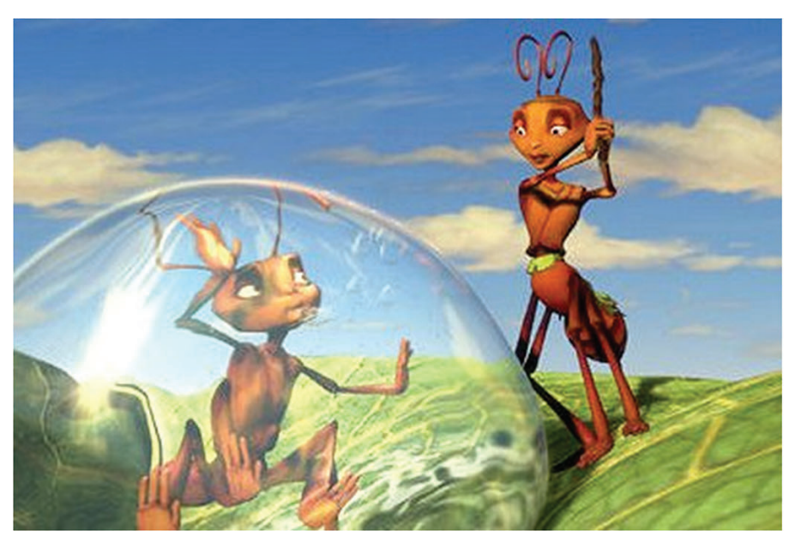
INTRODUCTION

Droplet-based microfluidic technology has, in recent years, found numerous applications in biology, chemistry, materials synthesis and process engineering applications. For example, it has been used in, among others, DNA analysis, enzyme assays, protein crystallisation and particle synthesis[1–2]. Microdroplets in microfluidic channels can act as multiple, self-contained and discrete micro-reactors when surrounded by another continuous immiscible fluid, whereby the reagents and reactions are contained and confined within the dispersed phase (droplets). Miniaturised flow systems are predominately dominated by surface forces due to the Scaling Law (**Figure 1**).



Scaling Law:

$$\frac{\textit{surface forces}}{\textit{volume forces}} \propto \frac{L^2}{L^3} = L^{-1} \xrightarrow[L \to 0]{} \infty$$

Figure 1: Surface forces dominate over volume forces in microsystems (image credit: DreamWorks[3])

Table 1: Important dimensionless numbers and scaling laws for two-phase microfluidic flows[4]

Dimensionless number	***Equation***	***Significance (force ratio)***	***Scaling law***
Bond (Bo)	$\rho g L^2 / \sigma$	gravitational/ interfacial	L^2
Capillary (Ca)	$\mu V / \sigma$	viscous/ interfacial	L
Ohnesorge (Oh)	$\mu / \sqrt{\rho \sigma L}$	viscous/ interfacial	$L^{-1/2}$
Peclet (Pe)	VL / D	convection/ diffusion	L^2
Reynolds (Re)	$\rho V L / \mu$	inertial/ viscous	L^2
Weber (We)	$\rho V^2 L / \sigma$	inertial/ interfacial	L^3
D-diffusion coefficient, ρ – density, L – length scale, σ – interfacial tension, μ – viscosity, V – flow velocity			

AIM

To simulate the evolution of interface and topology during droplet formation in a microfluidic flow-focusing junction using the COMSOL Multiphysics (version 3.5a) software program.

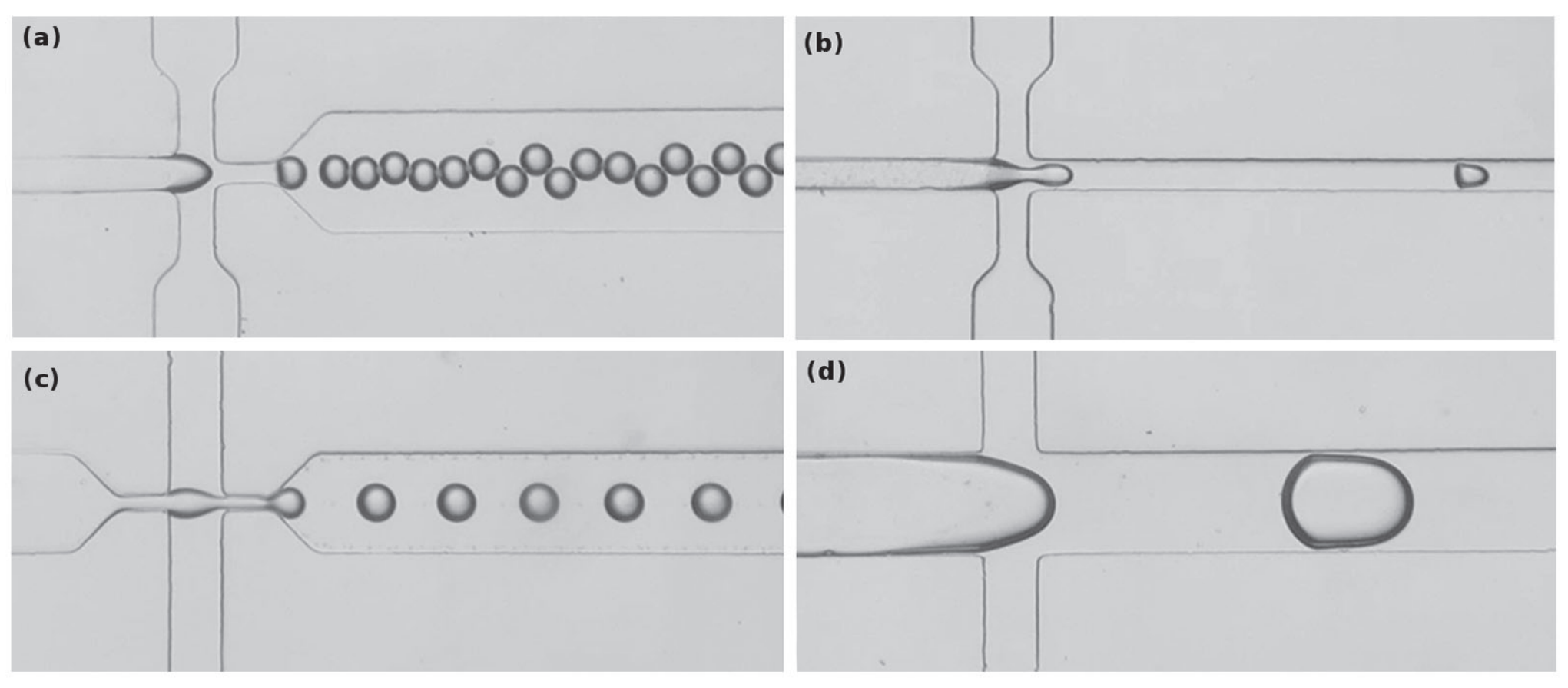


Figure 2: Droplet formation in variants of flow-focusing microfluidic channels

GOVERNING EQUATIONS

The Navier-Stokes equations and the level set (LS) equation are solved simultaneously;

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla \cdot \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T] + \nabla p = \rho \mathbf{g} + \mathbf{F}_\sigma \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{2}$$

$$\frac{\partial \varphi}{\partial t} + \mathbf{u}\nabla\varphi = \gamma\nabla \cdot [\varepsilon\nabla\varphi - \varphi(1-\varphi) \cdot \hat{\mathbf{n}}] \tag{3}$$

$$\mathbf{F}_\sigma = \sigma\delta\kappa\hat{\mathbf{n}},\ \delta = 6|\nabla\varphi||\varphi(\varphi-1)|,\ \kappa = \nabla\hat{\mathbf{n}},\ \hat{\mathbf{n}} = \frac{\nabla\varphi}{|\nabla\varphi|}, \tag{4}$$

where κ is the local interfacial curvature, δ is Dirac delta function and γ is a parameter controlling the interface thickness and approximated to the mesh size. The interface is reinitialised using the ε parameter which is approximated to the maximum velocity of the flow. The properties of the fluid were determined using a smeared out Heaviside's function across the interface.

$$\rho = \rho_1 + (\rho_1 - \rho_2)\varphi \tag{5}$$

$$\mu = \mu_1 + (\mu_1 - \mu_2)\varphi \tag{6}$$

RESULTS

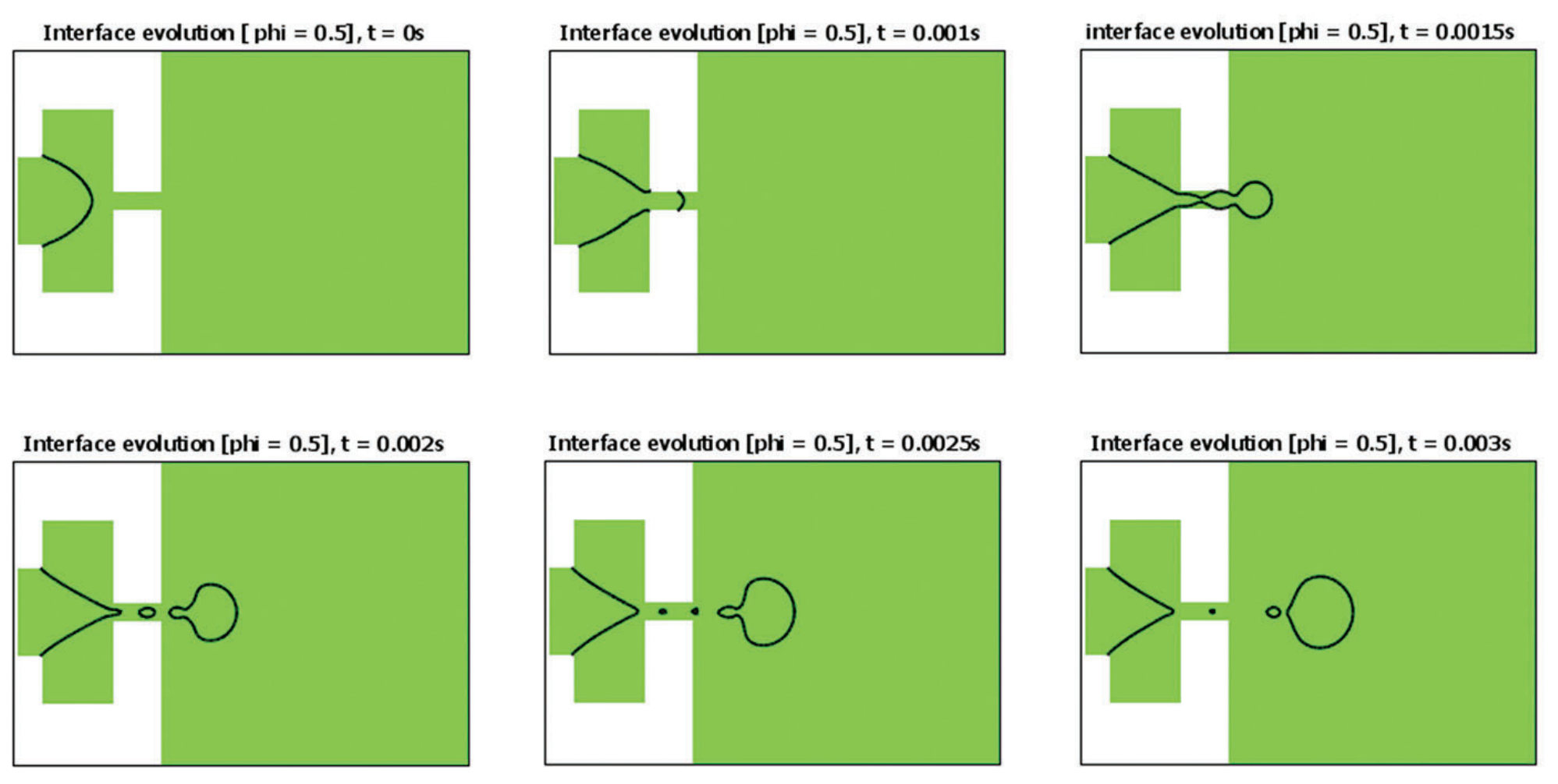


Figure 3: Simulation of droplet formation in flow-focusing microfluidic channel using a FE-based method

CONCLUSION

The evolution of the interface during microfluidic droplet formation can be captured with the LS method. Reinitialisation of the interface can be used to improve the mass conservation of the LS method in COMSOL Multiphysics.

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Alongside experimental work, numerical tools, such as computational fluid dynamics (CFD), allow us to study and analyse the behaviour of immiscible fluids within microchannels. Good understanding of these microfluidic flows provides us with leverage when utilised in chemical and biological applications.

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