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Investigation of pressure profile evolution during confined microdroplet formation using a two-phase level set method

Shazia Bashir [a], Julia M. Rees [a,*], Willam B. Zimmerman [b]

[a] School of Mathematics and Statistics, University of Sheffield, Hicks Building, Hounsfield Road, Sheffield S3 7RH, UK
[b] Department of Chemical and Biological Engineering, University of Sheffield, Newcastle Street, Sheffield S1 3JD, UK

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ABSTRACT

The formation of droplets at a T-junction in a microchannel network is primarily influenced by the pressure difference across the interface in the squeezing regime. Accurate measurements of droplet velocity and pressure profiles are difficult to obtain experimentally, yet these are the basic parameters required for understanding the physics governing the droplet formation process and for shaping the optimum design of microfluidic devices. The current work presents predictions from two dimensional numerical simulations of microdroplet generation at a T-junction. The simulation results are validated with the experimental observations. Detailed profiles of the predicted pressure evolution across the channel upstream of the T-junction indicate that the pressure variation is sensitive to small changes in the wetting properties of the continuous phase.

1. Introduction

Microfluidic reactors offer advantages associated with high surface-to-volume ratios, often by several orders of magnitude, compared to those of macroscale devices. Therefore, transfer processes can occur across a greater interfacial surface area, leading to increased heat and mass transfer rates. Consequently, the final equilibrium state may be attained from a lower energy consumption. Fluid behavior on micron scale dimensions is influenced by viscous effects rather than by inertial properties as the flow is essentially laminar, i.e. the Reynolds number, $Re < 1$ (Teh et al., 2008), with mass transfer and mixing processes being dominated by diffusion rather than by convection as in the macroscale case. In the case of single phase flow in a microchannel, the dispersion of solutes occurs along the length of the channel, which can lead to dilution and cross-contamination of injected samples. The confinement of chemical mixtures inside liquid droplets, or plugs, surrounded by an immiscible fluid in a microchannel has been shown to overcome these problems (Song et al., 2006; Leshansky and Pismen, 2009). More efficient transverse mass and heat transfer rates may be achieved due to the presence of recirculation zones within the liquid plugs.

Precise control of the generation of droplets is desirable in droplet-based microfluidics. This provides our motivation to better understand the dynamics of the droplet formation process. T-shaped microchannel are now widely used for generating microdroplets. The mechanism involves the shearing off the dispersed phase by the continuous phase which enables the generation of highly monodispersed microdroplets. In contrast to droplet formation in macroscale systems, droplets formed in microdevices tend to be stable, free from coalescence and do not break up as they propagate downstream. A microfluidic device for generating uniform sized water droplets within an oil phase incorporating a T-junction was first introduced by Thorsen et al. (2001). They suggested that the dynamics of the droplet breakup process is determined by the balance between the tangential shear stress and the interfacial tension. Nisisako et al. (2002) described a procedure for generating pico/nanoliter sized water droplets within an oil-based continuous phase using a T-junction microchannel. They succeeded in controlling the droplet diameter reproducibly by varying the flow velocity of the continuous phase. Van der Graaf et al. (2005) used a T-shaped microchannel to investigate unconfined droplet breakup as a model for membrane emulsification. A similar microfluidic device was used by Husny and Cooper-White (2006) to examine the influence of liquid viscosities and elasticity on the mechanism of droplet breakup. A detailed study of the formation of droplets and bubbles in a T-junction microchannel was carried out by Garstecki et al. (2006). They identified that, in the squeezing regime, the droplet breakup process is dominated by the pressure drop across the droplet as it emerges and proposed a scaling law for the length of the confined droplet that depends only on the flow rate ratio of the two immiscible fluids.

* Corresponding author. Tel.: +44 0 114 2223782.
E-mail addresses: shazia@pieas.edu.pk (S. Bashir), j.rees@shef.ac.uk (J.M. Rees), w.zimmerman@shef.ac.uk (W.B. Zimmerman).

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Xu et al. (2008) investigated scaling laws for controlling the range of droplet sizes within the squeezing and dripping regimes in T-junction microfluidic devices. Christopher et al. (2008) reported on a detailed experimental study of droplet breakup in the squeezing-to-dripping transition in T-shaped microfluidic junctions. They found that the dimensionless lengths of the stable droplets produced depended qualitatively on flow rate, capillary number and the ratio of the widths of the inlet channels, which controls the degree of confinement of the droplets. Link et al. (2004) repeatedly subdivided liquid plugs in a sequential network of T-junctions in order to create emulsions. Okushima et al. (2004) used sequential breakup through two T-junctions for the controlled production of monodisperse double emulsions.

Liquid droplets generated at T-junctions are particularly well-suited for biochemical reactions where each droplet can serve as an individual chemical reactor (Song et al., 2006; Stone et al., 2004; Breslauer et al., 2006). Mixing in these liquid droplets has been thoroughly studied (Song et al., 2003; Tice et al., 2003; Bringer et al., 2004). Other applications of droplet based microfluidic systems include multiphase dispersion (Okushima et al., 2004) and protein crystallization (Zheng et al., 2004; Leng and Salmon, 2009).

Compared to experimental observations, relatively few studies have been made that use numerical techniques to investigate multiphase flows in microfluidic devices. Recent advances in computational fluid dynamics (CFD), in particular for multiphase flows, have made the prediction of local parameters of the flow regime within a microfluidic device, such as velocity profiles, temperature and pressure gradients, and interface configurations, more accessible. Better understanding of these features is important for improving the design and control of microfluidic devices. Such data may be difficult or even impossible to extract from experiments. Sang et al. (2009) investigated the effect of viscosity on droplet formation in T-shaped microchannels using numerical and analytical methods. Qian and Lawal (2006) studied the gas–liquid slug flow regime in T-junction microchannels using the volume-of-fluid (VOF) based commercial CFD package FLUENT. The predicted lengths of slugs at various operating conditions were found to be in good agreement with experimental observations. Van der Graaf et al. (2006) used the Lattice Boltzmann method (LBM) to model the droplet breakup process at a T-junction and derived a semiempirical model for estimating the droplet volume in terms of flow rate and capillary number. Based on numerical simulations using a phase field method, De Menech et al. (2008) categorized the droplet breakup process into three different regimes: squeezing, dripping and jetting. The squeezing regime occurs at low values of the continuous phase capillary number ($Ca \lesssim 0.01$). The droplet is confined by the geometry of the channel. Droplet breakup occurs solely due to the build up of upstream pressure. Shear is the dominating force in the dripping regime ($Ca \gtrsim 0.02$). Breakup occurs when the viscous shear exerted by the cross-channel flow dominates over the interfacial tension. The jetting regime concerns droplet breakup into an unbounded fluid, which occurs at high values of *Ca*. The precise value of *Ca* above which transition from dripping to jetting occurs is presently unknown, and is almost impossible to explore, as the jetting regime could transform to that of a stable jet at any value of *Ca* above $\sim$0.1.

The velocity gradient in the vicinity of a droplet induces additional viscous stresses on the droplet. The interfacial tension at an oil–water interface gives rise to a pressure drop across the interface. A pressure drop is required to induce a flow along a microchannel of aqueous droplets in water–oil emulsions. This pressure drop is important even if the viscosity of the oil is small, as it contributes to increase the overall pressure drop in the microchannel. Therefore, in order to achieve precise manipulation of droplets, a key goal is to investigate the pressure profiles in the vicinity of the droplet.

The four key phases of droplet formation are (a) intrusion, where the dispersed phase begins to penetrate into the main channel, (b) blocking, where the dispersed phase could extend across the whole width of the main channel, (c) squeezing or elongation, where the emerging droplet is stretched in the downstream direction, and (d) breakup, when the droplet finally detaches from the inlet stream (Fig. 1).

De Menech et al. (2008) performed a systematic study of the pressure profile in relation to variations in interfacial tension. However, they did not investigate the dependency of the pressure profile with respect to the flow rate of the continuous phase or contact angle. Garstecki et al. (2006) investigated the evolution of the continuous phase pressure P_c in a study that assumed that the dispersed phase pressure P_d remained constant during the droplet breakup process.

In our recent work (Bashir et al., 2011), it was predicted using numerical simulations that the droplet length in the squeezing regime is influenced by the contact angle. In this article, numerical simulations are used to predict the effects of the continuous phase flow rate, *Qc*, interfacial tension and wettability on the pressure profiles, thus providing a more complete description of the underlying physics of the droplet formation process. The numerical model is described in Section 2. The system setup and a grid convergence study are presented in Section 3. The experimental details are described in Section 4. Results are presented in Section 5 and conclusions are summarized in Section 6.

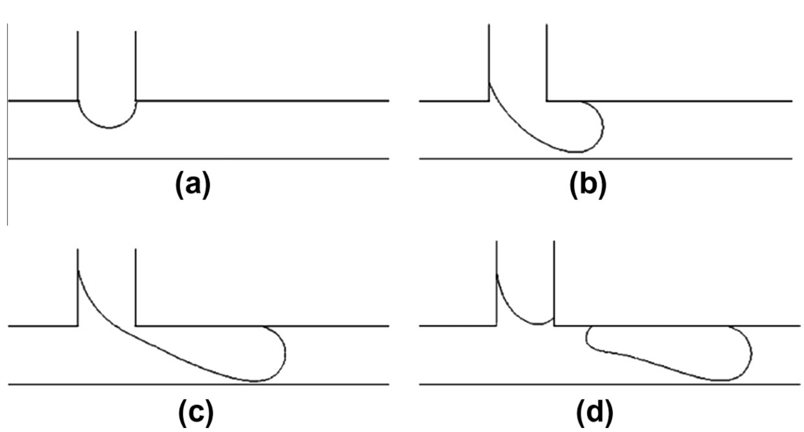

Fig. 1. Schematic illustrating the four phases of droplet formation: (a) the dispersed phase penetrates into the main channel; (b) the discontinuous stream nearly blocks the main channel; (c) the emerging droplet elongates downstream into the main channel; (d) the droplet separates from the inlet stream.