

Droplet Generation Modeling in Microfluidic Emulsifying Devices with Expansion Regions

Samuel Nyarko Osei¹, Petru S. Fodor¹

1. Department of Physics, Cleveland State University, Cleveland, OH, USA.

Abstract

The generation of monodisperse droplets using microfluidic emulsification devices has emerged as a powerful platform supporting broad applications in biomedical engineering, drug delivery encapsulation, materials synthesis, and chemical processing. However, optimizing the performance of these systems remains challenging due to the presence of multiple flow regimes and the strong sensitivity of both the droplet size, as well as size uniformity, to operating parameters such as flow rates, phase viscosities, and emulsifying region geometry. To address these challenges, we are developing computational models that allow the mapping of the emulsifying regimes as a function of the controlling parameters, and enable more efficient prototyping of emulsifying devices. In particular, we are exploring the effect on the droplet formation and uniformity, when expansion sections are used to control the shear rates in the emulsifying region where droplet formation and breakup occur. The models use the CFD Module from COMSOL Multiphysics to solve the Navier-Stokes equations in laminar flow systems, together with interface tracking models to visualize the evolution of the boundaries between the immiscible fluids, that define the droplets.

Keywords: microfluidics, emulsifiers, droplet generation, computational fluid dynamics.

Introduction

The ability to generate microsize emulsified droplets efficiently and with high uniformity is important for a variety of applications ranging from controlled encapsulation of ingredients (flavors, drugs, vitamins) in the food, pharmaceuticals, or cosmetic industries, to materials engineering applications, such as 3D printing stock, coatings, and scaffolds [1-3]. To this end, for many applications, microfluidic emulsification devices are seen as a viable strategy to enable the controlled generation of monodisperse droplets through the manipulation of immiscible fluids within microscale channels [4-5]. In these systems, droplet formation is governed by interactions among viscous forces, interfacial tension, and flow conditions [6-8]. Variations in parameters such as flow rates, fluid viscosities, and channel geometries result in different flow regimes, including squeezing, dripping, and jetting, which directly affect droplet size, uniformity, and production efficiency. Given the complexity of the flow structures in these devices, their prototyping would benefit greatly from accurate computational modeling that could efficiently map the droplet formation regimes for a broad array of parameters and geometries. In this study we use simulations to better understand how the generation of droplets in microfluidic devices is impacted by different flow-rate ratios across three microfluidic designs involving a simple cross-junction, a linear expansion, and a hyperbolic expansion region, respectively.

Methods

Emulsifier Design

The geometries of the microfluidic emulsifiers modeled in this work include two lateral inlets for the continuous phase (oil in this case) and one inline inlet for the dispersed phase (polymer). The three inlets meet at a junction where the emulsification of the polymer in droplets occurs due to the combined effect of the surface tension between the two liquids and the flow focusing present in this region. Besides the base case of a simple cross-junction emulsifier, in this study we investigate the effect of the addition of an expansion region placed immediately after the convergence point between the two liquid phases. Prior work in using expansion regions in the emulsification zone, shows that they can be a viable strategy to provide control over the droplet break-off process [9]. In our designs we used both a linear expansion region as well as one defined by a rectangular hyperbola. The later geometry is particularly attractive as it maximizes extensional flows along the center of the channel and also ensures that the deformation energy goes purely into stretching the fluid elements [10]. These unique characteristics of the flow through hyperbolic constrictions have already been exploited for applications from biomedical testing [11] to polymer processing [12] and microfluidic mixers [13]. For emulsifiers, the velocity profiles present this type of geometry, could mitigate the generation of secondary flows near the break-off point, which could help avoid inconsistencies in the separation

dynamics between different droplets, as well as the possible formation of secondary droplets.

For all the designs the inlets and outlet are channels with 100 μm in both width W_{channel} and height H_{channel} . Further dimensional details are provided in Figure 1. For the rectangular hyperbola design the edges of the expansion region are defined by the function:

$$y = \frac{b}{(a+x)} \quad (1)$$

with:

$$a = \frac{L_{\text{expansion}} W_{\text{expansion}}}{(W_{\text{channel}} - W_{\text{expansion}})} \quad (2)$$

$$b = \frac{L_{\text{expansion}} W_{\text{expansion}} W_{\text{channel}}}{2(W_{\text{channel}} - W_{\text{expansion}})} \quad (3)$$

where $W_{\text{expansion}} = 300 \mu\text{m}$ and $L_{\text{expansion}} = 300 \mu\text{m}$ are the maximum width and the length of the expansion region.

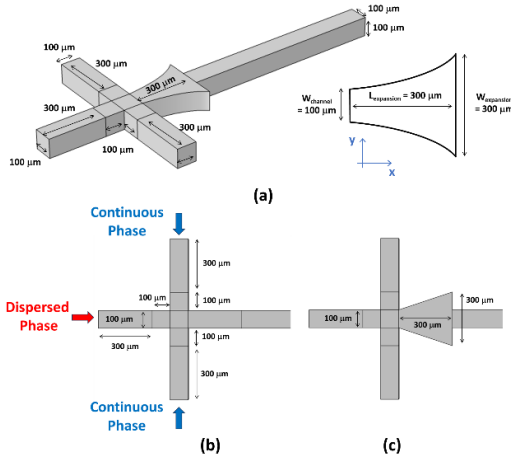


Figure 1. Geometry of the three emulsifiers designs studied: (a) with hyperbolic expansion; (b) simple cross-junction; and (c) linear expansion.

Governing equations

The prototype emulsifiers are modeled by numerically solving the Navier-Stokes equations (momentum conservation and continuity) for a two-phase fluid system under the assumption that the fluids are incompressible and Newtonian:

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right] = -\nabla p + \eta \nabla^2 \mathbf{u} + \mathbf{F} \quad (4)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (5)$$

where $\mathbf{u}$ [$\text{m}\cdot\text{s}^{-1}$] is the velocity vector, ρ [$\text{kg}\cdot\text{m}^{-3}$] is the fluid density, η [$\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$] is the fluid viscosity,

t [s] is the time, p [Pa] is the pressure, and the force term $\mathbf{F}$ [N/m^3] includes only the surface tension.

To track the interface between the two immiscible fluids a conservative level-set method is used [14-16]:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon \nabla \phi - \phi(1-\phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \quad (6)$$

where ϕ is a smoothing function that varies between values of 0 for one of the fluids and 1 for the other fluid, with the interface between the two phases corresponding to the 0.5 contour of the function ϕ . The parameters γ and ε are stabilization parameters.

Thus, the function ϕ allows the fluid properties to be defined as smooth spatial function:

$$\rho = \rho_{\text{oil}} + (\rho_{\text{polymer}} - \rho_{\text{oil}}) \phi \quad (7)$$

$$\eta = \eta_{\text{oil}} + (\eta_{\text{polymer}} - \eta_{\text{oil}}) \phi \quad (8)$$

For both fluid components the density used is 1000 [$\text{kg}\cdot\text{m}^{-3}$], while for the dynamic viscosity the values used for the two components are $\eta_{\text{oil}} = 0.002$ [Pa·s] and $\eta_{\text{polymer}} = 0.008$ [Pa·s], respectively.

COMSOL Multiphysics

The two-fluid phases level-set model is implemented in the Computational Fluid Dynamics (CFD) Module in COMSOL Multiphysics (COMSOL, Inc., Burlington, MA, USA). The simulations are carried on a three-dimensional domain meshed with $\sim 150,000$ tetrahedral mesh elements to ensure enough resolution to capture the fluid-fluid interfaces. The Navier-Stokes equations (4) and (5), and the level-set equation (6) are solved simultaneously. All the walls except the inlets and outlet are set to no-slip boundary conditions. The flow rate for the dispersed phase (polymer) inlet is set at $Q_d = 9$ [$\mu\text{L}/\text{min}$] while the flow rate for the individual inlets for the continuous phase (oil) is varied from $Q_c = 4.5$ to 36 [$\mu\text{L}/\text{min}$] to study the size and droplet dynamics dependence on the flow ratio Q_c/Q_d . The outlet of the microfluidics channel is set to zero pressure.

COMSOL Multiphysics is also used to analyze the data. Specifically, the integration feature over the volume fraction of fluid is used to estimate the effective diameter of the droplets produced.

Results & Discussion

Representative results for the velocity field overlapped with the streamline plots are shown in Figure 2. The results illustrate the effect of the expansion regions near the droplet formation and separation location. For both the linear and hyperbolic designs, respectively, the junction region is characterized by large velocity gradients.

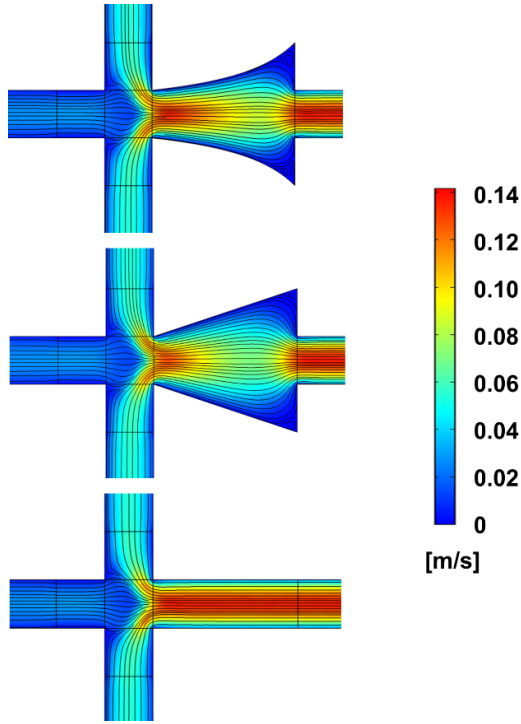


Figure 2. Cross-sectional velocity fields and streamline plots for emulsifiers with different expansion regions ($Q_c = 36$ [$\mu\text{L}/\text{min}$])

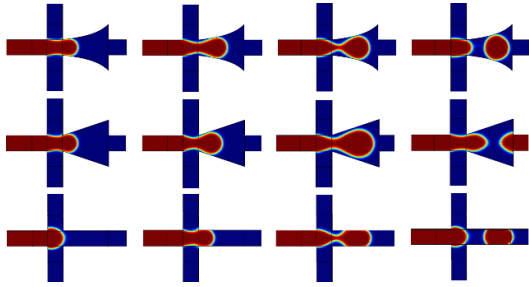


Figure 3. Dynamics of the droplet breaking process in the three emulsifier designs investigated ($Q_c = 9$ [$\mu\text{L}/\text{min}$])

In the expansion designs, the presence of the velocity gradient in the flow direction, which is maximum around the junction region, limits the region in which droplet breakup can occur. This in turn can support a more consistent break-off dynamics between subsequent droplets. For the flow magnitudes and ratios studied, the dynamics in the three designs shows that all three operate in the dripping regime where monodisperse droplets are formed (Figure 3). It is to be noted though, that careful inspection of the fluid dynamics immediately after the droplet separation indicates that while in the expansion designs the recovery of the fluid interface is rapid, that does not seem the case for the simple cross-junction design (Figure 4).

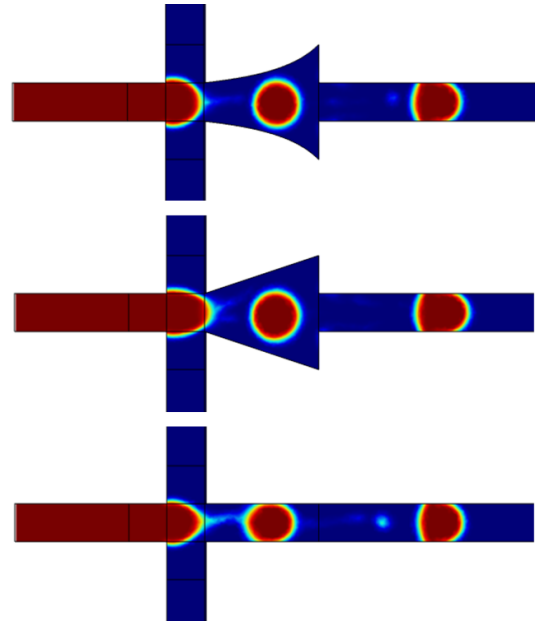


Figure 4. Snapshots of the droplet generation process captured immediately after the droplet separation in the emulsifying region ($Q_c = 36$ [$\mu\text{L}/\text{min}$])

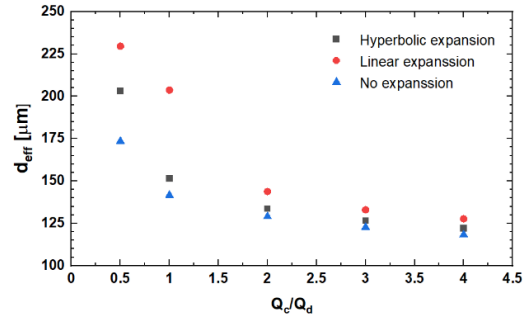


Figure 5. Effective diameter dependence on the flow ratio for the three designs.

In the later there are noticeable streamers between the inlet stream and the newly formed droplet. Moreover, these seem to coalesce into relatively sizable residual satellite droplets which would lead to a wider final droplet size distribution.

A size analysis over multiple droplets, was also performed by integrating over the volume fraction of the dispersed phase. The results show a clear dependence of droplet size on the dispersed to continuous phase flow ratios for all three geometries. In general, increasing the flow rate ratio Q_c/Q_d from 0.5 to 4.0 resulted in a decrease in droplet size (Figure 5). The linear expansion produced consistently the largest droplet sizes ranging from around 230 μm at the lowest flow ratio to about 130 μm at the highest flow ratio. Over the same range the simple cross-junction design shows the smallest

range in droplet sizes from around 170 μm to about 120 μm . The sample size in terms of the number of droplets is too small to be able to assess the level of monodispersity, although based on the above observed breakage dynamics that would be expected to be the highest in the expansion designs.

Conclusions

A computational model has been developed for the prototyping of microfluidic emulsifiers. The results confirm that the numerical simulations can capture key droplet formation behaviors, including stable dripping and near pinch-off dynamics under varying flow conditions. Future work will focus on further discretization of the droplet break-off region to further identify if the use of hyperbolic expansions designed to maximize elongational flows, allow for a more controlled pinch-off of the droplets with better size control and mitigation of the generation of satellite droplets.

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