Droplet Generation by means of a Two-Fluid Probe

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Introduction

Digital microfluidics is a technique based on the generation, handling, and measurement of droplets. Droplet generation is a necessary step for most high-throughput digital microfluidics applications. The standard droplet generation hardware generates droplets by injecting an aqueous solution into the immiscible oil at a T-junction in a microfabricated chip. Indeed, the T-junction type droplet generation device serves as an example in the model library of the COMSOL Chemical Engineering module.

A COMSOL simulation of a two-fluid probe for droplet generation is the focus of the work presented here. In Figure 1, the operating principle of the probe is shown, a Teflon tubing is placed inside a larger tube. A syringe pump draws fluid into the Teflon tubing at a flow rate greater than oil is pumped into the outer tubing. Thus some cell medium is drawn into the Teflon tubing in the form of droplets. Lemke et al. [1] patented a two-fluid probe that offers significant advantages over the T-junction type droplet generation device. Firstly, the probe is immersed in cell culture medium in a beaker, so that the medium can be mixed quite homogeneously by a simple magnetic stirrer. The concentration of the cells or microorganisms in the droplet can be fine tuned to give a high probability of having one cell or microorganism per droplet that is necessary for many biomedical applications. In a microfabricated droplet generator, such as a T-junction, cells are more likely to aggregate together or be trapped at surface inhomogeneities, e.g., at connectors, before they arrive at the T-junction. Secondly, it is relatively simple to fabricate this type of two-fluid probe and, in comparison with microfabricated droplet generators, no expensive clean rooms are required.

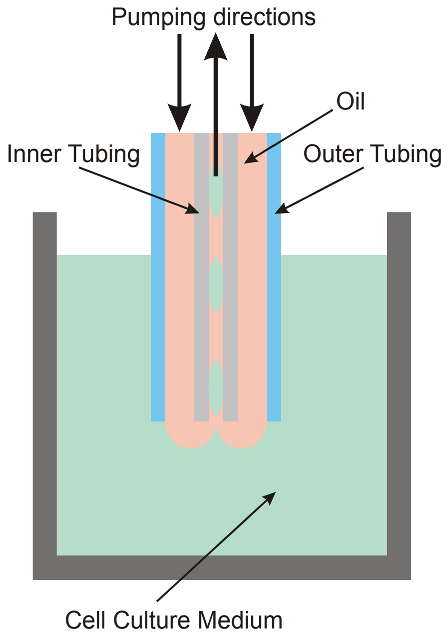

Figure 1: A schematic diagram of the two-fluid probe

[1] K. Lemke, G. Gastrock, A. Grodrian, R. Römer, M. Quade, M., D. Roscher (2008) Anordnung und Verfahren zum Erzeugen, Manipulieren und Analysieren von Kompartimenten. Patent DE 10 2008 039 117.4

Use of COMSOL Multiphysics

The geometry of the problem can be simplified quite easily by making use of two-dimensional axial symmetry. The flow in the system is at all times laminar and we chose to implement phase field version of the two-phase flow application mode of the Chemical Engineering module of COMSOL Multiphysics. Nevertheless it will be necessary to implement the level-set version, so that we can ascertain to which extent the results of the simulation are dependent on the choice of model.

Water	
Density	1000 kg/m^3
Viscosity	1.0×10^{-3} kg/(ms)
Tetradecane	
Density	773 kg/m^3
Viscosity	3.2×10^{-3} kg/(ms)
Surface Tension	44.2×10^{-3} N/m

Table 1. Properties of the fluids used in the simulation.

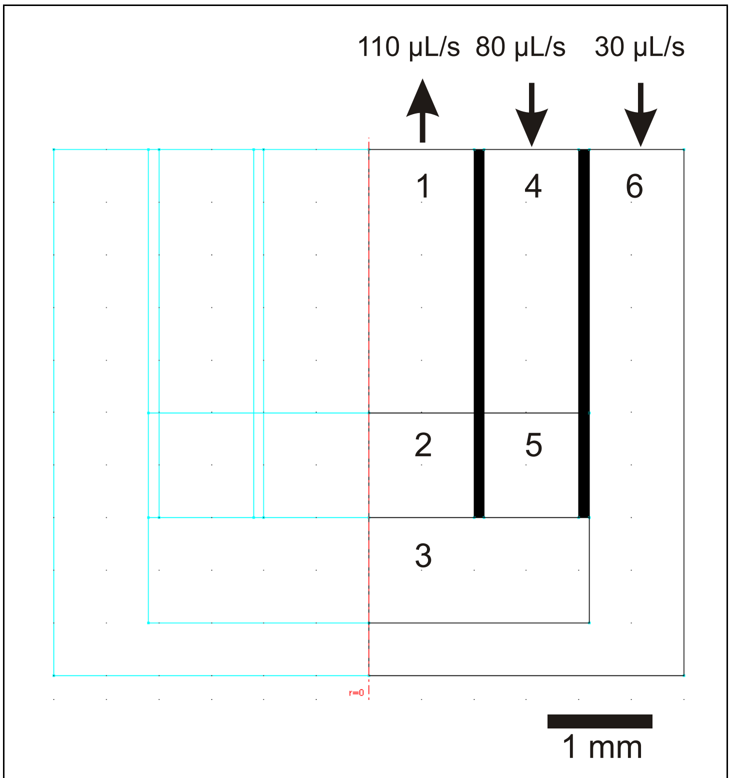

Figure 2: Geometry of the simulation model two-fluid probe

We chose to use the geometry shown above in Figure 2 with water initially filling subdomains 1, 2 , 3 and 6 and tetradecane filling subdomains 4 and 5. The fluid properties of water and tetradecane are given in Table 1. The boundaries of the tubings are defined as wetted walls. The inner tubing is in practice always Teflon tubing, we assigned a contact angle of 120°. In two separate simulations we assigned a contact angle of 60° and 120° as the contact angle of the walls of the outer tubing. The walls of the beaker are defined by the no-slip boundary condition. The initial fluid boundary is between the subdomains 3 and 5. The red line above defines the axis of symmetry. The arrows in figure 2 show the laminar outlet and inlet flow rates.

Expected Results

In Figure 3, the formation of a droplet and its transport through the inner tubing is illustrated from the results of a preliminary simulation. This allows the calculation of droplet size by the extrusion of the results of the 2D simulation to a 3D representation and then the performance of a subdomain integration of the volume fraction of the aqueous medium within the inner tubing.

The volume of aqueous medium in the inner tubing (subdomains 1 and 2 from Figure 2) in the first second of droplet generation is shown for two cases in Figure 4. The first case is for an outer tubing with a contact angle of 60° (hydrophilic) and the second case with a contact angle of 120° (hydrophobic). The results show how the surface energy of the materials used can affect the size and frequency of droplet generation. In Figure 3 it can be seen how the more hydrophilic outer tubing draws a small amount of aqueous media into the outer tubing so that the phase boundary is drawn a little closer to the inner tubing. In this way droplet breakup happens slightly more quickly so that as the blue curve in Figure 4 shows the droplets are smaller and are generated at a higher frequency than if the outer tubing is made of a more hydrophobic material.

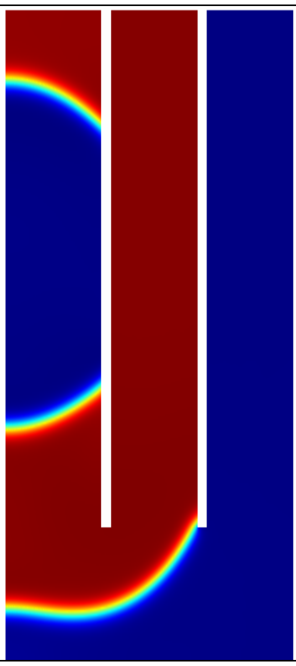

Figure 3. A frame of the simulation showing the passage of a water droplet through the inner tubing

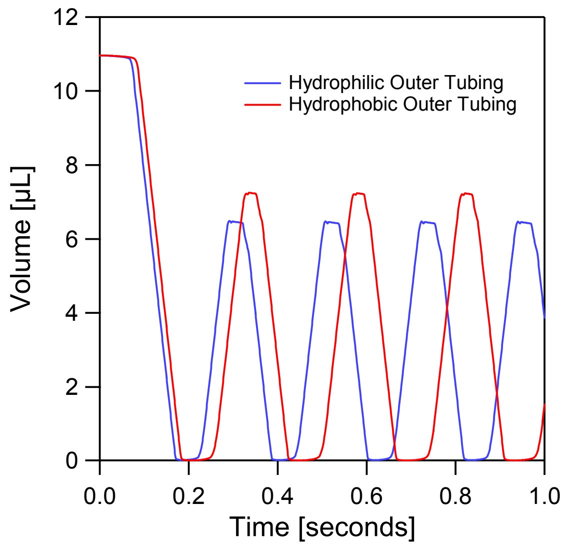

Figure 4. Comparison of the volume of water in the inner tubing as a function of time for the cases where the outer tubing is hydrophobic (red curve) and hydrophilic (blue curve.

We expect that this model will allow us to determine the effect of changing the output and input flow rates, the geometry of the probe, the choice of media (density, viscosity and surface tension) in addition to the contact angle of the materials out of which the probe is made. This simulation serves to complement ongoing practical work that experimentally evaluates the functioning of this two-fluid probe.

Conclusion

Droplet generation is a fundamental tool for digital microfluidics. In order for digital microfluidics to achieve maturity it is necessary to reliably control the generation of droplets. The two-fluid probe offers a way to generate droplets with an optimally mixed cell concentration directly from a beaker. This simulation offers a way to ascertain the size and spacing of droplets in tubing under various flow conditions in a two-fluid probe.