Simulation of a 3D Flow-Focusing Capillary-Based Droplet Generator

David Conchouso Gonzalez
PhD Student at Electromechanical Microsystems and Polymer Integration Research Laboratory (EMPIRe)
October 24th, 2013
Deals with:

- Behavior
- Control
- Manipulation

Of small volumes of fluids (µL, nL, pL)
Droplet Microfluidics

• Balance between viscous and surface tension forces.
• Discrete Volumes (Nano to Femtoliter)

CP= Continuous Phase (medium) & DP= Disperse Phase (droplets)
Potential Applications

- High reaction parameter control
- High temperature control
- Gas-Liquid Reactions
- Exploration of dangerous reagents
  - Phosgene, Acrolein, Interhalogen compounds
- Drugs Crystallization
  - API - Active Pharmaceutical Ingredients
- Controlled stoichiometries of reagents
- Hazardous Products
  - Azides preparation/reaction
Capillary-Based Droplet Generators

Co-Flow

Capillary MFDG

Cross-flow

3D-Flow Focusing

(A) (Seong, 2005)

(B) (McQuade, 2005)

(C) (Utada, 2007)

3D Flow-Focusing & Co-flow Devices

(D) (Utada, 2007)
Capillary-Based Droplet Generators

(Chu, 2007)
Simulated Capillary-Based Device

- **2D Model**
  - Dimension: 375, 125, 250, 1000, 254

- **Solid of Revolution**

- **Physical Device**
  - Oil inlet
  - Water inlet
  - Glass capillaries
  - Model
  - Square channel
  - Output
Simulation Setup

• Laminar Two-phase flow, phase field method.
• Physics Controlled Mesh
• Boundary conditions:
  o Inlets: Fixed Flow Rates for Water and Oil
  o Outlet: Zero pressure, no viscous stress
  o Initial Interface
  o 2D Axisymmetric
Simulation

Oil Flow Rate (Red) = 15μL/min
Water Flow Rate = 15μL/min

Oil Flow Rate (Red) = 20μL/min
Water Flow Rate = 40μL/min
Normalized droplet diameter \((D/D_h)\) versus flow rate ratio, at different total flow rates.

Frequency of generation (in droplets per second) versus flow rate ratio, at different total flow rates.
Future Work

• Through this simulation one could able to design generators in **series** to produce multiple emulsions with specific parameters:
  - Size,
  - Core-shell thickness,
  - Number of Daughter Droplets,
  - Synchronization of generation

(Chu, 2007)
Conclusions

• We have successfully simulated a 3D Flow focusing device using a 2D axisymmetric model (fast convergence <15min.)
• CFD can help to save time with fabrication and testing of the devices.
• This model will allow us to design multiple droplets with desired characteristics.
• At higher flow rates, droplet diameter decreases, and frequency of generation increases.
Thank you!
References


# Fluid Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Oil (DP)</th>
<th>Water (CP)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (Kg/m$^3$)</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>Dynamic viscosity (mPa\cdot s)</td>
<td>6.71</td>
<td>1.95</td>
</tr>
</tbody>
</table>
Laminar Phase Field Method

- The multiphase flow is described by the parameter $\phi$. One fluid element is defined as $\phi = 1$, whereas the second fluid element is $\phi = 0$. The interface between them (phase field) is the set of values $1 < \phi < 0$. 

(Bhadeshia)
Motivation

• Droplet formation depends on the liquids properties (viscosity and interfacial tension between the phases), and flowing rates. (Capillary Number)

• Unknown expected droplet size and hence core-shell thickness.

• Proper synchronization is needed to create multiple droplets

• Fabrication is challenging (especially the tapered wall and assembly process)

• Expensive cameras are required to characterize at high generation frequencies
Interdisciplinary Field