Computational Fluid Dynamical Simulations of Droplet Flow and Merger in Microfluidic Channels

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why miniaturize?

benefits of miniaturization

• cost economies through micromachining
• reduced sample/reagent and power consumption
• portability (e.g. point-of-care/in-the-field applications)
• superior analytical performance \((speed, efficiency \text{ and } control)\)
• facile process integration and automation \((c.f. \text{ microelectronics})\)
• high analytical throughput
• functionality

why chose microfluidics?

• scale dependence of heat and mass transfer
• improved performance \((speed/efficiency/control/throughput)\)
• functional integration of components facile

*superior quality and rate of generation of chemical / biological information*
fluid flow on the small scale

- large surface area-to-volume ratios allow for highly efficient mass and heat transfer.
- mass and energy are transferred quickly when creating or homogenizing solute & temperature gradients.
- as system dimensions are reduced fluids are increasingly influenced by viscosity rather than inertia, which results in laminar flow.
- the importance of diffusion and convective bulk flow for mass transport is controlled by flow velocity and system dimensions.
- high surface area-to-volumes ensure that surface tension influences fluid behaviour.

\[
Re = \frac{\rho v \delta}{\mu} \quad Pe = \frac{v \delta}{D} \quad Ca = \frac{v \mu}{\gamma}
\]
droplet-based microfluidics

- discrete liquid droplets are encapsulated by a carrier fluid that wets the channel surface and forms the continuous phase.
- droplets are isolated and form the dispersed phase in which reactions may occur.
- droplet size is well-defined (monodisperse).
- mass transport occurs without dispersion.
- droplets can be dosed with varying amounts of input reagents.
- droplets can be generated at kHz frequencies.
- droplets easily generated using flow-focusing and tee-junctions.
- can be achieved for both L/L and G/L systems.

unit operations: controlled droplet fusion
droplet manipulations: dilution on the microscale

passive dilution structure is based on L/L and L/channel structure hydrodynamic interactions

mother droplet is deformed and subjected to a back pressure due to surface tension

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23 output droplets access 4 orders of magnitude of concentration (100 µM - 36 nM)

c_{output} \propto \left(1 - \frac{V_d}{V_m}\right)^n
Physics of the Fluid 1
Physics of the Fluid 2

\[ \text{Re} = \frac{\rho UL}{\mu} \]

- Reynolds number (dimensionless #)
  - Ratio of inertial forces to viscous forces
- Re<1
  - Viscous > Inertial
  - Laminar Flow
  - More controllable and predictable environment
The Navier-Stokes equation is used to model the fluid velocity profile of a Newtonian fluid through a channel subjected to a pressure gradient $\nabla p$. This equation balances the inertial component of the fluid against pressure and shear stress.

$$\rho \left[ \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right] = -\nabla p + \mu \nabla^2 \vec{u}$$

The fluid being examined adheres to the conservation of mass:

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

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For microfluidic systems, the following simplifications can be made to the Navier-Stokes Equation:

- Low Reynolds number \( \text{Re} \ll 1 \) allows the convective term to be neglected
  \[
  (u \cdot \nabla)u = 0
  \]

- Assuming steady state inlet conditions, the fluid velocity field will not vary with time.
  \[
  \frac{d\vec{u}}{dt} = 0
  \]

These simplifications lead to an equation that describes Poiseuille flow:

\[
\mu \nabla^2 \vec{u} - \nabla p = 0
\]

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Experimental Results: Flow Focusing Junction

- **Flow Focusing Junction**
- **Oil (Carrier Phase)**
- **Aqueous Droplet**

Images:
- **A** $t' = 0 \text{ ms}$
- **B** $t' = 1.875 \text{ ms}$
- **C** $t' = 3.125 \text{ ms}$
2-D Geometry Modeling: Droplet Merger

Pillar Induced Merging

- $t' = 0$ ms
- $t' = 2.5$ ms
- $t' = 5$ ms
- $t' = 7.5$ ms

Merging In Expansion Chamber
Computational Fluid Dynamics Calculations

- Use 12 node, 24 processor computer cluster:
  - Linux based O/S
  - Red Hat shell allows for parallel processing
- Calculations performed on COMSOL Multiphysics software.
  - Can design device, set up boundary conditions.
  - Allows for solving simultaneous partial differential equations, e.g. Navier-Stokes for fluid flow, can couple to diffusion, temperature gradient, etc.
Droplet formation at flow focusing junction: experimental vs. 2-D modeling
3-D Geometry

- Change from 2-D Geometry: T-Junction and Merging Chamber Combined
Schematic of T-Junction

Inlet 1 composed of oil

Inlet 2 composed of water

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$w_f$</td>
<td>$50,\mu m$</td>
</tr>
<tr>
<td>$L2$</td>
<td>$300,\mu m$</td>
</tr>
<tr>
<td>$L1$</td>
<td>$1000,\mu m$</td>
</tr>
<tr>
<td>$h$</td>
<td>$100,\mu m$</td>
</tr>
<tr>
<td>Water:Oil</td>
<td>2:1</td>
</tr>
</tbody>
</table>
Schematic of Pillar Induced Merging Chamber

\[
\begin{array}{|c|c|}
\hline
w_o &= 40\mu m \\
w &= 50\mu m \\
w_p &= 20\mu m \\
\hline
\end{array}
\]

\[
\begin{array}{|c|c|}
\hline
p &= 40\mu m \\
w_c &= 220\mu m \\
w_c &= 50-70\mu m \\
\hline
\end{array}
\]
## Fluid Properties

### Re Number for Fluid 1 (oil)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volumetric Flow Rate</td>
<td>1.11e-10 m³/s</td>
</tr>
<tr>
<td>Fluid 1 density ( (\rho) )</td>
<td>1e³ [kg/m³]</td>
</tr>
<tr>
<td>Fluid 1 dynamic viscosity ( (\mu) )</td>
<td>1.95e-3 Pa·s</td>
</tr>
<tr>
<td>Velocity</td>
<td>2.22e-2 m/s</td>
</tr>
<tr>
<td>Re</td>
<td>11.4</td>
</tr>
</tbody>
</table>

### Re Number for Fluid 2 (water)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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<tbody>
<tr>
<td>Volumetric Flow Rate</td>
<td>5.55*10⁻¹¹ m³/s</td>
</tr>
<tr>
<td>Fluid 2 density ( (\rho) )</td>
<td>1e³ kg/m³</td>
</tr>
<tr>
<td>Fluid 2 dynamic viscosity ( (\mu) )</td>
<td>6.71e-3 Pa·s</td>
</tr>
<tr>
<td>Velocity (longer channel)</td>
<td>1.11E-2 m/s</td>
</tr>
<tr>
<td>Re</td>
<td>0.497</td>
</tr>
<tr>
<td>Interfacial Tension</td>
<td>5e⁻³ N/m</td>
</tr>
</tbody>
</table>
Droplet formation in 3-D chamber
Future Work

- Vary parameters such as: oil Reynold’s numbers, dimensions of pillar array, fluid velocity, etc. to get droplet merger.
- Model droplet merger in the merging chamber.
- Model sequential merging (3 or more droplets merging).
- Compare to recent experimental results at the ETH.
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