Control the poly-dispersed droplet breakup mode inside a microfluidic flow-focusing device by external electric field

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Objective of this study:
• Capture the droplet breakup modes by level-Set method;
• Test the capability of using electric field to control the droplet breakup mode.

Introduction:
(1) droplet-based microfluidics;
(2) droplet generator; breakup regimes and breakup modes;
(3) control the droplet breakup by electric fields

Numerical methods
(1) Conservative level-set & Electrostatics;
(2) Simulation setup

Results from simulations

Questions and Discussions
Introduction to droplet-based microfluidics

• The droplet-based microfluidics overcomes the drawbacks of the conventional single-phase microfluidics.

• **Approach**: introduce an immiscible carrier fluid (continuous phase) to encapsulate the reagents (secondary phase) inside discrete droplets / slugs.

• **Advantages**: Rapid mixing; no dispersion; minimized surface fouling.

• **Applications**:
  1. Nano-particle (NP) synthesis;
  2. In-situ kinetic measurement;
  3. Various other applications in chemistry and biology.

• **Challenges**:
  1. Control the droplet breakup to obtain droplets of desired sizes and distributions.
  2. Obtain “mono-dispersed” droplet sizes.

References:
Passive droplet / slug generation:
(1) Utilize device geometry and fluid flow;
(2) Three types of generators:
I. Co-flow device;
II. Cross-flow device (T-junction);
III. Hydrodynamic flow-focusing device.

Droplet breakup dynamics:
(1) Three forces:
Pressure force, viscous shear and surface tension force;
(2) Breakup regimes: Squeezing, Dripping, Jetting;
(3) Critical parameters:
   Capillary number \( (Ca = \mu_c U_c / \sigma) \)
   Flow ratio \( (Q = Q_c / Q_d) \)
   Viscosity ratio \( (\lambda = \mu_d / \mu_c) \)

References:
Droplet breakup modes

- Mono-dispersed breakup: uniform droplets, size variation < 2%;

- Poly-dispersed breakup: droplets of broad size distributions

- Typical poly-dispersed breakup modes:
  I. Single secondary (satellite) droplet after the primary droplet;
  II. Multiple secondary droplet after the primary droplet.

Poly-dispersed breakup mode seen in experiments (Anna, 2003)

Conclusions from literatures and previous simulations:
I. Poly-dispersed breakup mode is governed by the non-linear dynamics.
II. Initiation: imbalance of the three forces;
III. Two mechanisms: end-pinching & capillary instability;
IV. Comsol can capture these two modes and the wave shape.
V. Capillary instability needs time to develop.

Reference:
Electric field has been coupled with conventional droplet-based microfluidics to enhance the droplet manipulations (breakup, coalescence, sorting and etc).

- The different electric properties (permittivity, conductivity) induce electric charges on the fluid interface.
- The interactions between electric field and the induced charges generate electric forces (Maxwell stress) on the fluid interface.
- The electric force has shown the ability to control the droplet sizes.

Hypothesis: The electric field can control the droplet breakup mode in droplet-based microfluidics.
Fluid flow: Conservative Level-Set Method (LSM)

\[ \frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \nu \nabla \cdot \left( \epsilon \nabla \phi - \phi (1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right) \]  
(3)

\[ \hat{n} = \frac{\nabla \phi}{|\nabla \phi|} \]  
(4)

\[ \kappa = -\nabla \cdot \hat{n} \mid_{\phi=0.5} \]  
(5)

\[ F_{sf} = \sigma \kappa \delta \hat{n} \]  
(6)

\[ \delta = 6 |\nabla \phi| |\phi (1 - \phi)| \]  
(7)

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \]  
(8)

\[ \frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot [\mu (\nabla u + \nabla u^T)] + F_{sf} + F_{ef} \]  
(9)

\[ \rho = \rho_1 + (\rho_2 - \rho_1) \phi \]  
(10)

\[ \mu = \mu_1 + (\mu_2 - \mu_1) \phi \]  
(11)

\[ \epsilon = \epsilon_1 + (\epsilon_2 - \epsilon_1) \phi \]

\[ F_{ef} = \nabla \cdot T_{MW} = -\frac{1}{2} (E \cdot E) \nabla \epsilon \]  
(11)

Electrostatics: Poisson equation

\[ \nabla \cdot (-\epsilon \nabla V) = \rho_f \]  
(1)

\[ E = -\nabla V \]  
(2)
Simulation setup

- Field configuration: high potential $V_0$ left, ground right.
- Strong field in the dispersed phase ($\varepsilon_2 < \varepsilon_1$).
- Electric force is induced on the fluid interface.
- Electric force “squeezes” the fluid neck.

<table>
<thead>
<tr>
<th>Property</th>
<th>Continuous phase</th>
<th>Dispersed phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density (kg/m$^3$)</td>
<td>1000</td>
<td>960</td>
</tr>
<tr>
<td>Viscosity (mPa*s)</td>
<td>1</td>
<td>10/20/50/100</td>
</tr>
<tr>
<td>Relative permittivity</td>
<td>78.5</td>
<td>2.8</td>
</tr>
<tr>
<td>$Q_c/Q_d$</td>
<td>10~100 (Qd = 0.04 mL/h)</td>
<td></td>
</tr>
<tr>
<td>$V_0$</td>
<td>0 ~ 150 V</td>
<td></td>
</tr>
</tbody>
</table>
Effect of flow ratio on poly-dispersed breakup mode (“poly-dispersed breakup window”)

Observations (Nie, 2008), without electric field:
• Poly-dispersed breakup mode occurs in certain ranges of flow ratios (“poly-dispersed breakup window”).
• When the flow ratio increases beyond critical values, the poly-dispersed mode shifts to mono-dispersed mode.
• The locations and size of “windows” are functions of viscosity ratio ($\lambda = \mu_d/\mu_c$).
• The span of “window” is large when the viscosity ratio is small.

Simulation results: droplet breakup without electric field

Observations from simulations:
- The numerical model (LSM) can capture the “poly-dispersed breakup window” qualitatively.
- Good agreement of primary droplet sizes with experiments (Nie, 2008).
Effect of flow ratio on breakup modes

Observations:
- Increase the flow ratio from 50 to 100 → total droplet breakup time is reduced from 13 ms to ~ 8.5 ms.
- Reduce droplet breakup time → suppress the development of capillary instability → mono-dispersed breakup mode
- Hypothesis: apply electric field to speed up the breakup process thus to suppress the capillary instability.

Poly-dispersed breakup mode

Mono-dispersed breakup mode

Measure the neck width in the orifice entrance

Neck width ($W_n$) as a function of time

Increase the flow ratio

0 2 4 6 8 10 12 14 16
0 10 20 30 40 50 60 70
$W_n$ (μm)

$Q_e/Q_d = 50$
$Q_e/Q_d = 100$

Poly-dispersed

Mono-dispersed
The electric force squeezes the fluid neck thus reduces the droplet breakup time.
When $V_0 = 120$ V is applied, the total droplet breakup time is reduced from 13 ms to ~ 7 ms.
As the capillary instability does not have sufficient time to develop, the poly-dispersed breakup mode is eliminated.
Conclusions

- The simulations using Comsol have captured the droplet breakup modes successfully.

- The poly-dispersed breakup mode occurs due to the effect of capillary instability.

- The capillary instability requires certain time to develop before it can take effect.

- By shortening the droplet breakup time, the capillary instability can be suppressed, which can avoid the poly-dispersed breakup mode.

- By applying the external electric field, the electric force is induced on the fluid interface. The electric force helps to reduces the droplet breakup time thus to avoid the poly-dispersed breakup mode.

- As the applied voltage exceeds certain threshold value, the droplet breakup mode shifts from the poly-dispersed to the mono-dispersed one.
Acknowledgement

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Questions?