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Presentation

Numerical Study of Droplet Formation inside a Microfluidic Flow-Focusing Device

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Outline

- Introduction to Microfluidic Flow-Focusing Device (MFFD)
- Numerical Method (conservative level-set)
- Results and Discussion
    - Model Validation
    - Effect of dispersed phase viscosity
    - Effect of geometry
- Conclusion
- Acknowledgements

Droplet-based microfluidics

- **Fundamental:** capsulate reagents inside droplets;

utilize microfluidic technology to offer superior control

- **Category:**

Passive method: co-flow, cross-flow and flow-focusing devices

Active method: atomization, sprays, membrane emulsification

- **Advantages:**

rapid mixing;

no dispersion;

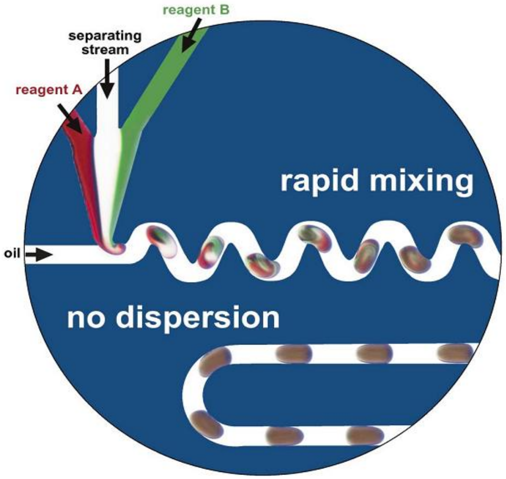
better control over flow and reactions

uniform size distributions

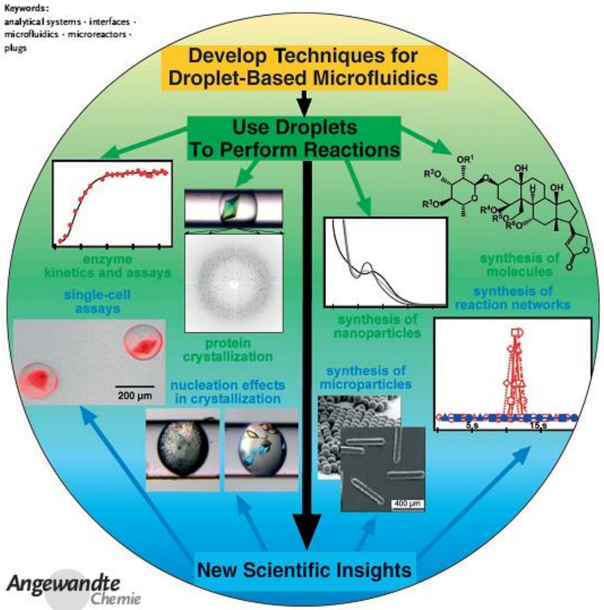
- **Applications:**

chemical analysis, material synthesis, time-resolved kinetic study …

Communications



Keywords:
analytical systems · interfaces · microfluidics · microreactors · plugs



Angewandte Chemie

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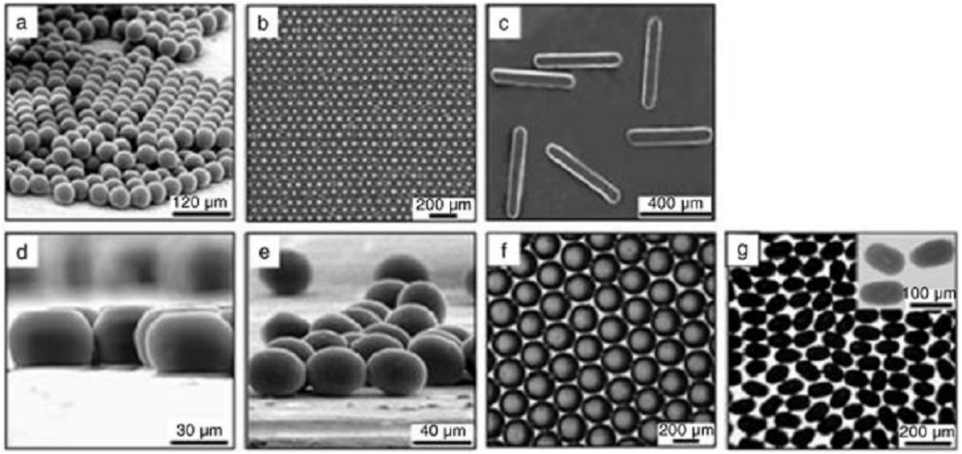
Applications on particle synthesis

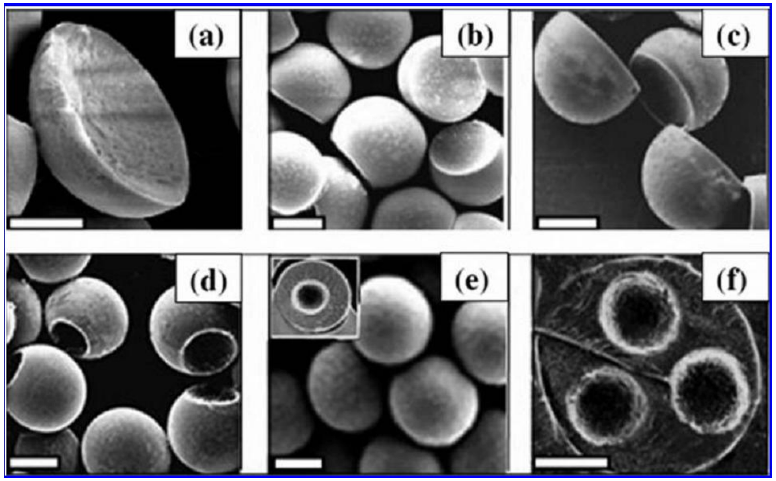
Polymer particles with controlled morphology

(S. Q. Xu, et al., 2005)



Polymer particles with core-shell structure

(Z. H. Nie, et al., 2005)



1. S. Q. Xu, Z. H. Nie, M. Seo, P. Lewis, E. Kumacheva, H. A. Stone, P. Garstecki, D. B. Weibel, I. Gitlin and G. M. Whitesides, *Angew. Chem.-Int. Edit.*, 2005, **44**, 724-728
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Microfluidic Flow-Focusing Device (MFFD)

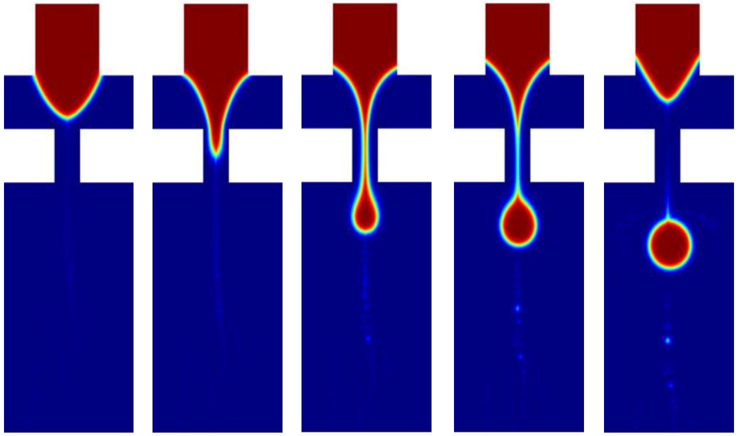
Fundamentals

(1) The dispersed phase is injected from the center channel while the continuous phase is injected from the two side channels.

(2) The two phases flow together through a contraction.

(3) Inside the orifice, the resulting elongation-dominated velocity field draws the dispersed phase into a thin jet that breaks into droplets.

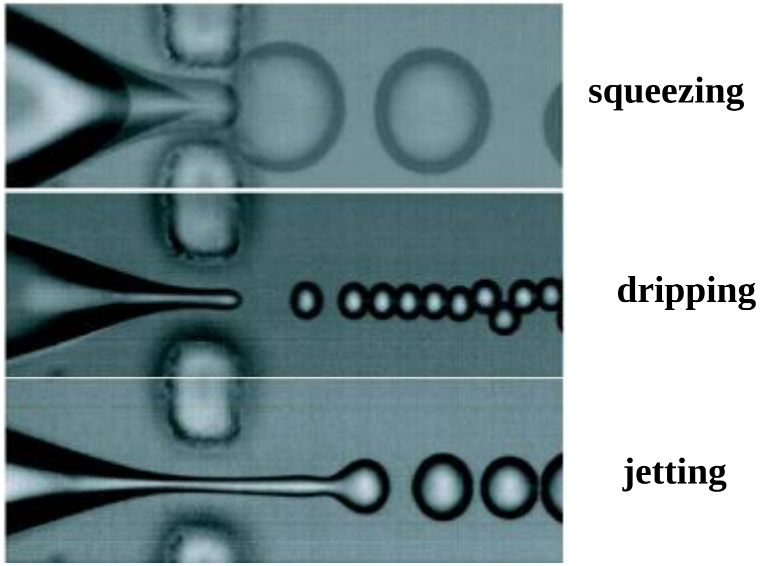
(4) The droplet sizes are comparable to the orifice width.



A typical droplet breakup process

Controlling Parameters

- Reynolds number (Re): $\mathrm{Re_c} = \frac{\rho_c U_c D}{\mu_c}$
- Capillary number (Ca): $\mathrm{Ca_c} = \frac{\mu_c U_c}{\sigma}$
- Volumetric flow ratio (φ): $\varphi = \frac{Q_c}{Q_d}$
- Viscosity ratio (λ): $\lambda = \frac{\mu_d}{\mu_c}$



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2. S. L. Anna and H. C. Mayer, *Phys. Fluids*, 2006, **18**.

Conservative level-set method

- Conservative level-set method

$$\frac{\partial\phi}{\partial t}+\vec{u}\cdot\nabla\phi=\gamma\nabla\cdot\left(\epsilon\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right)\qquad(1)$$

$$\hat{n}=\frac{\nabla\phi}{|\nabla\phi|}\qquad(2)$$

$$\kappa=-\nabla\cdot\hat{n}|_{\phi=0.5}\qquad(3)$$

$$\delta=6|\nabla\phi||\phi(1-\phi)|\qquad(4)$$

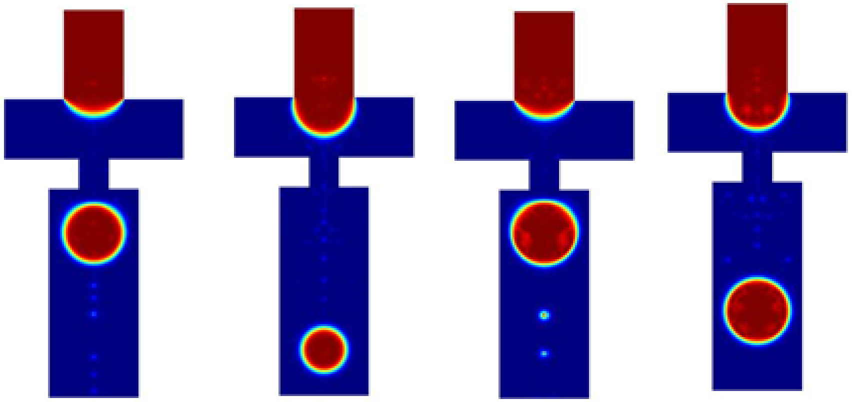
$$\rho=\rho_1+(\rho_2-\rho_1)\phi\qquad(5)$$

$$\mu=\mu_1+(\mu_2-\mu_1)\phi\qquad(6)$$

$$\vec{F}_{sf}=\sigma\kappa\delta\hat{n}\qquad(7)$$

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{u})=0\qquad(8)$$

$$\frac{\partial(\rho\vec{u})}{\partial t}+\nabla\cdot(\rho\vec{u}\vec{u})=-\nabla P+\nabla\cdot\left[\mu\left(\nabla\vec{u}+\nabla\vec{u}^T\right)\right]+\vec{F}_{sf}\qquad(9)$$



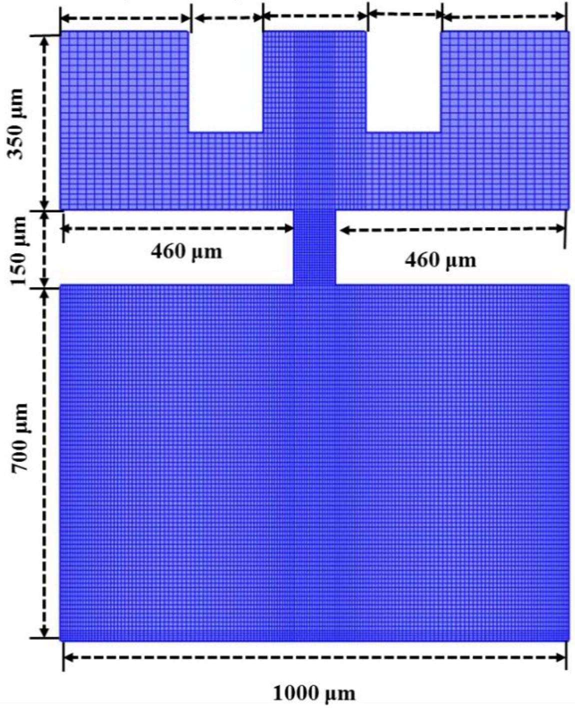
Non-conservative level-set **Conservative level-set**

Key findings

(1) Traditional level-set method (non-conservative form) converges faster but suffers from mass conservative issue.

(2) The conservative level set method has good mass conservation but takes longer computational time.

Simulation setup



2D computational domain with 13,000 elements

Fluid properties

Continuous phase: 2.0 wt% SDS aqueous solution
Dispersed phase: silicone oil

Liquids	Density ρ (kg/m^3)	Dynamic viscosity μ (cp)	Interfacial tension[a] σ (mN/m)
Silicone oil	930	10	3.3
	950	20	5.5
	960	50	4.8
	960	100	3.8
2.0 wt% SDS aqueous solution	1000	1000	N/A

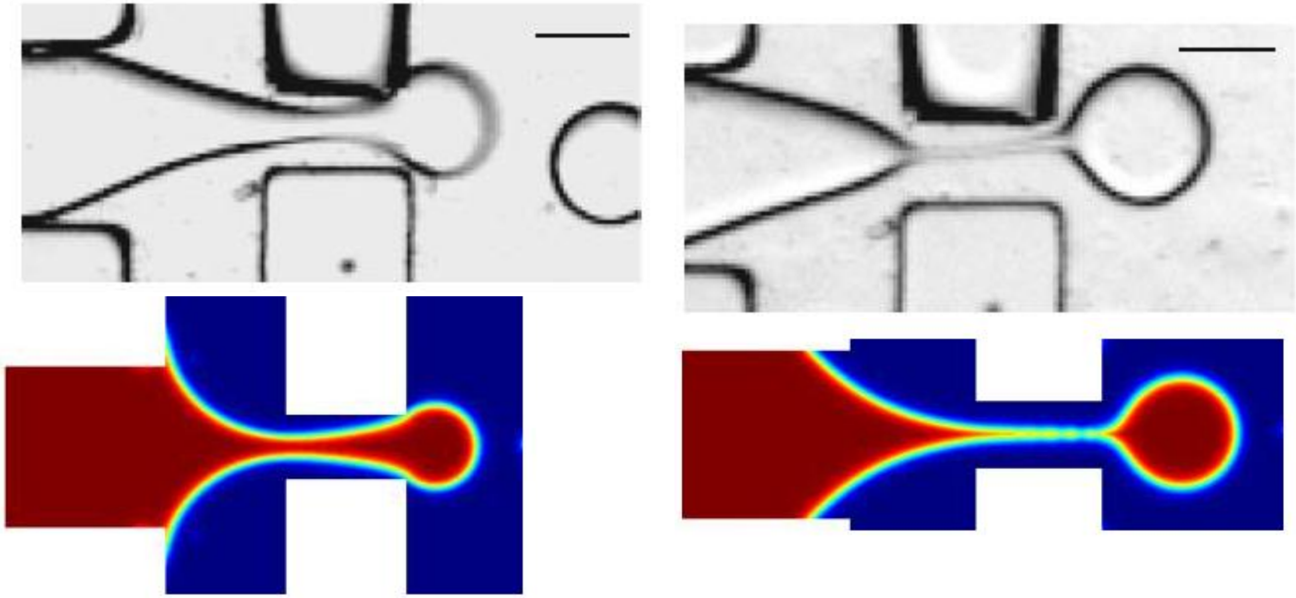
Operating conditions

Flow rate of the dispersed phase: 0.04 mL/h
Flow ratio: Q_c/Q_d = 10, 20, 50, 100
Re_c: 1.29~12.9
Ca_c: 0.005 ~ 0.05
Breaking regime: squeezing and dripping

Z. H. Nie, M. S. Seo, S. Q. Xu, P. C. Lewis, M. Mok, E. Kumacheva, G. M. Whitesides, P. Garstecki and H. A. Stone, *Microfluid. Nanofluid.*, 2008, **5**, 585-594.

Model Validation

Snapshots of droplets formed from silicone oil



Q_d=0.04 mL/h, Q_c/Q_d = 20, **μ_d = 20 cp**

Q_d=0.04 mL/h, Q_c/Q_d = 20, **μ_d = 100 cp**

Key findings

(1) At low μ_d, the dispersed phase effectively blocks the orifice and then the neck are squeezed.
(2) At high μ_d, the dispersed phase does not block the entire orifice but forms a long filament.
(3) The simulations qualitative agree with the experimental observations.

Z. H. Nie, M. S. Seo, S. Q. Xu, P. C. Lewis, M. Mok, E. Kumacheva, G. M. Whitesides, P. Garstecki and H. A. Stone, *Microfluid. Nanofluid.*, 2008, **5**, 585-594.

Squeezing breakup

Key findings

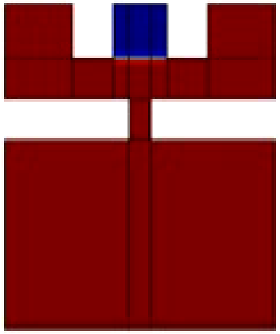
(1) Mono-dispersed breakup are observed at low μ_d and low Ca.

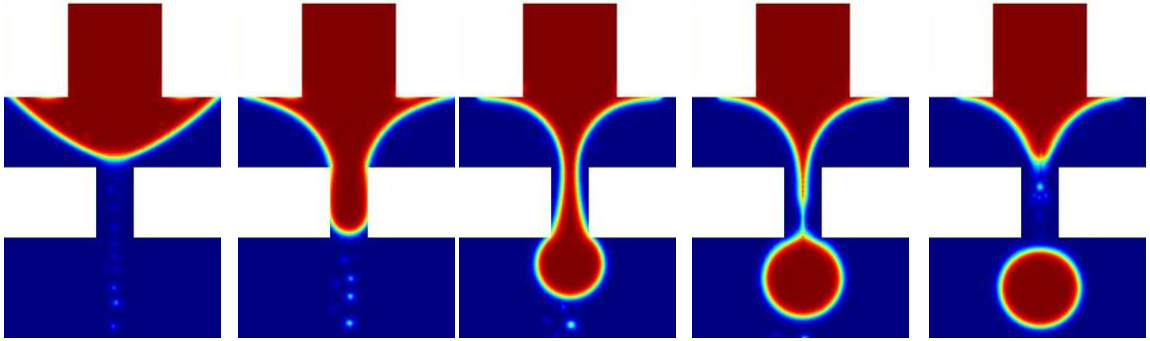
(2) The dispersed phase effectively blocks the continuous phase channel and orifice, building up a high pressure drop.

(3) The pressure squeezes the dispersed phase into a visible neck inside the orifice, and viscous shear force pinches a droplet.

(4) The surface tension force brings back the interface, and a new sequence starts.

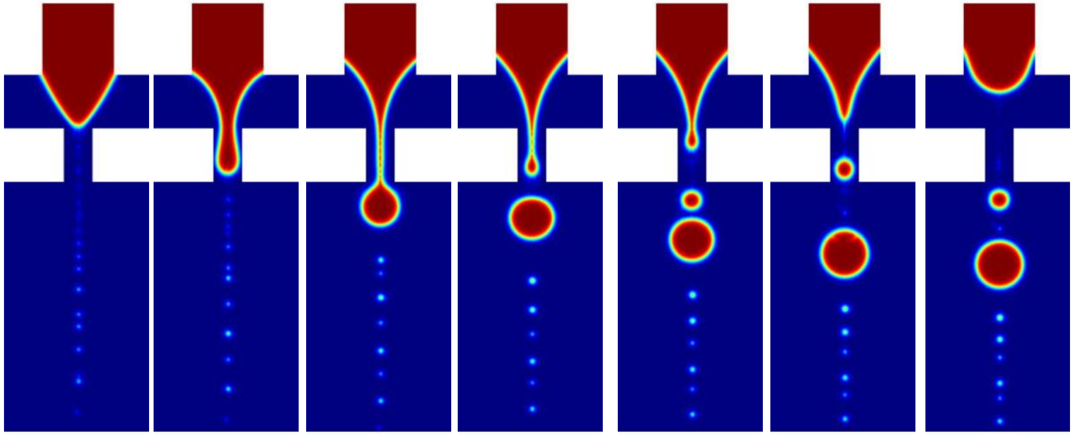
(5) Large droplets are obtained in squeezing regime.



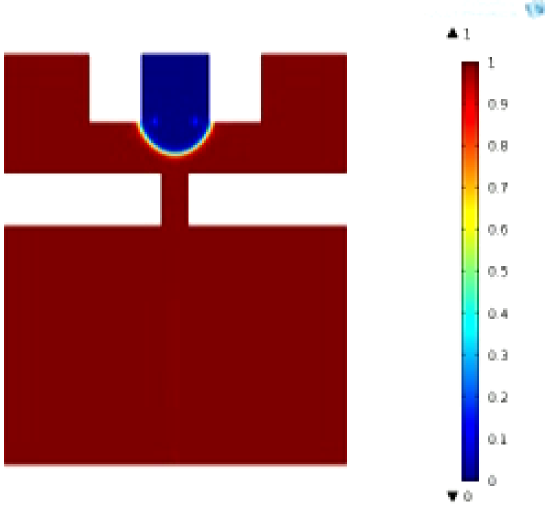


Q_d=0.04 mL/h, μ_d = 20 cp, $\mathbf{Q_c/Q_d}$ **=10**

Poly-dispersed dripping breakup



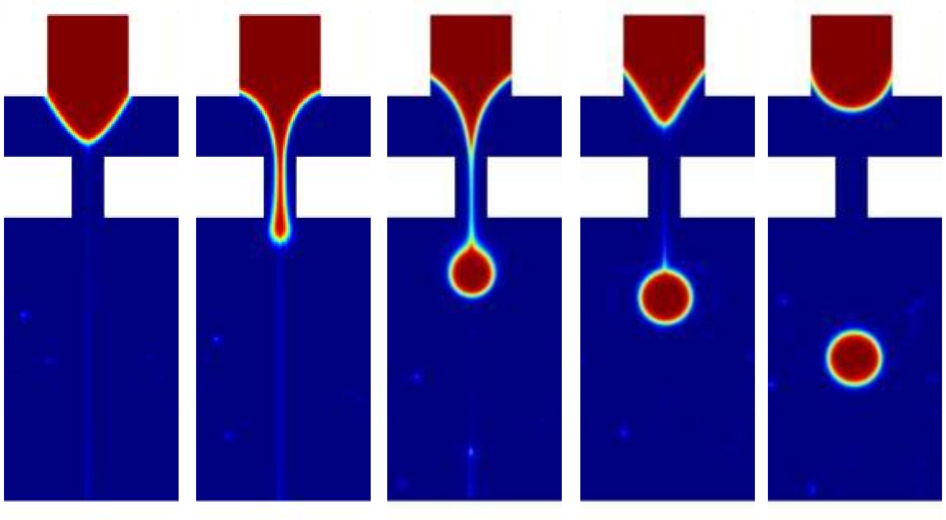
Q_d=0.04 mL/h, μ_d = 20 cp, **Q_c/Q_d =50**



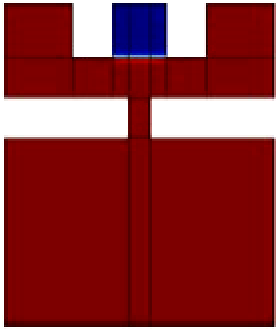
Key findings

(1) Dispersed phase does not block the entire orifice.
(2) When the primary droplet is pinched off from the dispersed phase, the dispersed phase continues to grow side the orifice, forming seconary droplets until all the dispersed phase in the orifice are separated.
(3) Primary droplet size is comparable to orifice width.
(4) Secondary (satellite) droplets are smaller than the primary droplets.

Mono-dispersed dripping breakup



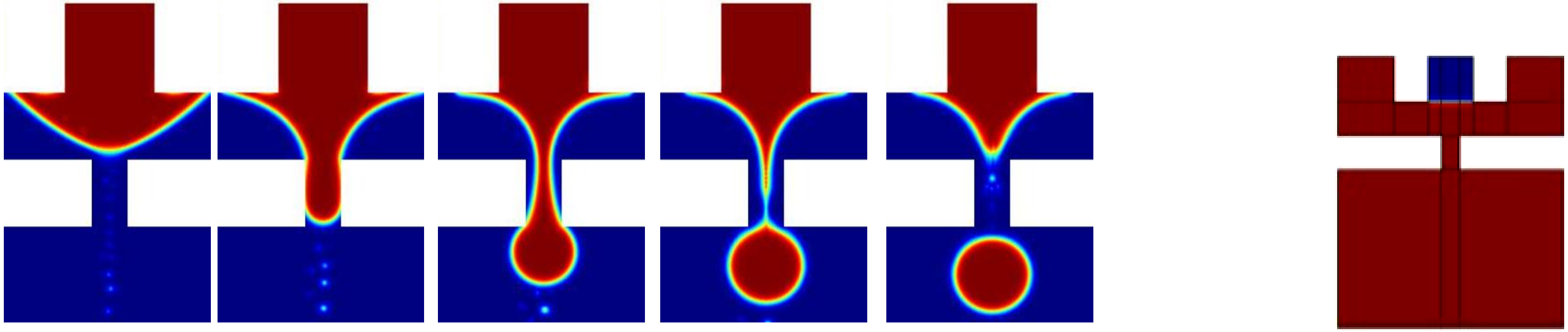
Q_d=0.04 mL/h, μ_d = 20 cp, **Q_c/Q_d =100**



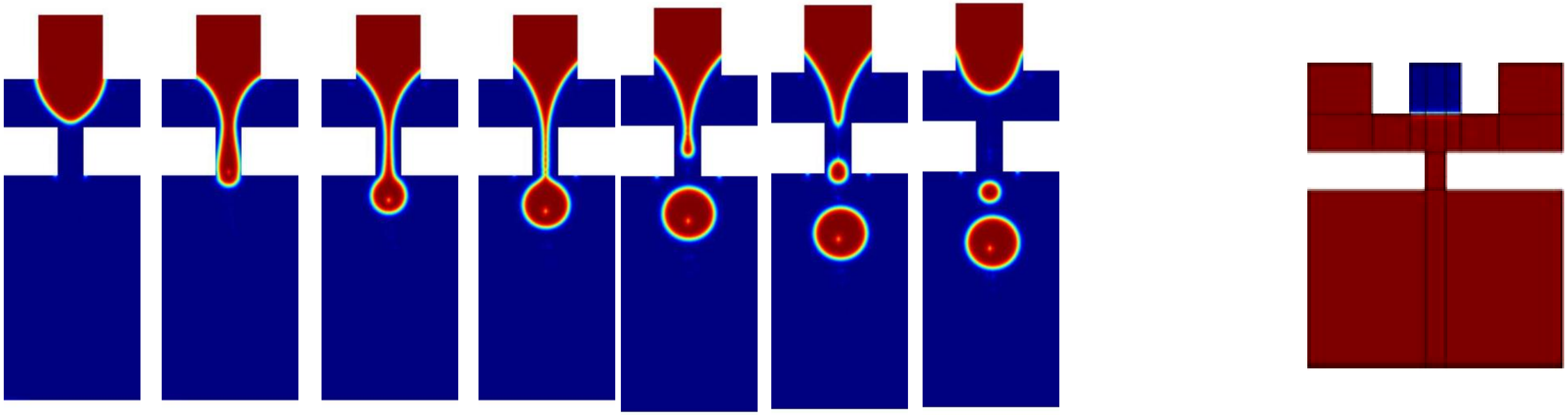
Key findings

(1) The strong shear force pinches off the entire thread from the dispersed phase.
(2) The dispersed phase does not continue growing inside the orifice.
(3) Small and mono-dispersed droplets are produced.

Effect of μ_d on breakup

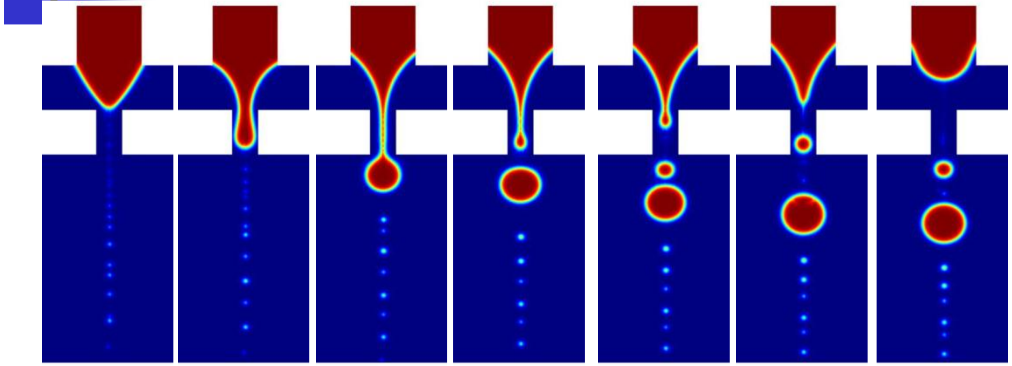


Q_d=0.04 mL/h, **μ_d = 20 cp,** Q_c/Q_d =10**,** D_p=168.75 μm

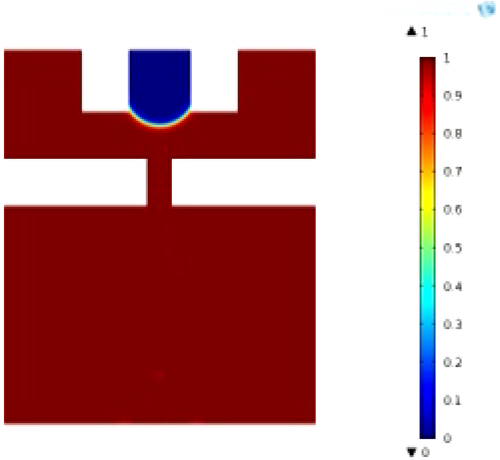


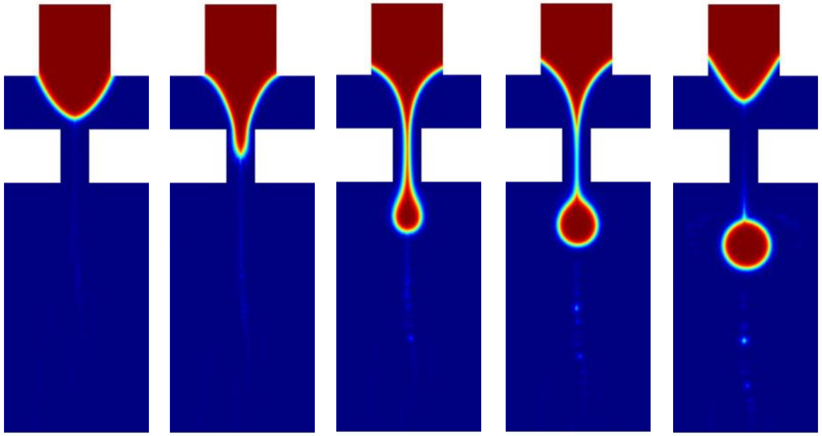
Q_d=0.04 mL/h, **μ_d = 100 cp,** Q_c/Q_d =10**,** D_p=155.43 μm

Effect of μ_d on breakup

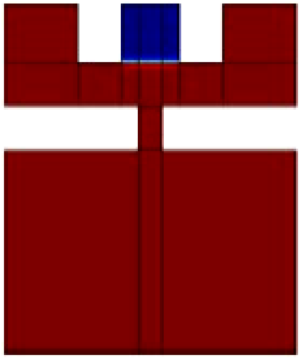


Q_d=0.04 mL/h, **μ_d = 20 cp,** Q_c/Q_d =50**,** D_p=119.7 μm



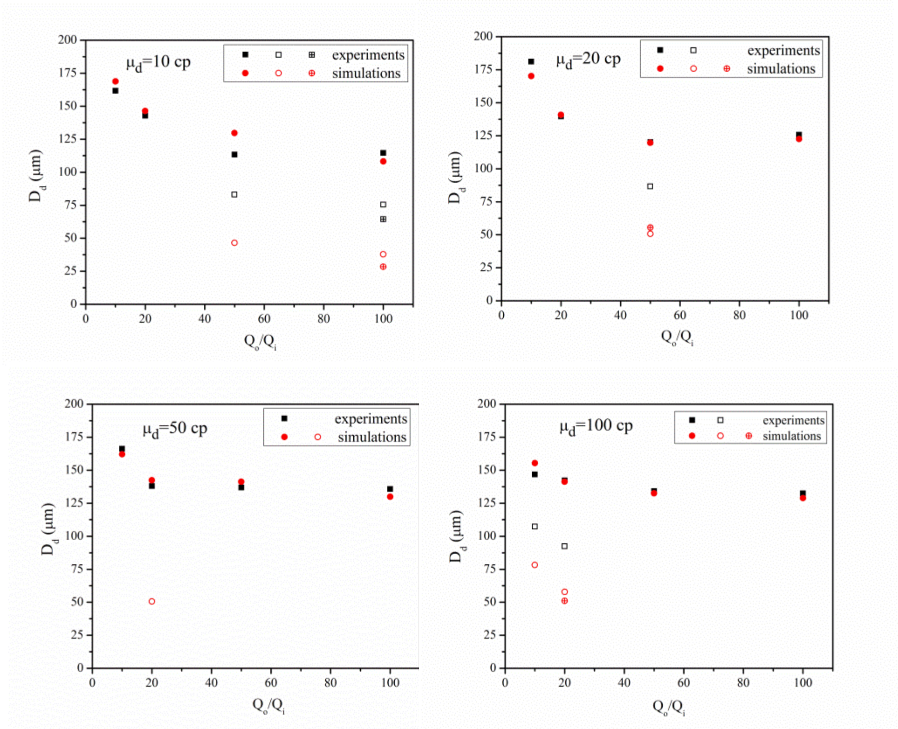


Q_d=0.04 mL/h, **μ_d = 100 cp,** Q_c/Q_d =50**,** D_p=132.47 μm



Model Validation

Comparison of predicted droplets sizes with experimental observations



Z. H. Nie, M. S. Seo, S. Q. Xu, P. C. Lewis, M. Mok, E. Kumacheva, G. M. Whitesides, P. Garstecki and H. A. Stone, *Microfluid. Nanofluid.*, 2008, **5**, 585-594.

Key findings

(1) Quantitative match with the experimental observations

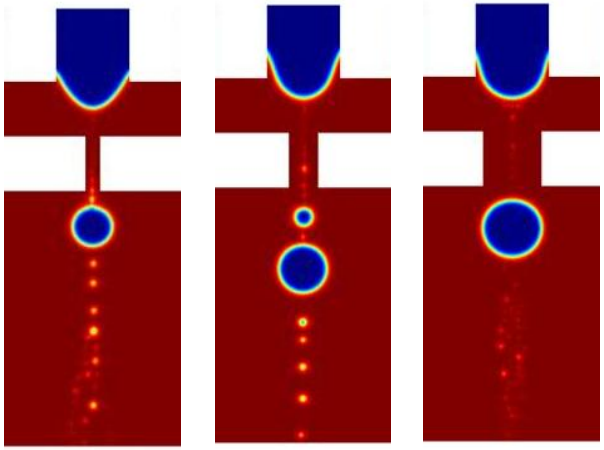
(2) Poly-dispersed droplet breakup is observed only within a range of flow ratio (Ca).

(3) The region of poly-dispersed breakup is affected by μ_d.

(4) At high μ_d, poly-dispersed breakup is observed at low Ca.

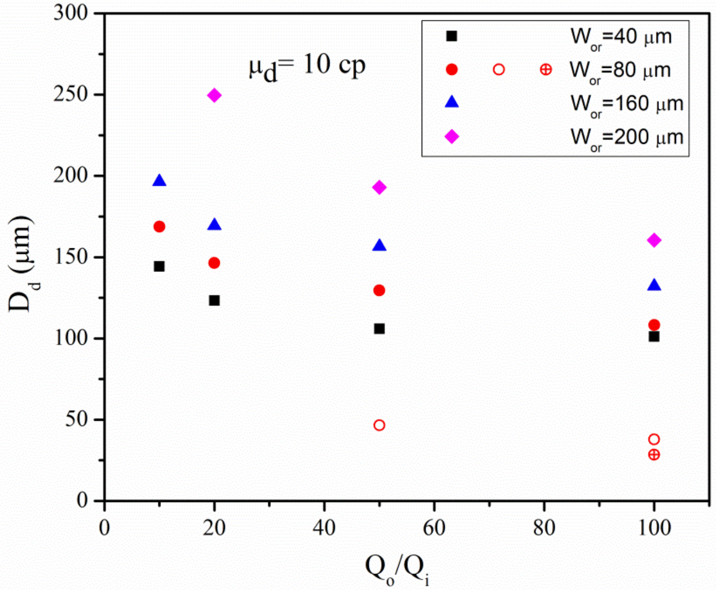
(5) The breakup is the competition between surface tension, pressure of the continuous phase and shear stress. Local flow field in the orifice region has strong influence on droplet breakup.

Effect of orifice width



W_{or} = 40 µm W_{or} = 80 µm W_{or} = 160 µm

$\mu_d = 10$ cp, $Q_c/Q_d = 50$



Droplet size as a function of flow ratio at various orifice width

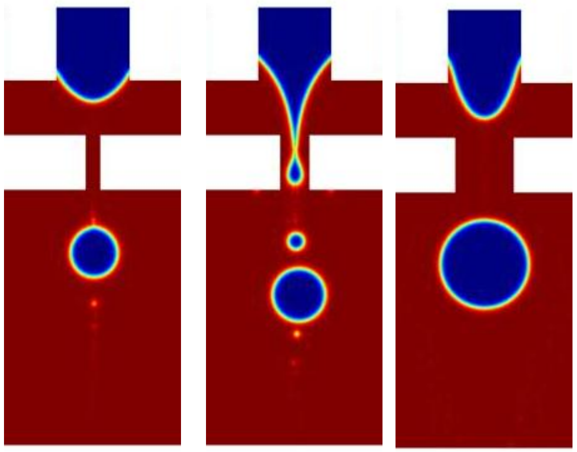
Key findings

(1) The orifice width controls the local shear force, pressure in the orifice region; therefore, it affects the breakup mechanism.

(2) Increasing orifice width leads to mono-dispersed and large droplets in all the explored flow ratios. The droplet size reduces significantly with the increase of flow ratio.

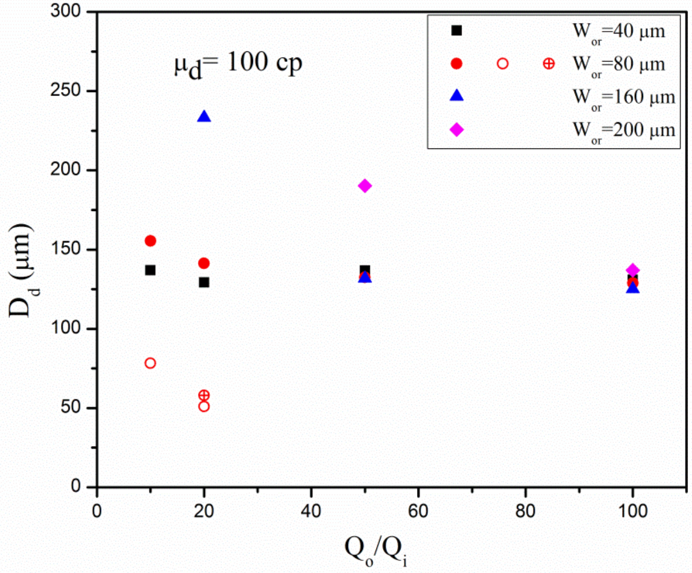
(3) Reducing orifice width leads to mono-dispersed and smaller droplets. The droplets sizes do not have significant change.

Effect of orifice width



W_{or} = 40 μm **W_{or} = 80 μm** **W_{or} = 160 μm**

μ_d = 100 cp, Q_c/Q_d = 20



Droplet size as a function of flow ratio at various orifice width

Key findings:

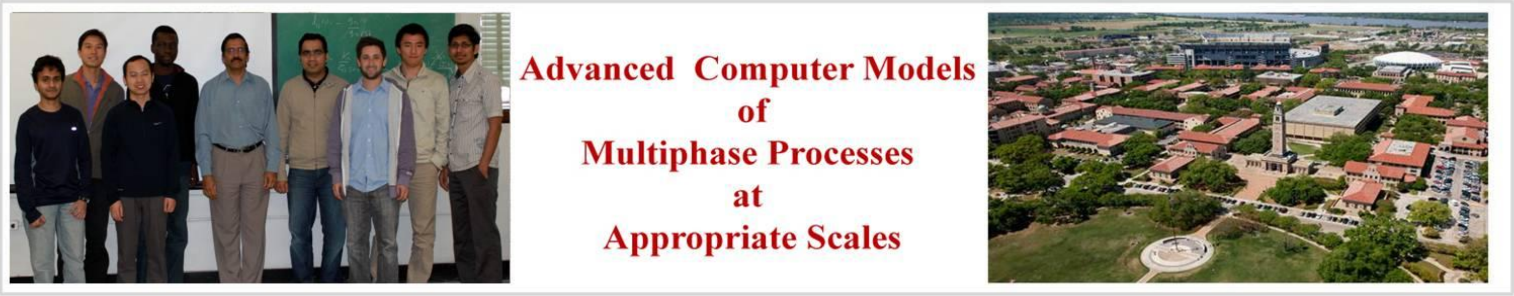
(1) Similar to low μ_d, mono-dispersed droplets are produced with very narrow and wide orifice.
(2) At low flow ratio, wide orifice results in significantly large droplets.
(3) The droplet sizes do not have remarkable different for small orifice width. (W_{or} = 40 and 80 μm)

Conclusion

- The effects of dispersed phase and the geometric dimensions (orifice width and the width of the inlet channel of the dispersed phase) on droplet breakup are analyzed.
- At low flow ratio, the breakup is dominated by squeezing where large and mono-dispersed droplets are produced.
- At high flow ratio, dripping dominates the breakup, producing small droplets.
- Poly-dispersed droplets are observed within a certain range of the flow ratios. This range is controlled by the viscosity of the dispersed phase.
- The width of the orifice is critical in droplet breakup. Wide orifice leads to large and mono-dispersed droplets; very narrow orifice produces small and mono-dispersed droplets; poly-dispersed droplets are only produced with a suitable orifice size for the explored flow ratios.
- The width of the inlet channel of the dispersed phase has a significant effect on droplet sizes.

Acknowledgement

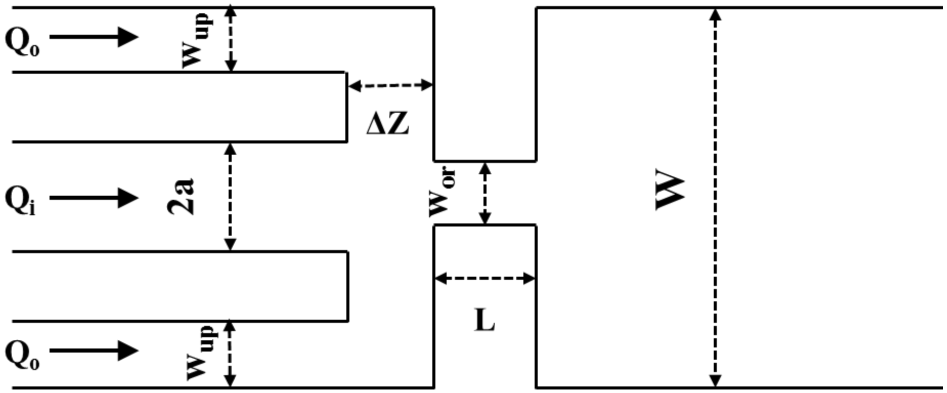
- Cain Chair Program at Chem. Engg. Dept., LSU
- Louisiana Optical Network Initiative (LONI)
- High Performance Computing (HPC) at LSU.
- Research Group Members.



Thank you for your attention!

Questions?

Effect of geometric dimensions of droplet formation



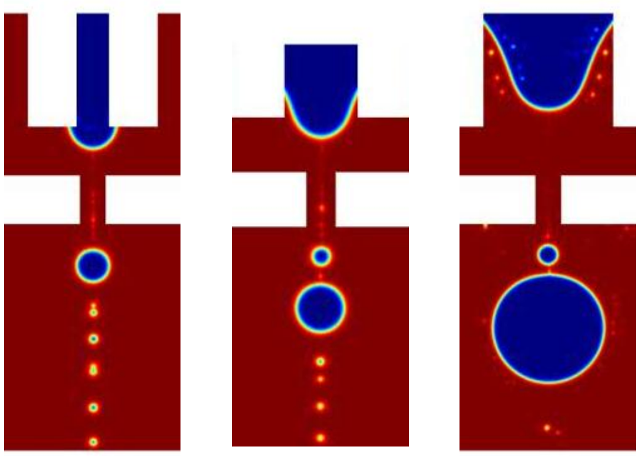
Effective Ca:

$$Ca_e = \frac{\mu_c Q_c a}{\sigma h \Delta z}\left[\frac{1}{w_{or}} - \frac{1}{2w_c}\right]$$

The droplet formation dynamics are controlled by upstream geometric dimensions:

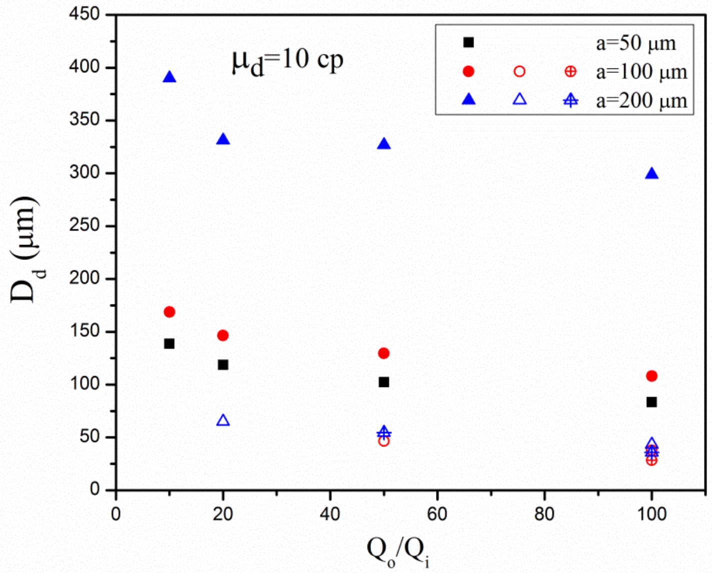
- Orifice width (W_{or})
- Inlet width of the dispersed phase (2a)
- Width of the focusing channel (ΔZ)

Effect of inlet width of the dispersed phase



2a = 100 µm **2a = 200 µm** **2a = 400 µm**

$\mu_d = 10$ cp, $Q_c/Q_d = 50$

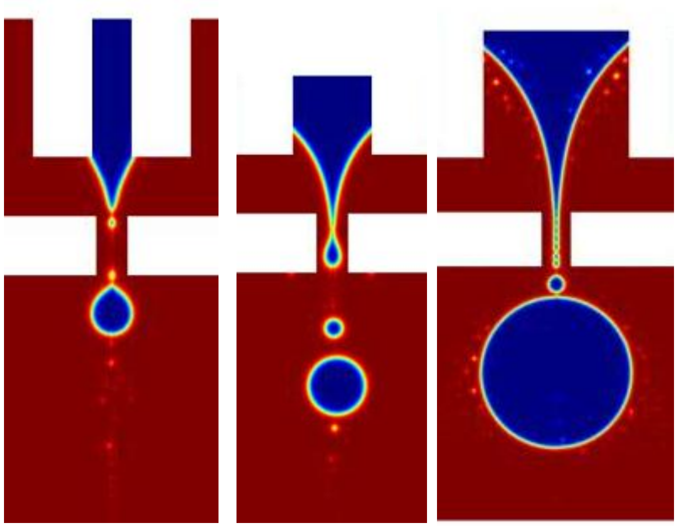


Droplet size as a function of flow ratio at various dispersed phase inlet width

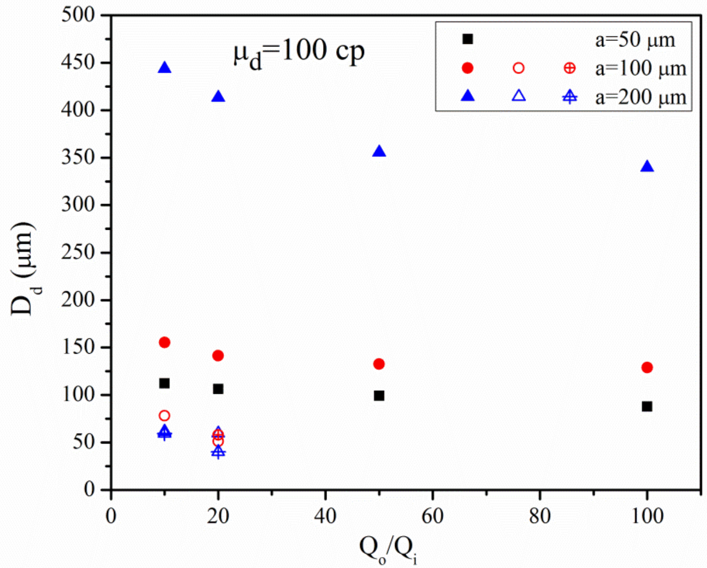
Key findings

1. The inlet width affects both droplet sizes and breakup mechanism.
2. Mono-dispersed droplets are observed at small 2a.
3. Large and poly-dispersed droplets are observed at large 2a.

Effect of inlet width of the dispersed phase



2a = 100 µm **2a = 200 µm** **2a = 400 µm**

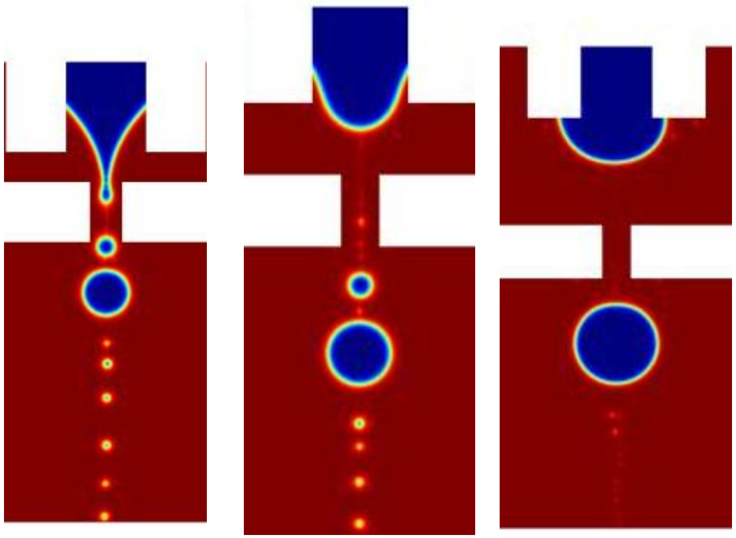


Droplet size as a function of flow ratio at various dispersed phase inlet width

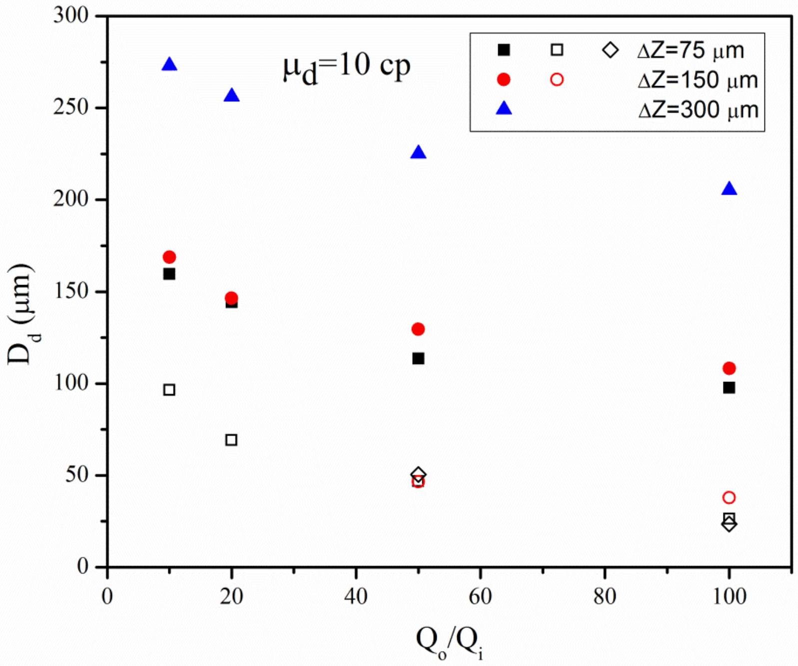
Key findings

(1) The inlet width affects both droplet sizes and breakup mechanism.
(2) Mono-dispersed droplets are observed at small 2a.
(3) Large and poly-dispersed droplets are observed at large 2a.

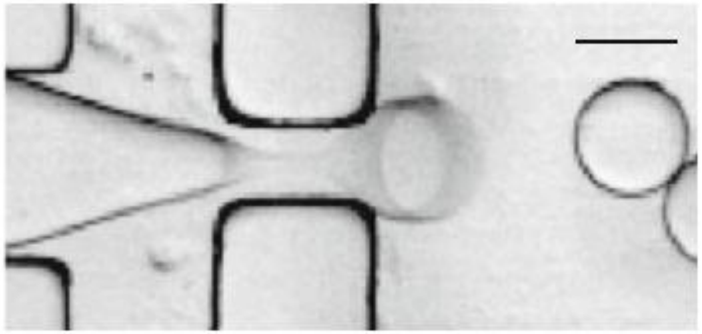
Effect of focusing channel

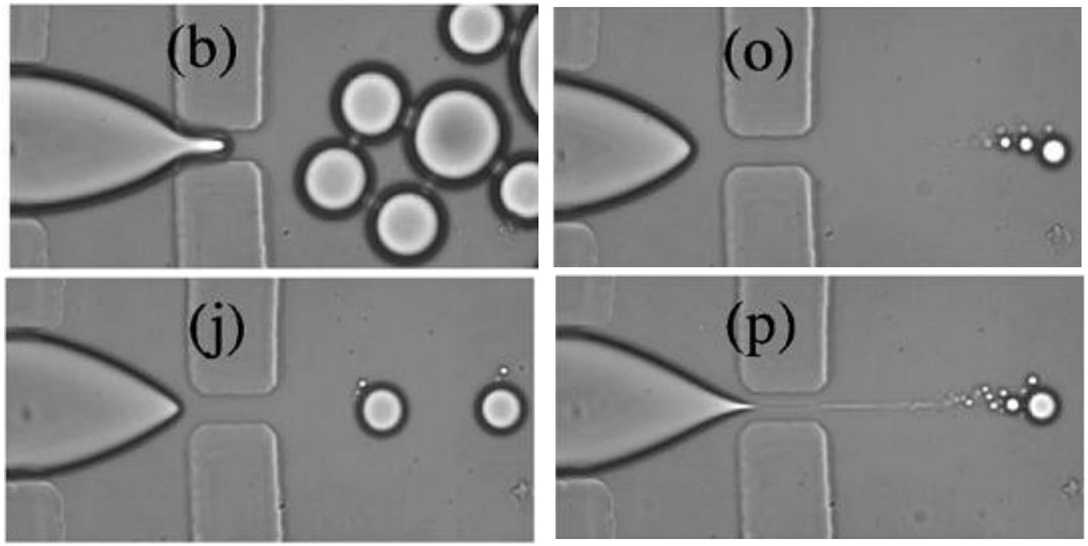


ΔZ = 75 µm **ΔZ = 150 µm** **ΔZ = 300 µm**



Coalescence of the droplets





Droplets may not coalescence

Droplets may not merge due to the surface properties, such as surface charge, surface tension …