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A Step towards Biosensors

Numerical Study of Shear-Thinning Droplet Breakup Dynamics at Microfluidics T-Junction using Level-Set Method

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OUTLINE

- **Introduction to Droplet Formation in Microchannel Network**
  - Research Background
  - Problem Statements
  - Research Scope
- **Numerical Model Setup**
  - Conservative Level-Set Method
- **Numerical Model Validation**
- **Results and Discussion**
- **Conclusion**
- **Acknowledgements**

RESEARCH BACKGROUND

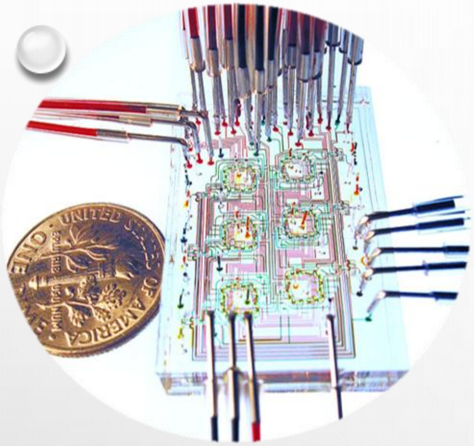
- **Emulsions:** contains a mixture of two immiscible liquids as one phase being dispersed throughout the other phase in small droplets.

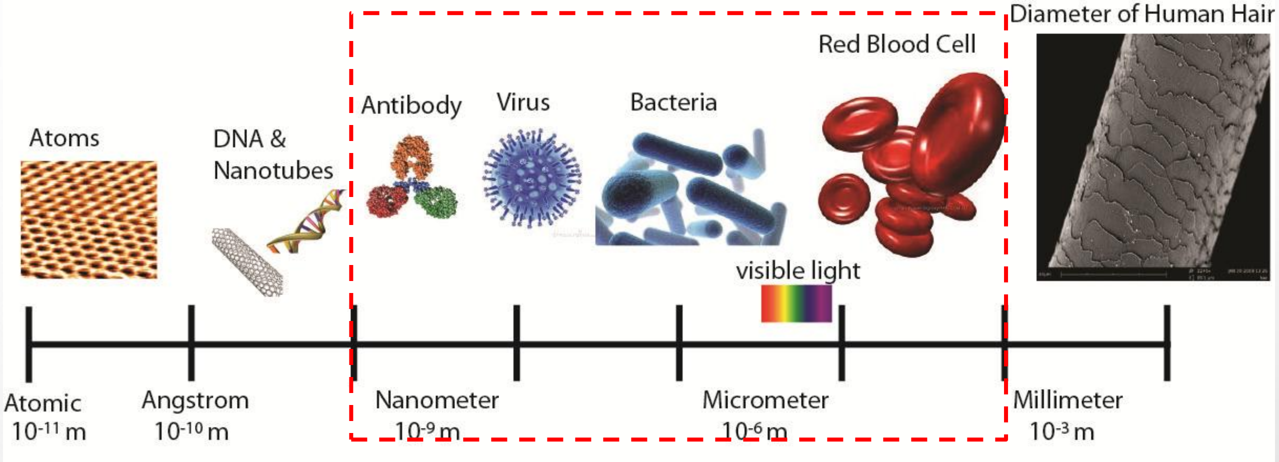
- Why are **emulsions** important?

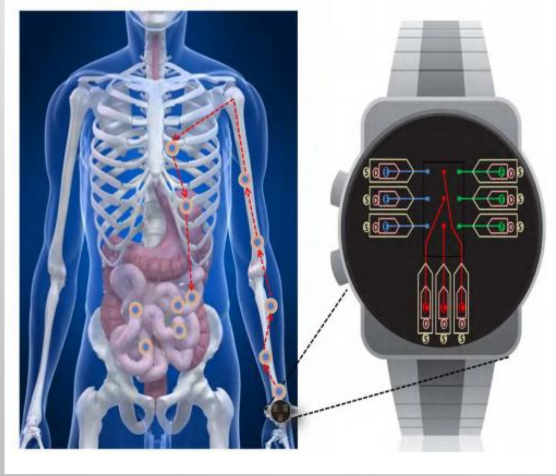
  In medical or pharmaceutics applications:
  - drug delivery systems
    - Administrating a pharmaceutical compound to achieve therapeutic effect
    - deliver vaccines and kill microbes

- **Microfluidic systems:** science and technology of systems that process or manipulate small amounts of fluids, using channels with micrometer length scales.

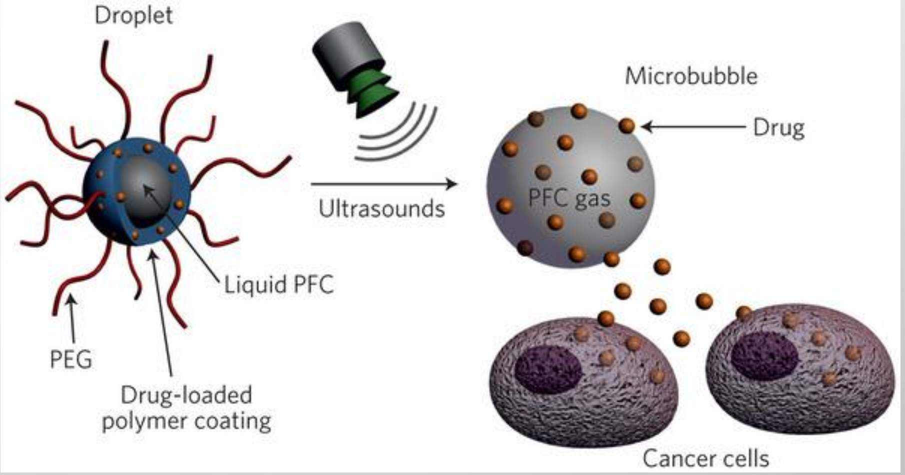
RESEARCH BACKGROUND







Chemotherapy Drug Delivery System[1]



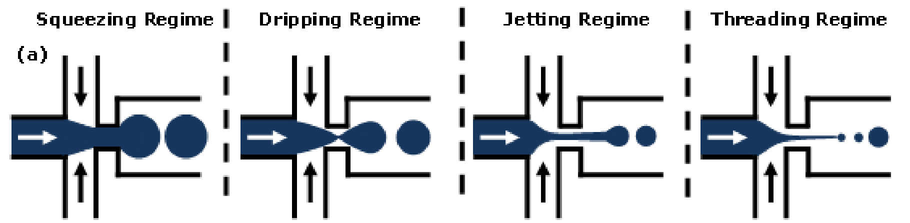
Drug delivery from echogenic perfluorocarbon (PFC)-containing nanoemulsions[2]

1. Adams, T., Yang, C.J., Gress, J., Wimmer, N., and Minerick, A (2012). Retrieved from http://cdn.intechopen.com/pdfs-wm/29689.pdf.
*2. Mura, S., Nicholas, J., and Couvreur, P. (2013). Nature materials, **12**, 991-1003.*

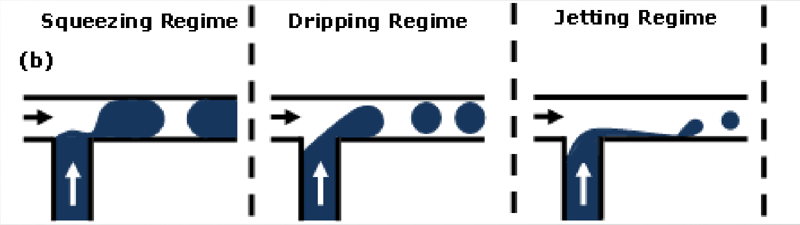
RESEARCH BACKGROUND

- **Microfluidic systems**: an alternative and versatile platform for microdroplets formation.

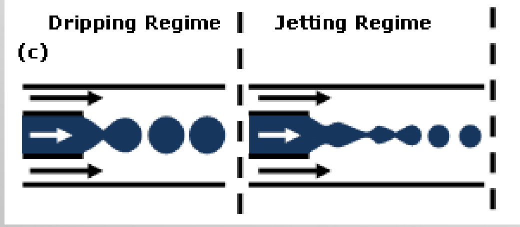
- Droplets can be generated via a number of methods.



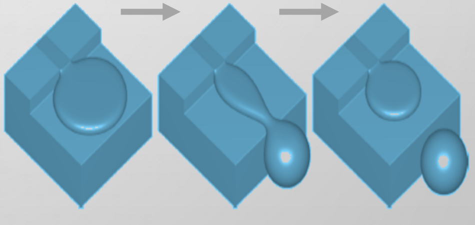
Breakup in Elongational Strained Flow



Breakup in Cross-Flowing Stream



Breakup in Co-Flowing Stream



Microchannel Emulsification[1]

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1. *Van der Zwan, E., Schroen, K., and Boom, R. (2009). Langmuir,* ***25****, 7320–7327.*

RESEARCH BACKGROUND

- **Scaling analysis** and **dimensionless numbers** are of key importance in designing and physics underlying in microfluidic devices.

- Provide importance of forces, energies, or time scale in presence and lead the way to simplification of complex systems.

- Dimensionless parameters associated with microfluidics are:

$$\boxed{\mathrm{Re} = \frac{\rho U L}{\mu} = \frac{inertial}{viscous}}$$

Reynolds

$$\boxed{Ca = \frac{\mu U}{\sigma} = \frac{\text{viscous}}{\text{interfacial}}}$$

Capillary

$$\boxed{We = \frac{\rho U^2 L}{\sigma} = \frac{\text{inertial}}{\text{interfacial}}}$$

Weber

$$\boxed{Wi = \tau_p \gamma = \frac{\text{polymerrelaxation time}}{\text{shear rate time}}}$$

Weissenberg

$$\boxed{De = \frac{\tau_p}{\tau_{flow}} = \frac{\text{polymerrelaxation time}}{\text{flow time}}}$$

Deborah

MICROFLUIDICS T-JUNCTION

- The tip of the dispersed phase enters the main channel.
- The disperse phase entering the T-junction is slowly convected downstream.
- A pressure increase in the continuous phase is expected. This action squeezes the neck of the dispersed thread and droplet is eventually generated[1].

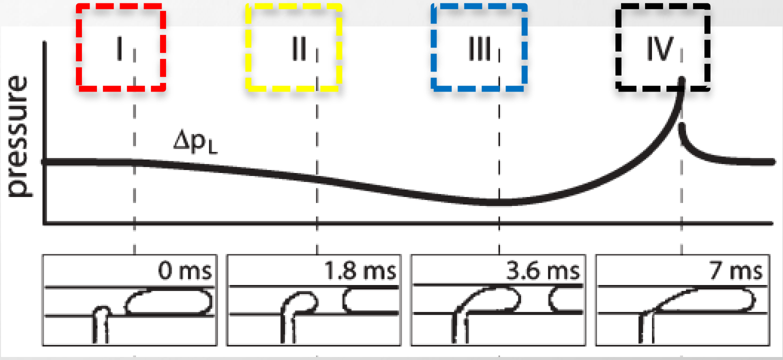


Figure 2: Postulated evolution of Laplace pressure during the droplet breakup process in a T-junction microchannel[2].

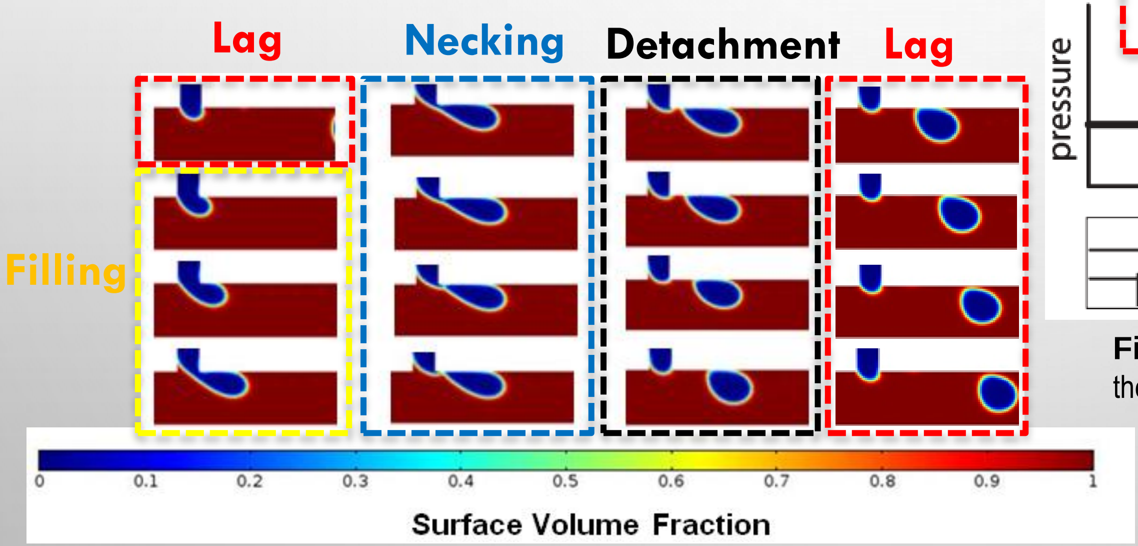
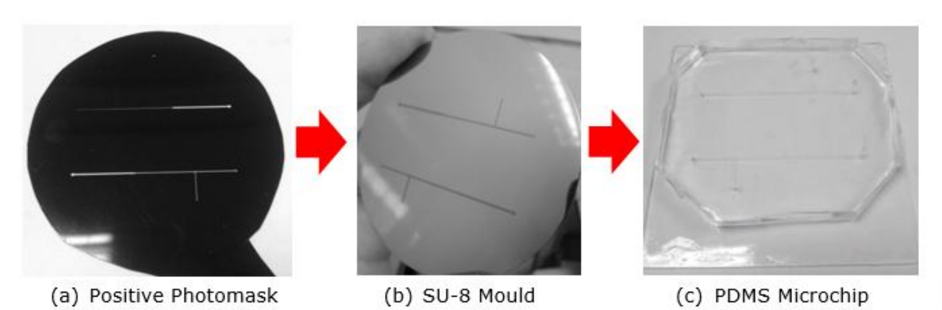
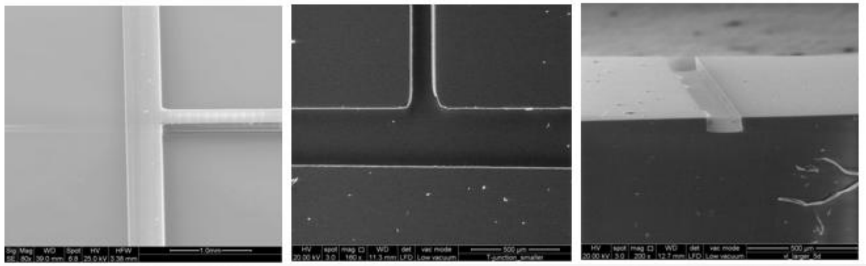


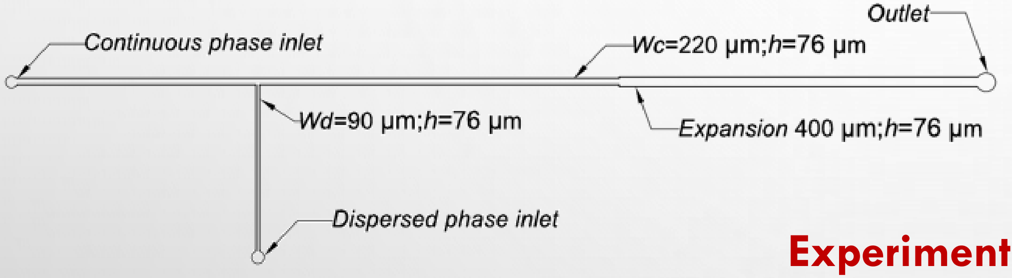
Figure 1: Snapshots of two-dimensional (2D) simulations of w/o droplet breakup process in microchannel (for system: Q=0.05, where continuous phase flow rate, Q_c =2.00 ml/hr, and dispersed phase flow rate, Q_d =0.10 ml/hr).

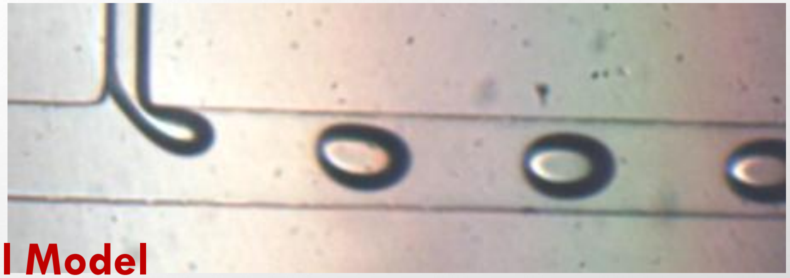
1. Glawdel, T., Elbuken, C., and Ren, C.L. (2012).*Physical Review*, **85**, 016323-1-016323-12.
2. *Garstecki, P., Fuerstman, M.J., Stone, H.A. and Whitesides, G.M. (2006). Lab Chip*, ***6***, *437-446.*

MICROFLUIDICS T-JUNCTION


(a) Positive Photomask (b) SU-8 Mould (c) PDMS Microchip

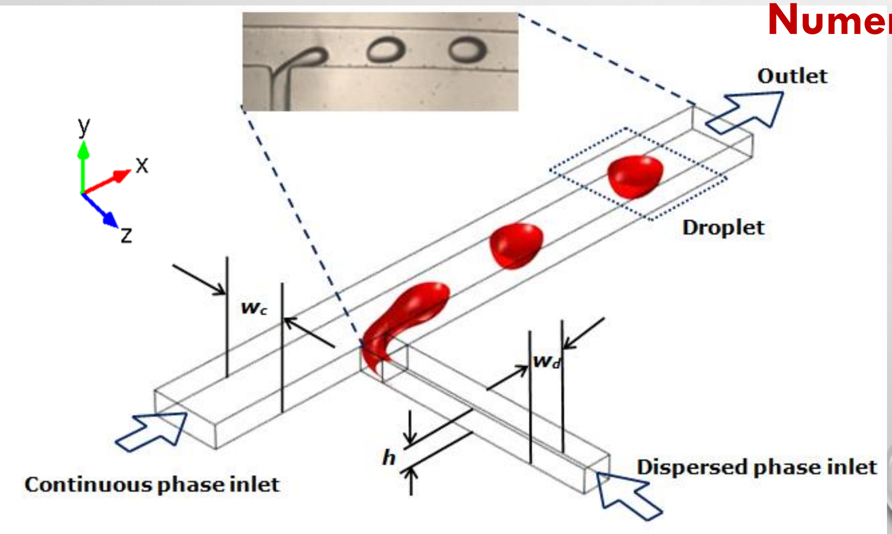


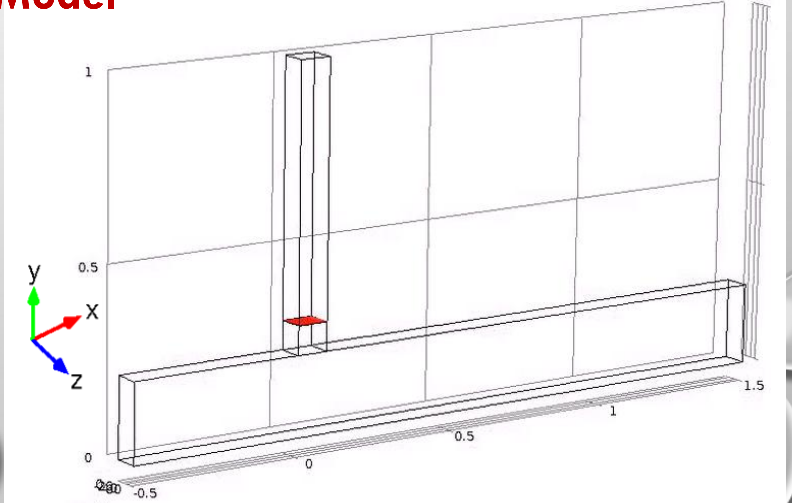




Experimental Model

Numerical Model





PROBLEM STATEMENTS

- Velocity profile for laminar **Newtonian** flow in a rectangular duct:

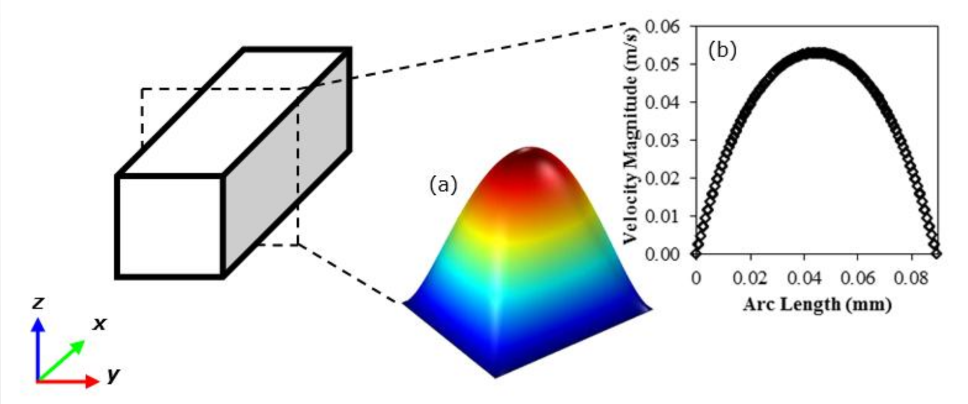


Figure 1: Velocity profile for laminar Newtonian flow: (a) Two-dimensional plot with velocity height expression, (b) One-dimensional plot with parabolic velocity profile in rectangular microchannel.

- Velocity profile for laminar **non-Newtonian shear-thinning** flow:

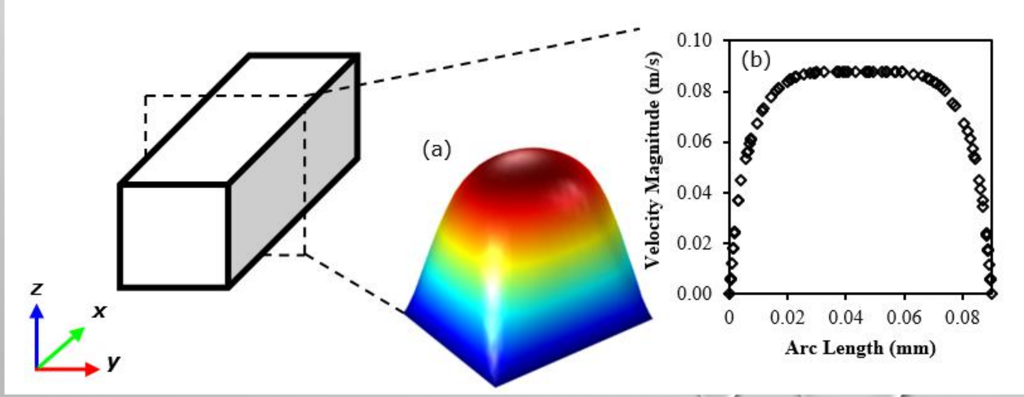
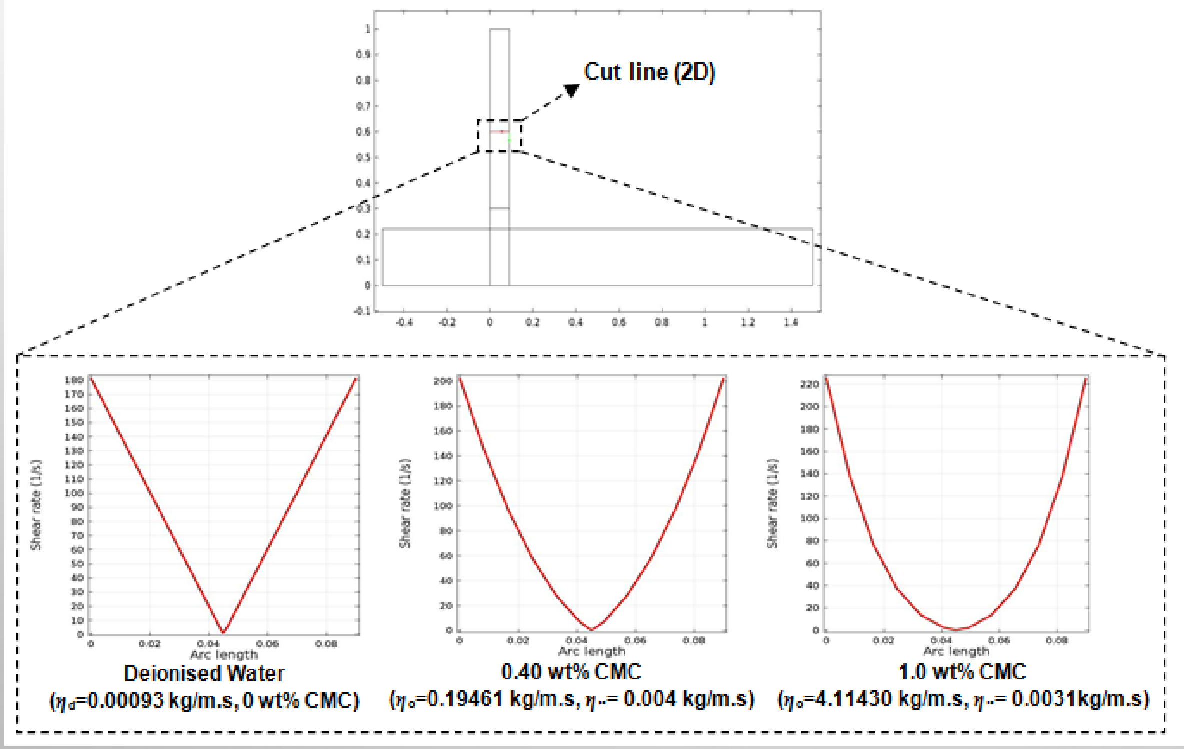


Figure 2: Velocity profile for non-Newtonian shear-thinning flow: (a) Two-dimensional plot with velocity height expression, (b) One-dimensional plot with blunted velocity profile in rectangular microchannel.

PROBLEM STATEMENTS

- Shear-rate profile for laminar **non-Newtonian shear-thinning** flow in a rectangular duct:

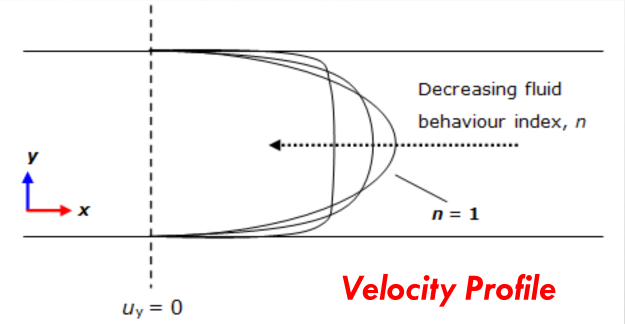


Deionised Water (η_d=0.00093 kg/m.s, 0 wt% CMC)

0.40 wt% CMC (η_o=0.19461 kg/m.s, η_∞= 0.004 kg/m.s)

1.0 wt% CMC (η_o=4.11430 kg/m.s, η_∞= 0.0031kg/m.s)

Figure 1*: Shear rate profile for Newtonian and non-Newtonian flow measured along the cut line 2D across the flow of dispersed phase in the microfluidic channel (for system: Q=0.05).*



- Apparent viscosity of shear-thinning fluid decreases as the shear rate increase;

- Velocity profile becomes increasingly blunt as *n* decreases.

RESEARCH SCOPE

Experimental I

Rheological Characterisation

- ➢ Newtonian and Non-Newtonian Fluids

Experimental II

PDMS Microchip Fabrication

- ➢ T-junction microfluidic device

Experimental III

Droplet Flow Experiment

- ➢ Applied Flow condition

Numerical I

Numerical Model Setup

- ➢ Conservative Level-Set Method

Numerical II

Model Validation

- ➢ d_{eff} Versus *Q*

Numerical III

Parametric Studies

- ➢ Effect of Dispersed Phase Concentration
- ➢ Effect of Continuous Phase Viscosity
- ➢ Effect of fixed dispersed to continuous phase viscosity ratio

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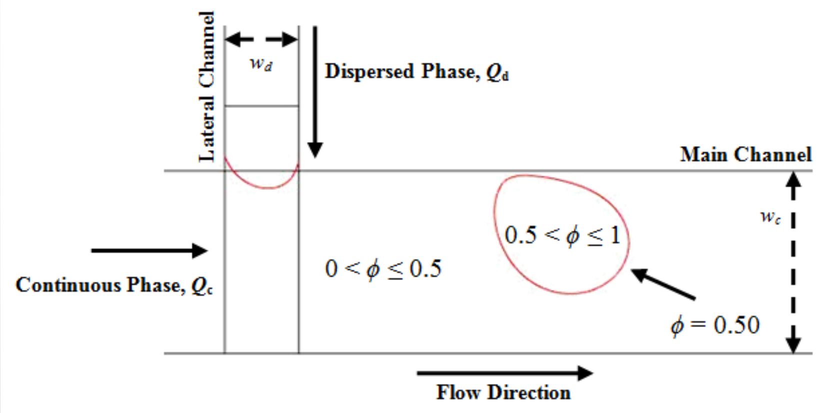
2D LAMINAR TWO-PHASE, LEVEL-SET



Geometry Modelling

- T-shaped configurations
- wc: 221 μm (continuous phase channel width)
- wd: 90 μm (dispersed phase channel width)
- d: 73.5 μm (depth of the channel)

Conservative Level-Set method[1]

To describe the interface between two immiscible fluids which is defined by the 0.5 contour of the level set (phase) function (ϕ).

Governing Equations

Incompressible Navier-Stokes (NS) equation:

$$\rho\frac{\partial \mathbf{u}}{\partial t}+\rho(\mathbf{u}\cdot\nabla)\mathbf{u}=\nabla\left[-pI+\eta(\nabla\mathbf{u}+(\nabla\mathbf{u})^{T}\right]+F_{st}$$

Continuity equation:

$$\nabla\cdot\mathbf{u}=0$$

Level-set equation:

$$\frac{\partial\phi}{\partial t}+\mathbf{u}\cdot\nabla\phi=\gamma\nabla\left[\varepsilon\nabla\phi-\phi(1-\phi)\frac{\nabla\phi}{|\nabla\phi|}\right]$$

$$F_{st}=\sigma k\mathbf{n}_{\Gamma}\delta_{sm}$$

where

$$k=-\nabla\cdot\mathbf{n}_{\Gamma}$$

$$\mathbf{n}_{\Gamma}=\frac{\nabla\phi}{|\nabla\phi|}$$

$$\delta_{sm}=6|\phi(1-\phi)||\nabla\phi|$$

The fluid properties of density and the dynamic viscosity across the interface

$$\rho=\rho_1+(\rho_2-\rho_1)\phi \qquad \eta=\eta_1+(\eta_2-\eta_1)\phi$$

Wall Boundary Conditions: Wetting wall

Complete Repulsion: **180°** contact angle

Inlet and Outlet Conditions

Inlet: Laminar inflow conditions with specified flow rate (ml/h) ($Q=Q_d/Q_c$)

Outlet: Pressure with no viscous stress (P= 0 Pa)

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[1] Olsson, E., and Kreiss, G. (2005). Journal of Computational Physics, **210**, 225-246.

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MESHED MODEL OF T-JUNCTION

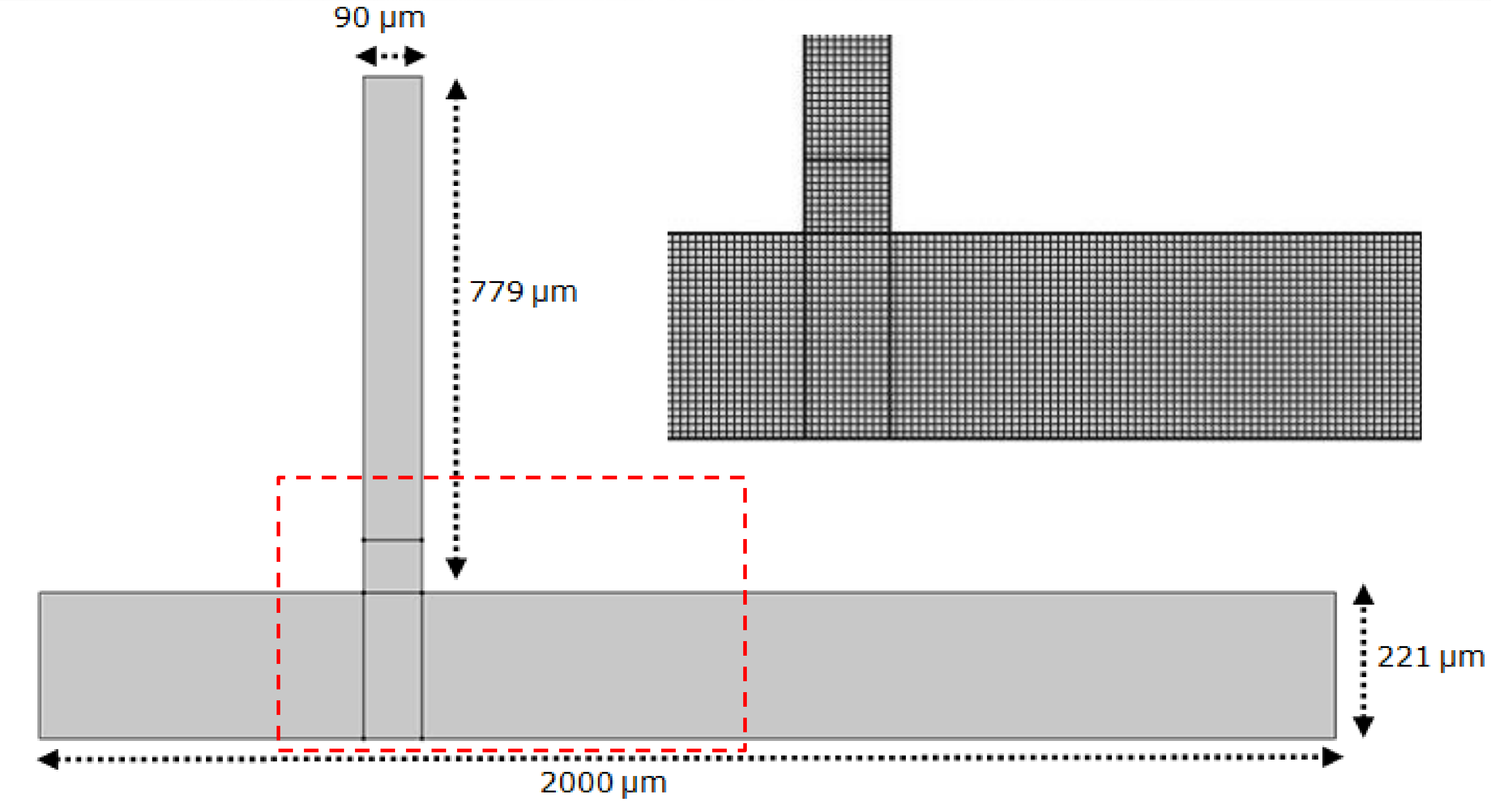

Figure 1:The geometry of microfluidics T-junction composed of five subdomains with prescribed dimensions in COMSOL simulation.

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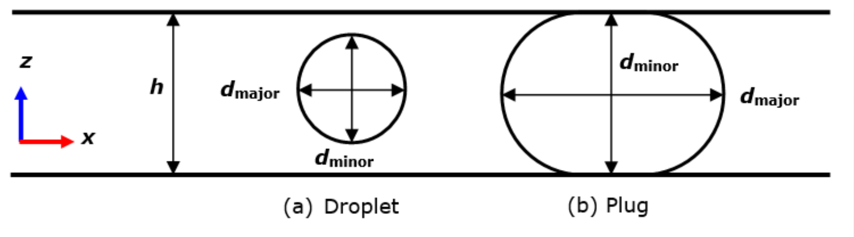
SIMULATION SETUP PARAMETERS

Table 1: General settings for the variables and parameter in COMSOL (for system: flow rate ratio, Q: 0.05).

Description	Expression	Unit
Volume Inlet 1*	2	ml/h
Volume Inlet 2*	0.1	ml/h
Effective Droplet Diameter*	d_{eff}	mm
Viscosity Fluid 1	0.068	kg/m.s
Viscosity Fluid 2(Water)	0.00093	kg/m.s
Viscosity Fluid 2 (Non-Newtonian)*	Rheological data	kg/m.s
Infinite shear viscosity*	Rheological data	kg/m.s
Zero shear viscosity*	Rheological data	kg/m.s
Relaxation time constant*	Rheological data	s
Fluid behaviour index*	Rheological data	1
Density Fluid 1	908.9	kg/m^3
Density Fluid 2 (Water)	998.2	kg/m^3
Density Fluid 2 (Non-Newtonian)*	Rheological data	
Surface Tension (Water)	0.02074	N/m
Surface Tension (Non-Newtonian)*	Rheological data	
Contact angle	180	degree
Depth of the channel	7.35e^{-5}	m

$$d_{eff} = 2 \cdot \sqrt{\frac{1}{\pi}\int_{\Omega}(\phi > 0.5)\,d\Omega}$$



(a) Droplet (b) Plug

Sodium Carboxymethylcellulose (CMC)

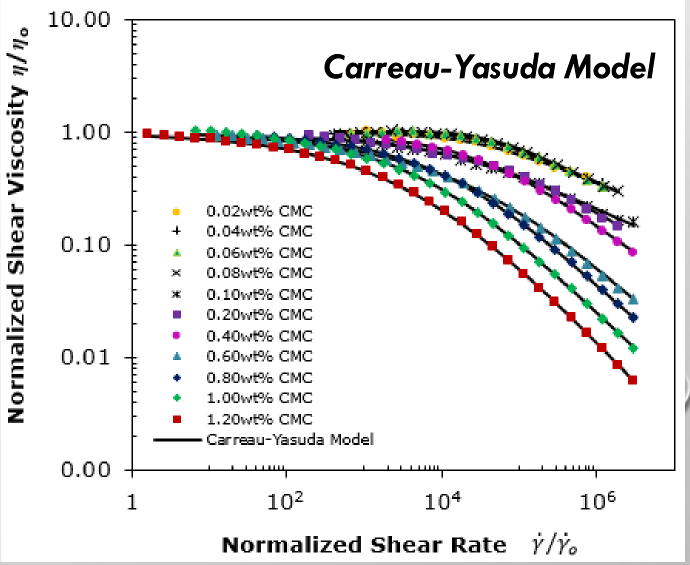


Figure 1: Normalized shear viscosity plotted against normalized shear rate for a series of CMC shear-thinning solutions with different concentrations.

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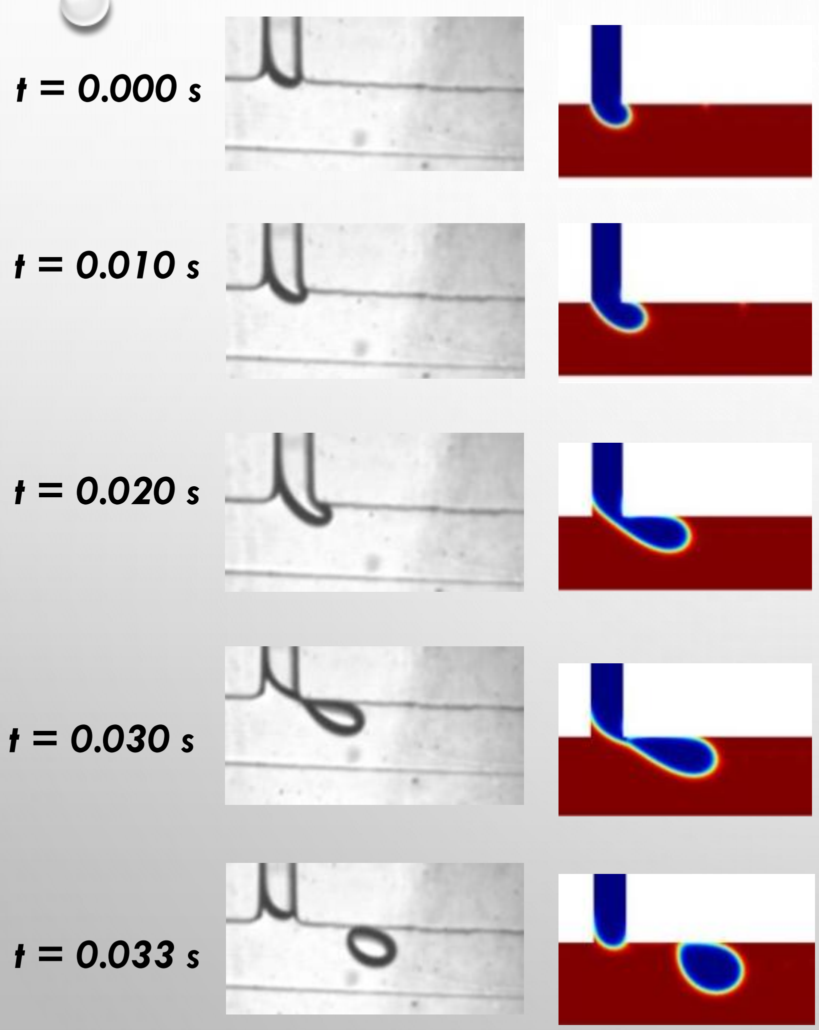
MODEL VALIDATION



Snapshots of 2D droplet breakup process at Q = 0.05

Table 1: Comparison of droplet diameter between numerical and experimental model (for system: flow rate ratio, Q: 0.05).

Qc (ml/h)	Qd (ml/h)	Qd/Qc	Error Percentage (%)
2	0.080	0.0400	1.10
2	0.100	0.0500	1.01
2	0.135	0.0675	5.04
2	0.200	0.1000	10.24
2	0.250	0.1250	9.96

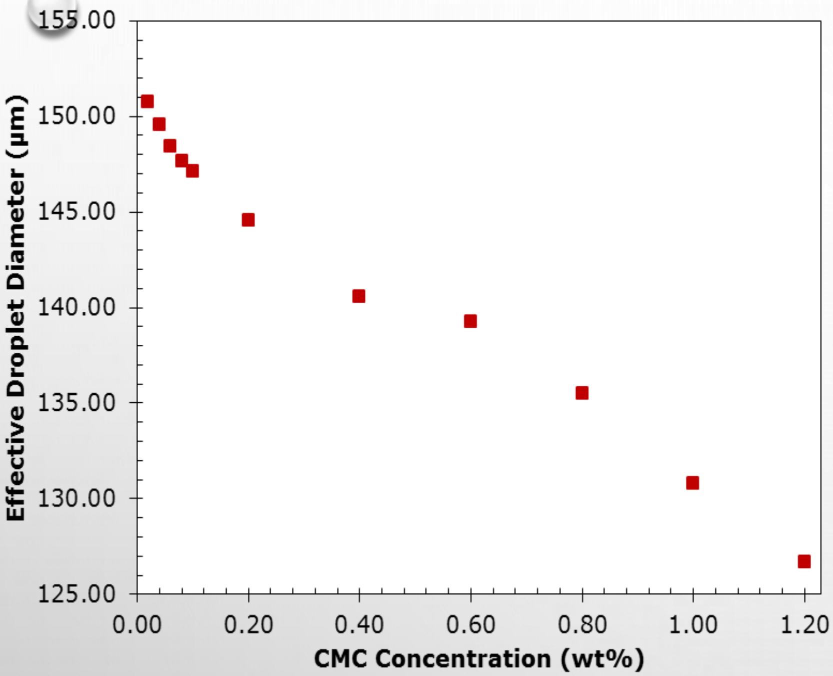
Q_c = Continuous Phase Flow Rate
Q_d = Dispersed Phase Flow Rate

Discrepancy between experimental and numerical[1]:

- Physical and rheological properties were affected by the room temperature fluctuations.
- Syringe pumps induced oscillation of flow rate.
- Difficulties of numerical dissipation in advection step of fluid simulation

[1] Wong, V.L.; Loizou, K.; Lau, P.L.; Graham, R.S.; and Hewakandamby, B.N. (2014). Numerical simulations of the effect of rheological parameters on shear-thinning droplet formation. Proceedings of the ASME 4th Joint US-European Fluids Engineering Division Summer Meeting, Chicago, Illinois, August 3-8, 9pp

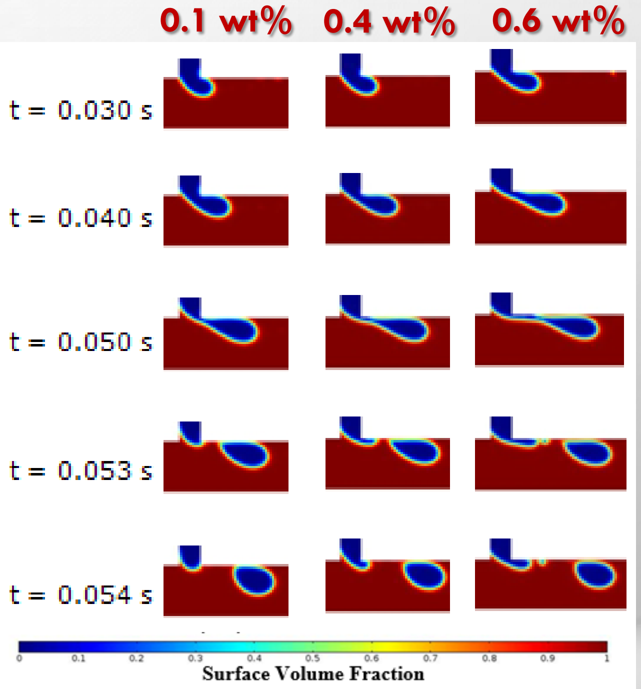
EFFECT OF DISPERSED PHASE CONCENTRATION



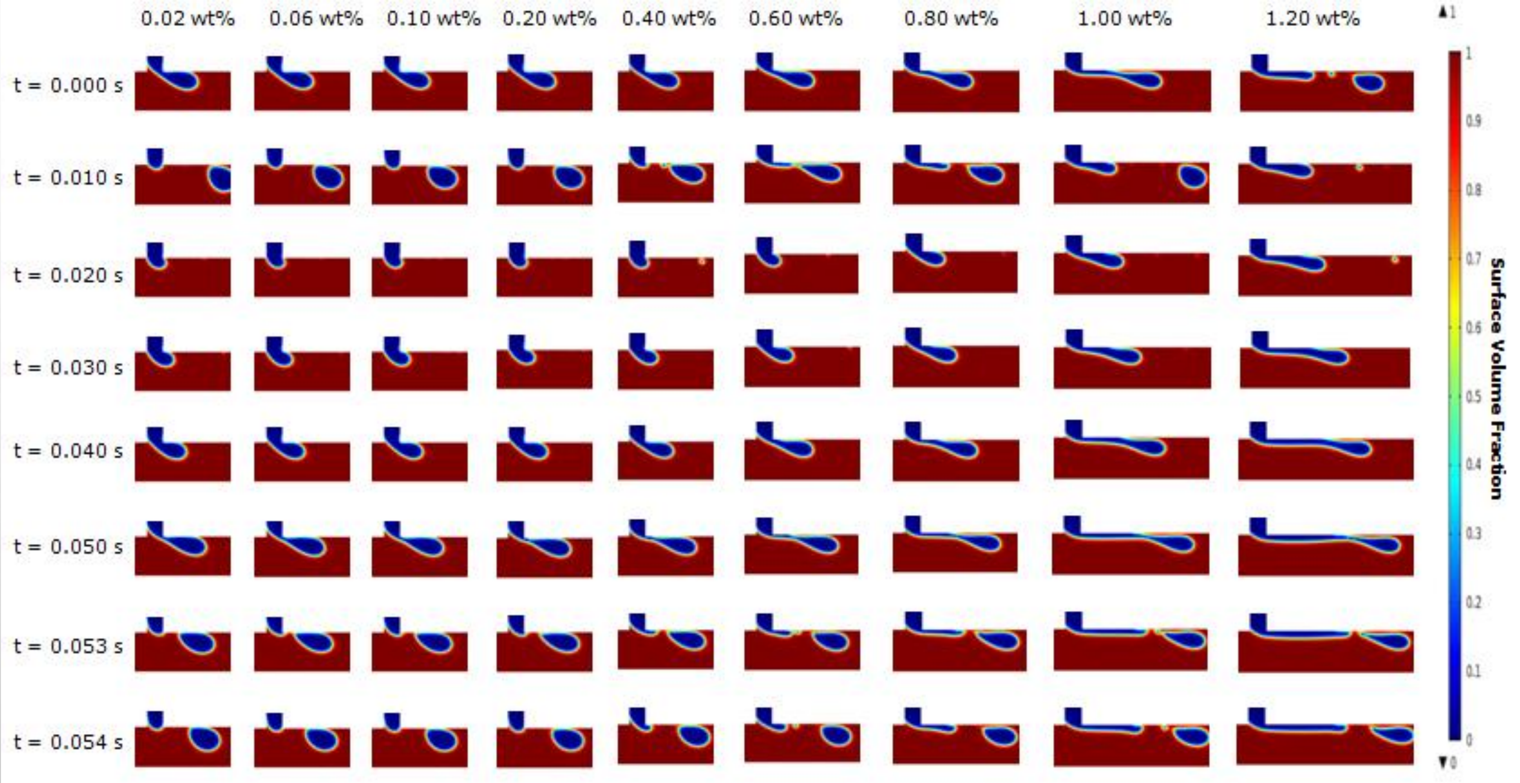
Parameter	**Effect of Dispersed Phase Concentration**
Continuous Phase	Olive Oil (η_c = 0.068 kg/m s)
Dispersed Phase	CMC Shear-Thinning Solution (0.02wt% to 1.20wt%)

1. Shear-Thinning Effect

- Larger shear-thinning effect will tend to reduce the resulting droplet length for higher viscosity.
- Greater shear-thinning effect exhibit decrease in viscosity upon the application of shear due to the inertial force.



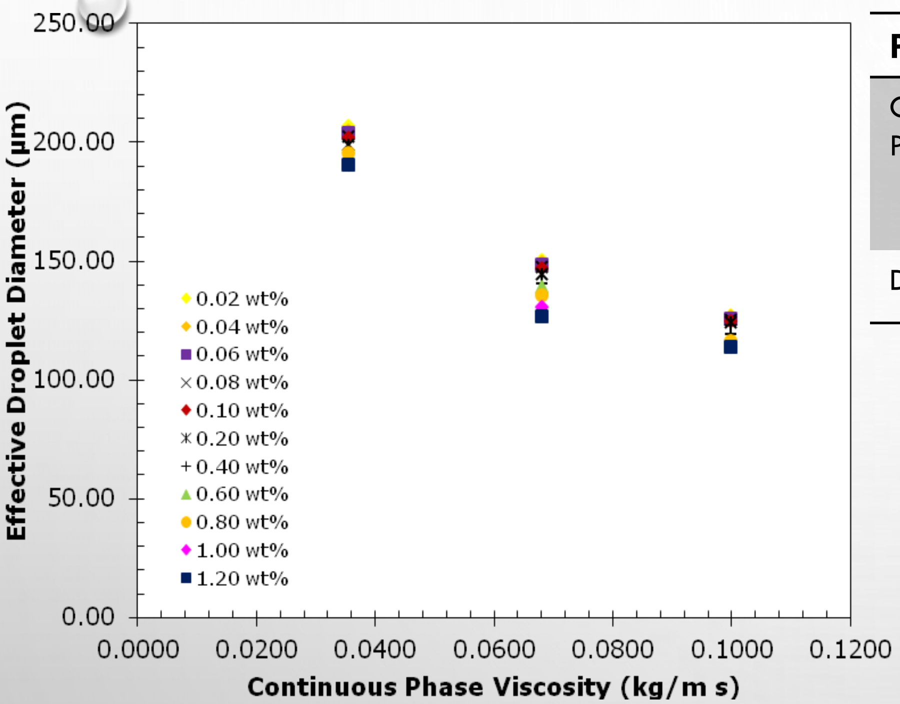
EFFECT OF DISPERSED PHASE CONCENTRATION



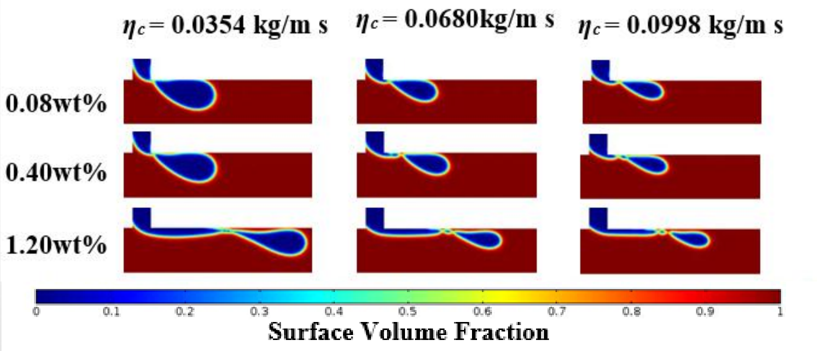
2. Viscosity Effect

- Viscosity of a polymer solution depends on its concentration and molecular weight of the dissolved polymer. When the SCMC liquid is more viscous (C*~0.4 wt%), the viscous pressure in dispersed thread becomes more dominant.
- Viscous pressure overcome the opposing capillary pressure→ Elongated dispersed thread

EFFECT OF CONTINUOUS PHASE CONCENTRATION



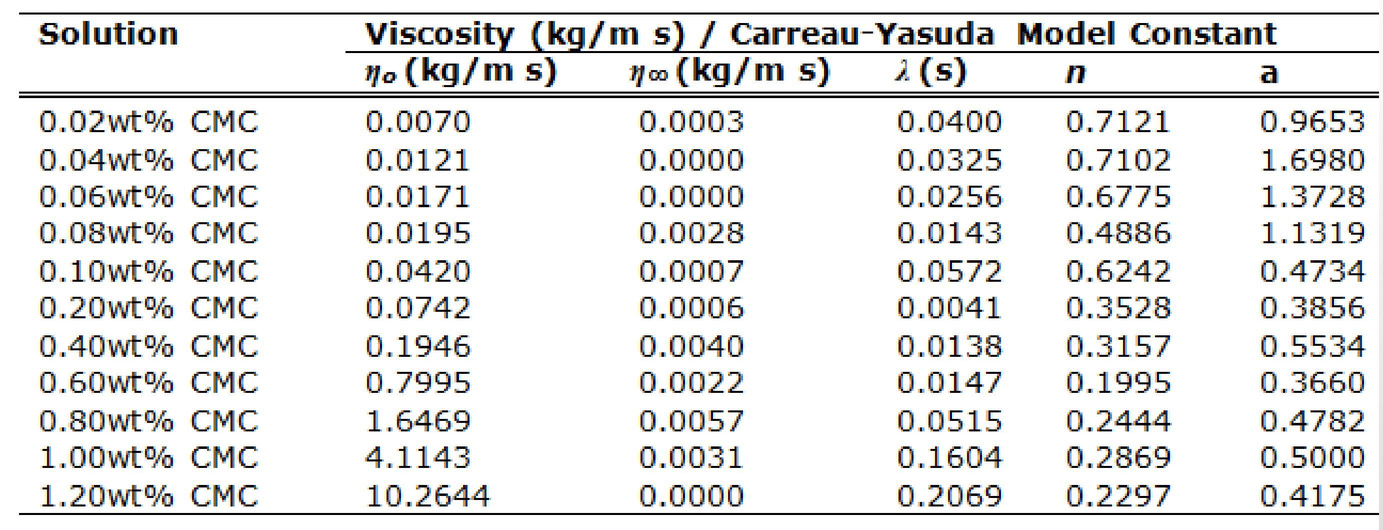
Parameter	Effect of Continuous Phase Viscosity
Continuous Phase	Mineral Oil (η_c = 0.0354kg/m s) Olive Oil (η_c = 0.068 kg/m s) Peanut Oil (η_c = 0.0998kg/m s)
Dispersed Phase	CMC Shear-Thinning Solution (0.02wt% to 1.20wt%)



Viscous Shear-Stress, $\tau \propto \eta_c Q_c$

- For lower η_c , viscous shear-stress appear to be minimised and surface tension becomes increasingly dominant on the breakup process →larger droplets are generated.
- Increasing the η_c generally gives rise to increasing shear force on penetrating dispersed phase thread→ smaller droplets are generated.
- Jetting phenomenon → force the droplet detachment point to move further downstream from the corner of T-junction, resulting in generation of smaller droplets.

EFFECT OF FIXED DISPERSED TO CONTINUOUS VISCOSITY RATIO



Solution	Viscosity (kg/m s) / Carreau-Yasuda Model Constant				
	η_o (kg/m s)	η_∞ (kg/m s)	λ (s)	n	a
0.02wt% CMC	0.0070	0.0003	0.0400	0.7121	0.9653
0.04wt% CMC	0.0121	0.0000	0.0325	0.7102	1.6980
0.06wt% CMC	0.0171	0.0000	0.0256	0.6775	1.3728
0.08wt% CMC	0.0195	0.0028	0.0143	0.4886	1.1319
0.10wt% CMC	0.0420	0.0007	0.0572	0.6242	0.4734
0.20wt% CMC	0.0742	0.0006	0.0041	0.3528	0.3856
0.40wt% CMC	0.1946	0.0040	0.0138	0.3157	0.5534
0.60wt% CMC	0.7995	0.0022	0.0147	0.1995	0.3660
0.80wt% CMC	1.6469	0.0057	0.0515	0.2444	0.4782
1.00wt% CMC	4.1143	0.0031	0.1604	0.2869	0.5000
1.20wt% CMC	10.2644	0.0000	0.2069	0.2297	0.4175

Parameter	**Effect of Fixed Dispersed to Continuous Phase Viscosity Ratio**
Continuous Phase	Adjusting η_c = zero shear viscosity (η_o) of CMC solution.
Dispersed Phase	CMC Shear-Thinning Solution (0.04wt% to 0.40wt%)

Carreau-Yasuda Model

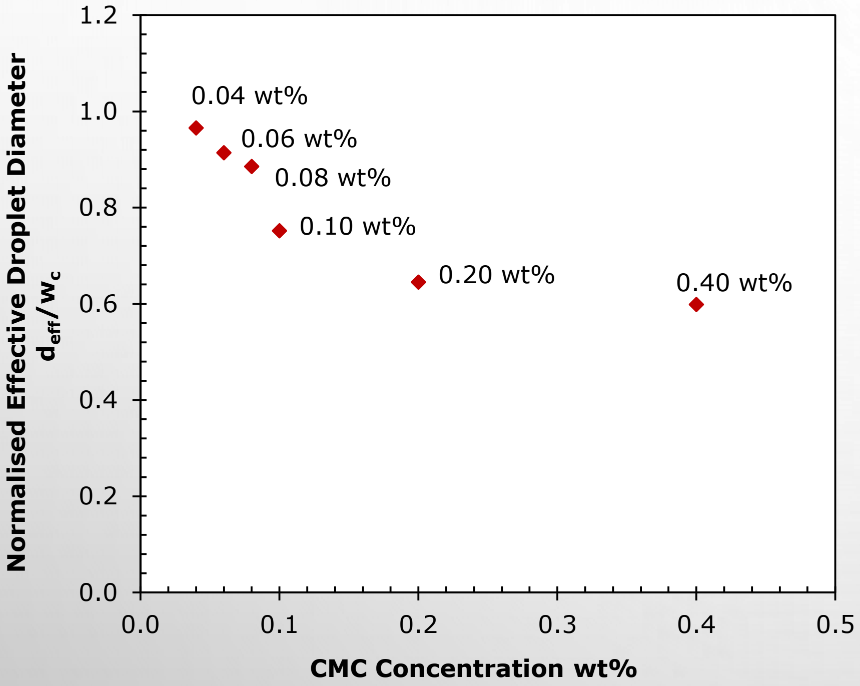
$$\eta(\dot{\gamma}) = \eta_\infty + (\eta_o - \eta_\infty)[1 + (\lambda_{CY}\dot{\gamma})^a]^{\frac{n-1}{a}}$$

η_o = zero shear-viscosity

η_∞ = infinite shear-viscosity

λ_{CY} = relaxation time constant

EFFECT OF FIXED DISPERSED TO CONTINUOUS VISCOSITY RATIO

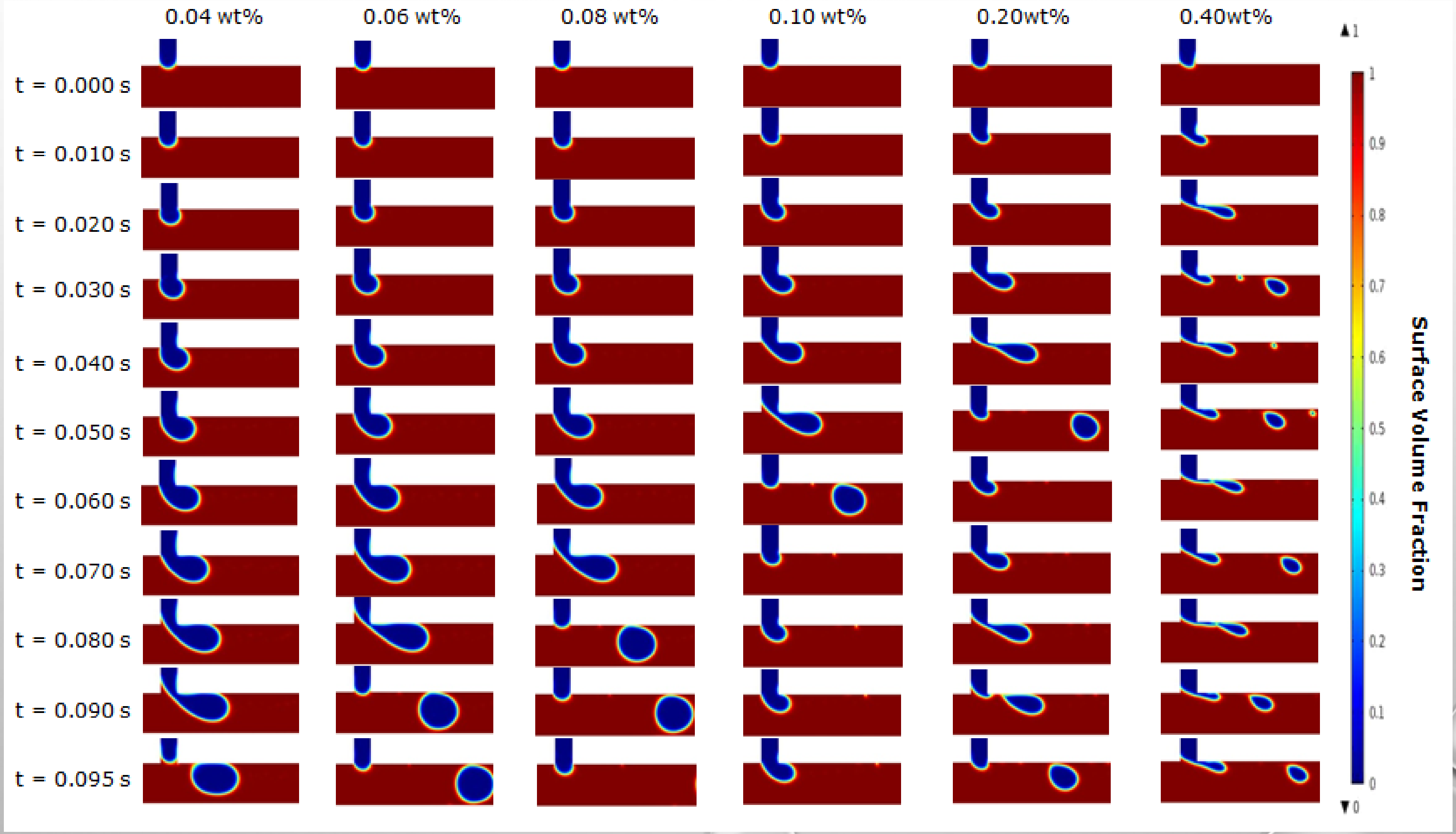


- Viscosity ratio (**$\lambda=\eta_o/\eta_c$**) →quotient of zero shear viscosity of dispersed phase (η_o) with the viscosity of continuous phase (η_c).
- Changing the CMC concentration= changes the η_o .
- The **η_c** is varied to **always match the η_o** of the dispersed phase. (λ=1)

Viscous Shear-Stress, $\tau \propto \eta_c Q_c$

- The η_c with the identical value of η_o always dominates the breakup process →η_c is constantly larger than the averaged η_d→shear-thinning behaviour.
- When $\eta_c >> \eta_d$, the viscous shear stress is a vital distorting force acting on the interface, becomes prevailing→ accelerate the breakup process→ formation of smaller droplets.

EFFECT OF FIXED DISPERSED TO CONTINUOUS VISCOSITY RATIO



CONCLUSION

- Droplet dynamics are governed by:
  - Viscous shear-stress exerted by the continuous phase.
  - Shear-thinning properties of dispersed phase.
- d_{eff} decrease as dispersed concentration increases. Theoretical predictions are found to be inconsistent to those previous empirical observations that focused on dispersed fluid with different non-Newtonian characteristic.
- Larger η_c was expected to induce higher viscous shearing force acts on penetrating dispersed phase thread, thus reducing the d_{eff}.
- Considering a fixed λ of 1, The resultant droplet diameter is markedly decreased by increasing the equivalent viscosity of both phases.

ACKNOWLEDGEMENTS

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Thank you for your attention.

Any Questions??