Chemical and Biological Engineering
UNIVERSITY OF COLORADO BOULDER

Experimental and Computational Analyses of Droplet Motion in Straight, Rectangular Microchannels

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Introduction

- Microfluidics can be leveraged for applications such as drug delivery, single-cell assays, “lab-on-a-chip”/μTAS (micrometer-scale total analysis system)
- Low Reynolds number regime (viscous dissipation ≫ inertial effects)
- **Objective:** quantify the steady-state velocity and deformation of droplets as a result of changing different parameters of the flow
  - Boundary-integral simulations
  - Macroscopic flow cell and computer vision code

$$Re = \frac{\rho U H}{\mu_e} = \frac{\text{inertial forces}}{\text{viscous forces}} \ll 1$$

Numerical Methods: Boundary-Integral Method with Moving Frame

- Numerical solution of the Boundary-Integral form of the Stokes equations
  - $\boldsymbol{u}(\boldsymbol{y}) \equiv$ velocity on drop surface
  - $\boldsymbol{q}(\boldsymbol{y}) \equiv$ density function on domain surface
- Only requires meshing of the interfaces (drop + channel)
- A moving frame is used to further reduce computational load
- For straight channels, the undisturbed flow is given by Boussinesq's solution

$$\boldsymbol{u}(\boldsymbol{y}) = \frac{2}{\lambda+1}\left[\boldsymbol{u}_\infty(\boldsymbol{y}) + \boldsymbol{F}(\boldsymbol{y}) + 2\int_{S_\infty} \boldsymbol{q}(\boldsymbol{x}) \cdot \boldsymbol{\tau}(\boldsymbol{x}-\boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{x}) dS_x\right] + \frac{2(\lambda-1)}{\lambda+1}\int_{S_d} \boldsymbol{u}(\boldsymbol{x}) \cdot \boldsymbol{\tau}(\boldsymbol{x}-\boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{y}) dS_x$$

$$\boldsymbol{q}(\boldsymbol{y}) = -\boldsymbol{F}(\boldsymbol{y}) - (\lambda-1)\int_{S_d} \boldsymbol{u}(\boldsymbol{x}) \cdot \boldsymbol{\tau}(\boldsymbol{x}-\boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{x}) dS_x - 2\int_{S_\infty} \boldsymbol{q}(\boldsymbol{x}) \cdot \boldsymbol{\tau}(\boldsymbol{x}-\boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{x}) dS_x - \frac{\boldsymbol{n}(\boldsymbol{y})}{S_\infty}\int_{S_\infty} \boldsymbol{q}(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x}) dS_x$$

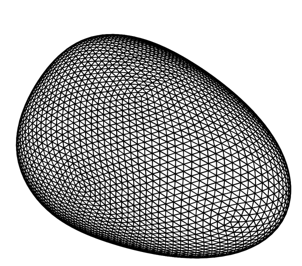


Figure 1. Drop mesh used for discretization

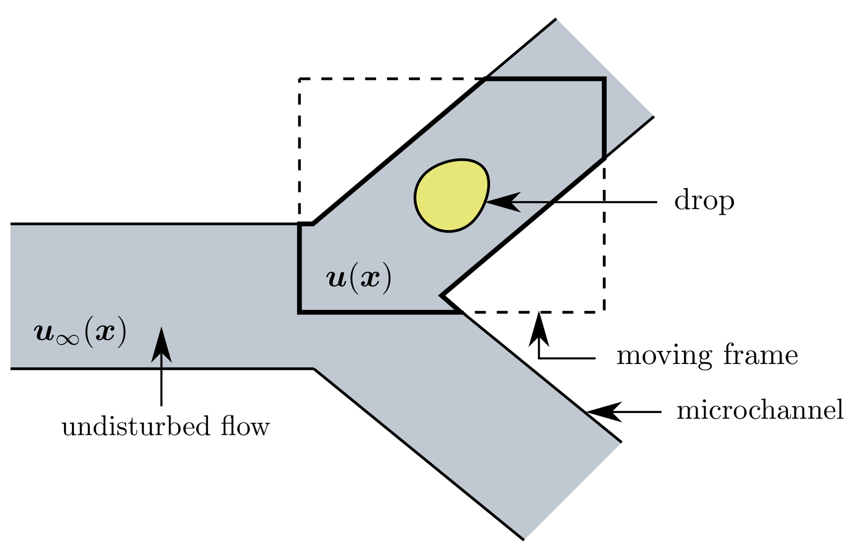
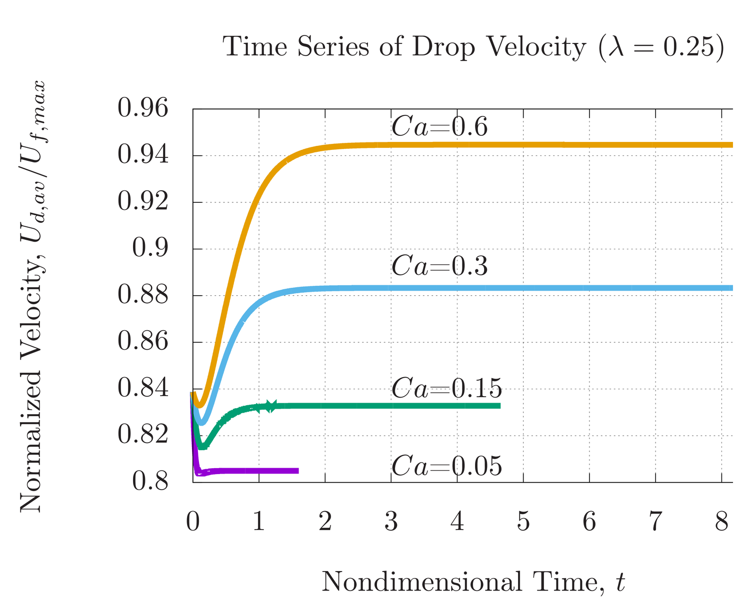


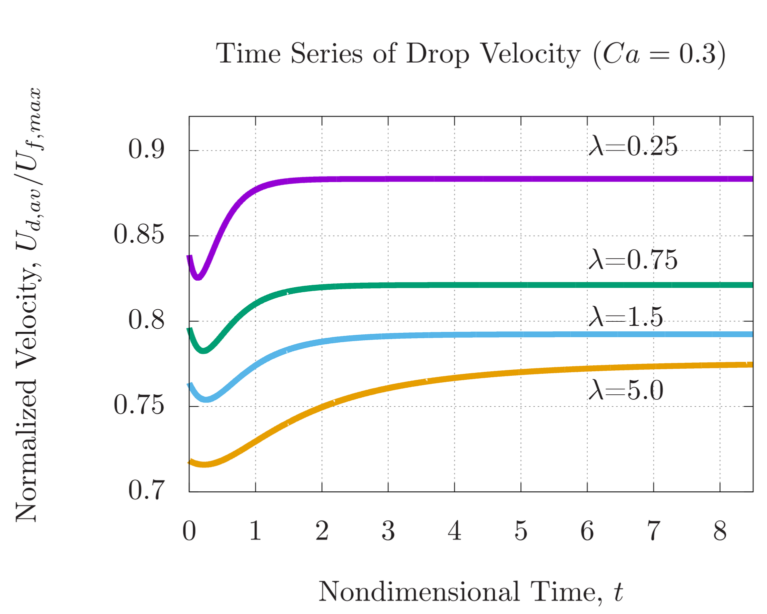
Figure 2. Moving-frame approach for the solution [1, 2]

Results: Simulated Droplet Motion and Deformation



$$Ca = \frac{\mu_e U}{\sigma} = \frac{\text{viscous forces}}{\text{surface forces}}$$

- As $Ca \nearrow$, more t to reach steady state
- As $Ca \nearrow$, higher steady state velocity
- As $Ca \nearrow$, more deformation $\Rightarrow$ more hydrodynamic shape



$$\lambda = \frac{\mu_d}{\mu_e} = \frac{\text{droplet viscosity}}{\text{fluid viscosity}}$$

- As $\lambda \nearrow$, more t to reach steady state
- As $\lambda \nearrow$, lower steady state velocity
- As $\lambda \nearrow$, more deformation

Methods: Macroscopic Flow Cell

- Droplet is introduced manually via a syringe. A syringe pump is used for the bulk fluid.
- Castor oil is used as the bulk fluid
- Droplets are made of PDMS or a Water + Glycerol mixture and then dyed

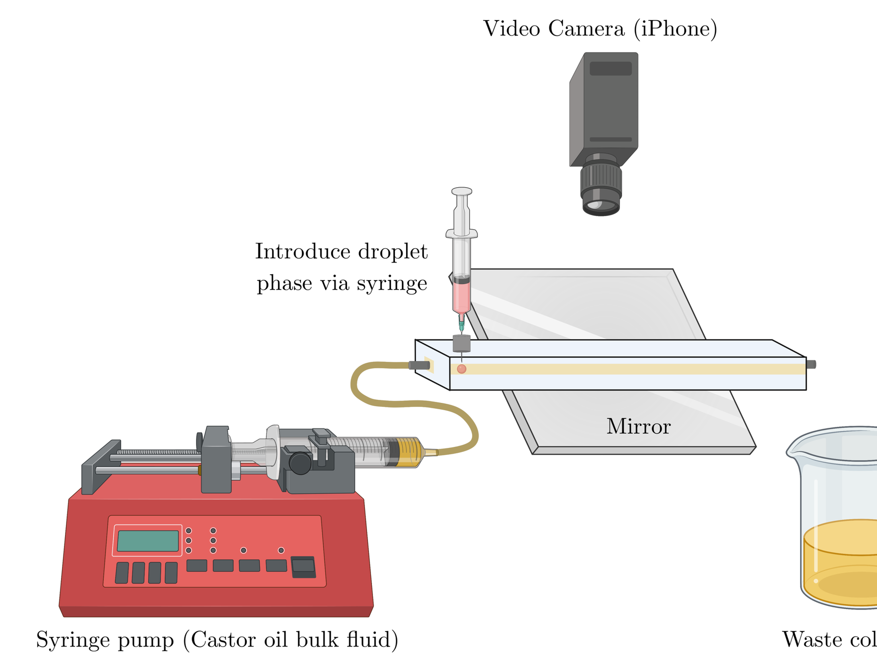
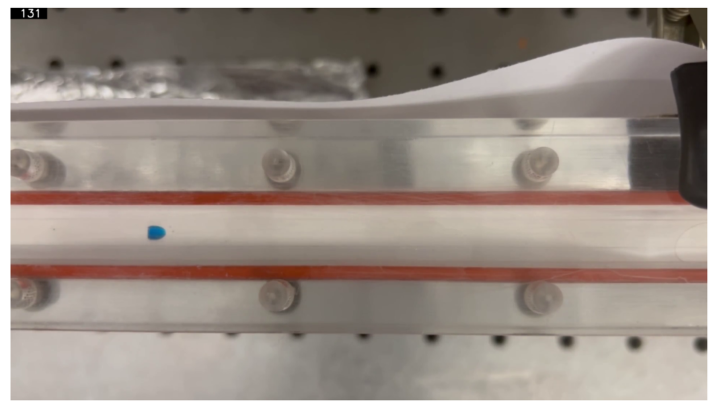


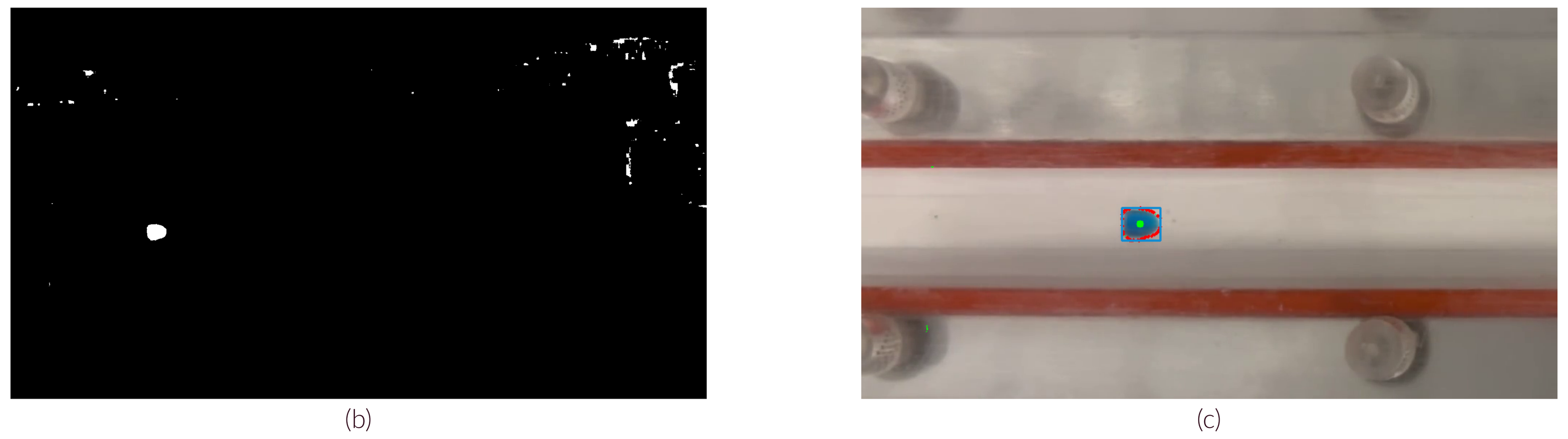
Figure 3. Diagram of experimental apparatus (created with BioRender.com)

Computer Vision Algorithm



(a)

- Used to calculate drop position and deformation
- Droplet center is calculated as a contour average
- Image correction is necessary to account for lens distortion [3]



(b) (c)

Figure 4. Implementation of the computer vision algorithm. The frames show (a) a video frame with the droplet, (b) the color mask, and (c) the contour and bounds generated by the algorithm

Results: Initial Experimental Results

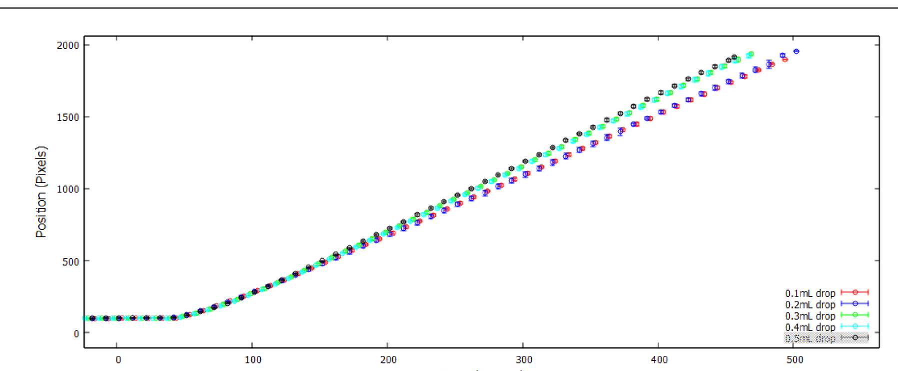
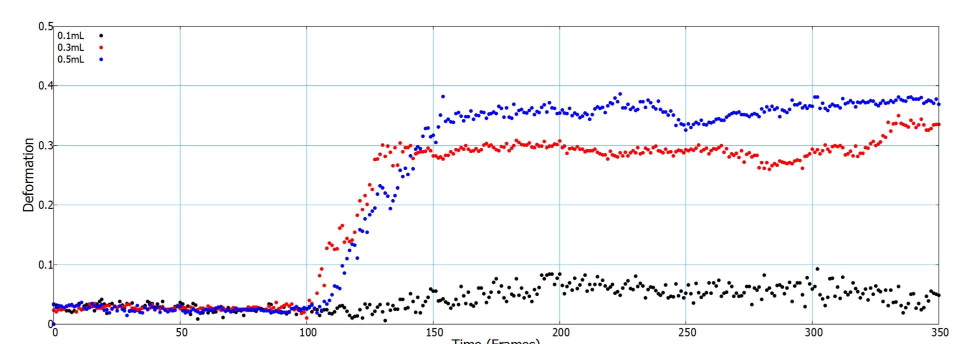


Figure 5. Droplet position over time for 15mL/min bulk flow (normalized so that droplet motion starts at same frame)



$$D_T = \frac{L_{maj} - L_{min}}{L_{maj} + L_{min}}$$

L_{maj} = major semiaxis

L_{min} = minor semiaxis

Figure 6. Droplet Taylor deformation parameter over time for 15mL/min bulk flow (0.1, 0.3 and 0.5 [mL])

Pendant Drop Experiments

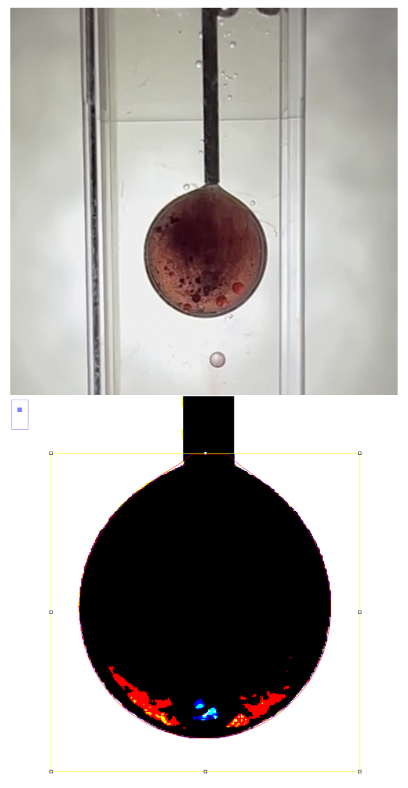


Figure 7. Single frame of pendant drop experiment video and binarization from FIJI

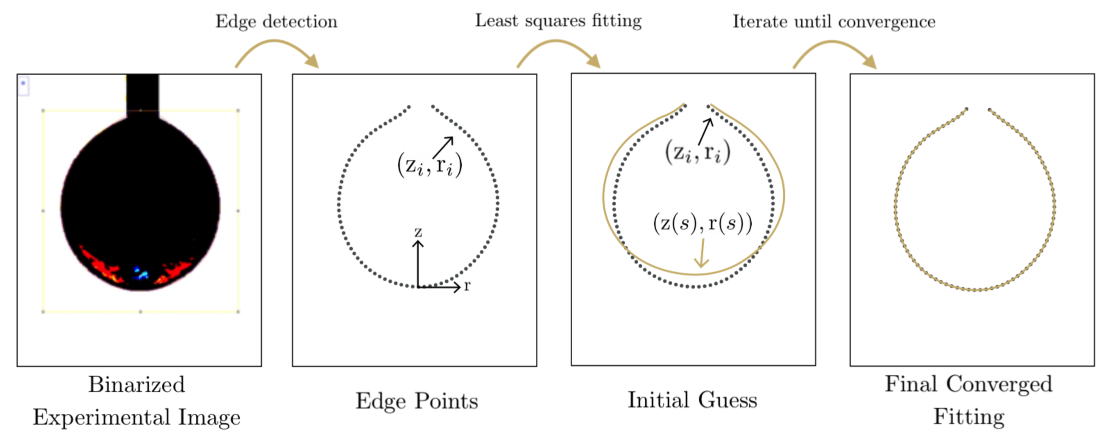


Figure 8. Outline of the drop tensiometry process, adapted from [4]

Drop Phase	Bulk Phase	σ $\left[\frac{\text{mN}}{\text{m}}\right]$	Uncertainty
Water	Air	77.7	± 5.8
PDMS	Air	22.5	± 3.3
PDMS	Castor Oil	18.0	± 3.1

Table 1. Initial interfacial and surface tension values

Water has a tabulated $\sigma = 72\frac{\text{mN}}{\text{m}}$

Concluding Remarks

- Boundary integral method is efficient in simulating viscous droplets flowing in straight microchannels
- As $\lambda \nearrow$, deformation $\nearrow$ and $U_{av,ss} \searrow$ (more resistance to flow + high viscous stress)
- As $Ca \nearrow$, deformation $\nearrow$ and $U_{av,ss} \nearrow$ (more hydrodynamic shape)
- Good qualitative agreement between simulations and experiments, and promising interfacial tension results

Future Plans

- FIJI $\rightarrow$ In-house code
  - Lens distortion correction for experimental videos
  - Isometric simulation videos
- Determine interfacial tension values of droplet fluids
  - In-house fitting code
- Simulate droplets with experimentally determined conditions
- Improve regularity and control in apparatus
  - Droplet origin and volume
- **Maybe?** $\rightarrow$ PDMS microfluidic chip (Ding lab in Mechanical Engineering)

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References

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[3] Zhang, Z. A flexible new technique for camera calibration. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 22(11):1330–1334, November 2000.

[4] Berry, J.D. and Neeson, M.J. and Dagastine, R.R. and Chan, D.Y.C. and Tabor, R.F. Measurement of surface and interfacial tension using pendant drop tensiometry. *Journal of Colloid and Interface Science*, 454:226–237, September 2015.

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