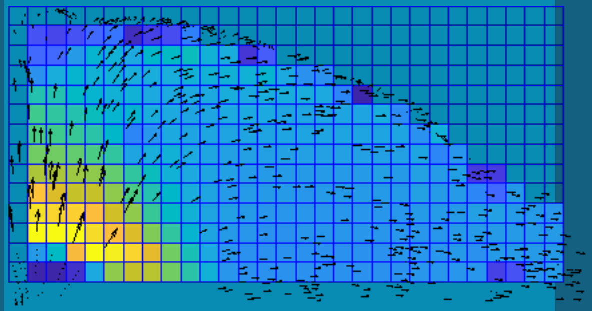
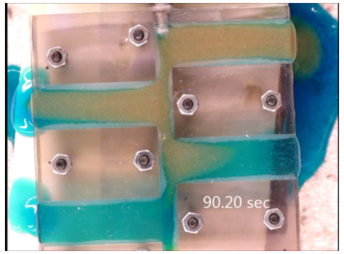
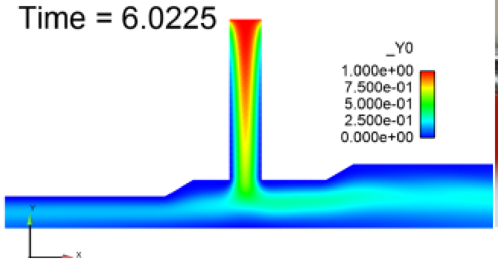
SAND2022-9439C

# Computational models and experimental studies of mold filling in thin channels with yield stress fluids



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15th World Congress on Computational Mechanics
Virtual Conference from Yokohama, Japan
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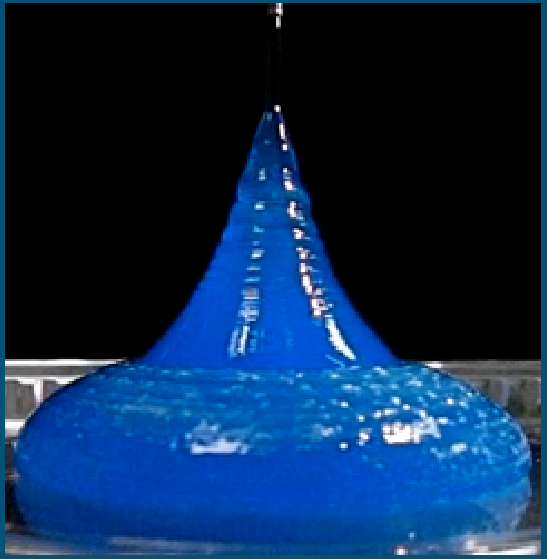
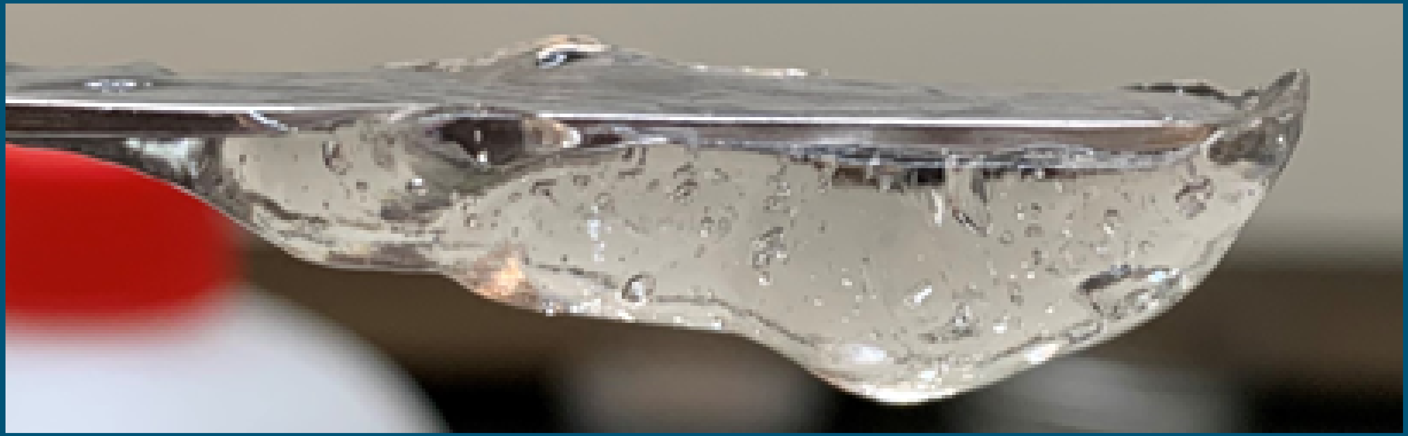
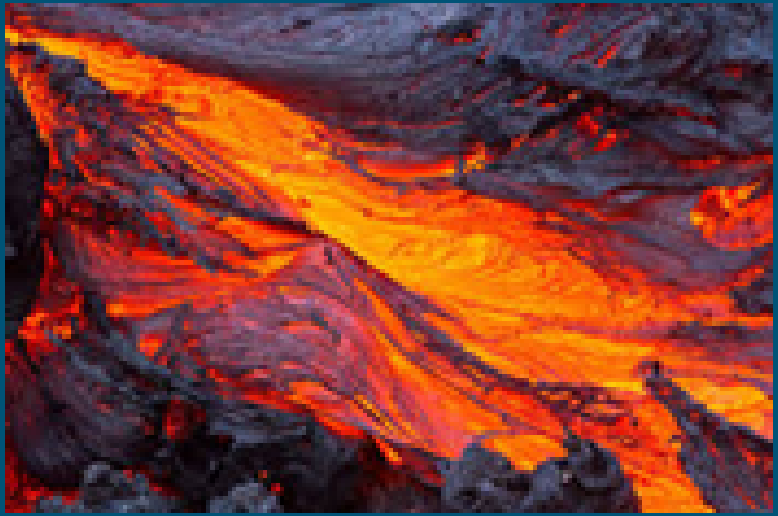
# Motivation for studying yielding fluids







Yield stress can be seen in wax, whipped cream, toothpaste, lava, ceramic pastes, and Carbopol

# Develop computational models for free-surface flows of yield stress fluids

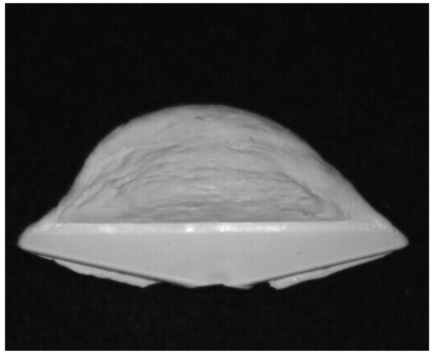
## Why is this needed?

- Accurate predictions of surface profiles and spreading dynamics for flowing systems

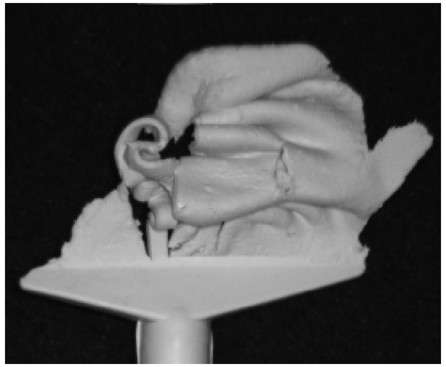
## Current state-of-the-art in production codes:

- Ramp viscosity arbitrarily high to “solidify” a fluid
- Does not accurately preserve the stress state that develops in the fluid
- One way coupling between fluid and solid codes

We propose developing numerical methods informed by novel experimental diagnostics that transition from solid-to-fluid, while accurately predicting the stress and deformation regardless of phase.

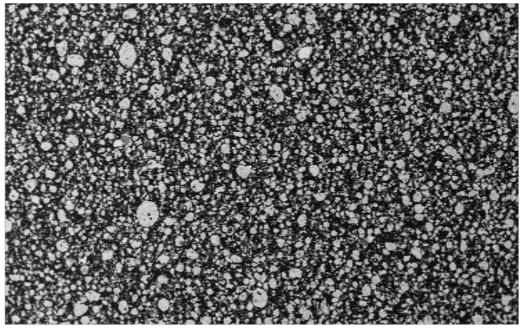


2.5 mm shot, 100% injection speed



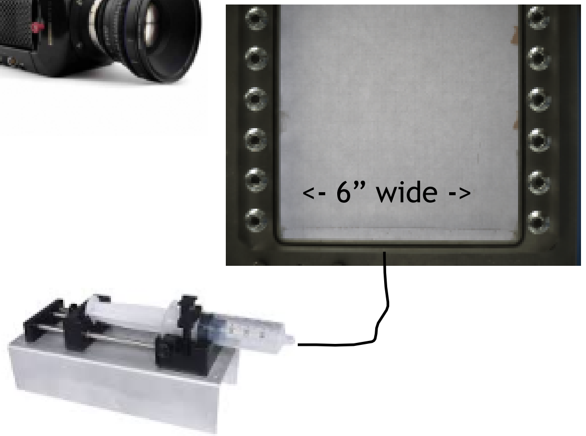
2.5 mm shot, 40% injection speed

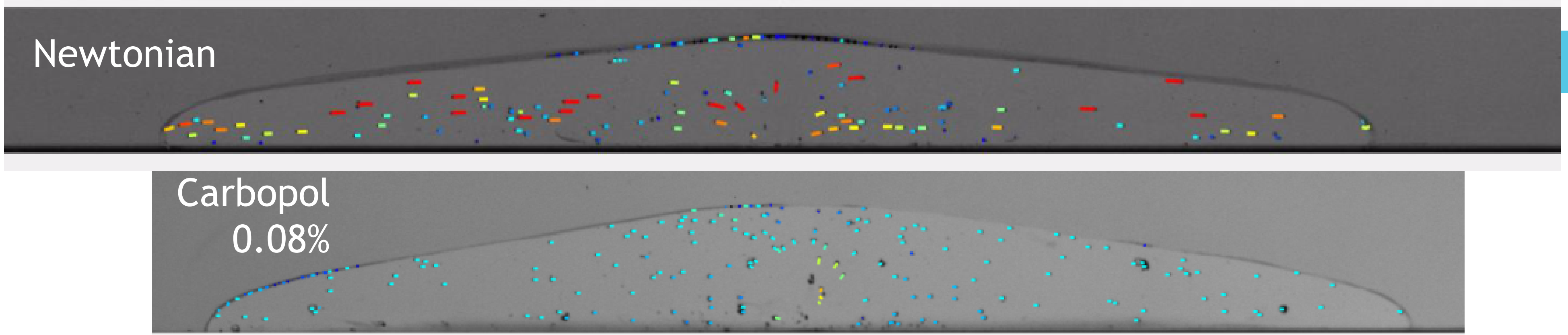
Green ceramic processing shows yield stress and both fluid and solid-like behavior

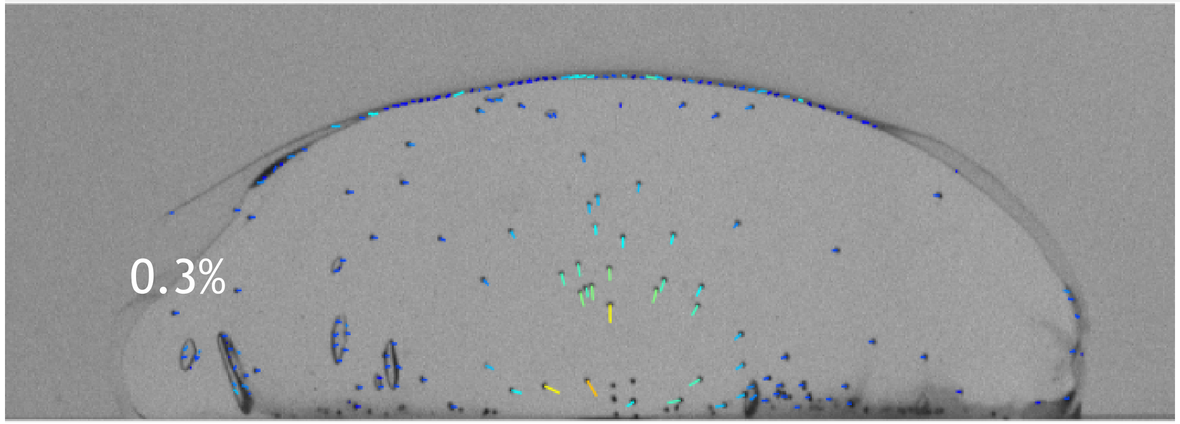


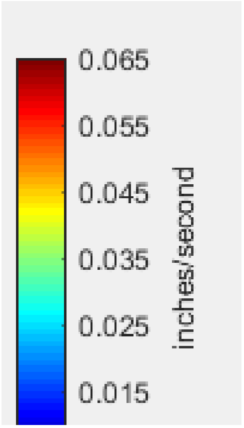
Target system: solidifying continuous phase with particles and droplets (e.g. polyurethane foams)

- Newtonian fluid shows evidence of Poiseuille flow across channel
- All Carbopol solutions show constant velocity across the channel
- Away from the inlet, there are regions of local arrest within the channel for the yield stress fluid not seen in the Newtonian fluid

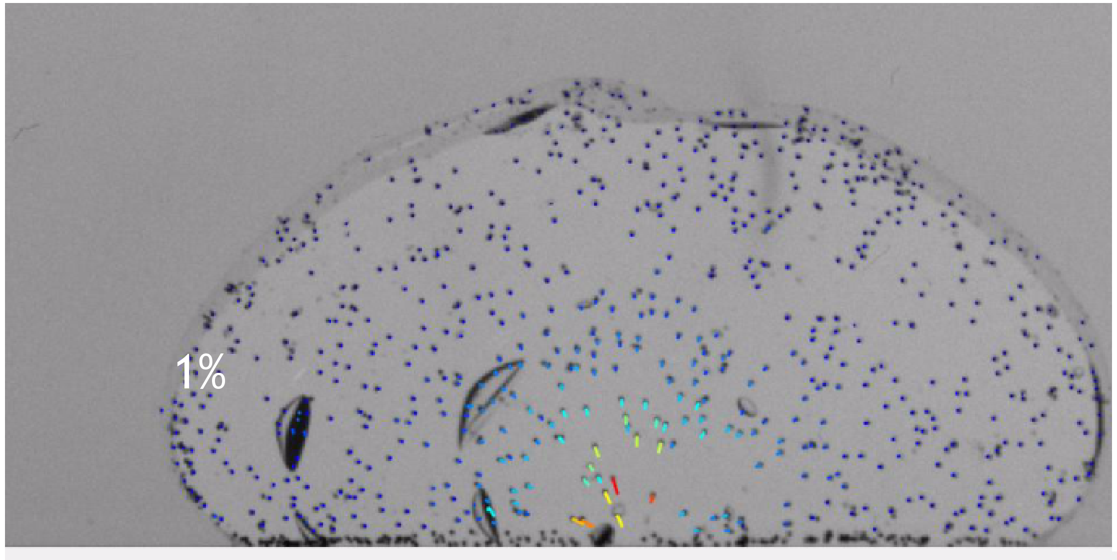


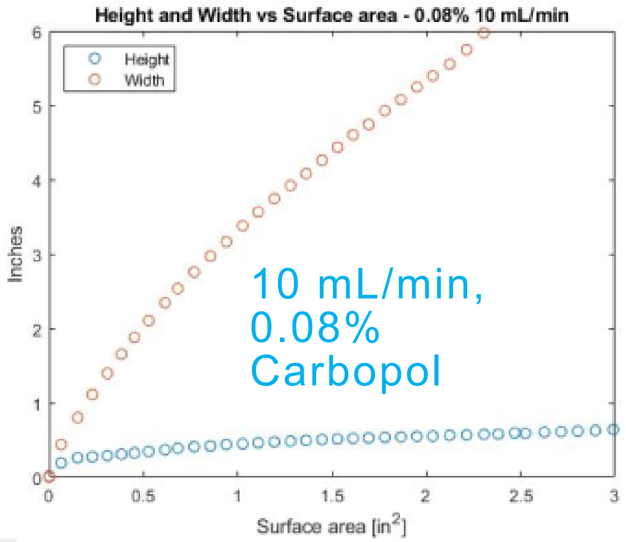



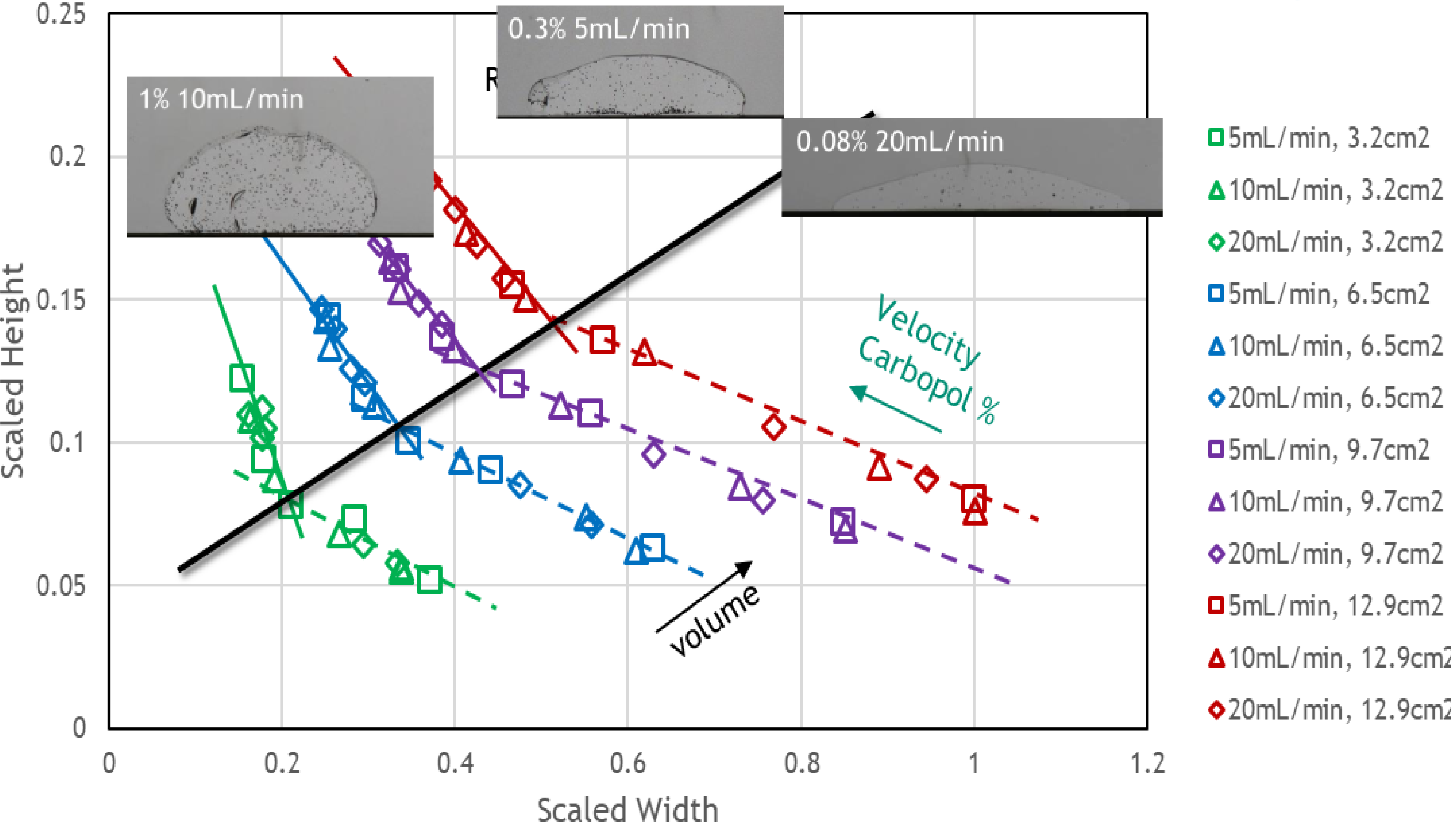

Injection speed 10 ml/min
Area = 6.5 $cm^2$



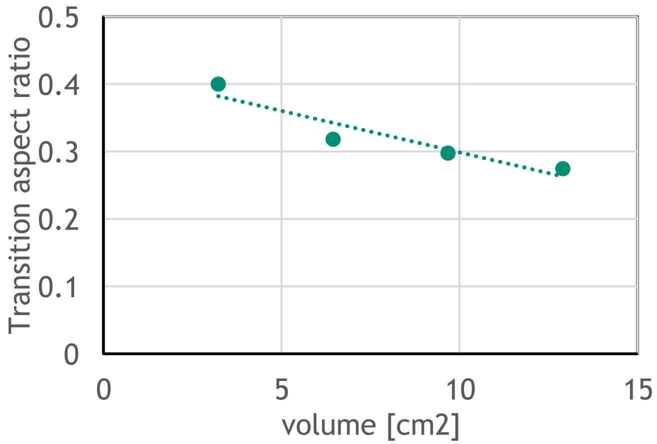



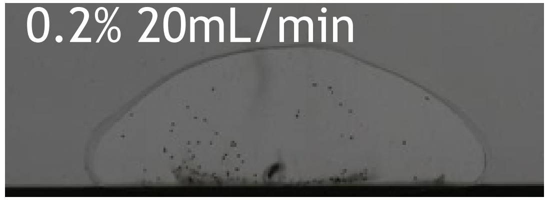
# Morphology of Injected Fluid Drop

$$R = \frac{\tau_Y + K\dot{\gamma}^n}{\rho g H}$$




- Change in morphology of the fluid domain from more triangular to round
- Drop morphology depends on the combination of yield and flow stresses
- Same aspect ratio is observed at higher speeds for lower Carbopol concentrations



# Transition from Triangular to Rounded: Collapse of Data

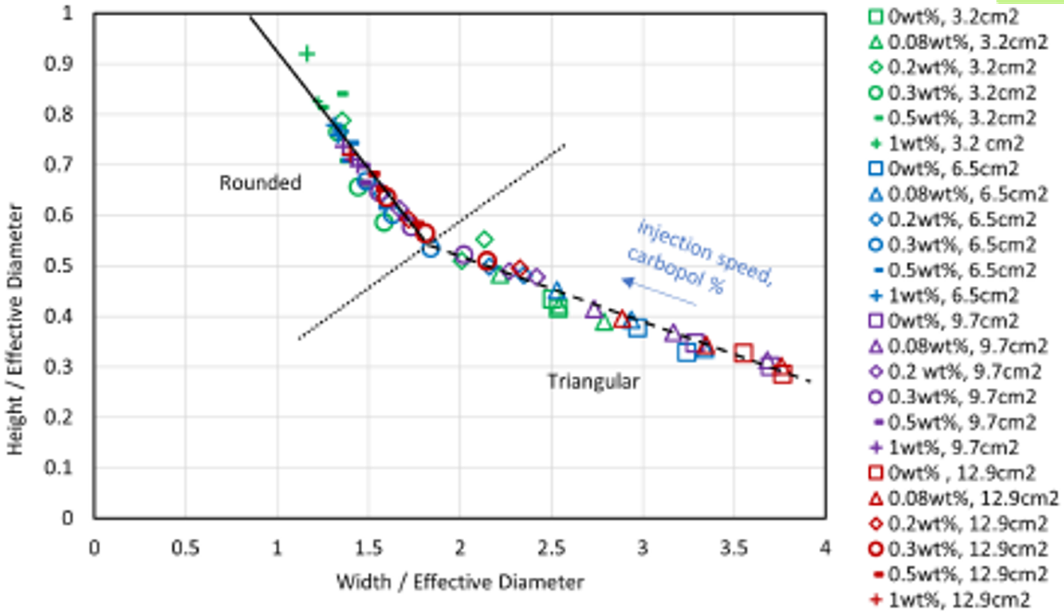
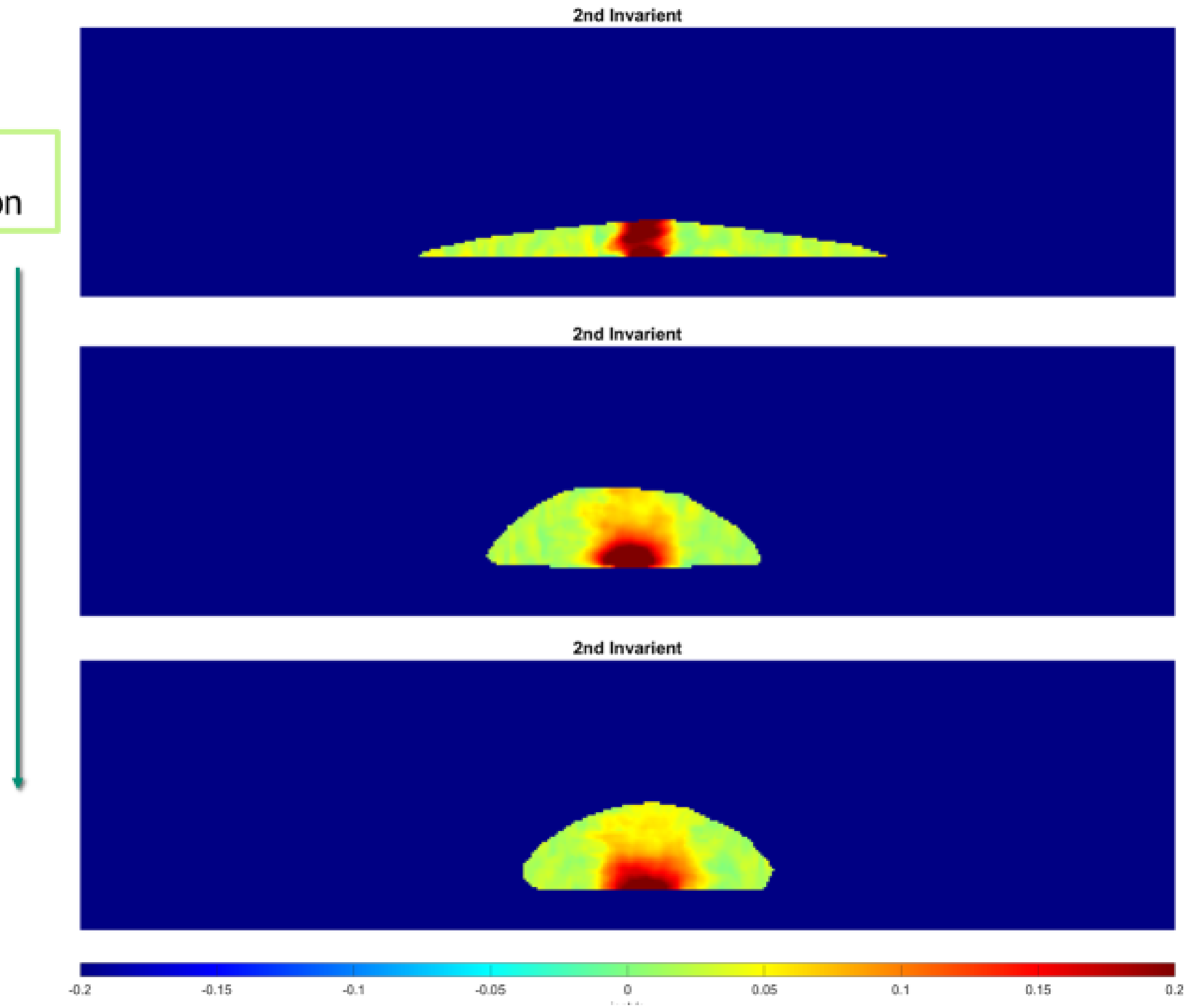



FIG. 5: Compilation of drop morphology results for 5, 10 & 20 mL/min injections speeds for various Carbopol concentrations (symbol) and drop sizes (color).

Carbopol concentration




- Collapse of data if we scale it to an effective width and diameter based on spherical drop
- Mechanism of flow changes with yield stress
- Triangular flows are inertial dominated while fluids with yield stress are rounded and flow dissipates in a circular manner

# Equations of motion and stress constitutive equations

Momentum and Continuity

$$\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u}\mathbf{u}\right) = -\nabla P + \nabla \cdot (2\mu\dot{\gamma}) + \nabla \cdot \boldsymbol{\sigma}$$

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

Oldroyd-B stress constitutive model + Saramito yield model

$$\frac{1}{G}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \overset{\nabla}{\boldsymbol{\sigma}}\right) + \left[\frac{1}{k|\boldsymbol{\sigma}_d|^{n-1}}\right]^{\frac{1}{n}} \mathcal{S}(\boldsymbol{\sigma}, \tau_y)\boldsymbol{\sigma} = 2\dot{\gamma}$$

Herschel-Buckley (HB)-Saramito yield model

$$\mathcal{S}(\boldsymbol{\sigma}, \tau_y) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right)^{\frac{1}{n}}$$

Solve with Finite Element Method for $\mathbf{u}$, $P$, $\boldsymbol{\sigma}$ and $\dot{\boldsymbol{\gamma}}$ tensors

Guénette, R. and Fortin, M. *Journal of Non-Newtonian Fluid Mechanics* (1995) 60: 1, 27-52.

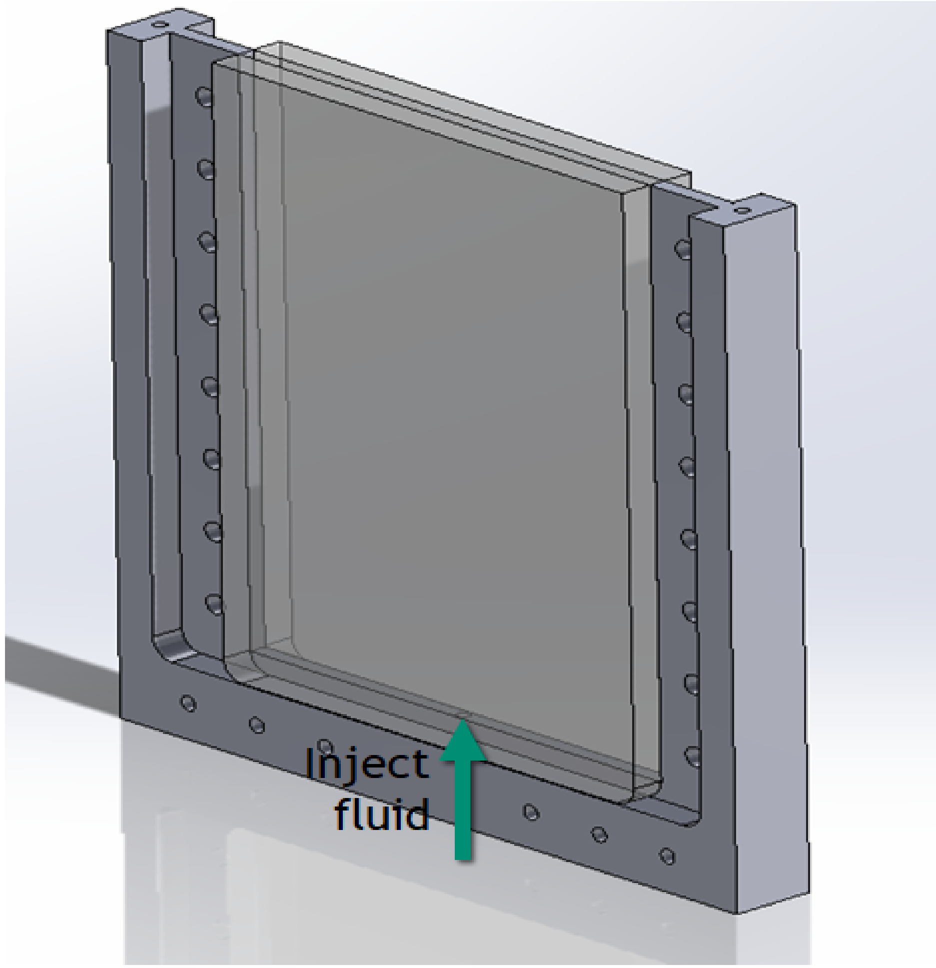
Saramito, P. *Journal of Non-Newtonian Fluid Mechanics* (2007) 145: 1, 1-14.

Fraggedakis, D et al. *Journal of Non-Newtonian Fluid Mechanics* (2007) 236, 104-122.

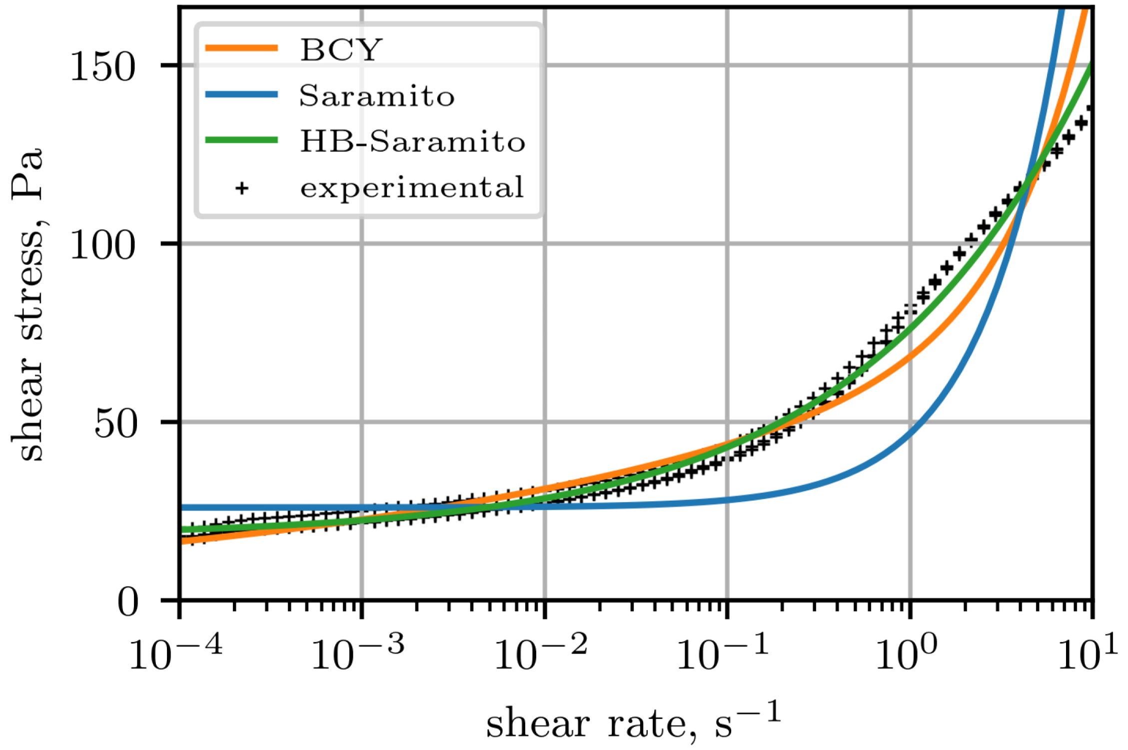
# Mold filling geometry: flow between two thin plates

## Apparatus dimensions

- Inlet diameter = 0.138 cm
- ($x$) Width = 15.2 cm
- ($y$) Height > Width
- ($z$) Gap between plates = 0.5 cm
  - This dimension is not resolved 2D in computations
  - Drag force due to unresolved stress needs to be modeled in some manner



# Characterization of Carbopol and parameter fitting




- Small amplitude stress vs. strain curve, gives the elastic modulus, *G.*
- Other rheological parameters were determined using a nonlinear least squares fit.

## Bingham-Carreau-Yasuda (BCY)

$$\mu = \mu_\infty + \left[\mu_0 - \mu_\infty + \tau_y \frac{1 - e^{-F\dot{\gamma}}}{\dot{\gamma}}\right]\left[1 + (b\dot{\gamma}^a)\right]^{\frac{n-1}{a}}$$

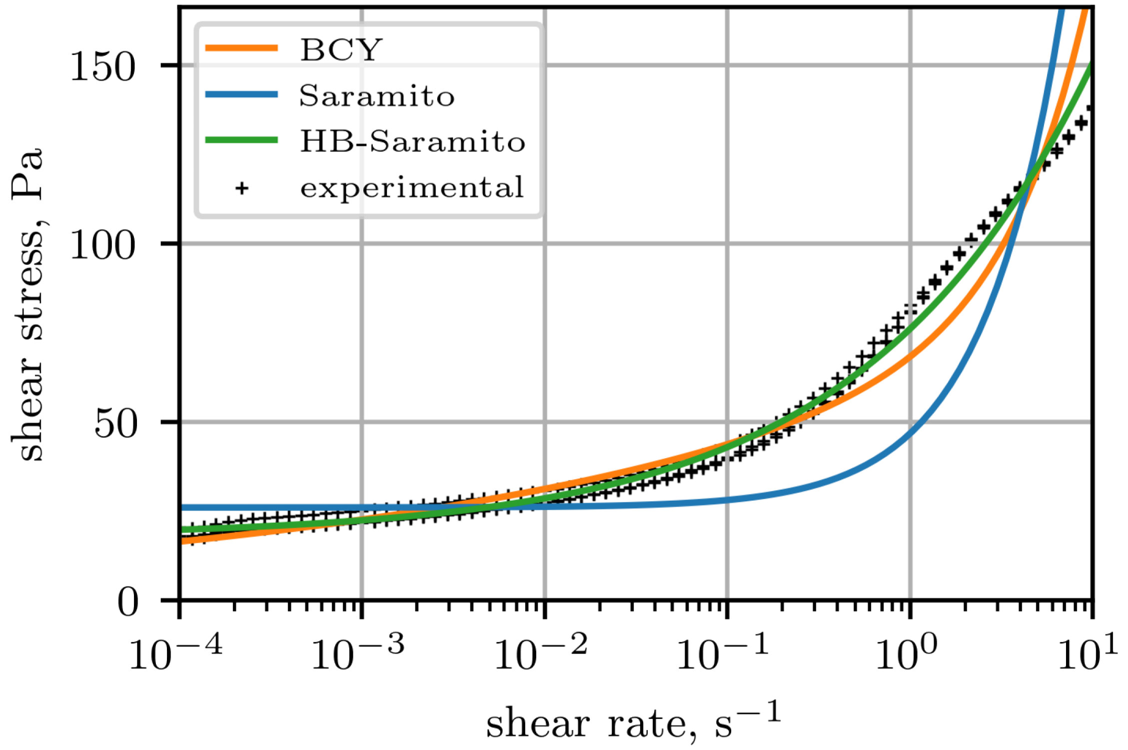
| $\mu_0$, (Pa•s) | $\mu_\infty$, (Pa•s) | $b$ ($s^{-1}$) | $a$ | $n$ | $\tau_y$, (Pa) | $R^2$ |
|---|---|---|---|---|---|---|
| 217.15 | 0.018 | 3.112 | 0.966 | 0.190 | 31.21 | 0.954 |

## Saramito-Oldroyd-B

$$\frac{1}{G}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \overset{\nabla}{\boldsymbol{\sigma}}\right) + \left[\frac{1}{k|\boldsymbol{\sigma}_d|^{n-1}}\right]^{\frac{1}{n}} \mathcal{S}(\boldsymbol{\sigma}, \tau_y)\boldsymbol{\sigma} = 2\dot{\boldsymbol{\gamma}}$$

| | $n$ | $k$, (Pa•$s^n$) | $\tau_y$, (Pa) | $G$, (s) | $R^2$ |
|---|---|---|---|---|---|
| Saramito | == 1 | 52.85 | 32.10 | 576.9 | 0.889(*) |
| HB-Saramito | 0.368 | 58.9 | 17.89 | 576.9 | 0.991 |

# Characterization of Carbopol and parameter fitting




- $^{(\star)}$Fit for constant viscosity Saramito model done with $\dot{\gamma} \leq 2\ s^{-1}$

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# 3D mold filling simulations

## Constitutive models

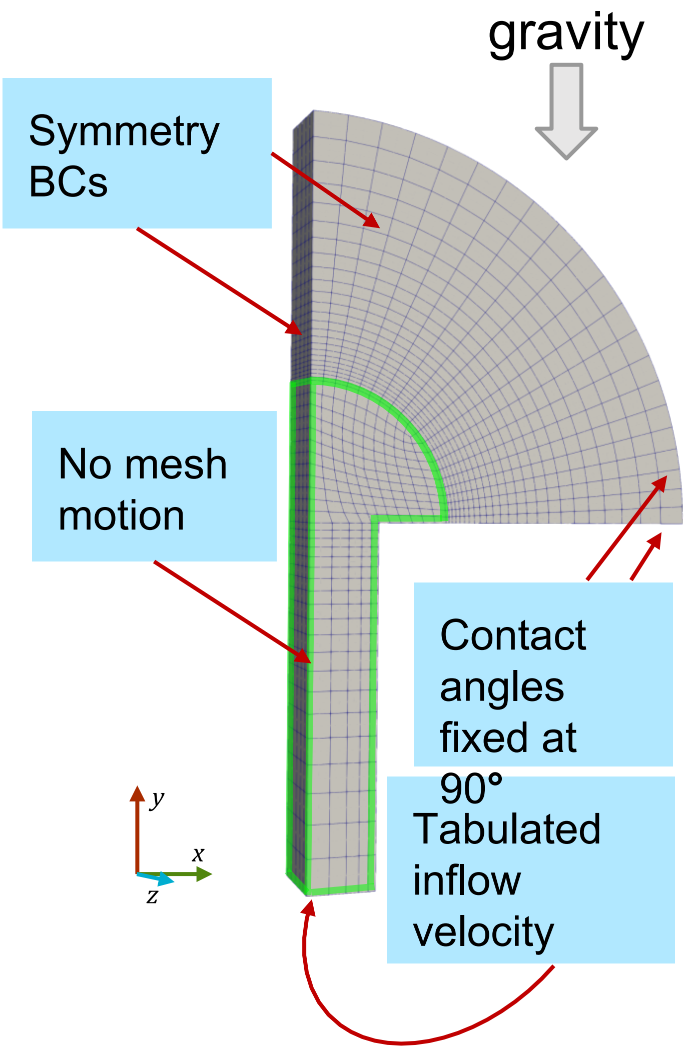
- Bingham-Carreau-Yasuda (generalized Newtonian)
- Saramito-Oldroyd-B
  - Constant viscosity
  - Herschel-Buckley (HB)

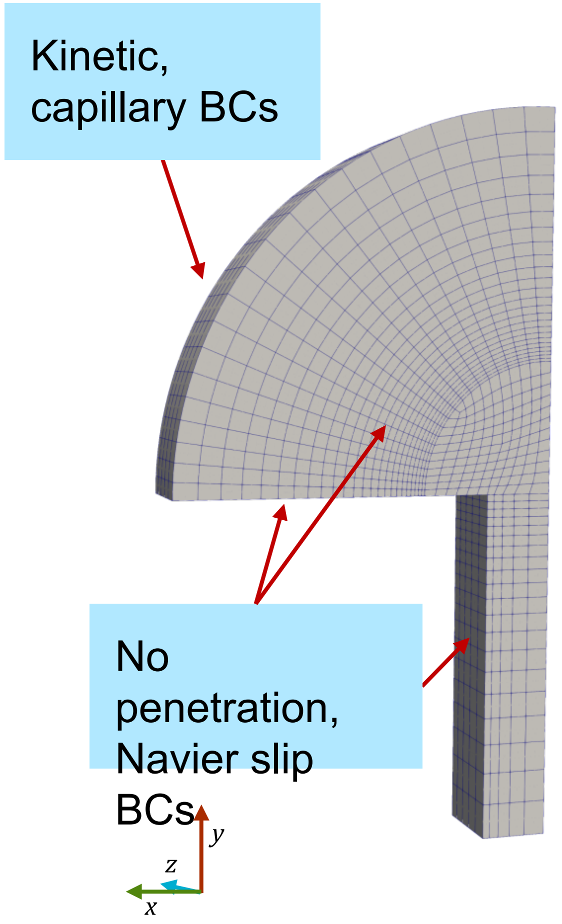
## Computations

- Finite element method in Goma
- Arbitrary Eulerian-Lagrangian moving mesh framework
- Remeshing done every ~30 timesteps

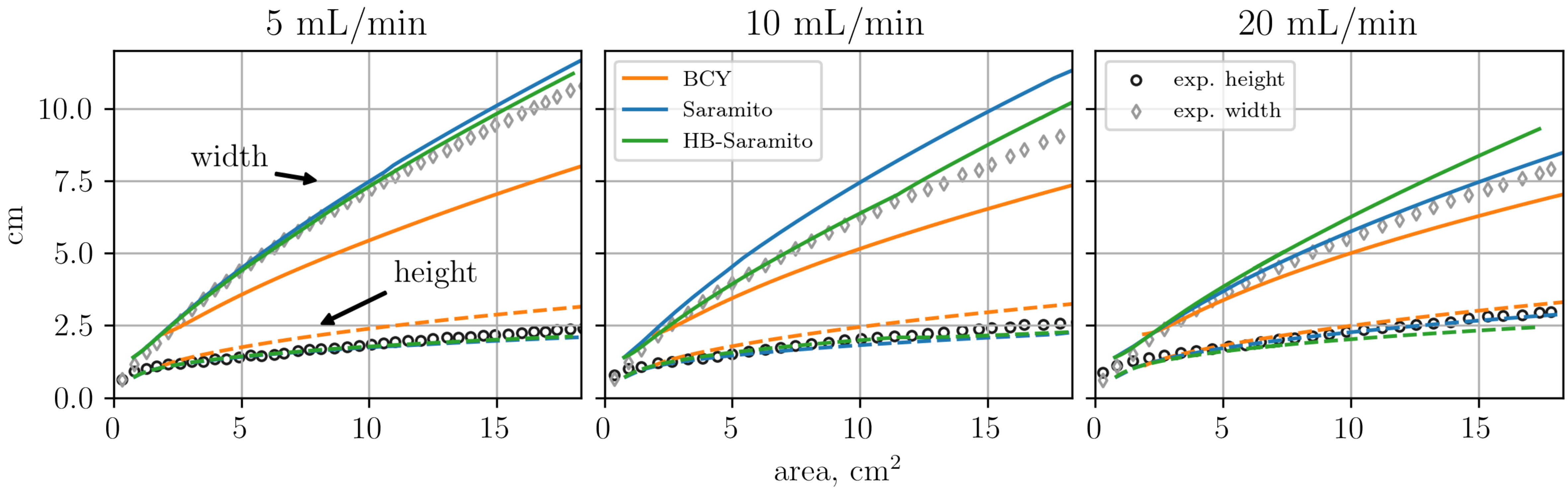
## Validation Experiments

- 0.3 wt.% Carbopol
- 5-20 mL/min flow rate



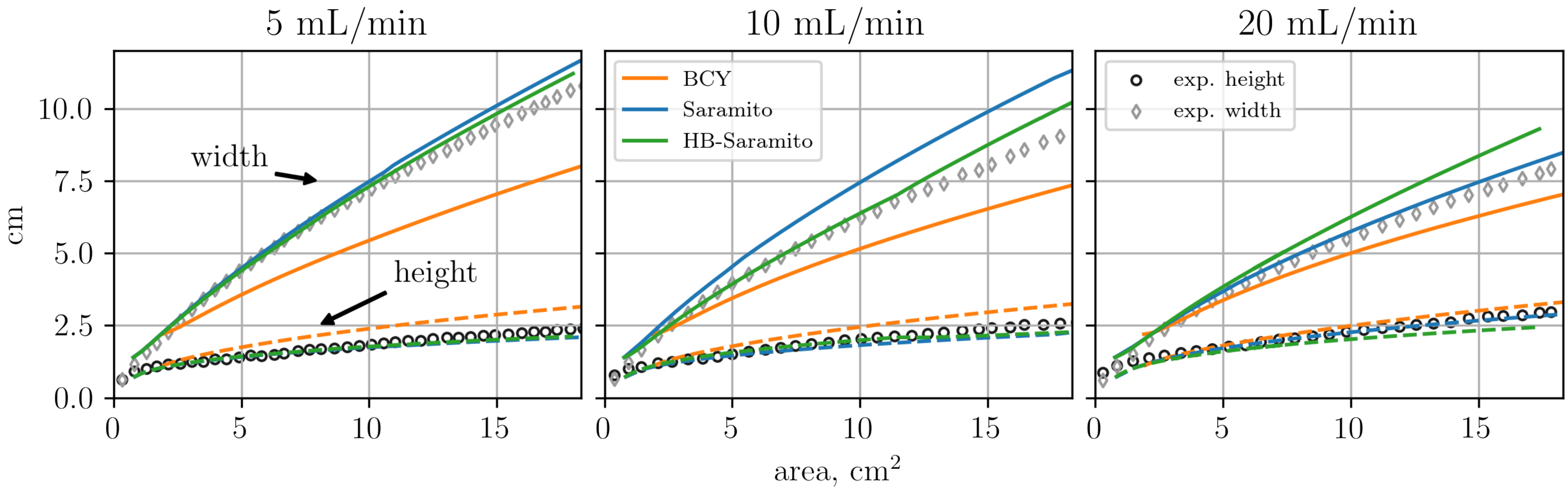



# Droplet dimensions computed from 3D simulations



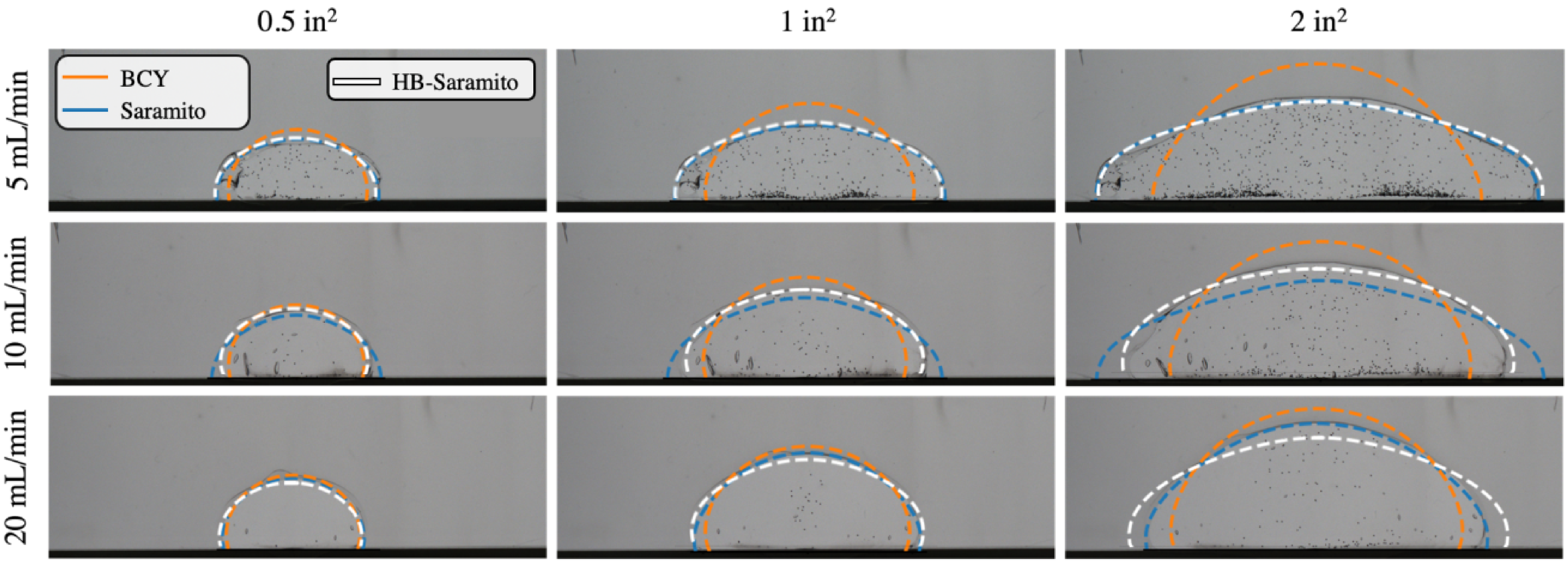

- Droplet height predictions for both flavors of the Saramito accurately capture droplet height.
  - Constant viscosity variant performs a bit better at the highest flow rate considered
- BCY model tends to overestimate droplet height

# Droplet dimensions computed from 3D simulations




- HB-Saramito model accurately predicts width for 5, 10 mL/min inflow, but overestimates at higher flow rates.
- BCY model substantially underestimates droplet width at low to moderate (5-10 mL/min) inflow.

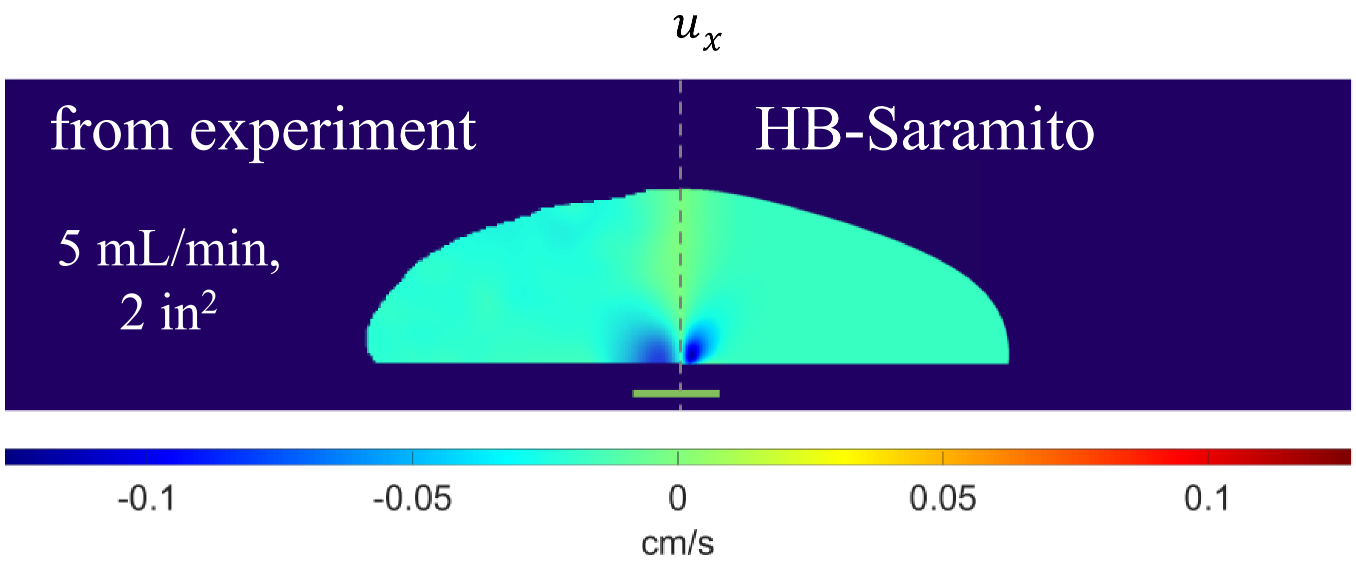
# Droplet shape computed from 3D simulations

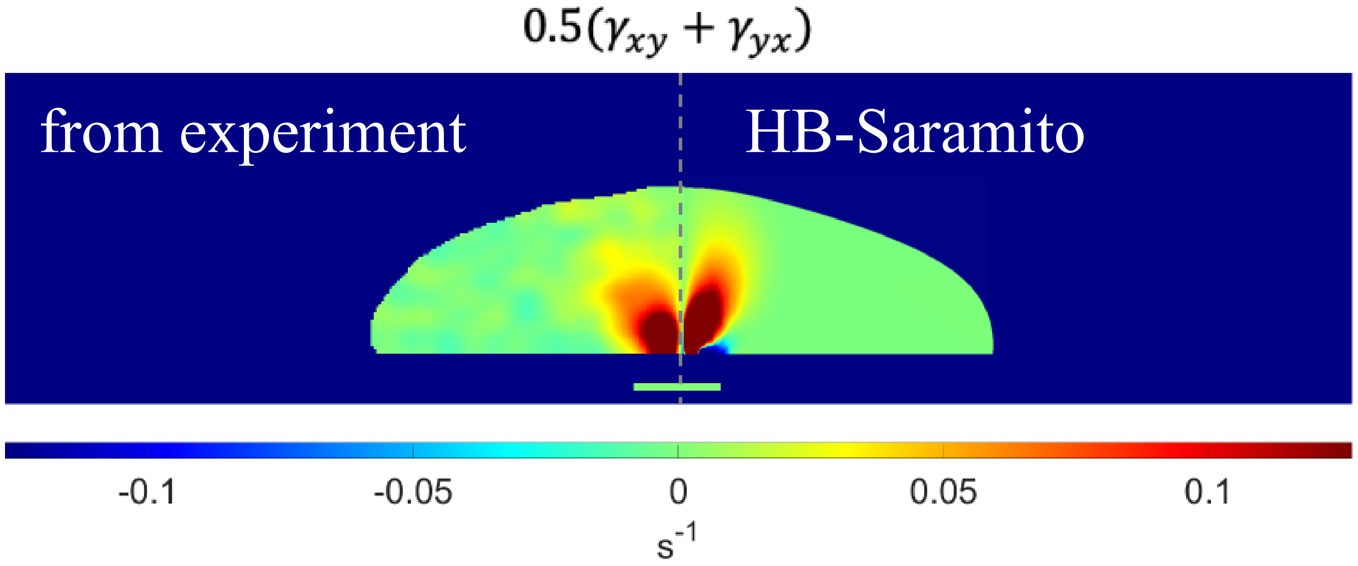



- Experimental droplet transitions from round triangular as volume is increased.
  - For a fixed droplet volume, higher flow rate leads to a rounder droplet.
- The Saramito and HB-Saramito models predict this behavior (though imperfectly).
  - BCY model struggles to show transition to a triangular shape at larger volumes.

# Comparison experimental shear and velocity maps to computations

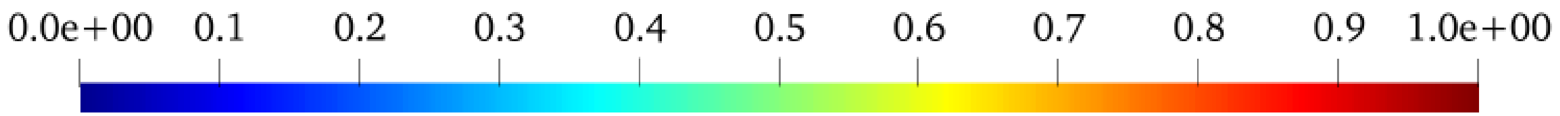
- For the available data, x-velocity and shear rate computed by the HB-Saramito model are generally in agreement with experimental values
- Differences manifest near the inlet region:
  - Near-wall velocity is underestimated
  - Computations predict a shear-rate reversal which is not observed experimentally
  - This indicates slip near the inlet is underestimated

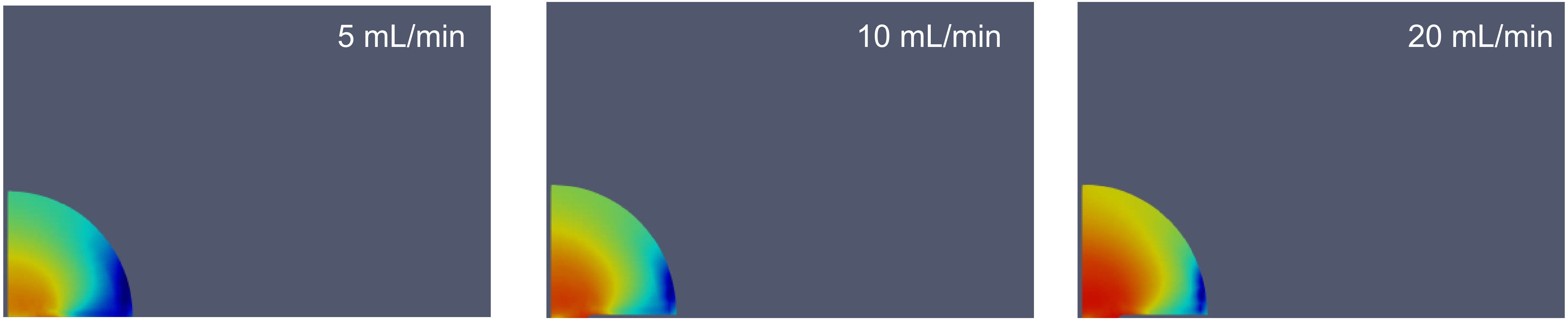


# Yield coefficient computed by HB-Saramito model

$$\mathcal{S}(\boldsymbol{\sigma}, \tau_y) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right)^{\frac{1}{n}}$$




- $S = 0$ indicates solid-like behavior, $S > 0$ → fluid-like
- Unyielded region ($S = 0$) appears near the edges of the droplet and grows at the volume increases
- Increasing flow rate associated with a larger degree of fluid-like behavior, particularly near the fluid inlet.

# Summary and conclusion

- Both Saramito and HB Saramito models yielded accurate predictions for droplet height.
  - Predicting droplet width is more difficult – both EVP models considered were more accurate than the BCY model, though neither Saramito-type model was decisively more accurate than the other.
  - Shear rate and horizontal velocity computed from the HB-Saramito model generally agree with available experimental data.
    - Noticeable differences near the fluid inlet likely due to underestimation of local fluid slip on boundaries.
- Ongoing efforts:
  - Hele-Shaw and level set implementations of EVP models
  - Computations over a range of fluid properties for the mold filling scenario
  - Confined free-surface flows over an obstruction

J. McConnell, et al., “Computational modeling and experiments of an elastoviscoplastic fluid in a thin mold-filling geometry,” to be published, JNNFM, June, 2022

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