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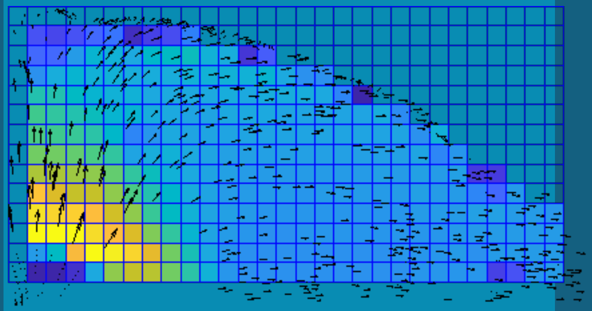
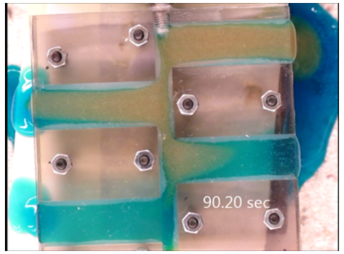
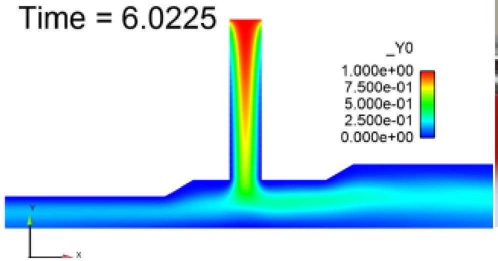
Numerical simulations of free -surface flows of a Carbopol solution







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U.S. DEPARTMENT OF ENERGY NNSA

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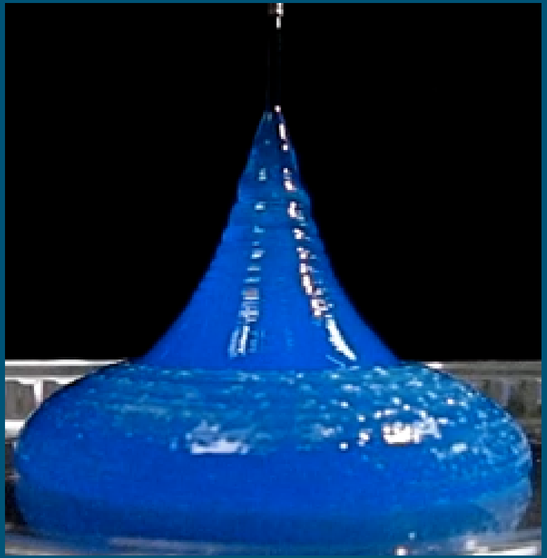
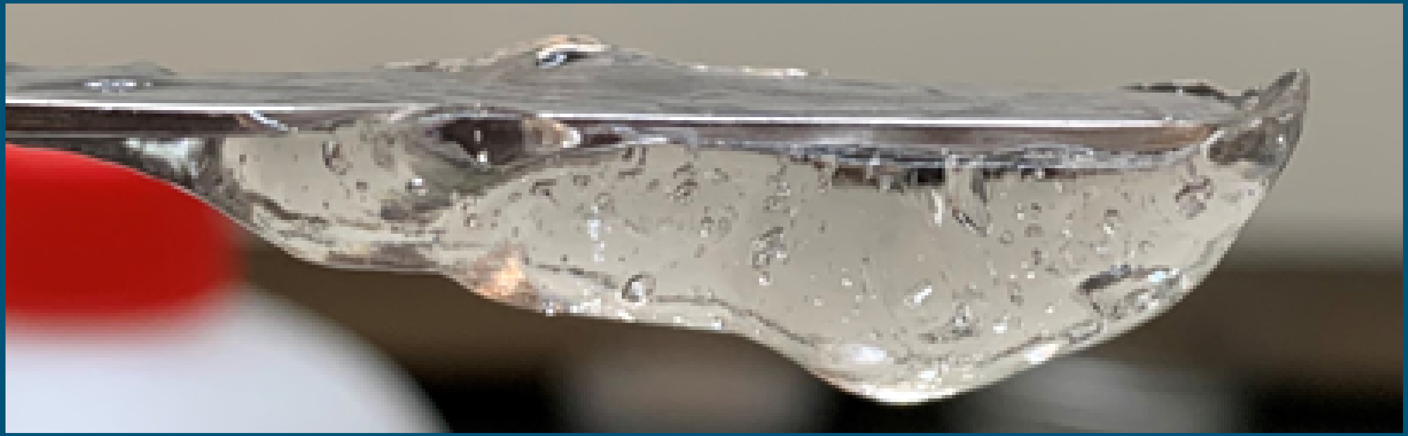
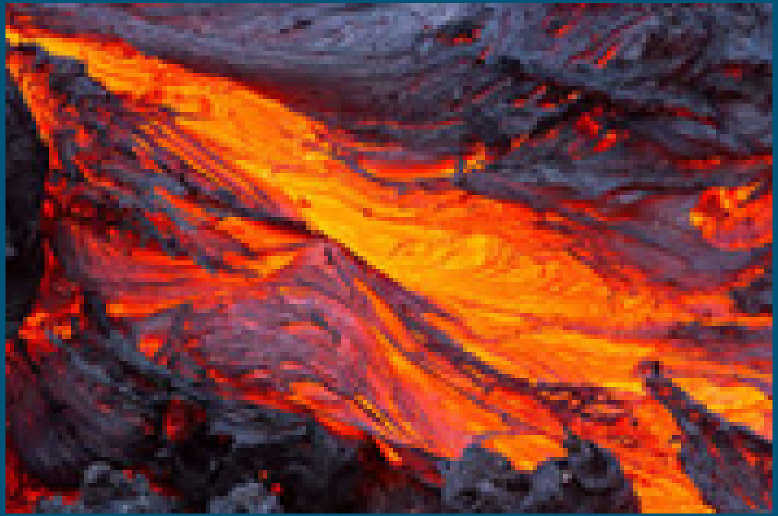
Motivation for studying yielding fluids







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

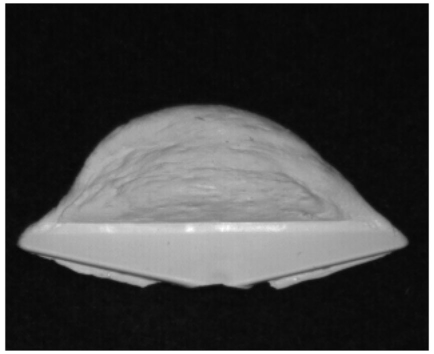
Why is this needed?

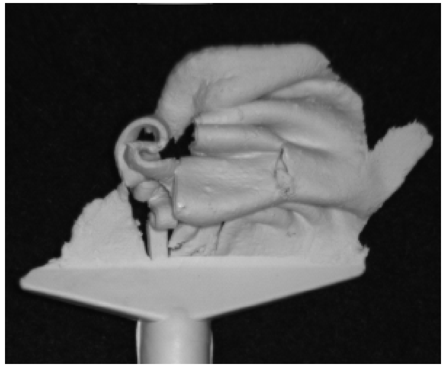
- Accurate predictions of surface profiles and spreading dynamics for flowing systems

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

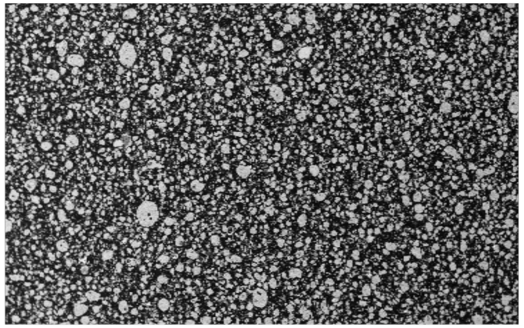
- Ramp viscosity arbitrarily high to "solidify" a fluid
- Does not accurately preserve the stress state that develops in the fluid
- One way coupling between fluid and solid codes

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

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

$$\frac{1}{G}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \overbrace{\mathbf{u} \cdot \nabla \boldsymbol{\sigma} - \nabla \mathbf{u} \cdot \boldsymbol{\sigma} - \boldsymbol{\sigma} \cdot [\nabla \mathbf{u}]^T}^{\overset{\nabla}{\boldsymbol{\sigma}}}\right) + \frac{1}{\eta}\mathcal{S}(\boldsymbol{\sigma}, \tau_y)\boldsymbol{\sigma} = 2\dot{\gamma}$$

$$\mathcal{S}(\boldsymbol{\sigma}, \tau_y) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right)$$ Saramito yield model

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.

2D mold-filling simulations

Constitutive models

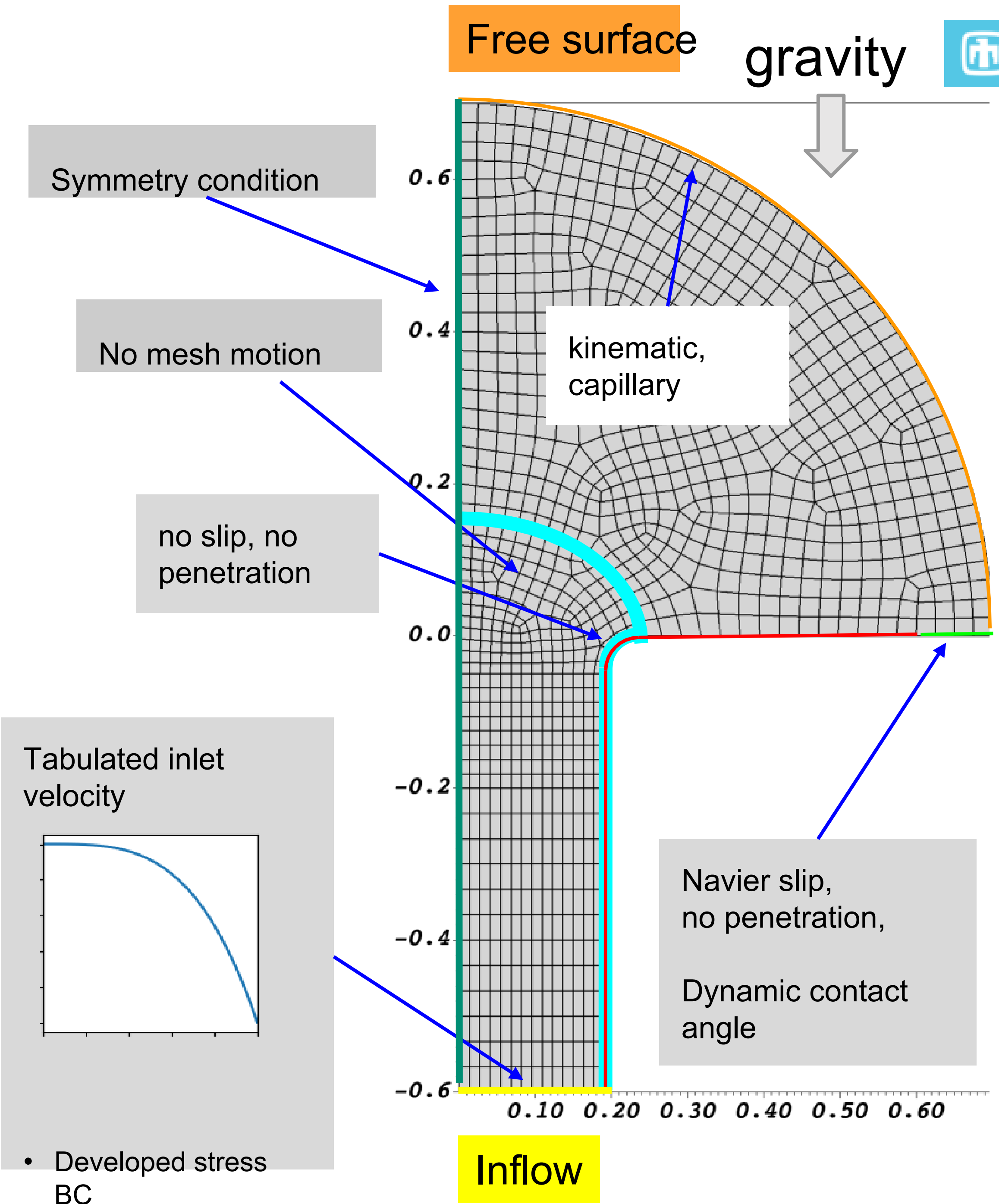
- Saramito-Oldroyd-B (EVP)
- Bingham-Carreau-Yasuda (generalized Newtonian)

Computations

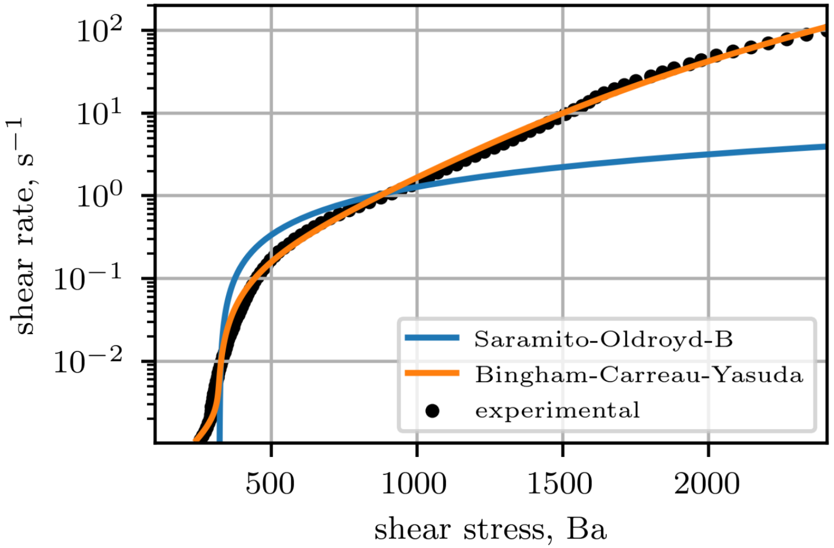
- Finite element method in Goma
- Arbitrary Eulerian-Lagrangian moving mesh framework

Validation Experiments

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



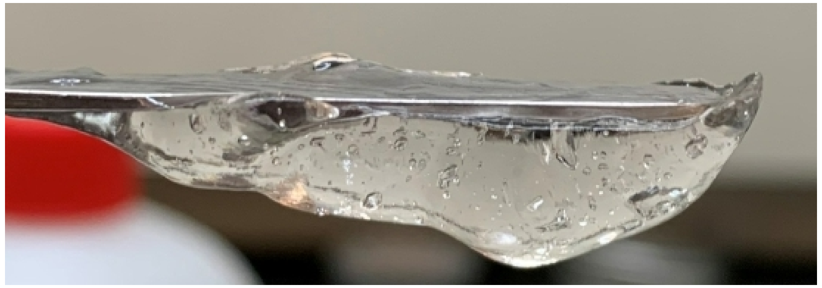
Characterization of Carbopol and parameter fitting



Bingham-Carreau-Yasuda (BCY)

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

Carbopol %	μ_0, (Pa•s)	μ_∞, (Pa•s)	b (s^{-1})	a	n	τ_y, (Pa)
0.3%	217.15	0.018	3.112	0.966	0.190	31.21



Saramito-Oldroyd-B

$$\frac{1}{G}\left(\frac{\partial \boldsymbol{\sigma}}{\partial t} + \overset{\triangledown}{\boldsymbol{\sigma}}\right) + \frac{1}{\eta}\mathcal{S}(\boldsymbol{\sigma}, \tau_y)\boldsymbol{\sigma} = 2\dot{\gamma}$$

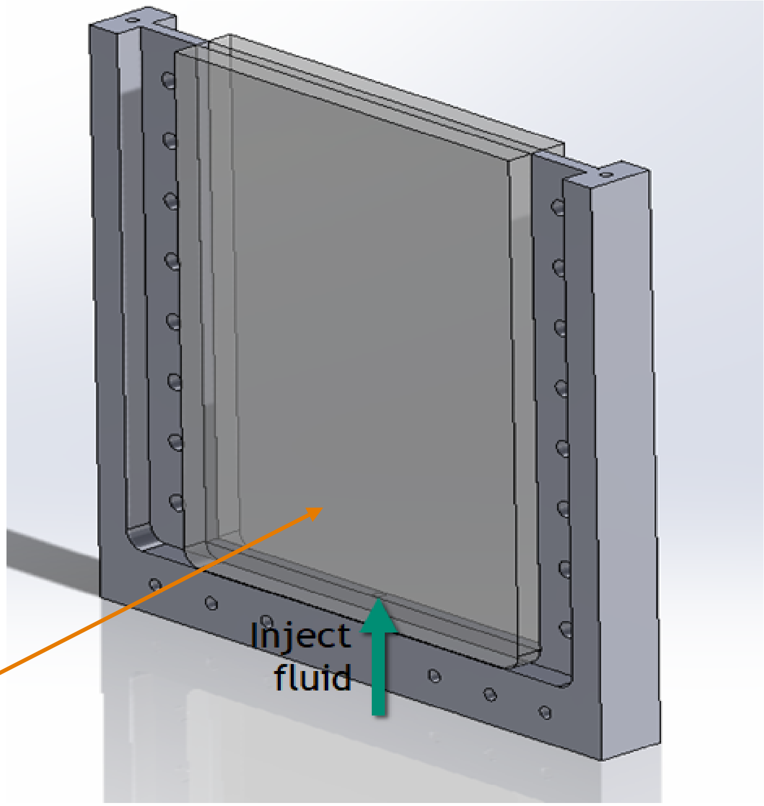
Carbopol %	η, (Pa•s)	τ_y, (Ba)	G, (s)
0.3%	52.85	32.10	576.9

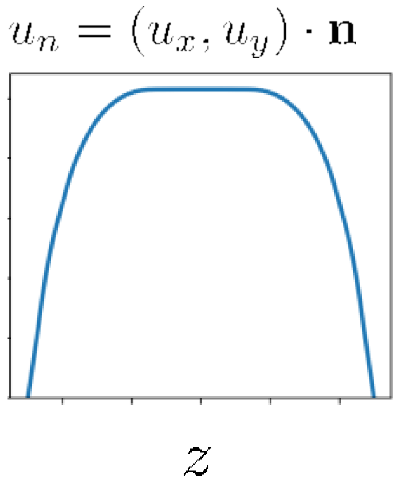
- Small amplitude stress vs. strain curve, gives the elastic modulus, *G.*
- Other rheological parameters were determined using a nonlinear least squares fit.

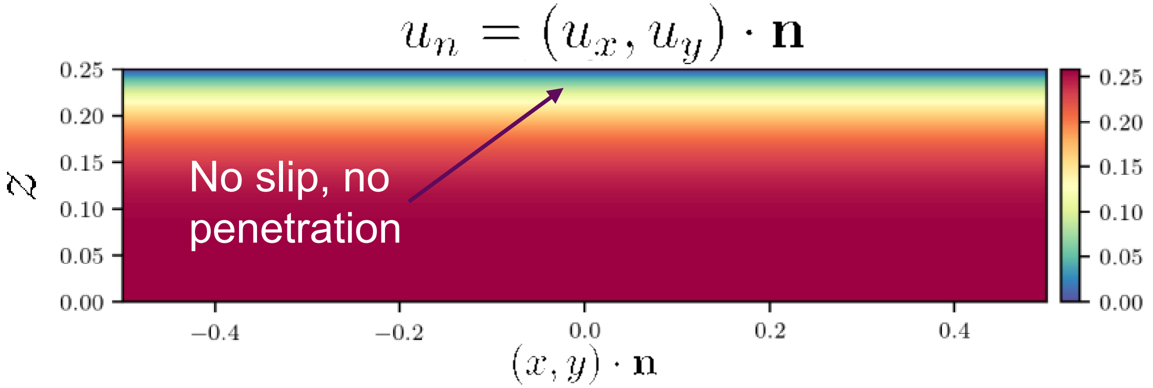
Mold-filling geometry: Flow between two thin plates

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 in computations
  - Drag force due to unresolved stress needs to be modeled







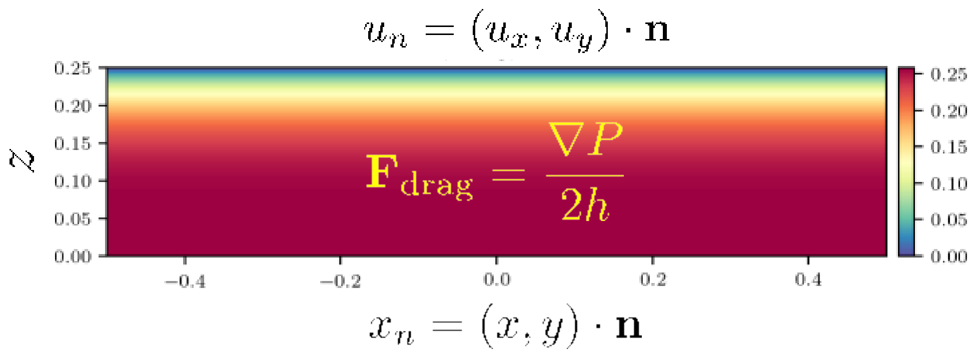
Drag model

- Drag model accounts for force due stress caused by the presence of a shear gradient in the unresolved dimension
- Included in flow model as a momentum source term and has the following form:

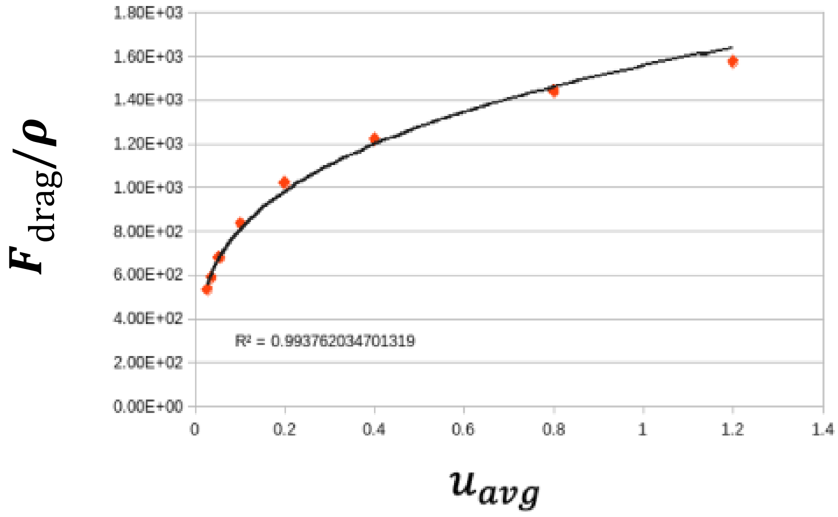
$$\mathbf{F}_{\mathrm{drag},i} = a\mathbf{u}_i\left(\sqrt{|\mathbf{u}|^2+\epsilon}\right)^{b-1}$$

a, b are fitted parameters, $\epsilon = 10^{-4}$

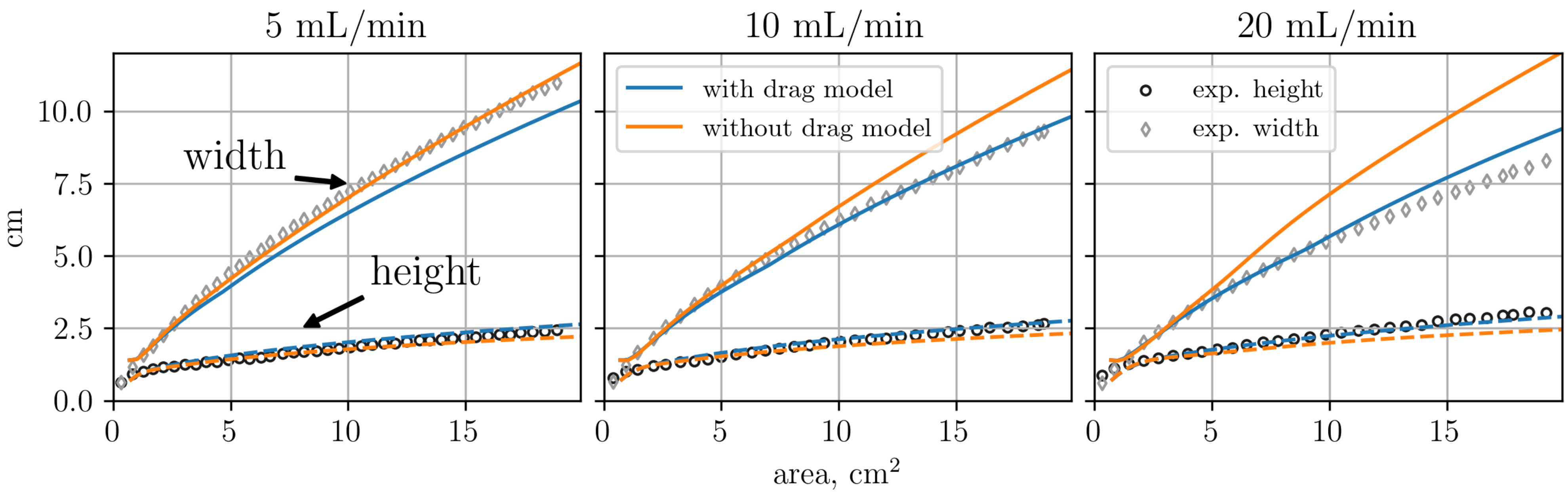
- Computations for obtaining drag model parameters are done with the Bingham-Carreau-Yasuda (BCY) generalized Newtonian model



1. Perform computations for a planar Poiseuille system over a range of ∇P values,
2. compute u_{avg} and average force due to shear stress, $\boldsymbol{F}_{\mathrm{drag}}$
3. Obtain values of a, b via regression to get $\boldsymbol{F}_{\mathrm{drag}}(u_{avg}; a, b)$

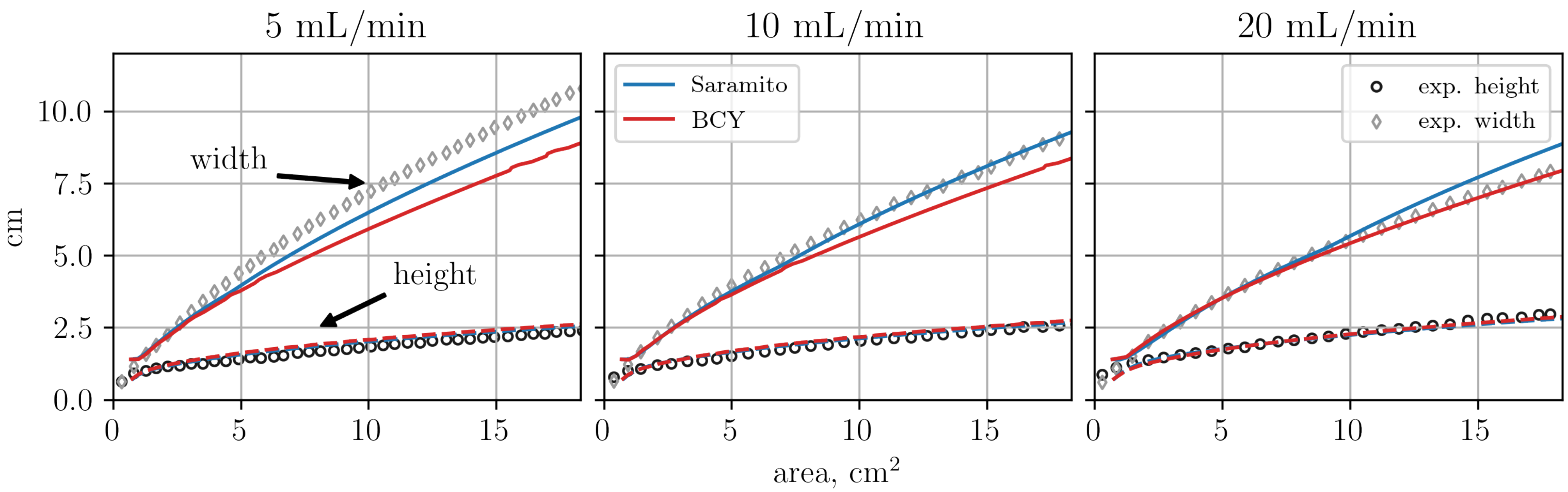


Comparing computed and observed blob dimensions



- Predicted droplet dimensions are more accurate when drag model is used for the 10 and 20 mL/min computations
  - 5 mL/min case performs worse with drag model; fitted BCY model likely overestimates the viscosity for this scenario

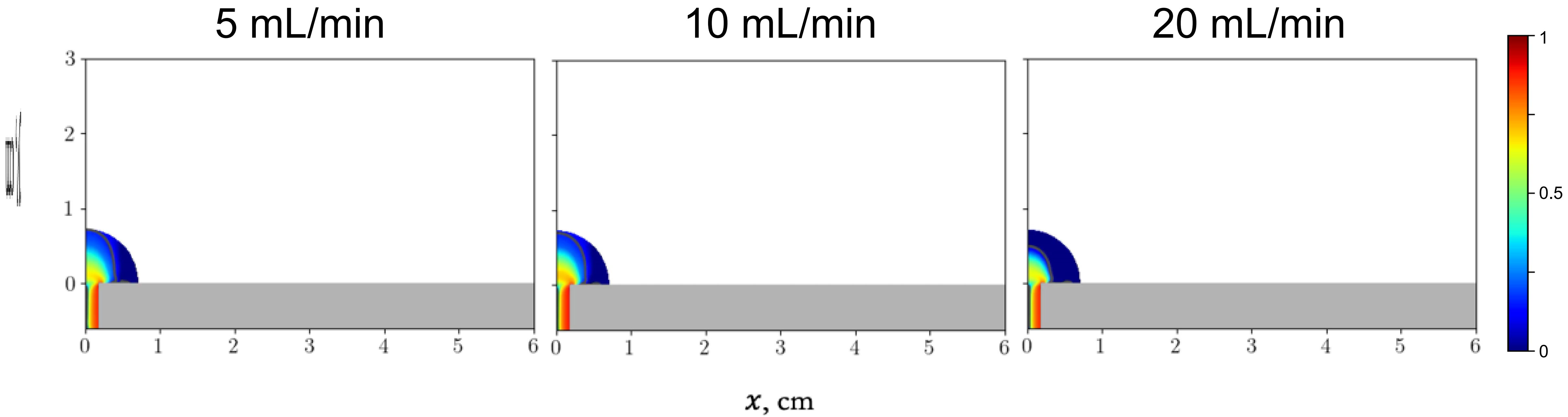
Comparing computed and observed droplet dimensions



- Dimensions computed the Saramito and BCY models are similar
  - Height computations are nearly indistinguishable
  - Width predicted by the Saramito model consistently larger (and more accurate) than BCY predictions

Computed yield coefficient

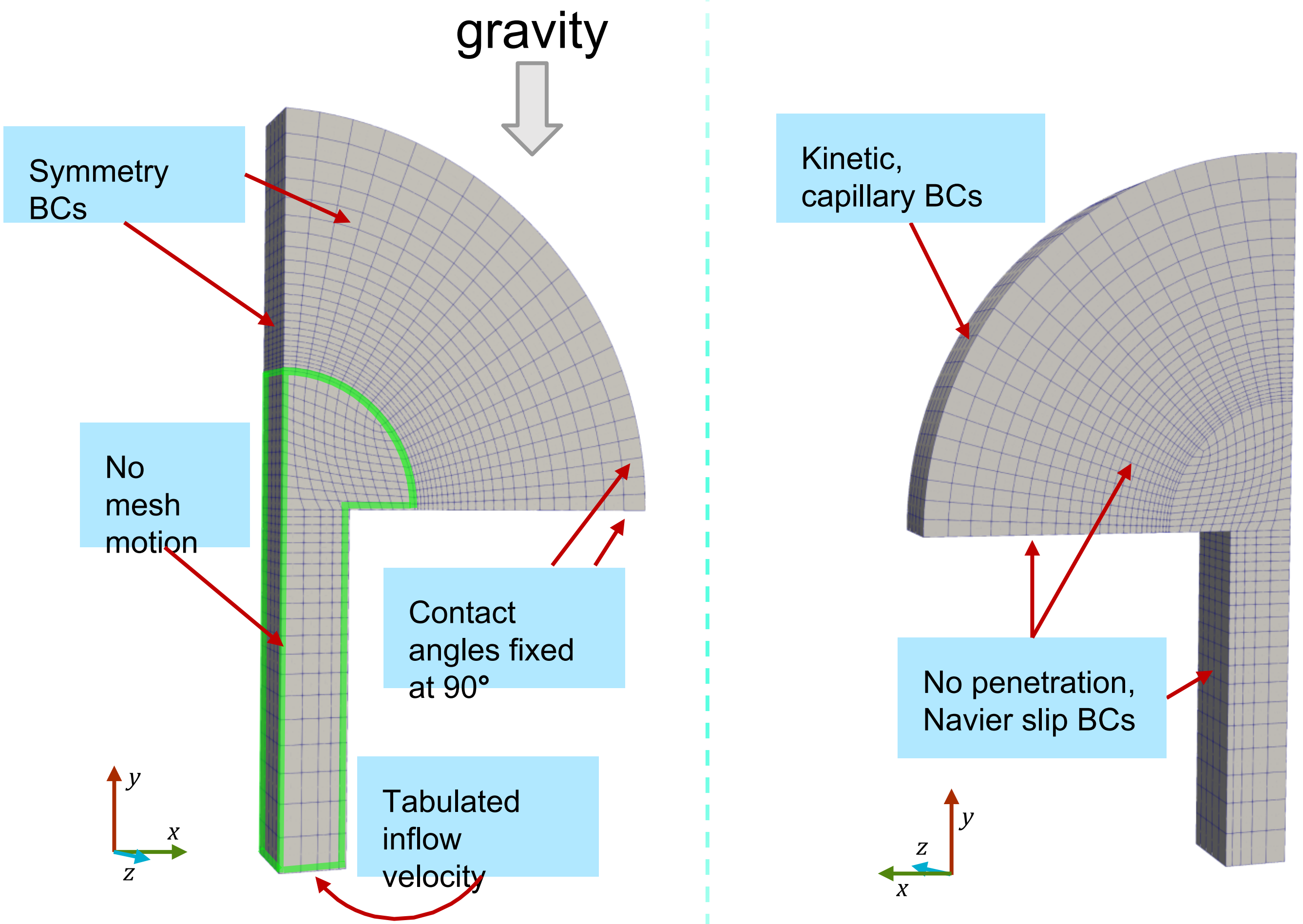
$$\mathcal{S}\left(\boldsymbol{\sigma}, \tau_{\text{yield}}\right) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_{\text{yield}}}{|\boldsymbol{\sigma}_d|}\right),$$



- Time is scaled by flow rate
- Gray lines indicate computed yield boundary

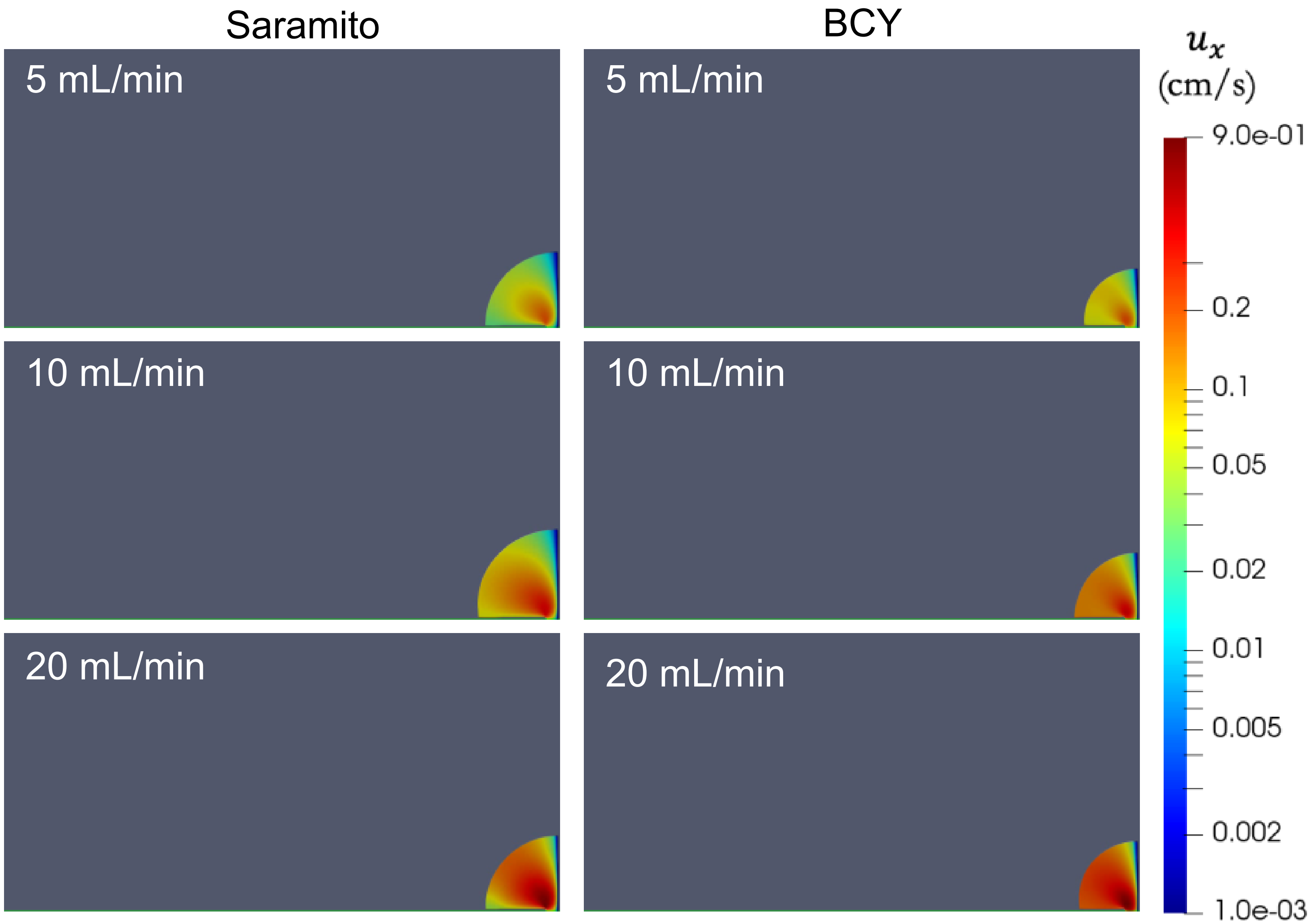
3D Mold-filling simulations

- 3D computations preclude the need for modeling unresolved stresses
  - Substantially more expensive than 2D simulations
- Boundary conditions imposed for 3D simulations are similar to 2D computations with the following key differences:
  - Navier slip condition imposed on all solid boundaries
  - Fixed contact angle imposed on all contact edges

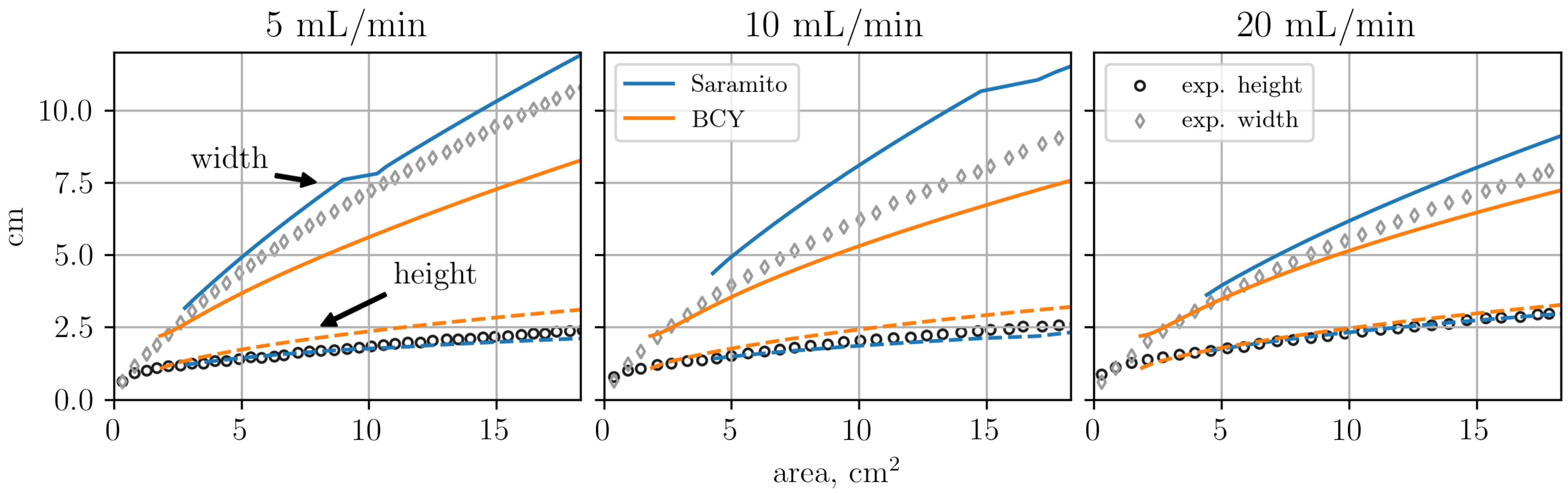


3D computations

- Pictured: x-velocity at droplet symmetry plane
- Time is scaled by flow rate
- In all instances, the Saramito model predicts a droplet shape that is shorter and longer than the BCY model
    - Differences in droplet dimensions between model in 3D is larger than what we see in 2D computations.



Droplet dimensions computed from 3D simulations



- Saramito model:
  - Height predictions are close to experimental values
  - Width is overestimated, sometimes substantially
    - Seems to be due to a lack of explicit shear thinning in model
- BCY model:
  - Height predictions are close, but often overestimate experimental values
  - Width is underestimated
    - Could be due to several factors, including a zero-shear viscosity that is too large, too much slip at solid surfaces, *etc.*

Confined free-surface flow around an obstruction

Constitutive model

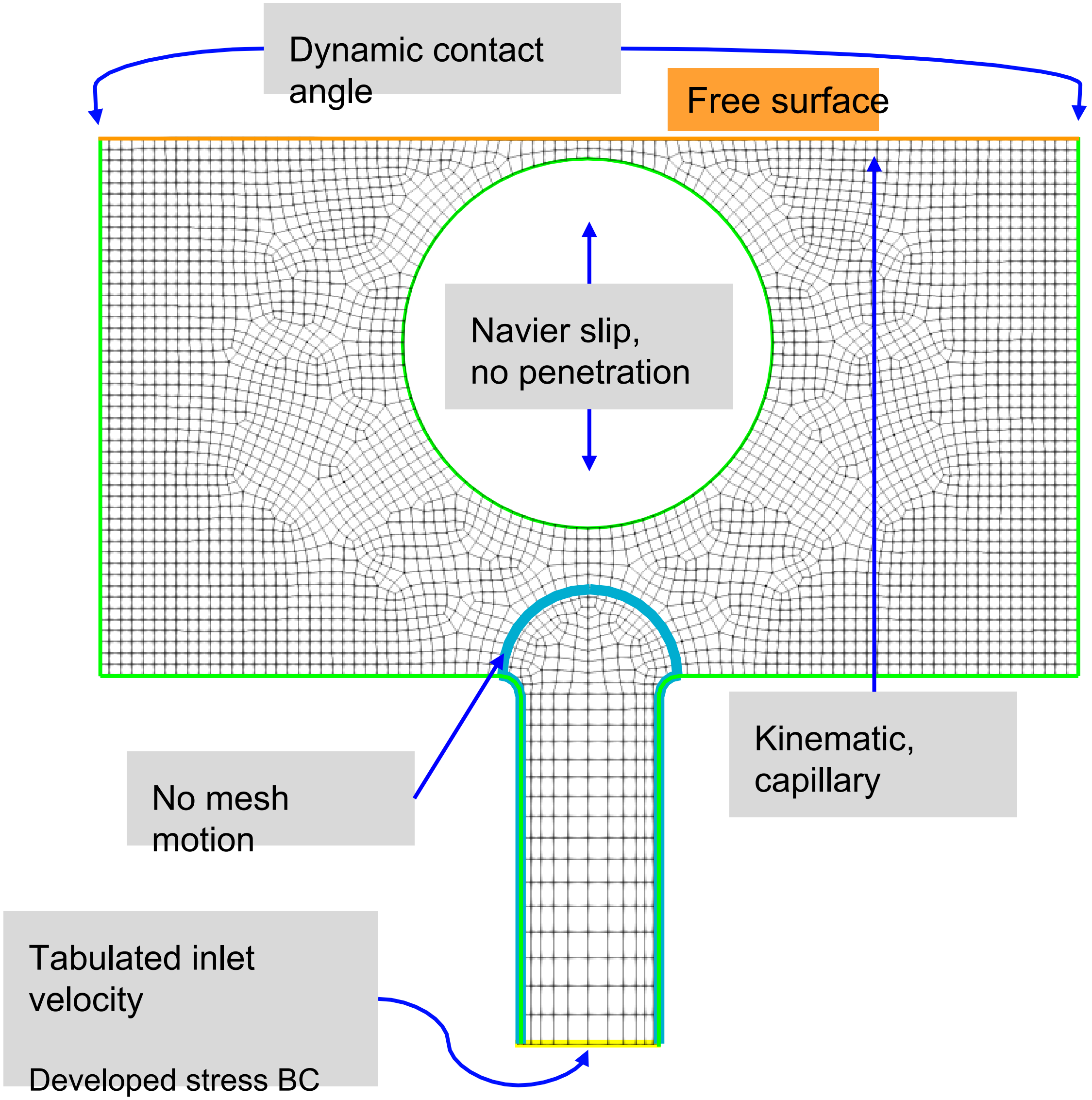
- Herschel-Bulkley Saramito-Oldroyd-B (EVP)

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

- Parameters (0.3% Carbopol):
  - $\tau_y = 21.35$ Pa
    $n = 0.495$,
    $k = 59.6$ Pa·s^n

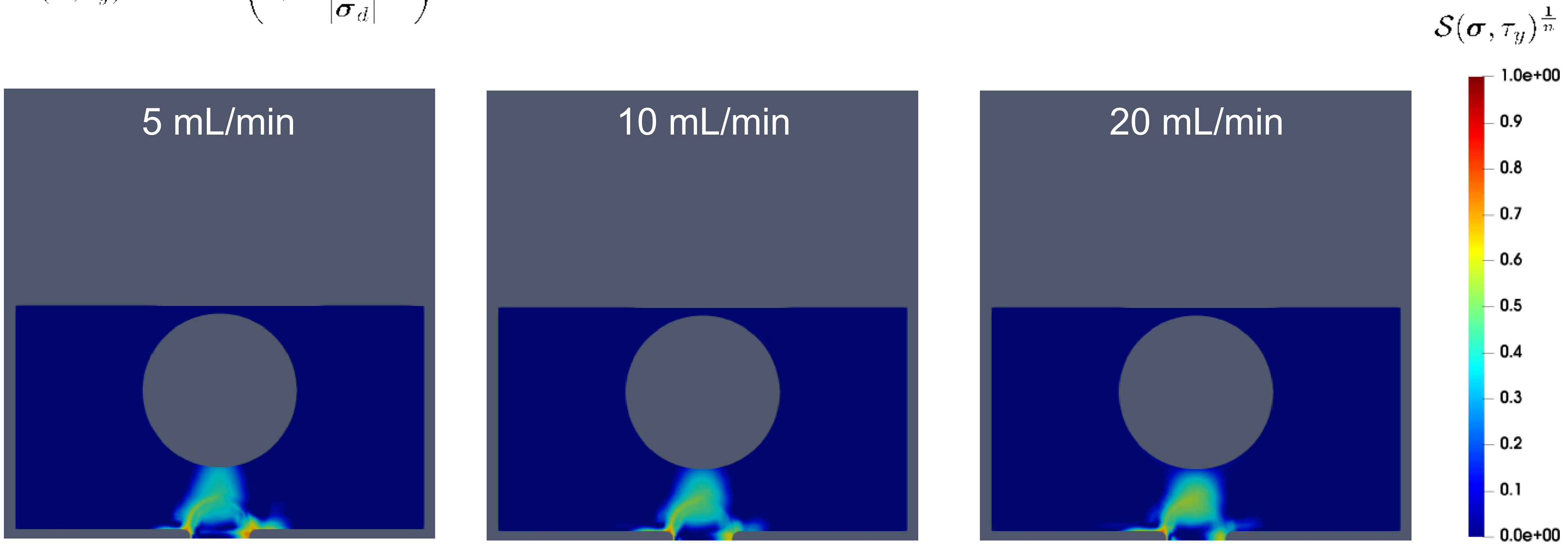
- Sphere diameter: 10 cm
- Domain width : 2.75 cm

Validation Experiments – *work in progress*



Confined free-surface flow around an obstruction

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



- Yielded regions within the domain shrink and eventually vanish as the flow rate is increased from 5 to 20 mL/min
- Computations suggest that a bubble forms near the top of the obstruction at elevated flow rates (>5 mL/min)

Conclusions and future work

- Demonstrated capability to simulate free surface (mold filling) flows of a yielding fluid
  - 2D:
    - Accuracy of droplet shape predictions in 2D are improved overall by including an unresolved drag model
    - Drag model worsened at the lowest flow rate considered, possibly due to underestimating fluidity at these flow rates
  - 3D:
    - Getting accurate flow behavior predictions is a continuing challenge – several factors have contributed to this including boundary condition complexity, lack of explicit shear thinning in implemented EVP model

- Working on:
  - Improving 3D mold-filling computations
    - Added explicit shear thinning to Saramito model – 3D simulations in progress
  - Computations over a range of fluid properties for the mold filling scenario
  - Confined free-surface flows over an obstruction