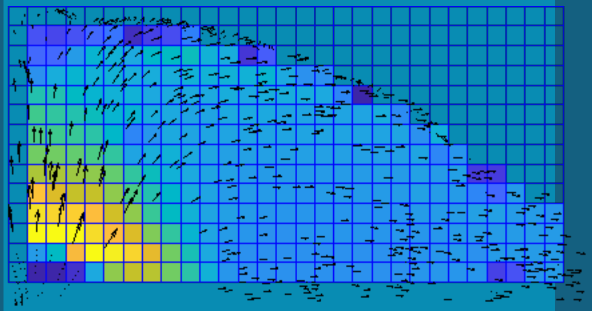
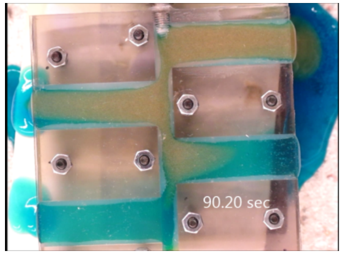
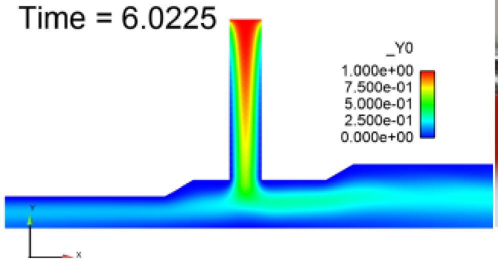
SAND2021-8875C

Sandia National Laboratories

Computational Models for Fluid-to-Solid Transitions in Yield Stress Fluids







Josh McConnell, Rekha Rao (SNL)
Pania Newell (University of Utah)
Weston Ortiz (UNM)

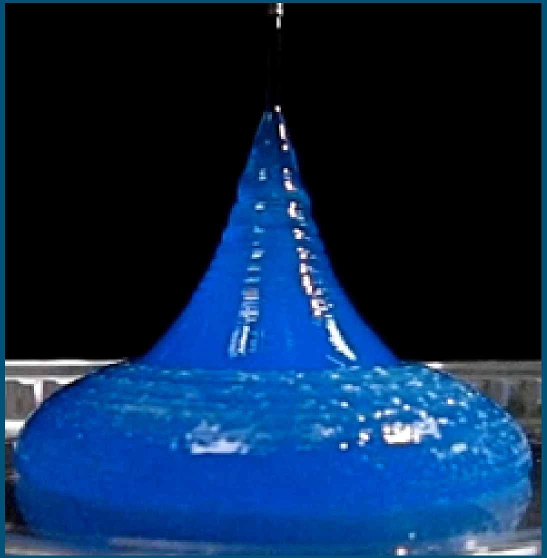
16th US National Congress on Computational Mechanics

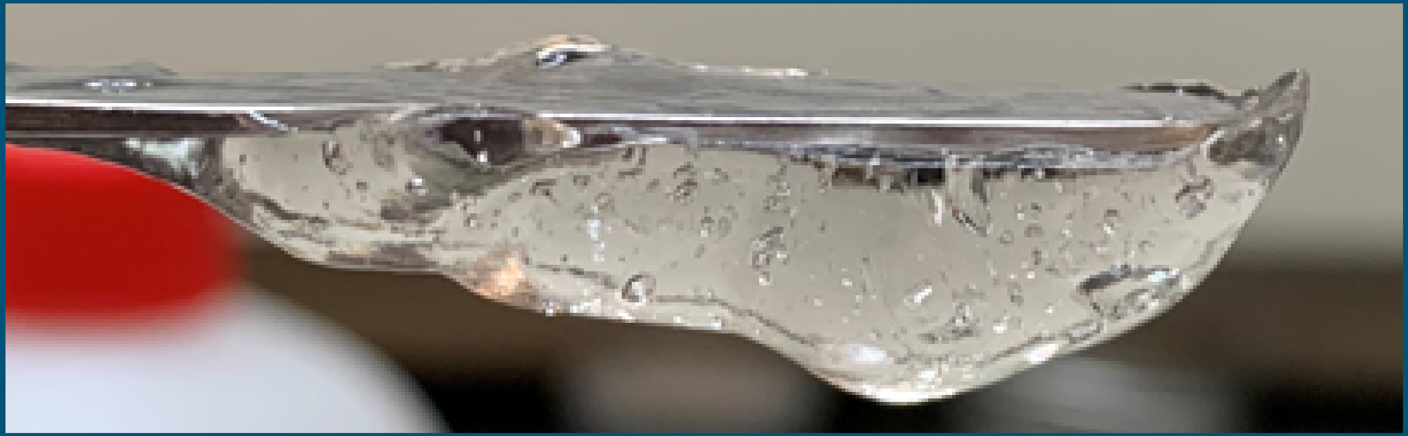
July 26, 2021

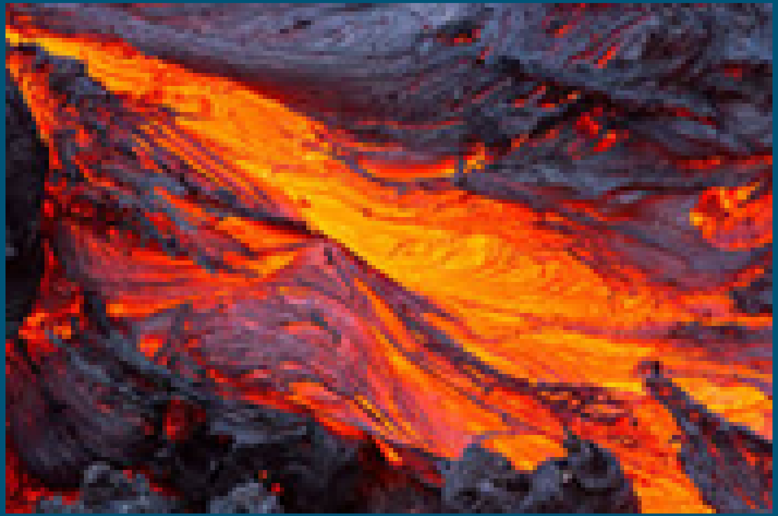
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

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

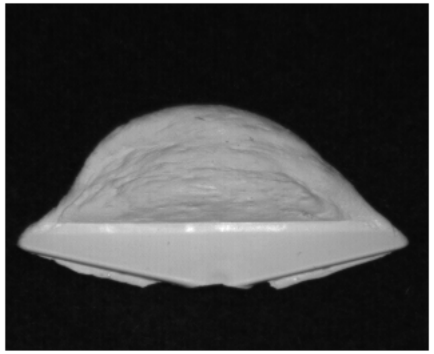
Why is this needed?

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

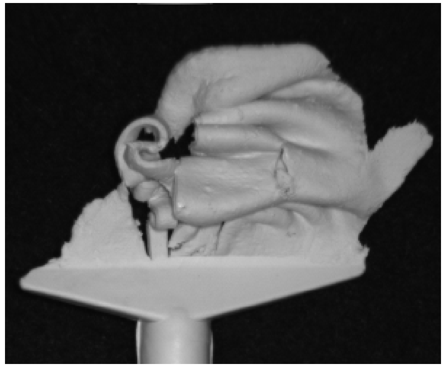
Current state-of-the-art in production codes:

- 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.

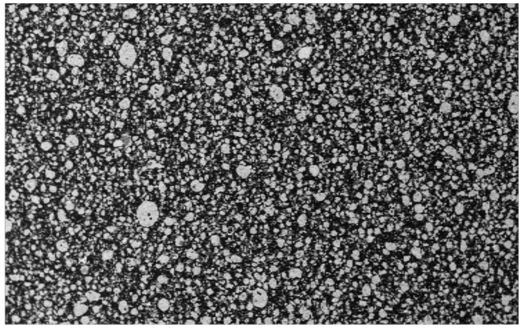


2.5 mm shot, 100% injection speed



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

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

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

Model validation: Planar Poiseuille flow

Analytical solution

$$\boldsymbol{\sigma}_{xy} = (\nabla_x P) y$$

$$\boldsymbol{\sigma}_{xx} = 2\lambda \frac{(\nabla_x P)^2}{\eta} y^2$$

$$|\boldsymbol{\sigma}_{\boldsymbol{d}}| = \sqrt{\boldsymbol{\sigma}_{xy}^2 + \boldsymbol{\sigma}_{xx}^2/4}$$

$$u(y) = \begin{cases} u_y(y) & |y| > y_c \\ u_y(y_c) & |y| \le y_c \end{cases}$$

$$y_c = \pm \frac{h}{a\sqrt{2}} \sqrt{\sqrt{1 + 4\left(\frac{a\tau_y}{h \nabla_x P}\right)^2} - 1}$$

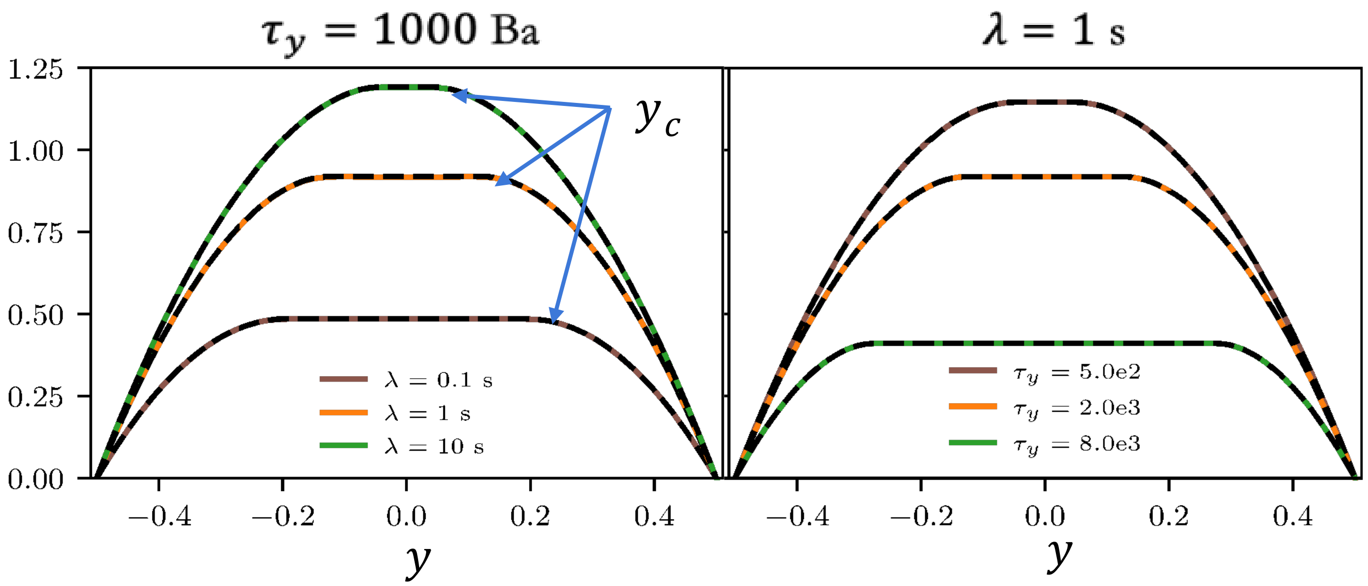
$$u_y = \frac{\nabla_x P}{2\eta}(y^2 - h^2) + \frac{\tau_y}{\lambda \nabla_x P}\left[\sinh^{-1}(ay/h) - \sinh^{-1}(a)\right].$$

$$a = \lambda h \nabla_x P / \eta$$

- Colorful lines are computed solutions, black dashed lines are exact solutions

$\nabla_x P = 1000$ Ba

$h = 0.5$ cm

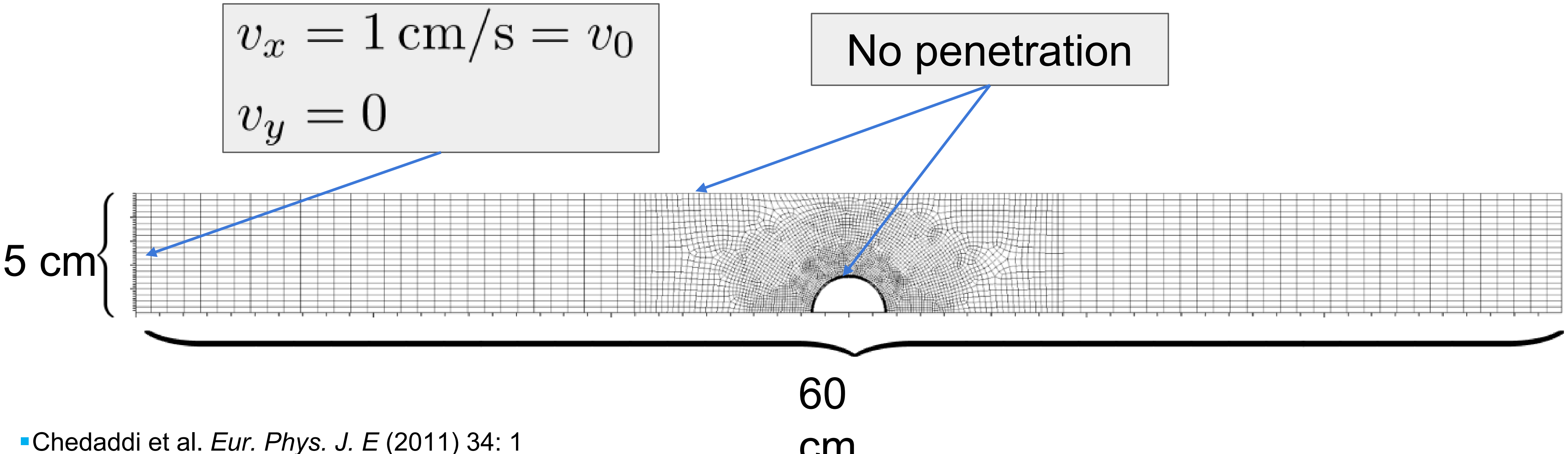


Model validation: flow past a cylindrical obstruction

- Quasi-two dimensional experiments presented from case in Cheddadi et al., 2011
- Fluid is a "wet foam," which has a yield stress, elasticity and also exhibits slip at solid boundaries

model parameters

η, (Ba•s)	τ_y, (Ba)	λ, (s)
2.6	26	0.2



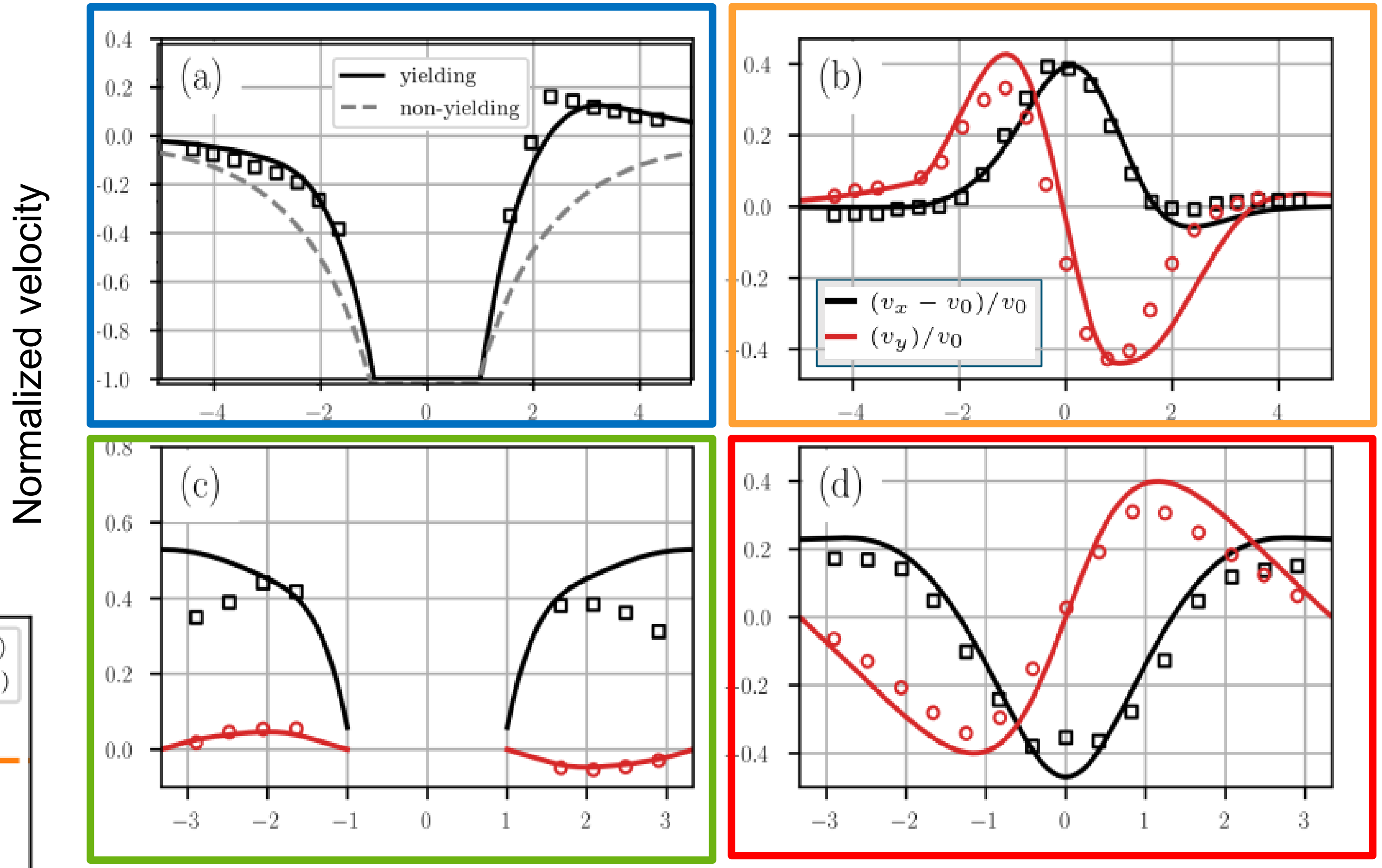
- Chedaddi et al. *Eur. Phys. J. E* (2011) 34: 1

Comparing computations to experimental observations

- Computed velocities match experiments for the most part.
- Velocity asymmetry observed for line-of-sight (a) is characteristic of a yielding fluid
- Symmetric result from the non-yielding computation (gray dashed line)

streamwise centerline

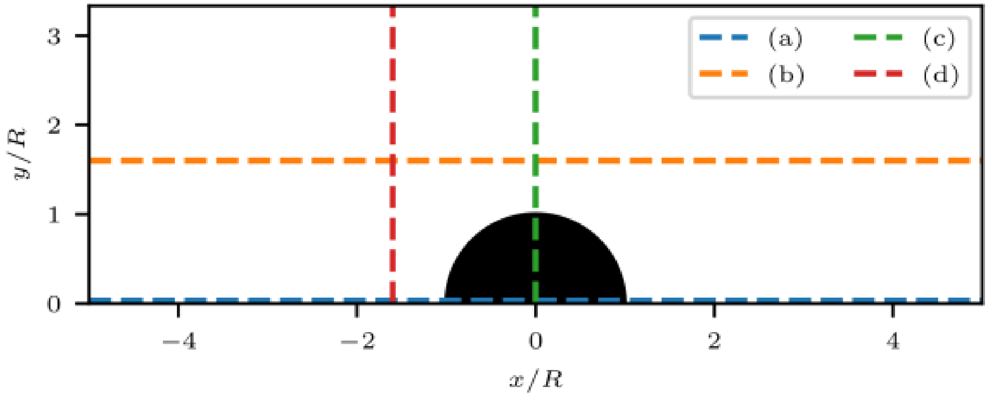
halfway to the wall



spanwise centerline

before sphere

Normalized spatial coordinate



- Chedaddi et al. *Eur. Phys. J. E* (2011) 34: 1

Mold Filling Simulation

Constitutive models

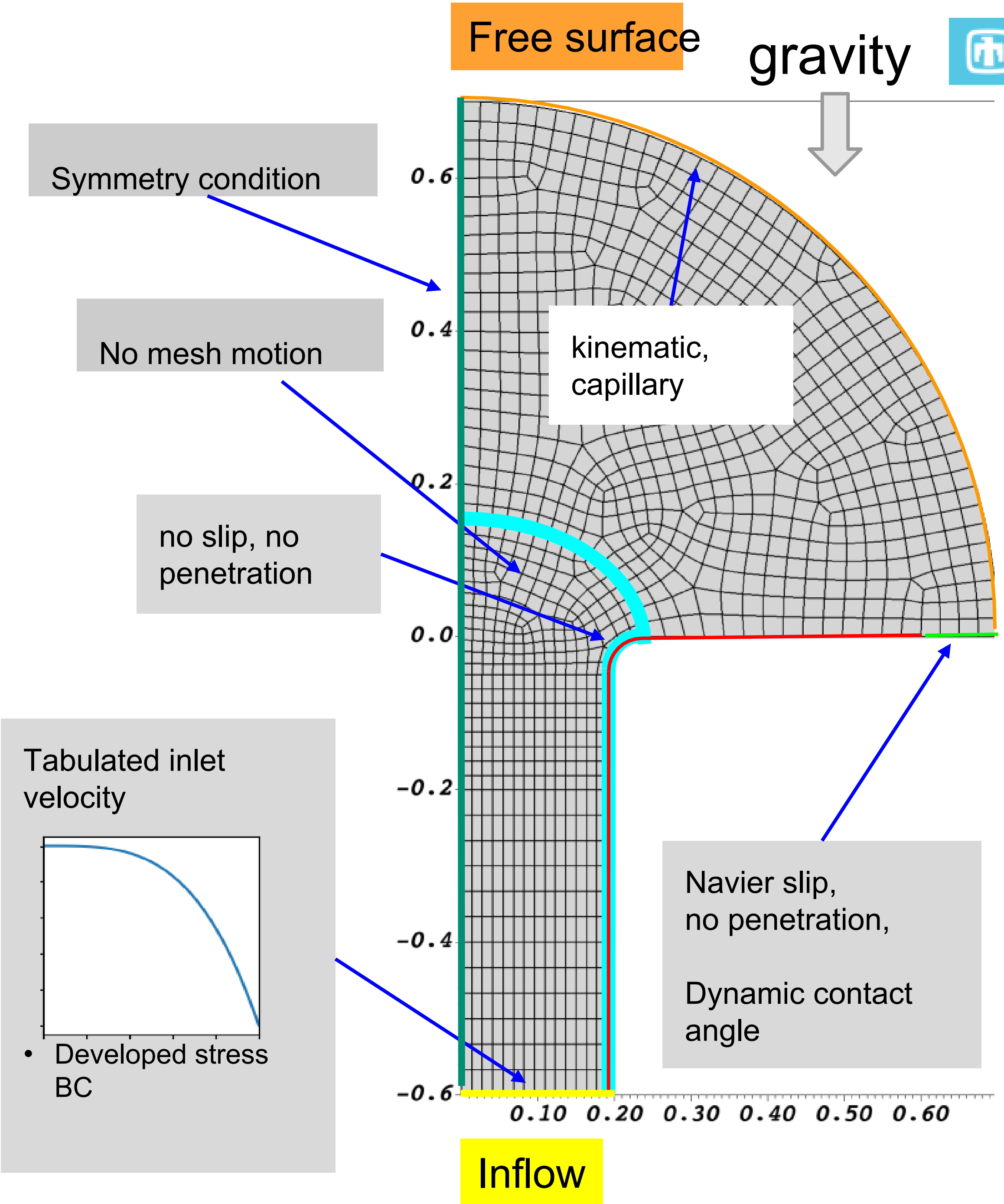
- Saramito-Oldroyd-B (EVP)
- Bingham-Carreau-Yasuda (generalized Newtonian)

Computations

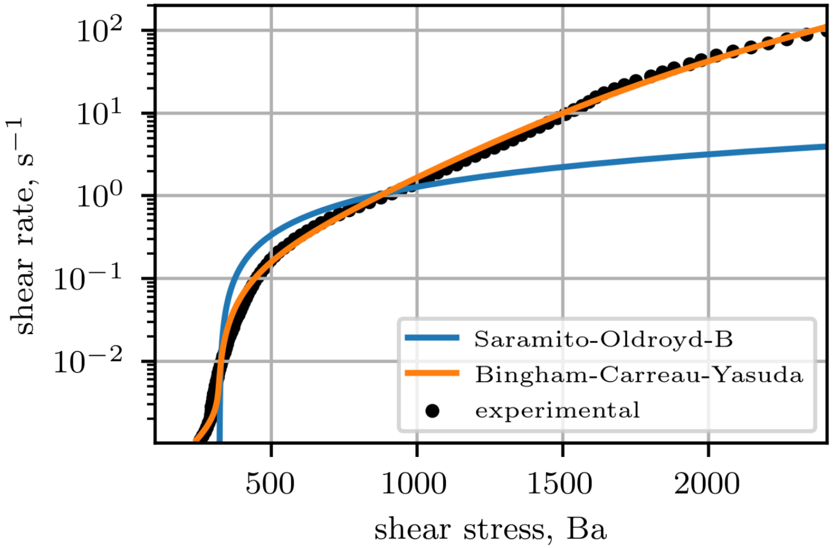
- Finite element method in Goma
- Arbitrary Eulerian-Lagrangian moving mesh framework

Validation Experiments

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



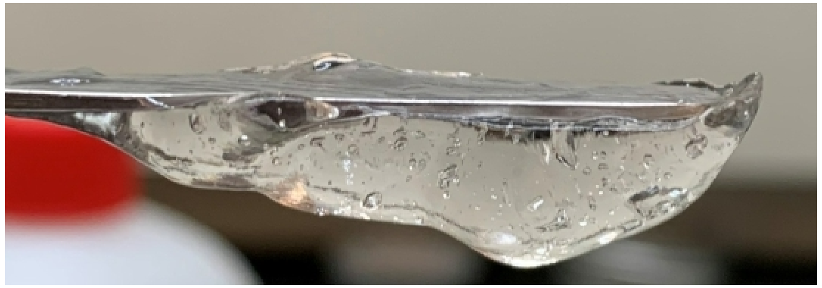
Characterization of Carbopol and Parameter fitting



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, (Ba•s)	μ_∞, (Ba•s)	b (s^{-1})	a	n	τ_y, (Ba)
0.3%	2171.5	0.18	3.112	0.966	0.190	312.1



Saramito-Oldroyd-B

$$\lambda\left[\frac{\partial \boldsymbol{\sigma}}{\partial t} + \mathbf{u}\cdot\nabla\boldsymbol{\sigma} - \boldsymbol{\sigma}\cdot\nabla\mathbf{u} - \nabla\mathbf{u}^T\cdot\boldsymbol{\sigma}\right] + \max\left[0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right]\boldsymbol{\sigma}$$

$$= \eta_{fluid}(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$$

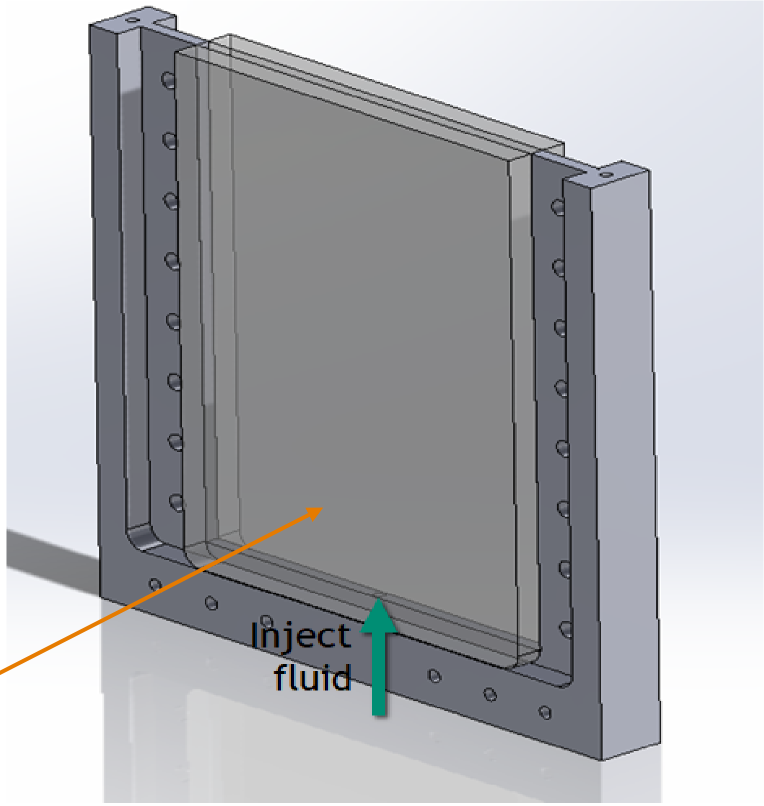
Carbopol %	η, (Ba•s)	τ_y, (Ba)	λ, (s)
0.3%	528.5	321.0	0.1102

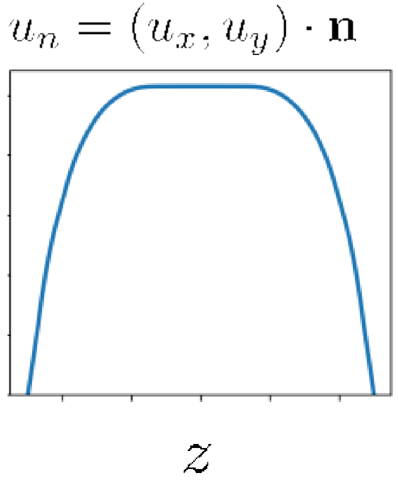
- Small amplitude stress vs. strain curve, gives the elastic modulus (G = 440 Pa).
- Other rheological parameters were determined using a nonlinear least squares fit.

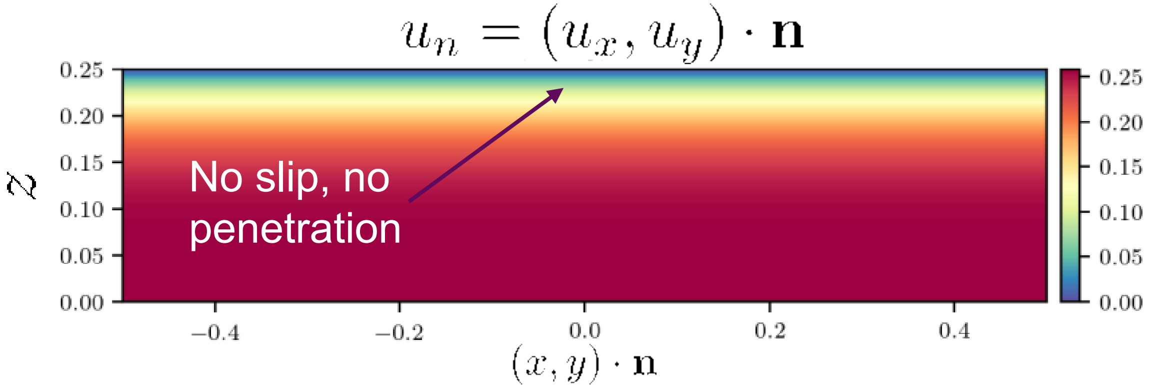
Mold filling geometry: Flow between two thin plates

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







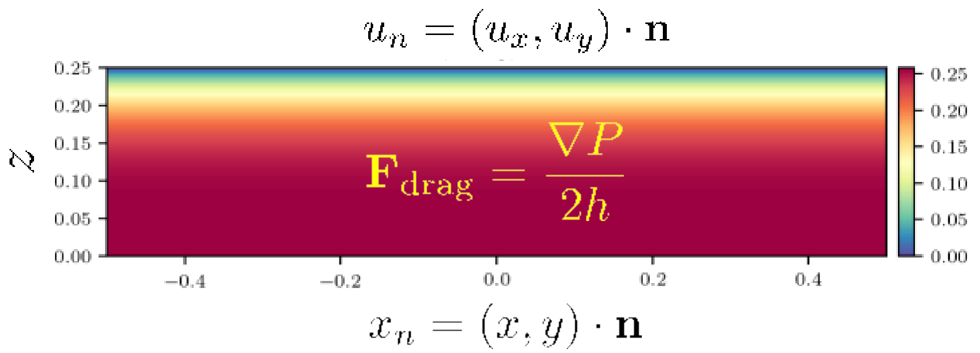
Drag model

- 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:

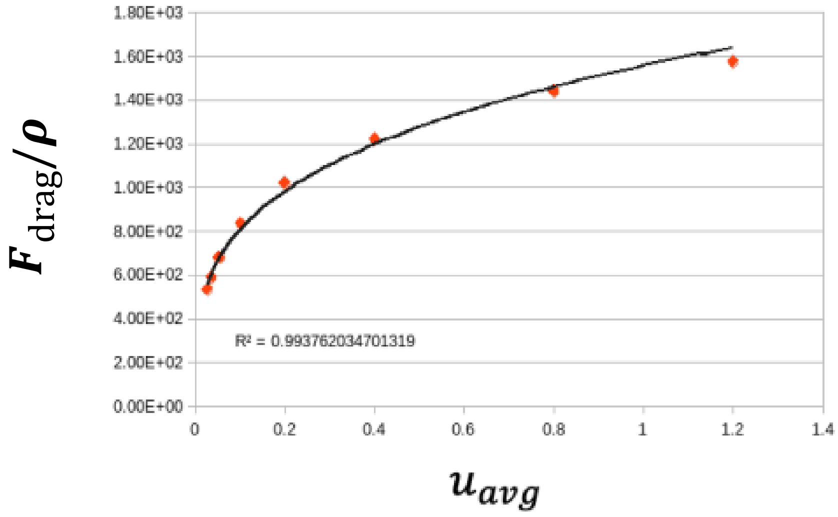
$$\mathbf{F}_{\mathrm{drag},i} = a\mathbf{u}_i \left(\sqrt{|\mathbf{u}|^2 + \epsilon}\right)^{b-1}$$

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

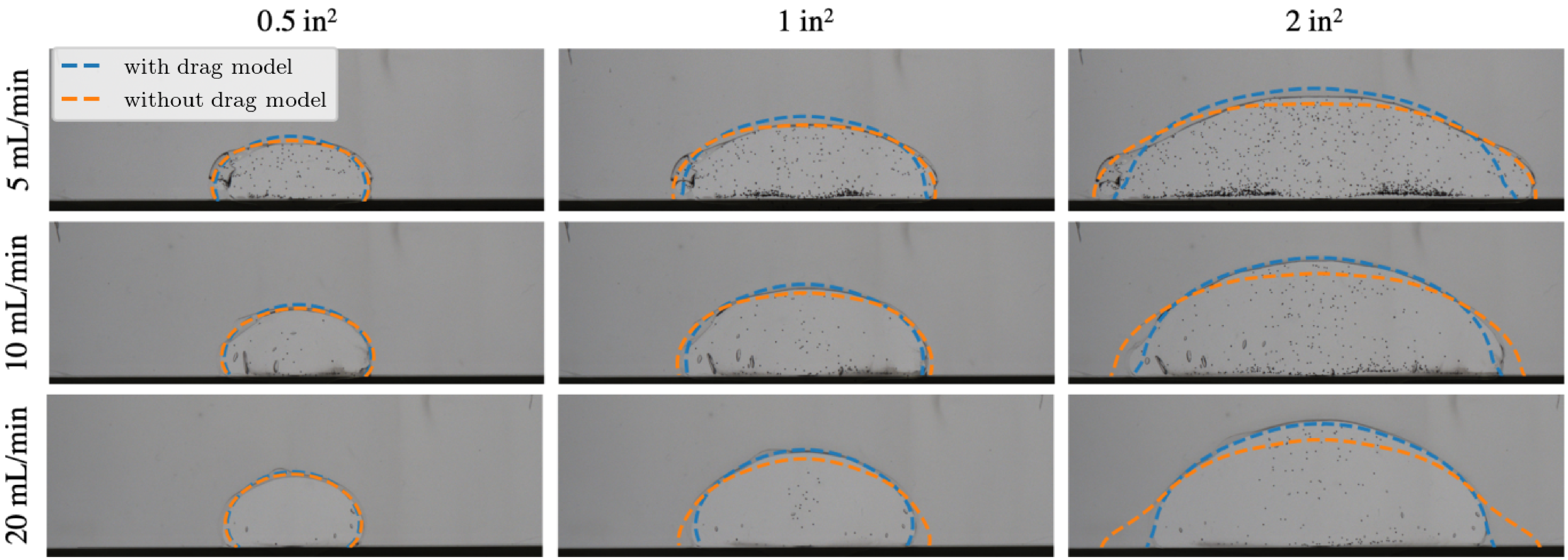
- Computations for obtaining drag model parameters are done with the Bingham-Carreau-Yasuda (BCY) generalized Newtonian model



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 $\boldsymbol{F}_{\mathrm{drag}}(u_{avg}; a, b)$

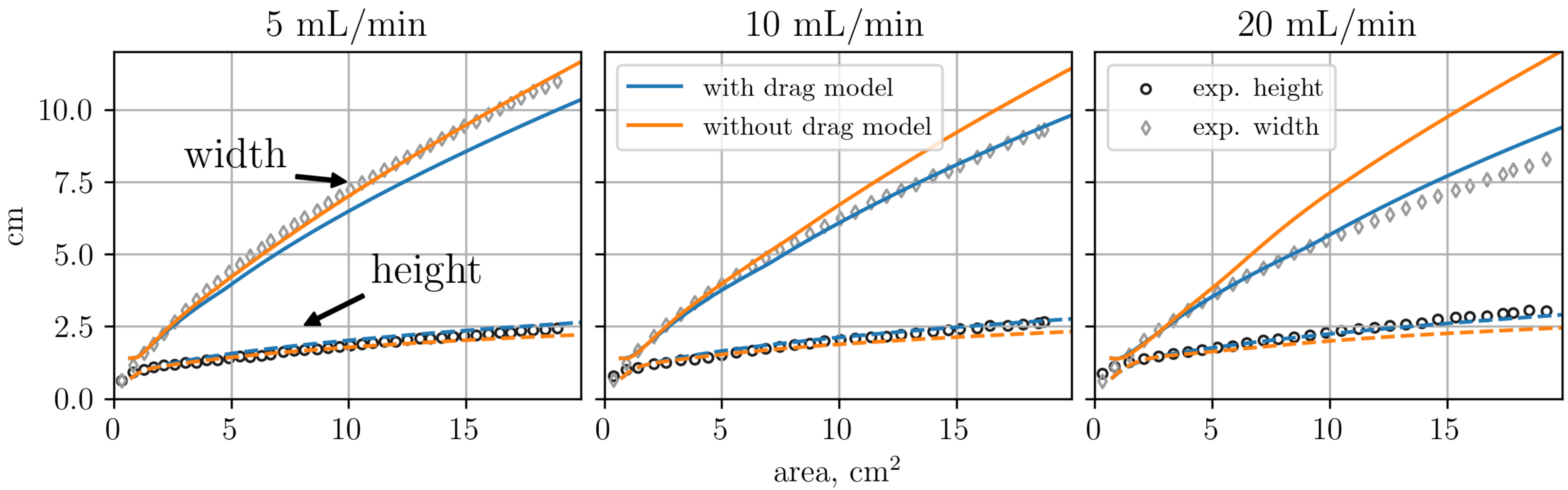


Comparing computed and observed droplet shapes



- Impact of including drag model is most apparent near the contact line
  - Drag model inhibits predicted fluid yielding near the contact line which inhibits droplet spreading
- Using the drag model improves accuracy of predicted shape for elevated flow rates

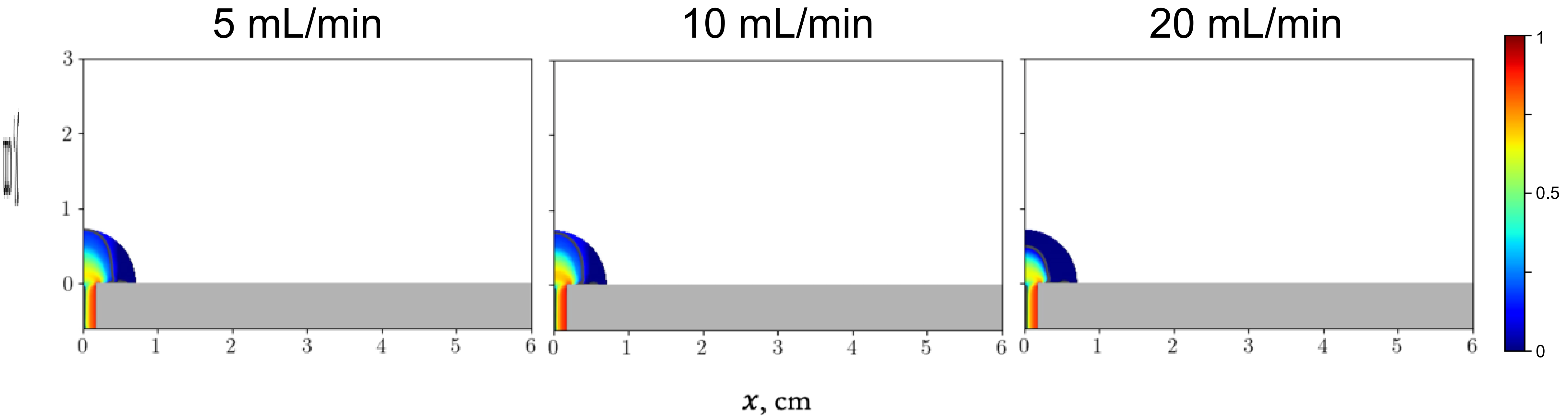
Comparing computed and observed blob dimensions



- 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

Computed Yield coefficient

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

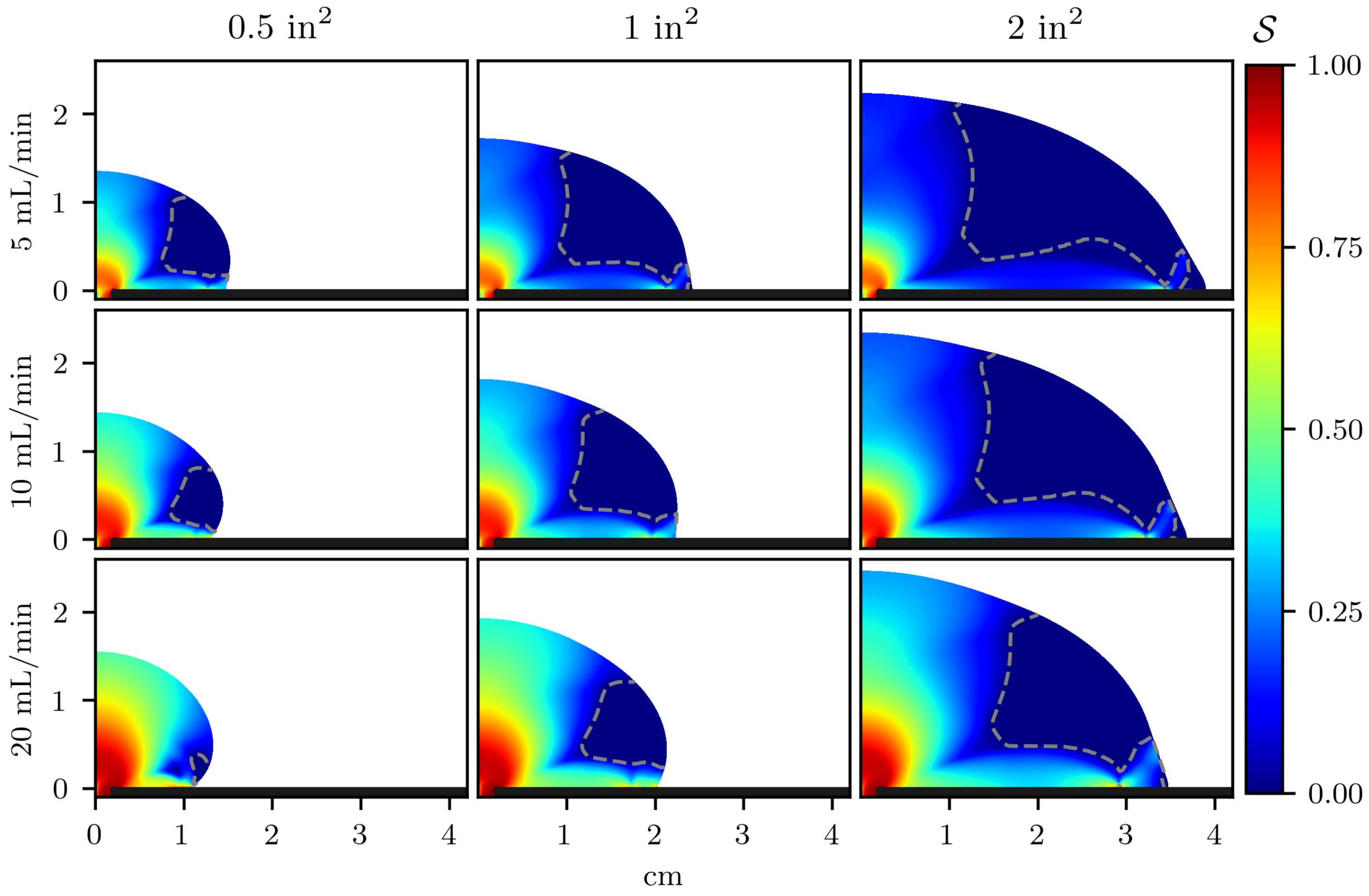


- Time is scaled by flow rate
- Gray lines indicate computed yield boundary

Computed yield coefficient

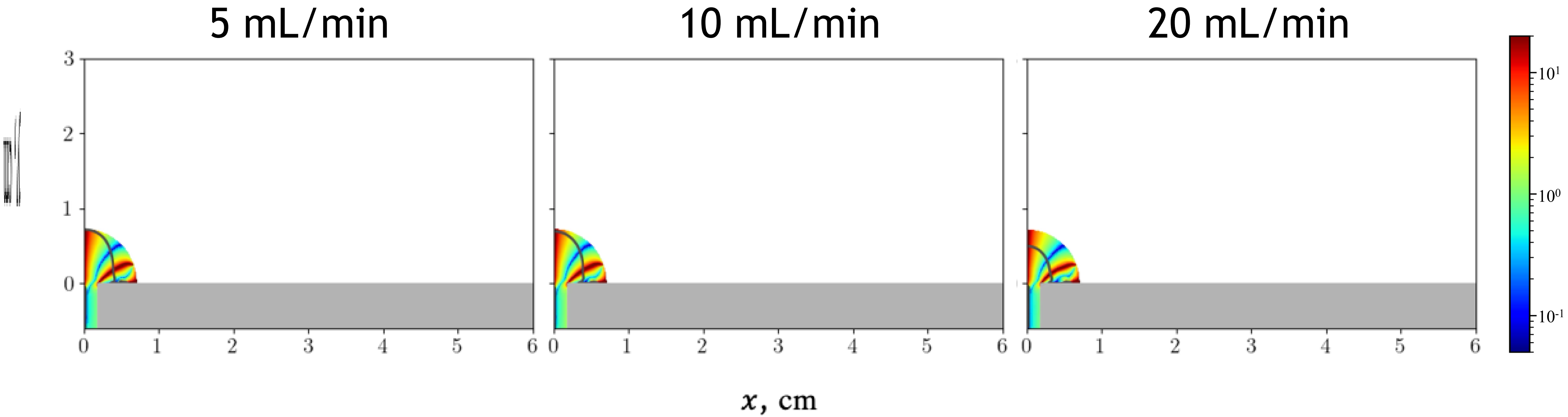
$$\mathcal{S}\left(\boldsymbol{\sigma}, \tau_{\text{yield}}\right) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_{\text{yield}}}{|\boldsymbol{\sigma}_d|}\right),$$

- For all scenarios, the unyielded fluid region within the droplet grows from the outer edge and upward as fluid is added to the domain
- Unyielded region remains at the outer edge of the droplet and above the high-shear region near the horizontal no-slip boundary



Local Weissenberg number

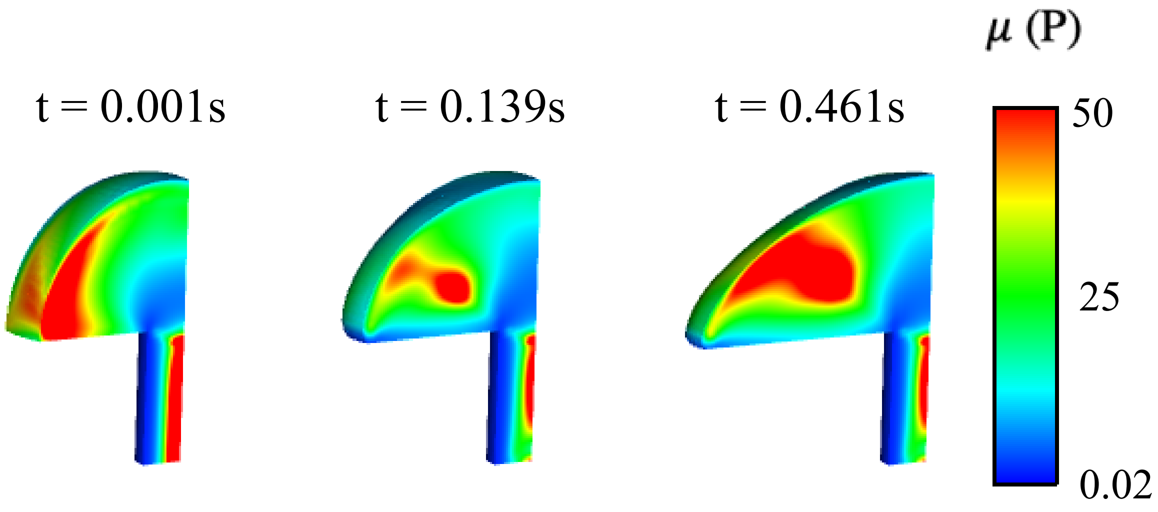
$$Wi = \frac{|\boldsymbol{\sigma}_{xx} - \boldsymbol{\sigma}_{yy}|}{|\boldsymbol{\sigma}_{xy}|}$$

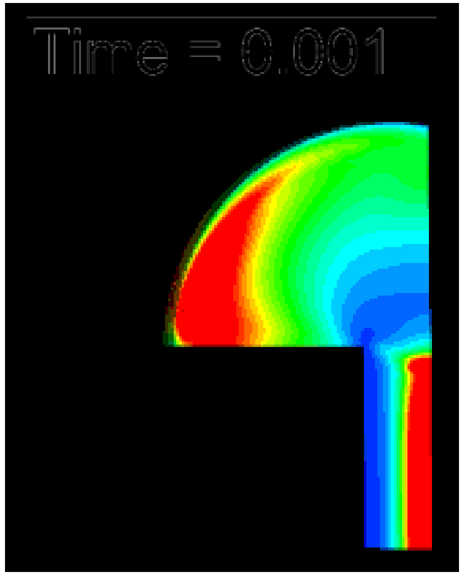


- Computations suggest that alternating regions of normal stress dominant behavior appear in growing droplets

Work in progress: 3D level set computations

- **Shown:** BCY model for 0.08% Carbopol
- All apparatus boundaries are resolved → wall drag model not necessary
  - Can be used to determine the efficacy of the drag model used in 2D computations
- In the future:
  - 3D Level set computations with the Saramito EVP model
  - 3D ALE computations





Conclusions and Future work

- Computations using Saramito stress model implementation agree with
  - Aanalytical solution to planar Poiseuille flow
  - Published experimental data
- Demonstrated capability to simulate free surface (mold filling) flows of a yielding fluid
  - Accuracy of blob shape predictions are improved overall by including an unresolved drag model
  - Drag model worsened at the lowest flow rate considered, possibly due to over predicting the viscosity
- Working on:
  - Computations over a range of fluid properties for the mold filling scenario
  - Coupling yield stress to local structure
  - Extending model to full three-dimensional analysis