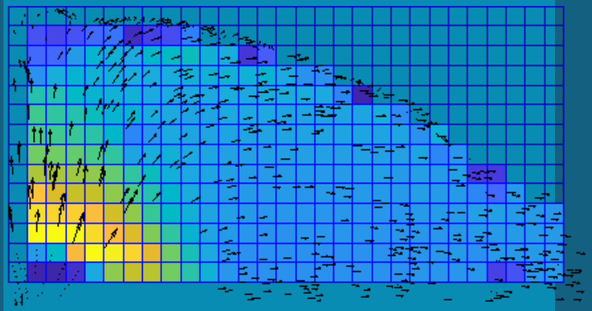
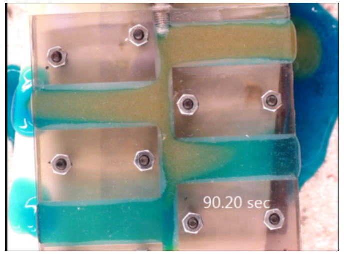
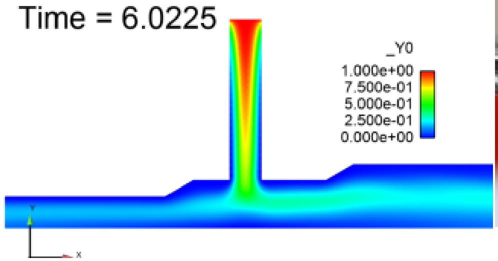
SAND2022-8130C

Sandia National Laboratories

Two- and three-dimensional simulations of an elastoviscoplastic material in a thin mold-filling geometry







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Austin, Texas

June 19-24, 2022

U.S. DEPARTMENT OF ENERGY NNSA

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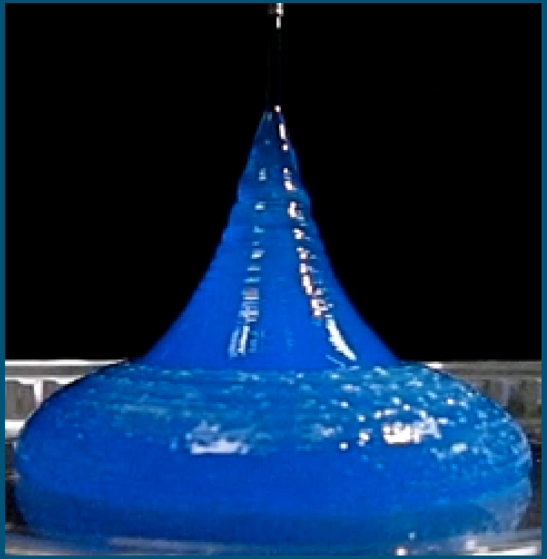
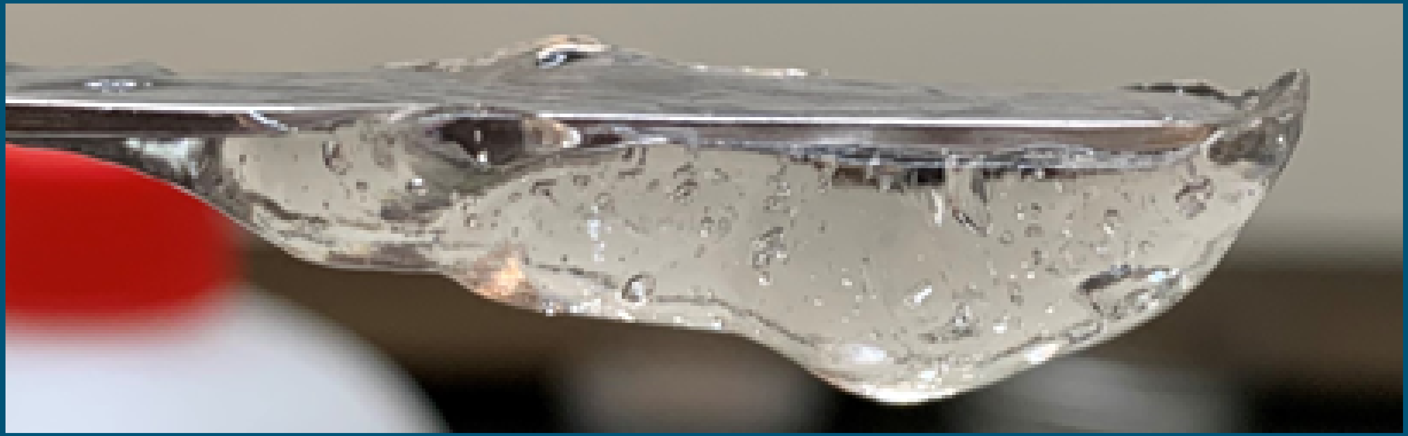
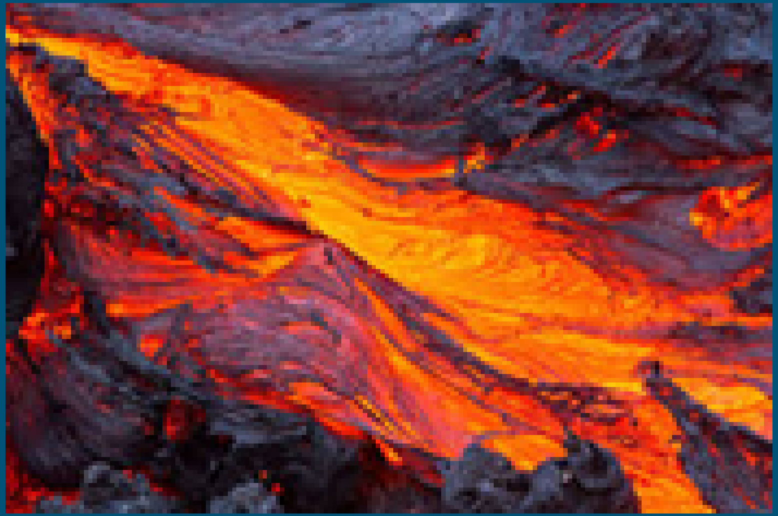
Motivation for studying yielding fluids







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

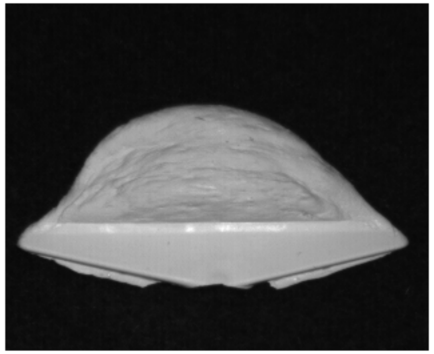
Why is this needed?

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

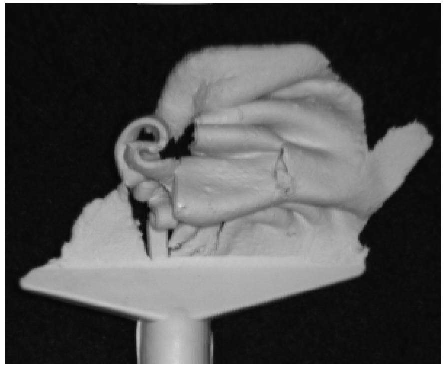
Current state-of-the-art in production codes:

- 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.

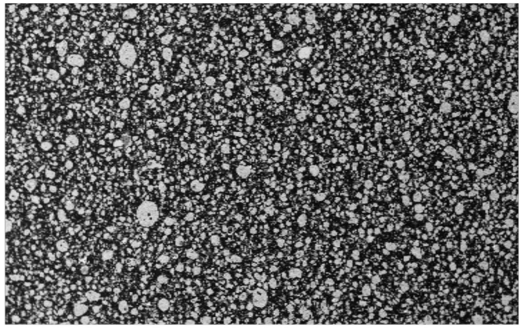


2.5 mm shot, 100% injection speed



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 (e.g. polyurethane foams)

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.

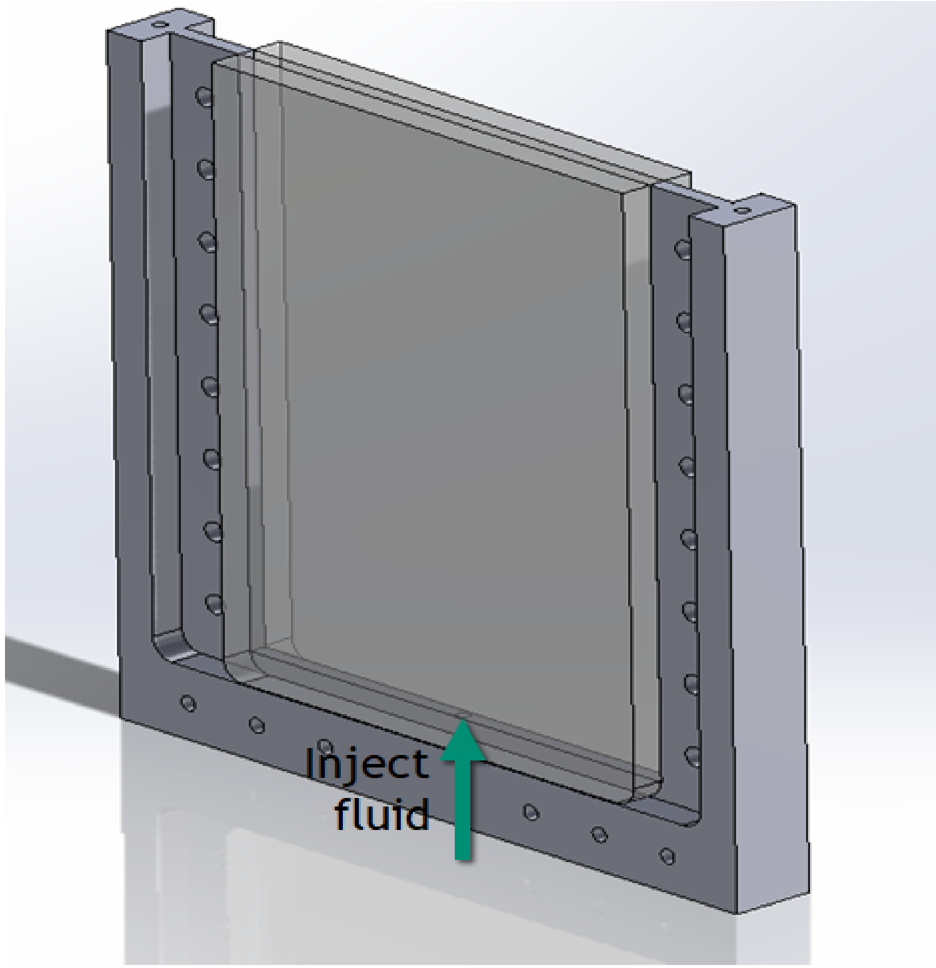
Saramito, P. *Journal of Non-Newtonian Fluid Mechanics* (2007) 145: 1, 1-14.

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

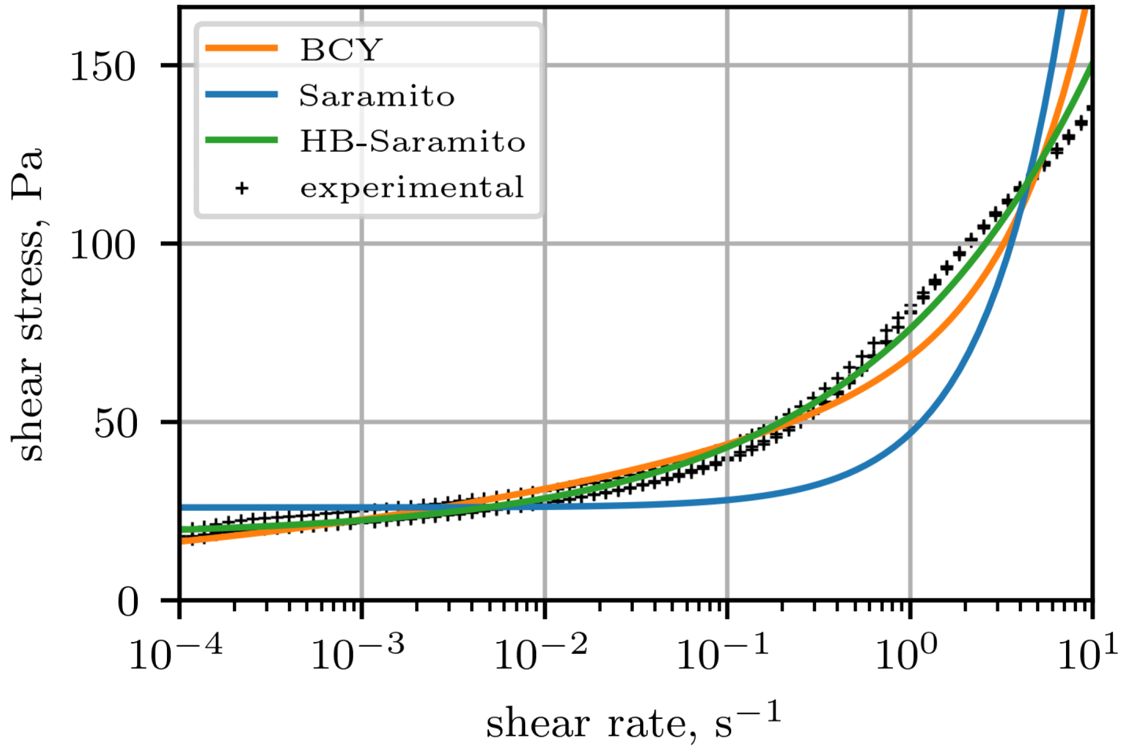
Mold filling geometry: flow between two thin plates

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)

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

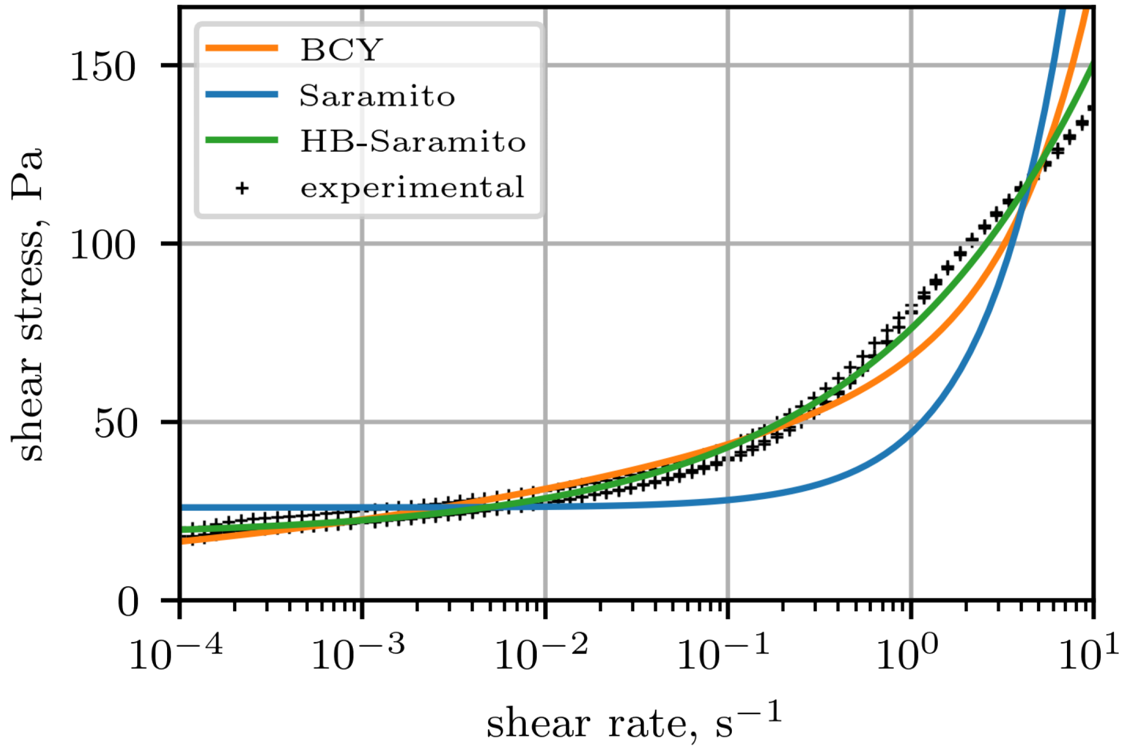
μ_0, (Pa•s)	μ_∞, (Pa•s)	b (s^{-1})	a	n	τ_y, (Pa)	R^2
217.15	0.018	3.112	0.966	0.190	31.21	0.954

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)	τ_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



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

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3D mold filling simulations

Constitutive models

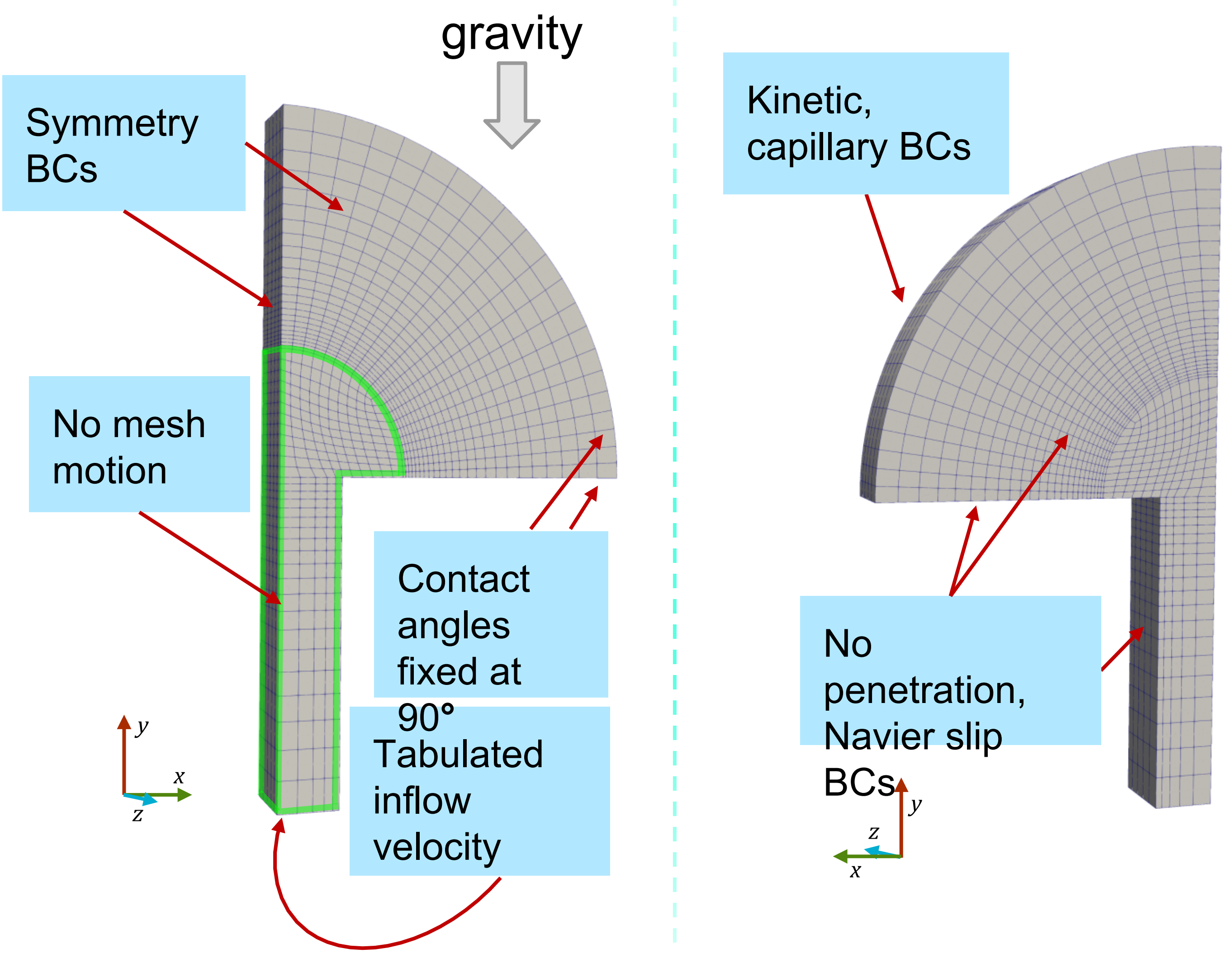
- Bingham-Carreau-Yasuda (generalized Newtonian)
- Saramito-Oldroyd-B
  - Constant viscosity
  - Herschel-Buckley (HB)

Computations

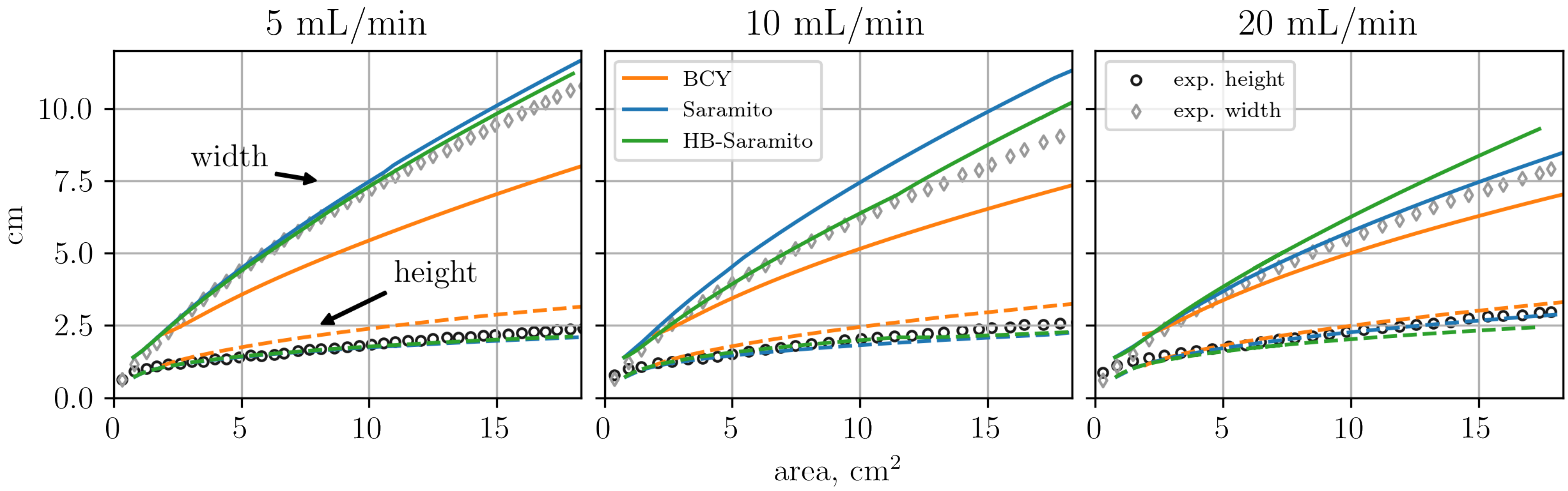
- Finite element method in Goma
- Arbitrary Eulerian-Lagrangian moving mesh framework
- Remeshing done every ~30 timesteps

Validation Experiments

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

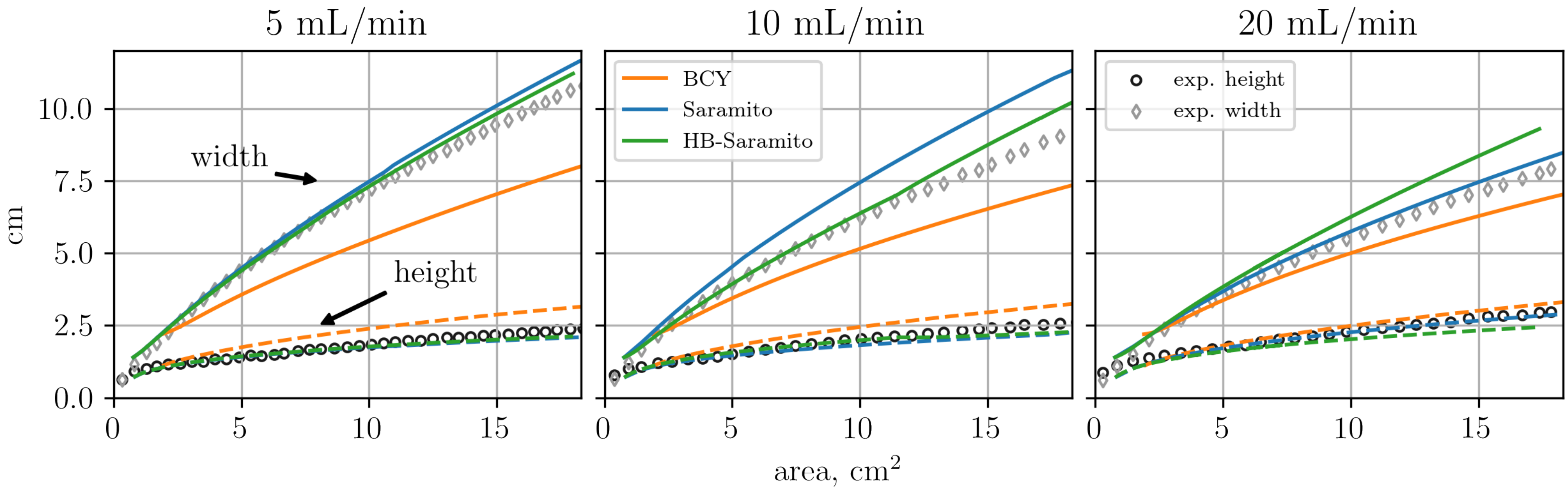


Droplet dimensions computed from 3D simulations



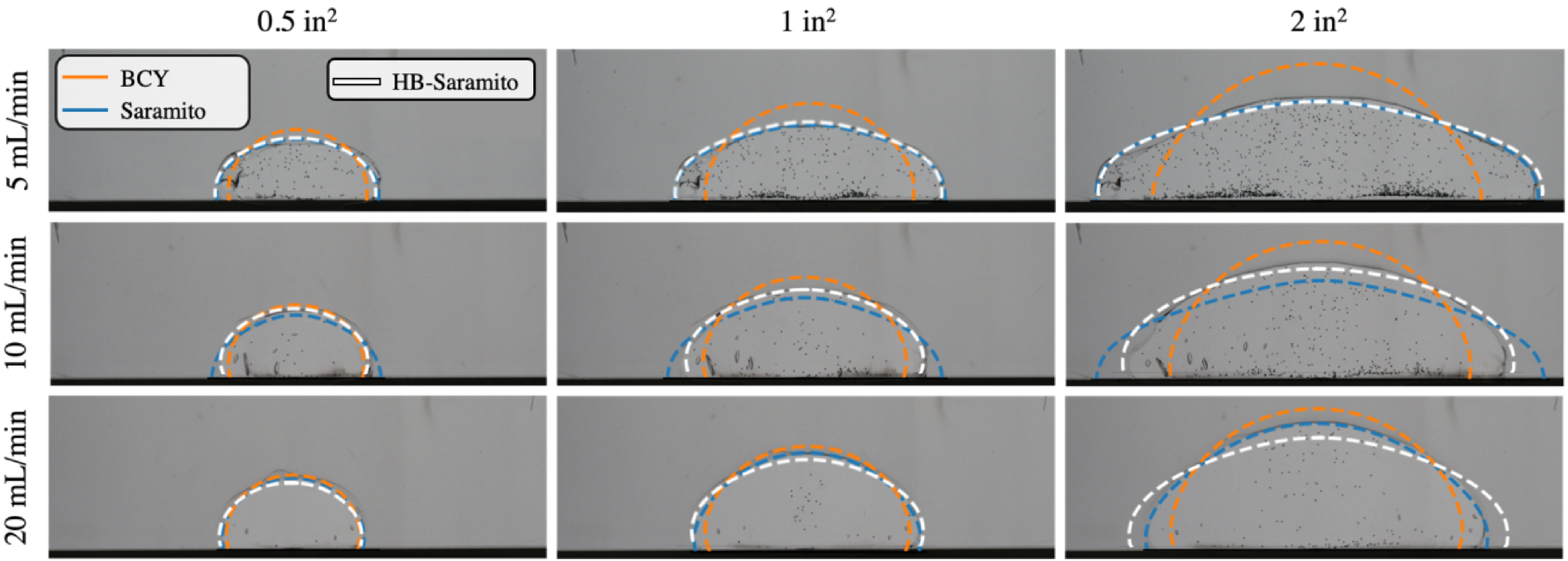
- Droplet height predictions for both flavors of the Saramito accurately capture droplet height.
  - Constant viscosity variant performs a bit better at the highest flow rate considered
- BCY model tends to overestimate droplet height

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.

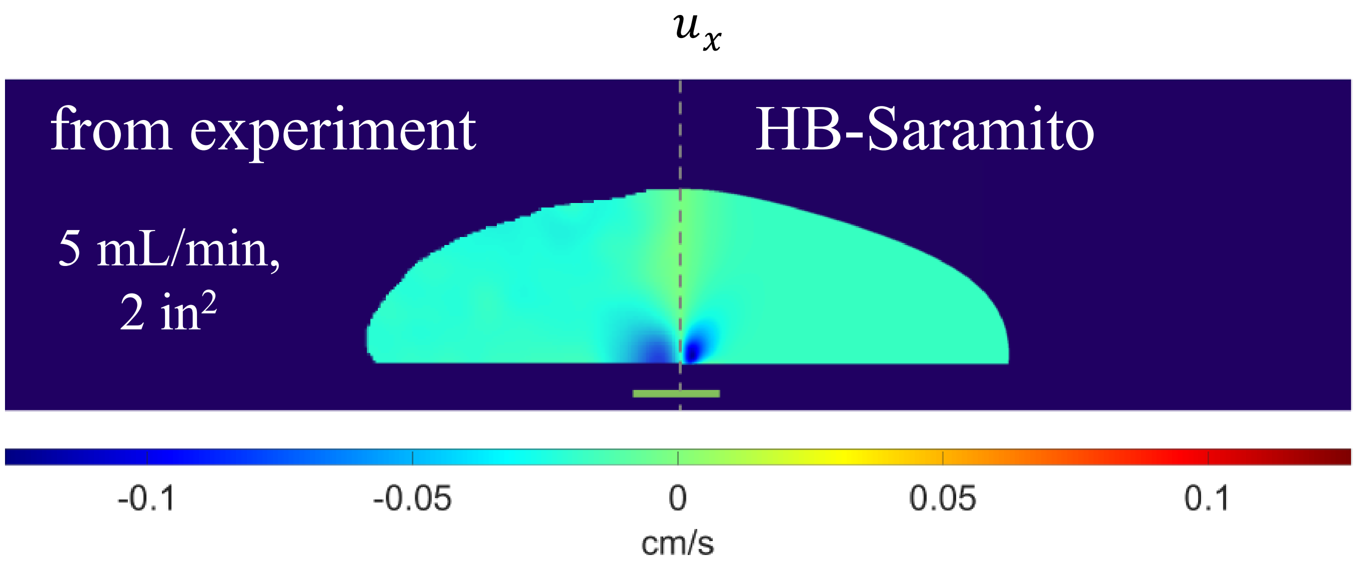
Droplet shape computed from 3D simulations

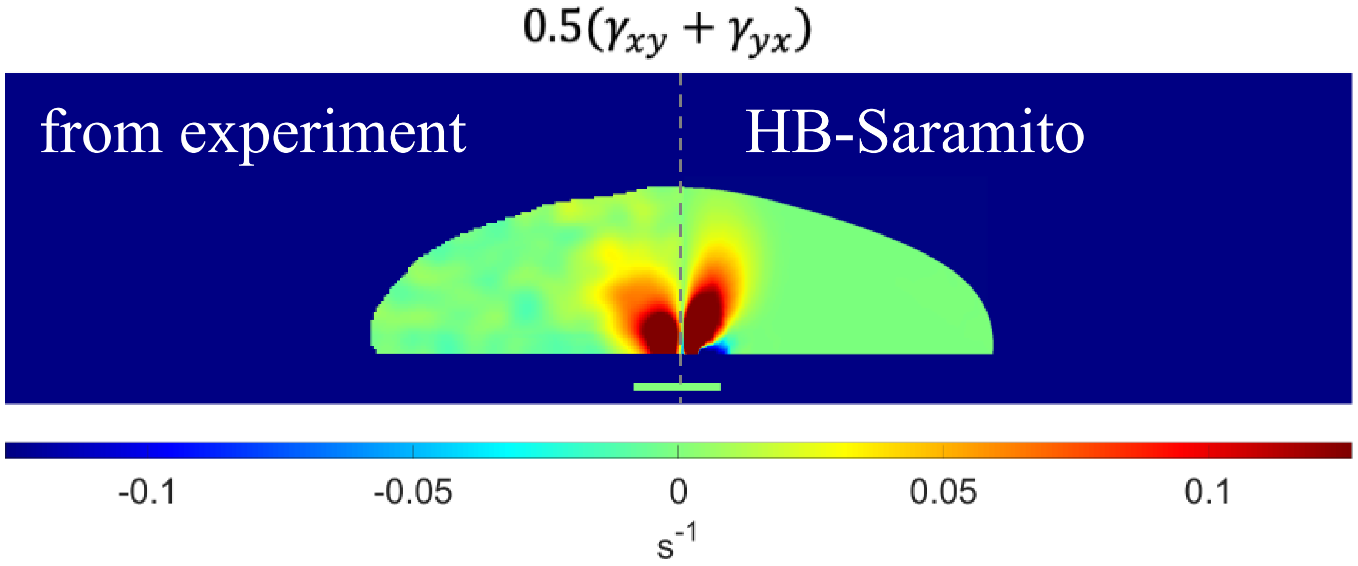


- Experimental droplet transitions from round triangular as volume is increased.
  - For a fixed droplet volume, higher flow rate leads to a rounder droplet.
- The Saramito and HB-Saramito models predict this behavior (though imperfectly).
  - BCY model struggles to show transition to a triangular shape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

Comparison experimental shear and velocity maps to computations

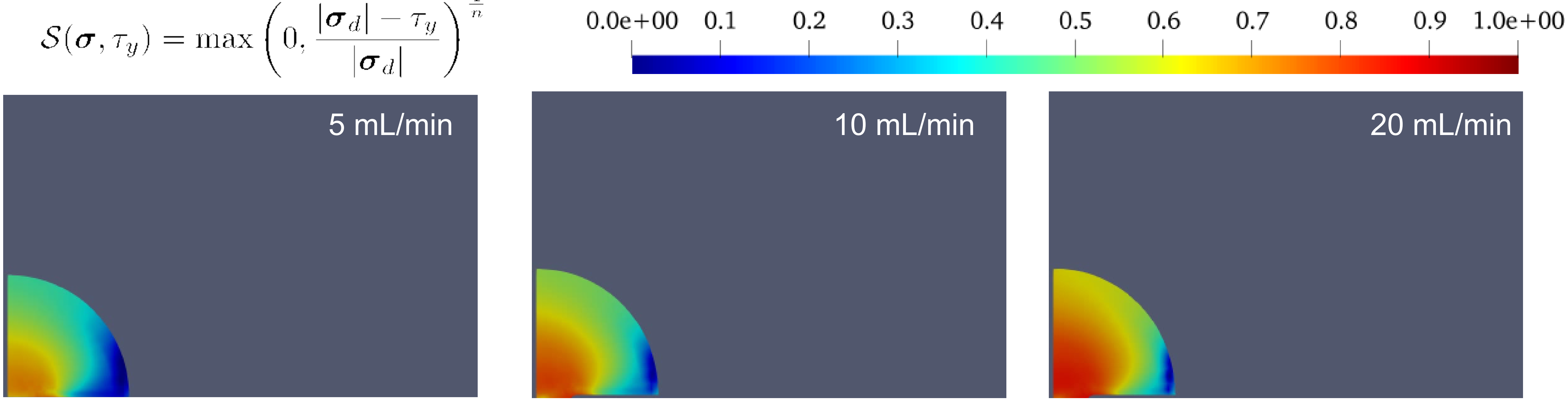
- For the available data, x-velocity and shear rate computed by the HB-Saramito model are generally in agreement with experimental values
- Differences manifest near the inlet region:
  - Near-wall velocity is underestimated
  - Computations predict a shear-rate reversal which is not observed experimentally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





Yield coefficient computed by HB-Saramito model

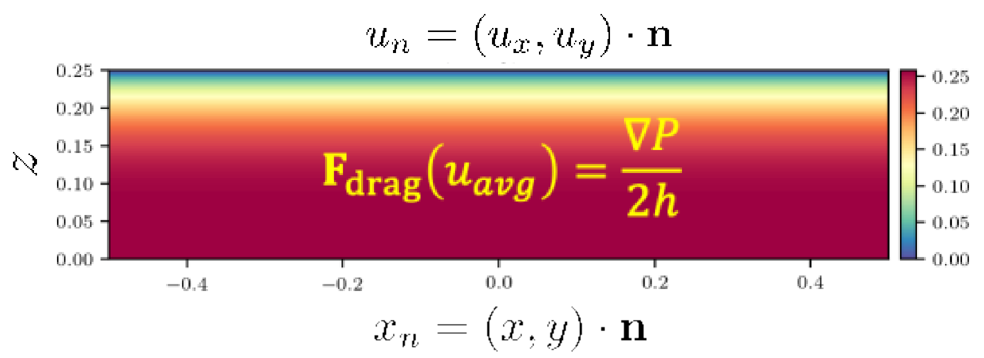
$$\mathcal{S}(\boldsymbol{\sigma}, \tau_y) = \max\left(0, \frac{|\boldsymbol{\sigma}_d| - \tau_y}{|\boldsymbol{\sigma}_d|}\right)^{\frac{1}{n}}$$



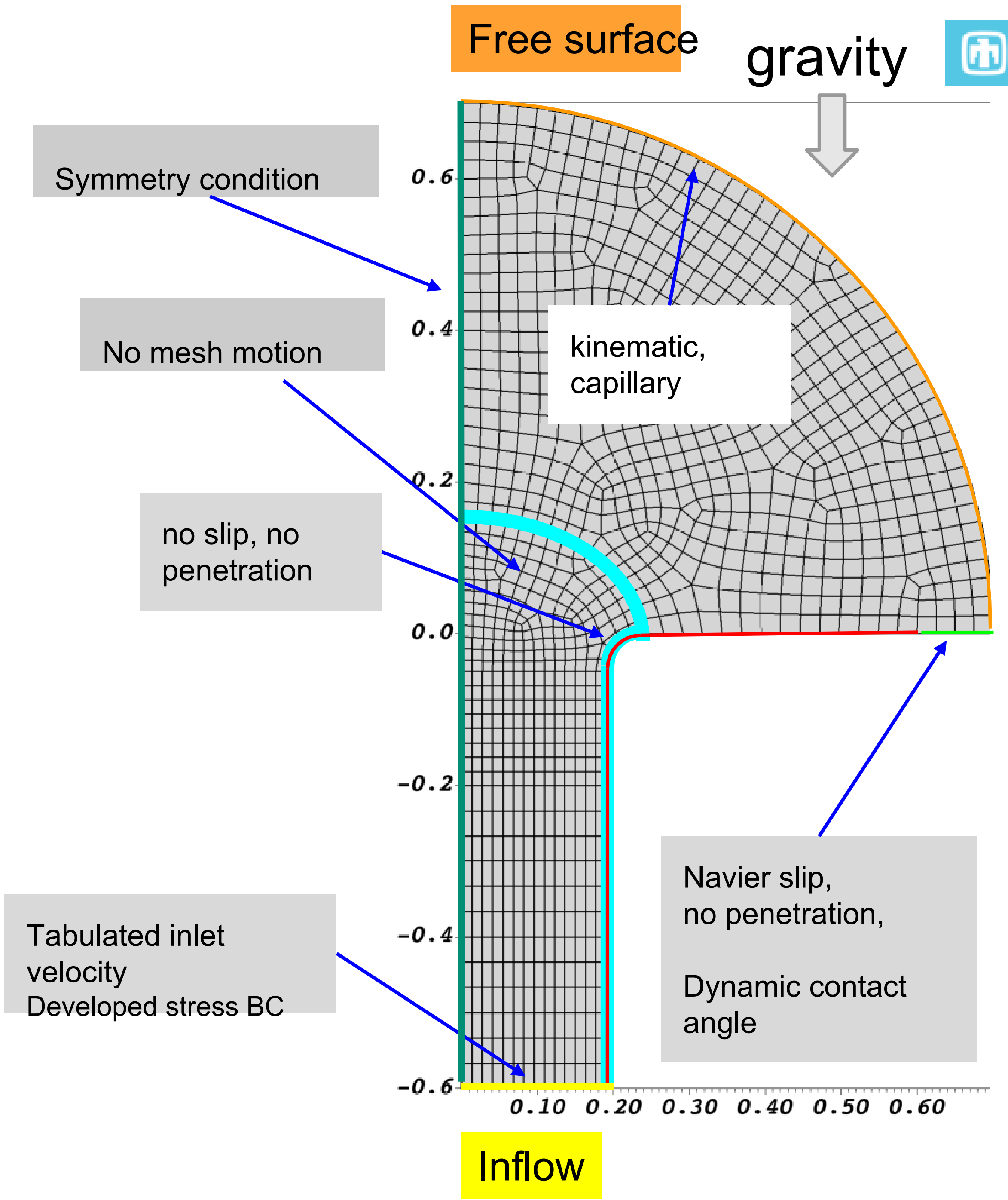
- $S = 0$ indicates solid-like behavior, $S > 0$ → fluid-like
- Unyielded region ($S = 0$) appears near the edges of the droplet and grows at the volume increases
- Increasing flow rate associated with a larger degree of fluid-like behavior, particularly near the fluid inlet.

2D mold filling simulations

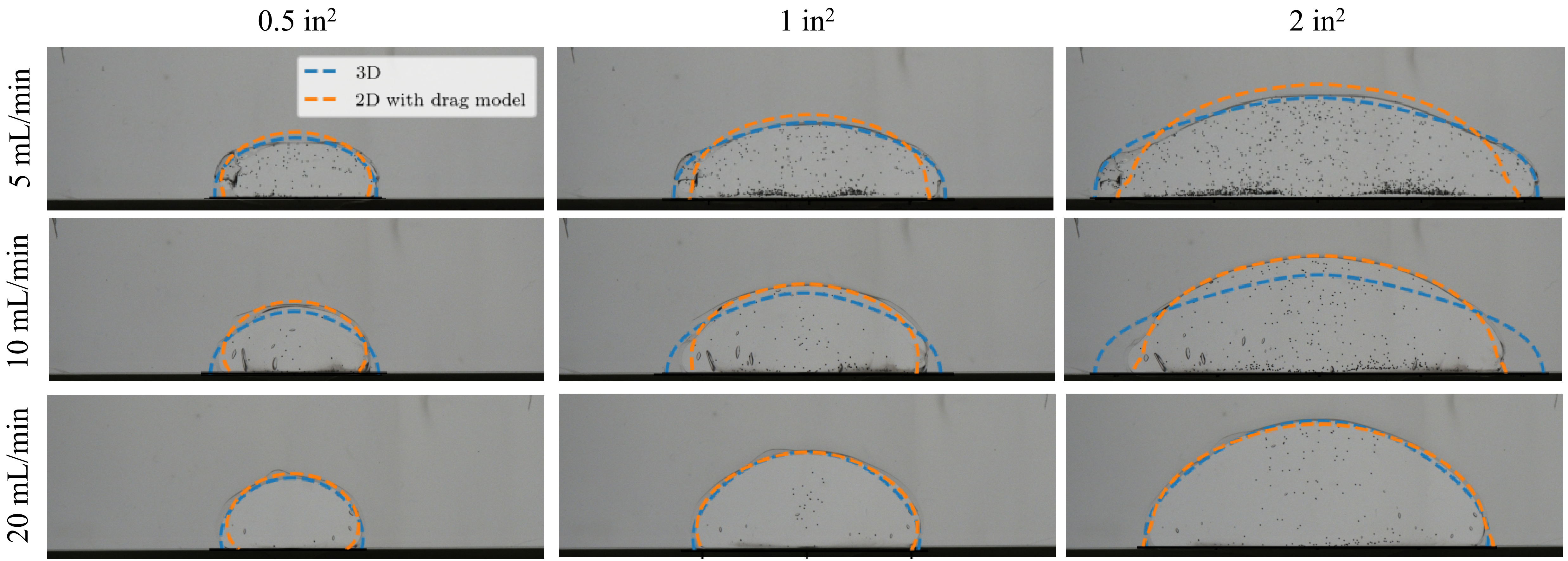
- 2D computations are substantially cheaper, but require a model for unresolved stresses – we model these stresses through a source term on the momentum equations ($\mathbf{F}_{\text{drag}}$)
- Model for $\mathbf{F}_{\text{drag}}$ calibrated from planar Poiseuille computations run over a range of ∇P values,



- Boundary conditions imposed for 2D simulations are similar to 3D computations



Comparing computed and observed droplet shapes (constant viscosity Saramito model)



- Accuracy of 2D computations with the drag model is similar to 3D results for less than 1/10 of the computational cost.

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

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.
- 2D computations with constant viscosity Saramito model + drag model work well
  - Yield droplet shapes comparable to analogous 3D computations at less than 1/10 the cost.
- 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

Extra slides

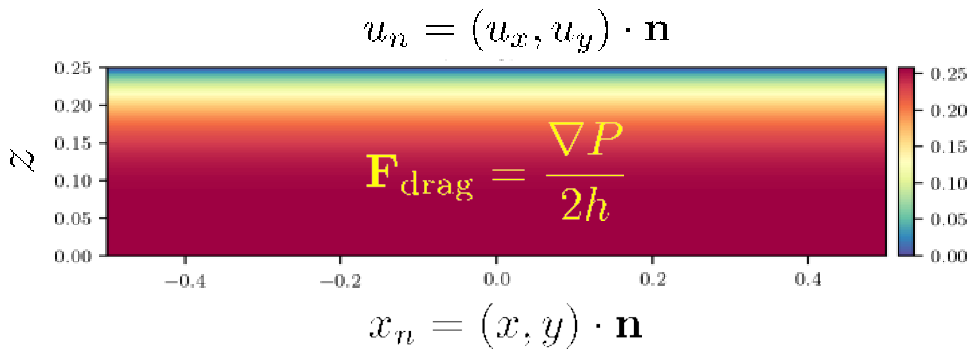
Drag model

- 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:

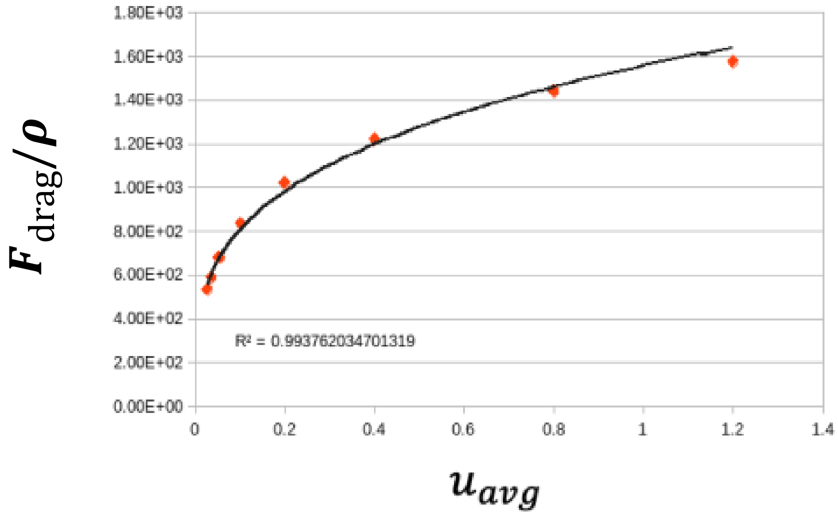
$$\mathbf{F}_{\mathrm{drag},i} = a\mathbf{u}_i \left(\sqrt{|\mathbf{u}|^2 + \epsilon}\right)^{b-1}$$

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

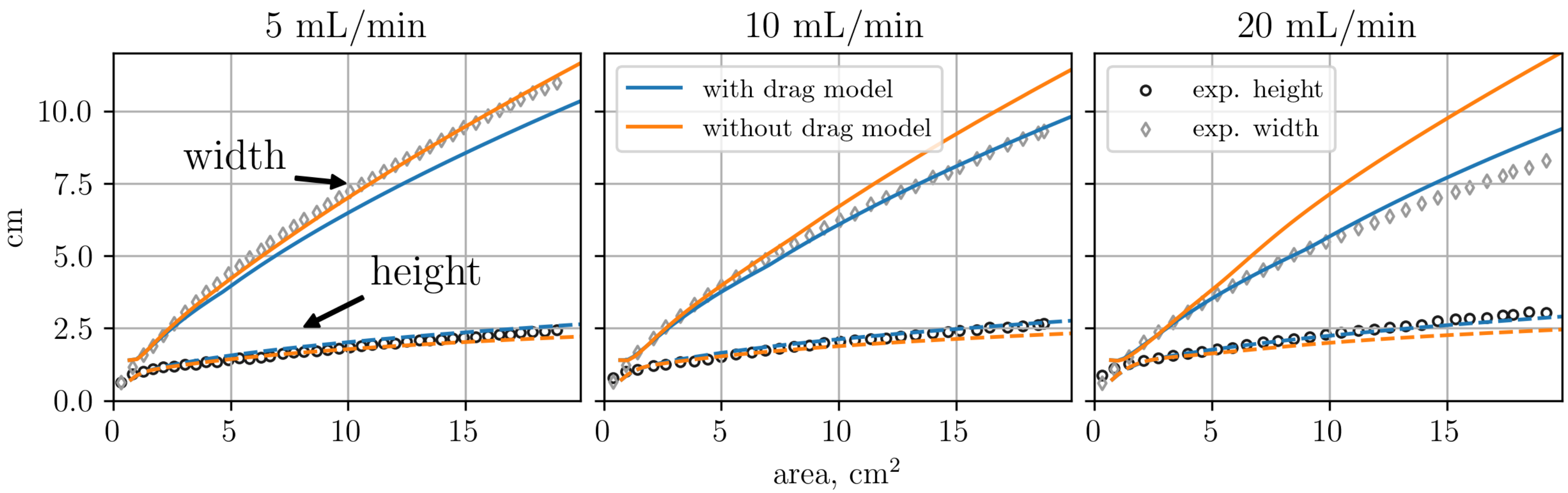
- Computations for obtaining drag model parameters are done with the Bingham-Carreau-Yasuda (BCY) generalized Newtonian model



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 (Saramito model)



- 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

Confined free-surface flow around an obstruction

Constitutive model

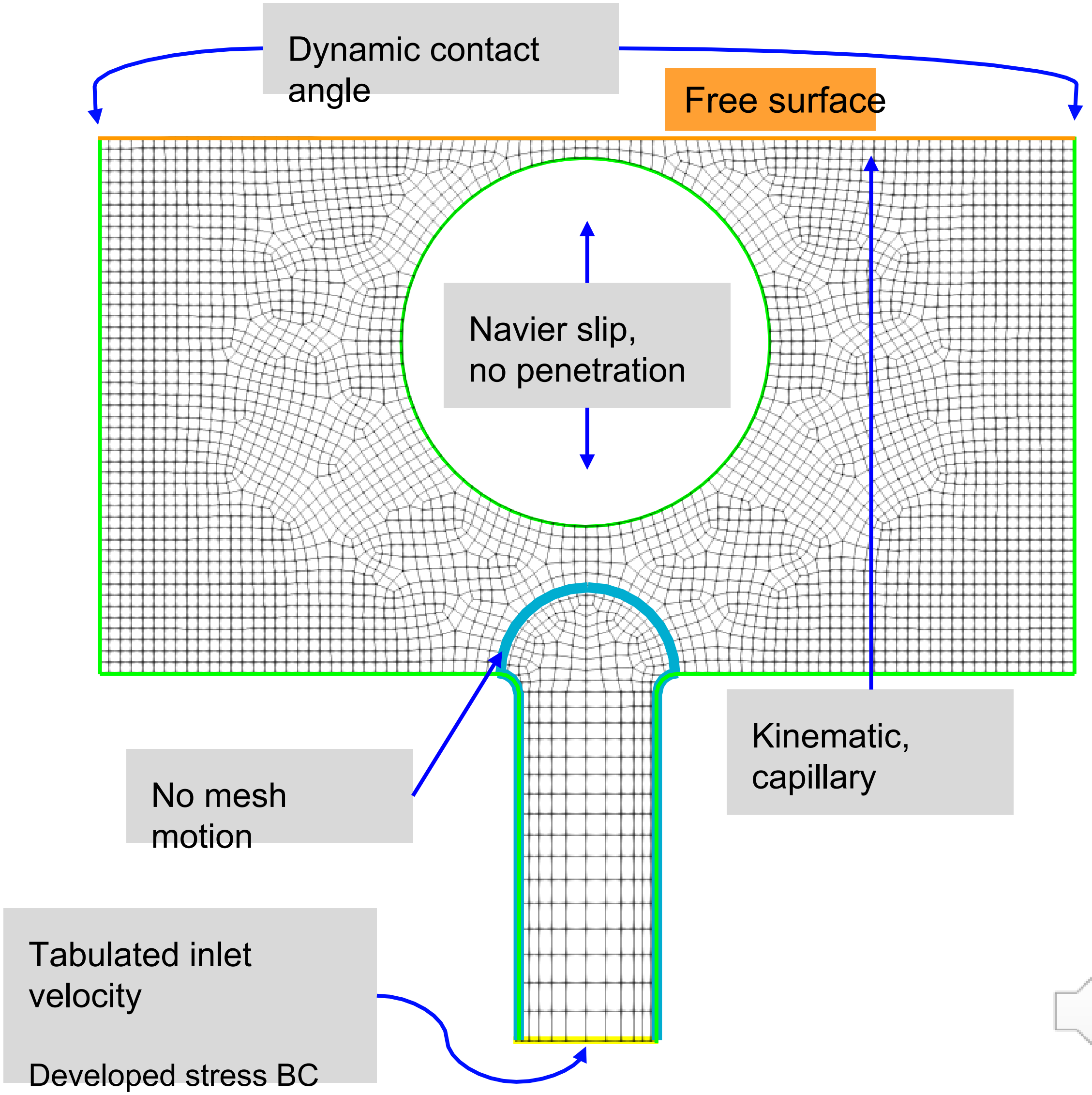
- Herschel-Bulkley Saramito-Oldroyd-B (EVP)

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

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

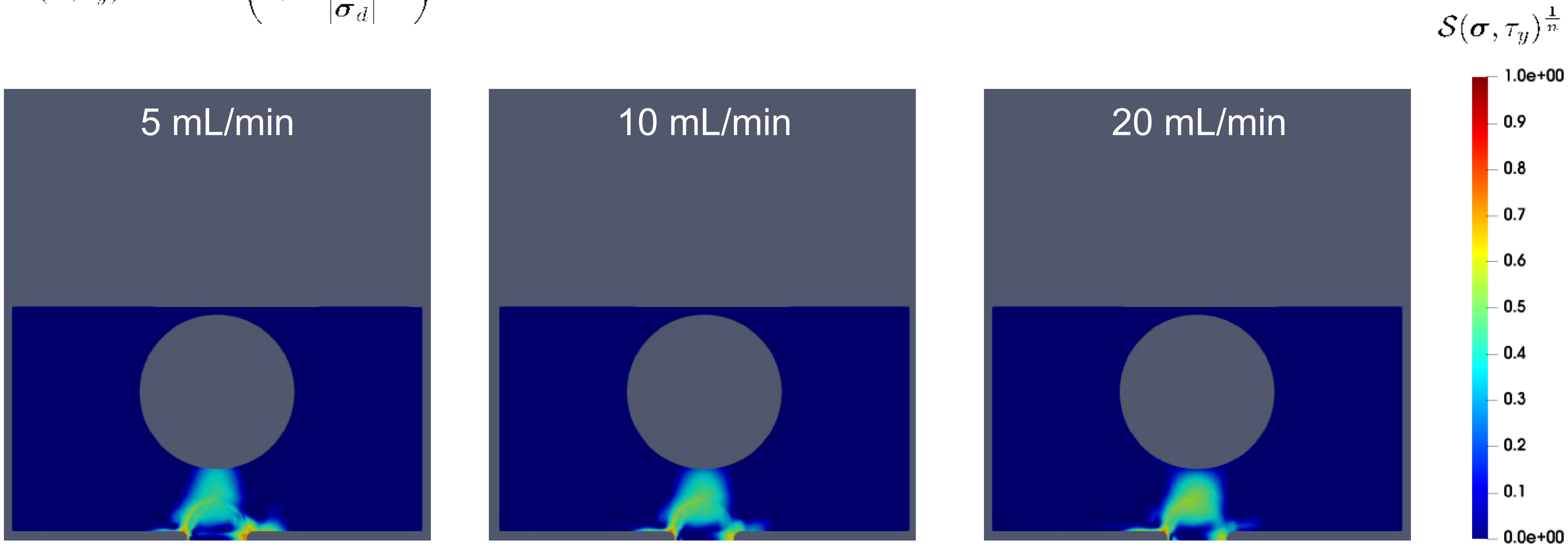
- Cylinder diameter: 10 cm
- Domain width : 2.75 cm

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)