SAND2022-13814C

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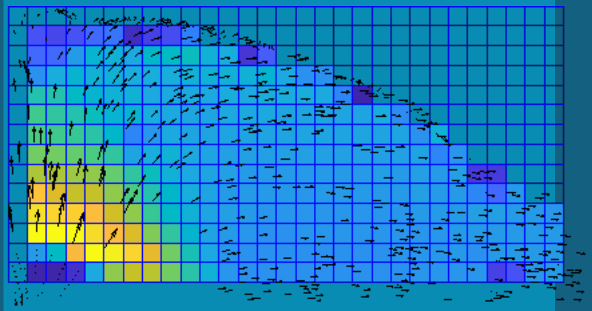
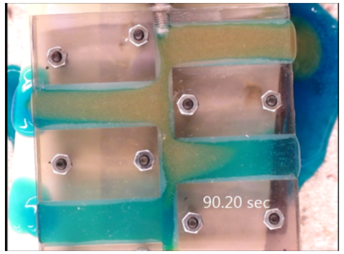
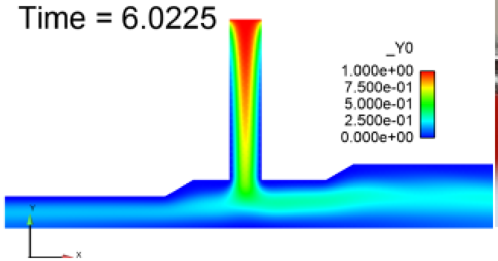
Numerical simulation and experiments of yield stress fluids filling a thin mold







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Society of Rheology 93rd Annual meeting

Chicago, Illinois

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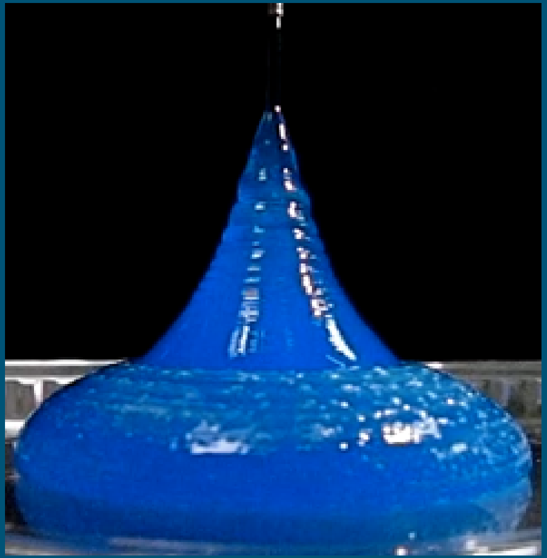
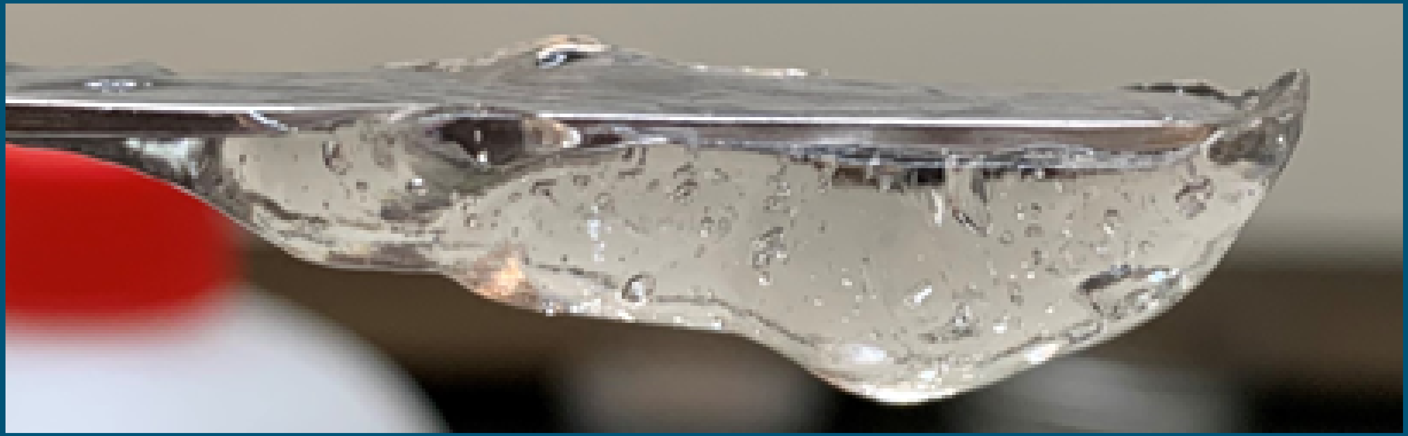
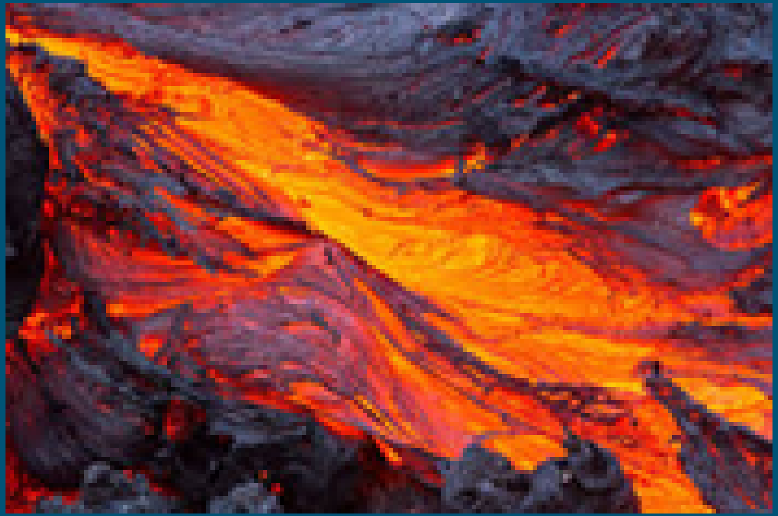
Motivation for studying yielding fluids







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

Objective: develop computational models for free-surface flows of yield stress fluids

Why is this needed?

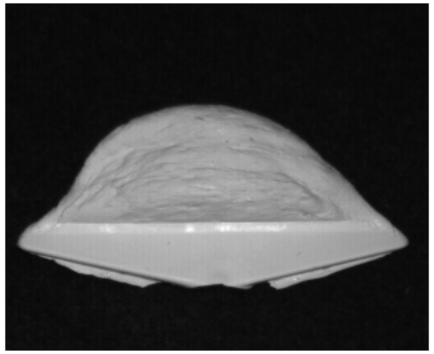
- Accurate predictions of surface profiles and spreading dynamics for flowing systems

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

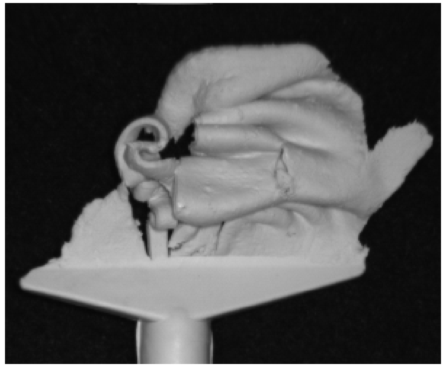
- Ramp up viscosity arbitrarily high to “solidify” a fluid
- Does not accurately preserve the stress state that develops in the material
- One way coupling between fluid and solid codes

Our approach:

- Develop and implement constitutive models that can represent both solid and fluid behavior

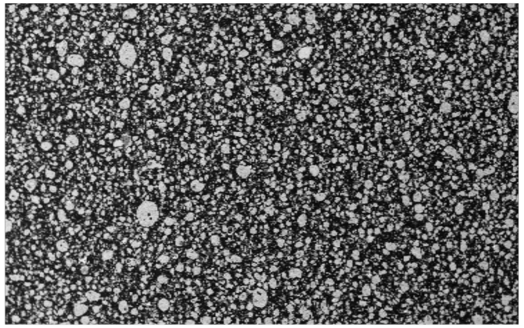


2.5 mm shot, 100% injection speed



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)

Models for Visco/elastic/plastic materials

- Viscoplastic (yield stress fluid) models
  - Bingham: $\sigma = \tau_y + \eta\dot{\gamma}$
  - Herschel Bulkley: $\sigma = \tau_y + k\dot{\gamma}^n$
- Viscoelastic models
  - Maxwell: $\lambda\dot{\sigma} + \sigma = 2\eta_p\dot{\gamma}$
  - Kelvin-Voigt: $\sigma = G\dot{\gamma} + \eta\ddot{\gamma}$
- Elastoviscoplastic (EVP) models
  - Saramito [1]: $\frac{1}{G}\dot{\sigma} + \max\left[\frac{|\sigma|-\tau_y}{k|\sigma|^n}\right]^{\frac{1}{n}}\sigma = 2\dot{\gamma}$
  - P&L model [2]: $\lambda\dot{\sigma} + \sigma = 2\eta_p(\dot{\gamma})\dot{\gamma}$
  - KDR [3]: $\lambda_1\dot{\sigma} + \sigma = \eta_p(\dot{\gamma})\dot{\gamma} + \lambda_2\ddot{\gamma}$

1. P. Saramito. *A new constitutive equation for elastoviscoplastic fluid flows.* J. Non-Newton. Fluid Mech., 145 (1) (2007), pp. 1-14
2. Y.S. Park, P.L.F. Liu. *Oscillitory pipe flows of a yield stress fluid.* . J. Fluid Mech. 658 (2010) 673-689
3. Kamani, Krutarth, Gavin J. Donley, and Simon A. Rogers. *Unification of the Rheological Physics of Yield Stress Fluids*. Phys. Rev. Lett. 126:21 (2021): 218002

Some recent numerical EVP fluid studies

- Particle sedimentation, oscillating, and elongational flow [1]
- 2-phase, buoyancy-driven flows [2]
- Dam-breaking for a range of fluid properties (yield stress, elastic modulus, *etc.*) [3]
- Collision of droplets with a vertical obstruction [4]
- Droplet spreading on a pre-wetted surface [5]

1. D. Fraggedakis, Y. Dimakopoulos, J. Tsamopoulos. *Yielding the yield stress analysis: A thorough comparison of recently proposed elasto-visco-plastic (EVP) fluid models.* J. Non-Newton. Fluid Mech., 236 (2016), p. 104-122
2. P. Moschopoulos, A. Spyridakis, S. Varchanis, Y. Dimakopoulos, J. Tsamopoulos. *The concept of elasto-visco-plasticity and its application to a bubble rising in yield stress fluids*. J. Non-Newton. Fluid Mech., 297 (2021), 104670
3. C.M. Oishi, R.L. Thompson, F.P. Martins. *Transient motions of elasto-viscoplastic thixotropic materials subjected to an imposed stress field and to stress-based free-surface boundary conditions.* Internat. J. Engrg. Sci., 109 (2016), pp. 165-201
4. C.M. Oishi, F.P. Martins R.L. Thompson. *Gravitational Effects in the Collision of Elasto-Viscoplastic Drops on a Vertical Plane.* Fluids (2020) *5*(2), 61
5. Jalaal M., Stoeber B., Balmforth N.J. *Spreading of viscoplastic droplets* J. Fluid Mech., 914 (2021), p. A21

Equations of motion and stress constitutive equations

Momentum and Continuity

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

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

Oldroyd-B stress constitutive model + Saramito yield model

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

Herschel-Buckley (HB)-Saramito yield model

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

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

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.

We also consider a generalized-Newtonian constitutive model

Momentum and Continuity

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

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

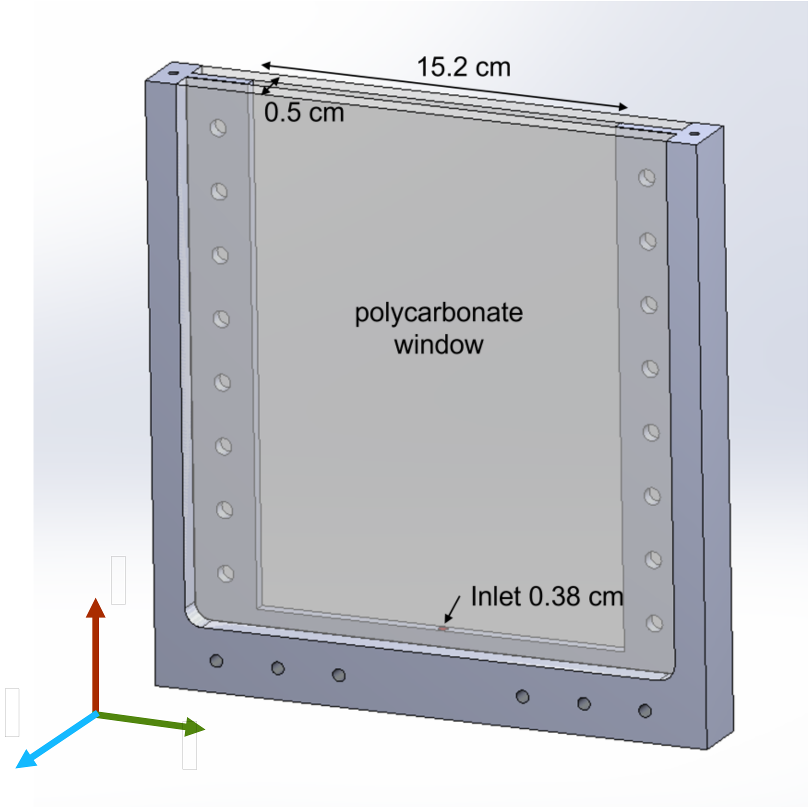
Bingham-Carreau-Yasuda model

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

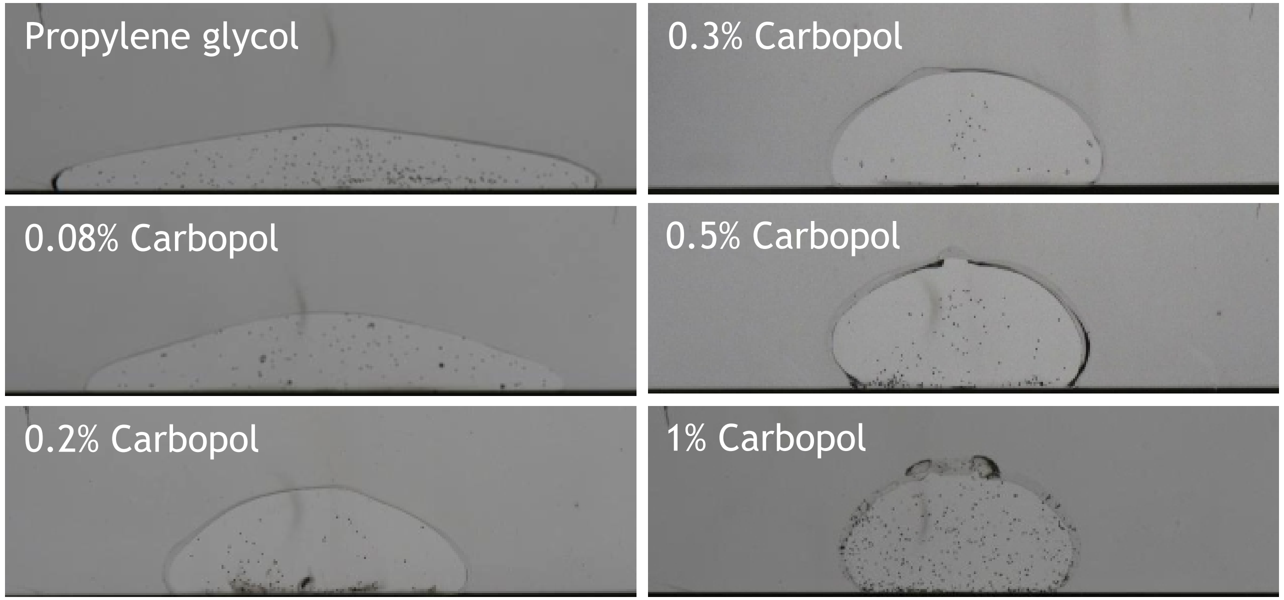
Solve with Finite Element Method for $\mathbf{u}$, P, and $\dot{\boldsymbol{\gamma}}$

Mold filling geometry: flow between two thin plates

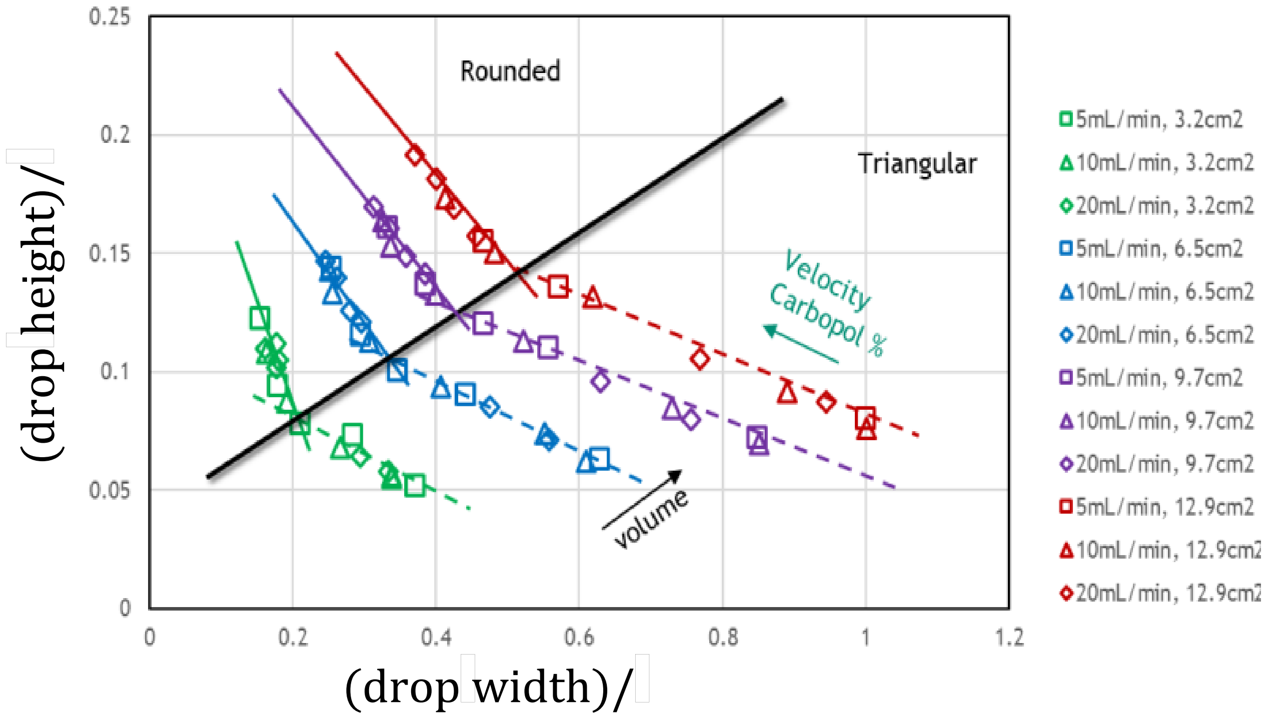
- **Apparatus dimensions**
  - Inlet diameter = 0.38 cm
  - (x) W = Width = 15.2 cm
  - (y) Height > Width
  - (z) Gap between plates = 0.5 cm

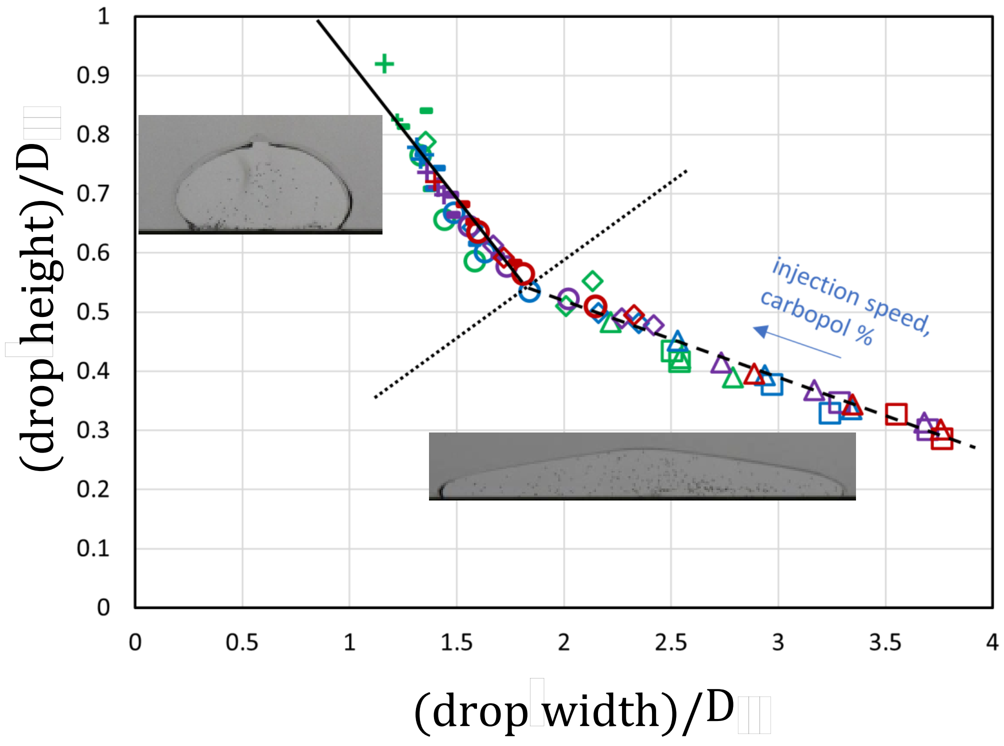


- **Experimental study considers**
  - inlet flow rate: 5-20 mL/min
  - 0-1 wt% Carbopol solutions



Trends for drop shape evolution





- Fluid drop changes from triangular to round with
  - increasing injection flow rate, Carbopol concentration
  - decreasing drop cross-sectional area

- Height, width collapse onto a single curve when scaled by effective diameter, D_{eff}

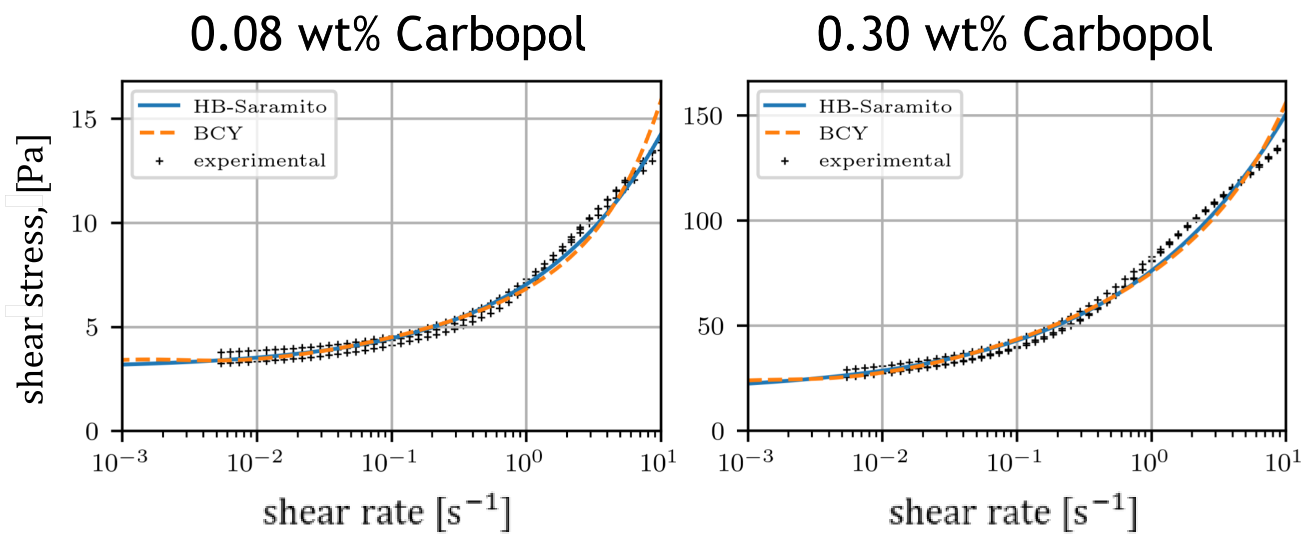
$$\frac{\pi}{4} D_{eff}^2 = \text{cross-sectional area}$$

Characterization of Carbopol and parameter fitting

HB-Saramito

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

[Carbopol]	[Pa · s [	[Pa]	] Pa]	n
0.08 wt%	4.04	25.2	3.01	0.446
0.30 wt%	58.92	479.7	17.89	0.368



Bingham-Carreau-Yasuda (BCY)

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

[Carbopol]	μ_0 [Pa · s]	μ_∞ [Pa · s]	τ_y [Pa]	λ [s]	a	n
0.08 wt%	6.73	0.018	1.53	1.12	1.0	0.22
0.30 wt%	241.71	0.001	31.21	3.11	1.0	0.19

- The elastic modulus, *G* is determined via small amplitude stress vs. strain data
- Other rheological parameters were determined using a nonlinear least squares fit

Mold filling simulations

Constitutive models

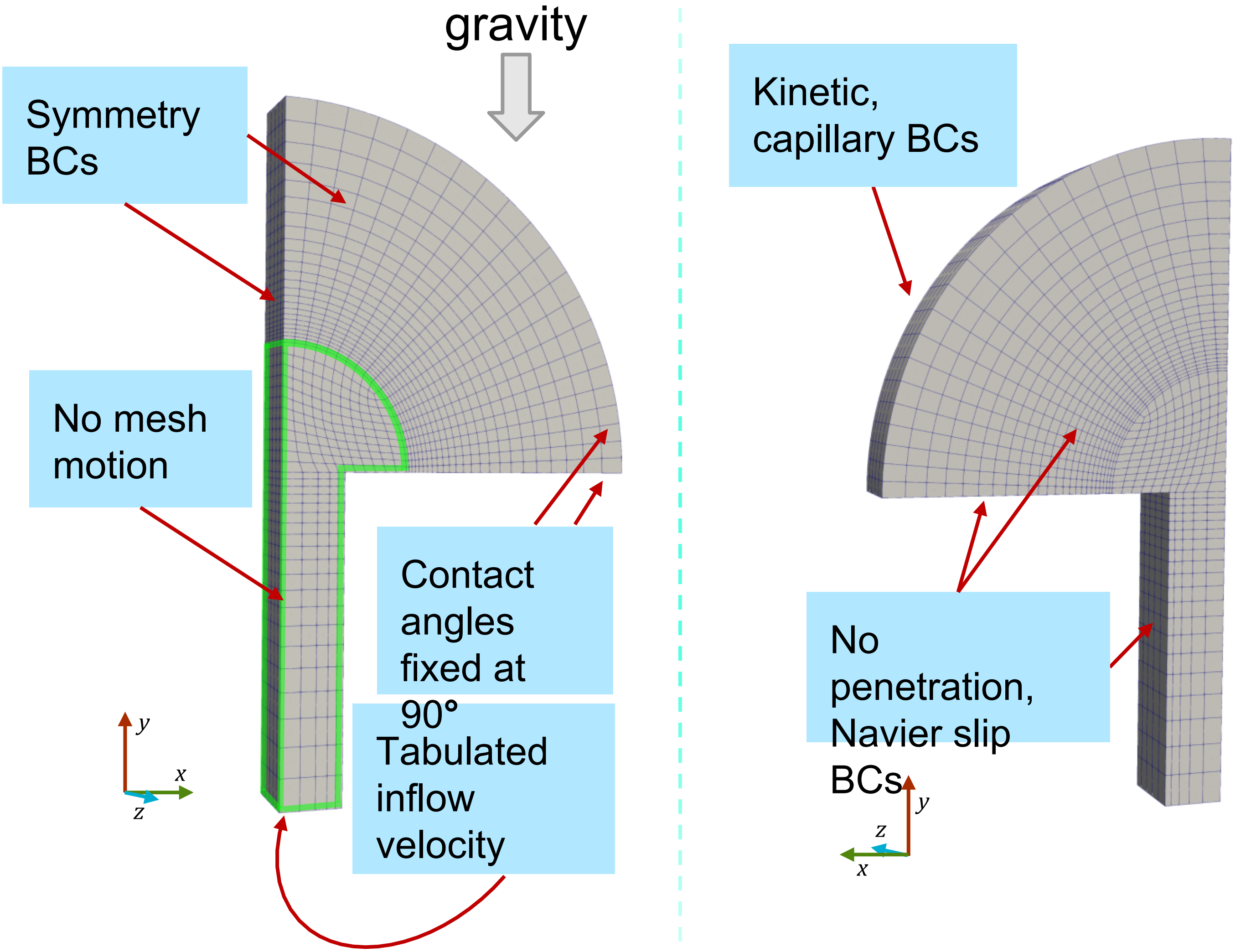
- Bingham-Carreau-Yasuda (generalized Newtonian)
- HB-Saramito

Computations

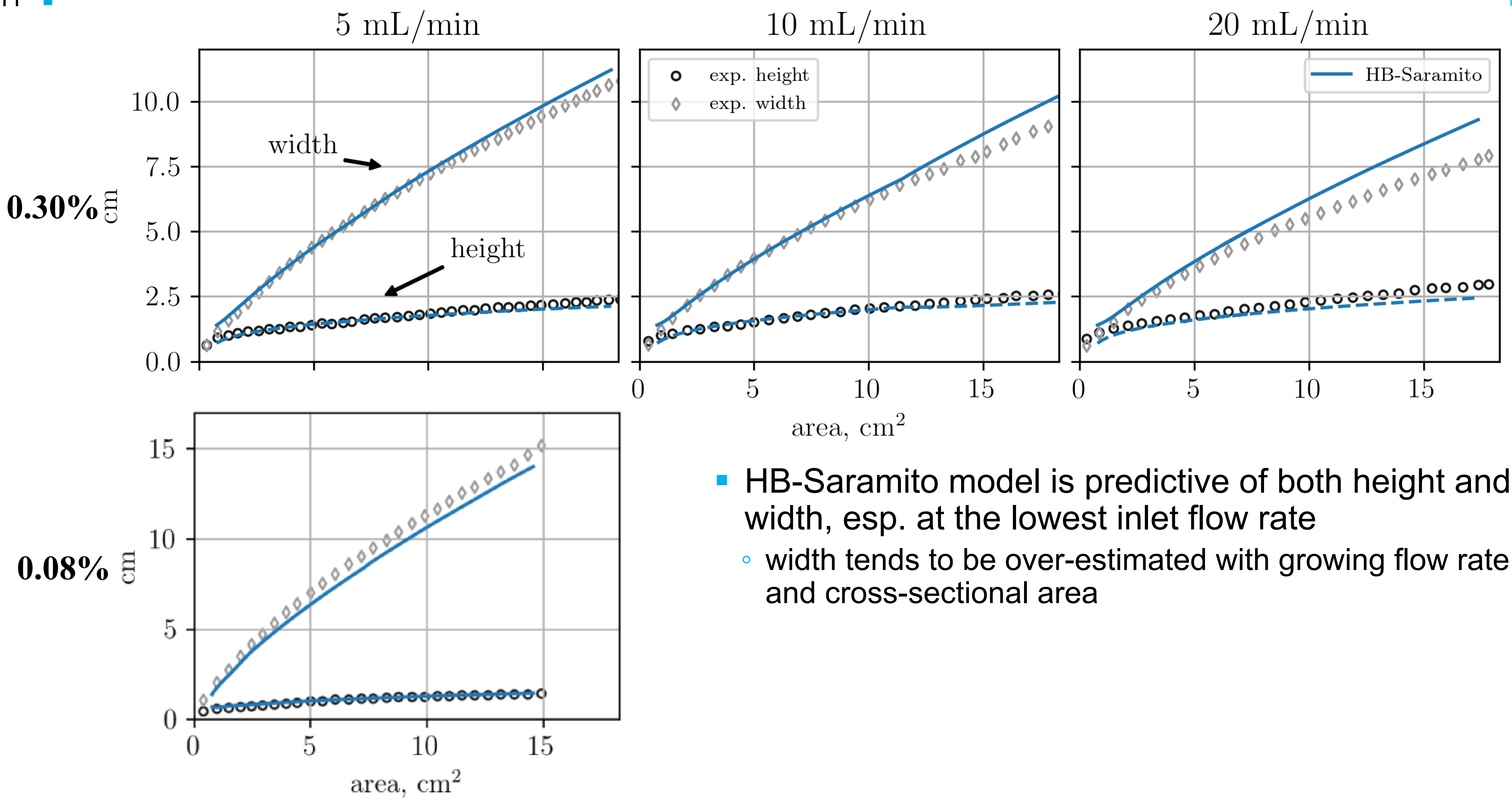
- Finite element method in Goma
- Arbitrary Eulerian-Lagrangian moving mesh framework
- Remeshing done every ~30 timesteps

Validation Experiments

- 0.08, 0.30 wt.% Carbopol
- 5-20 mL/min inlet flow rate

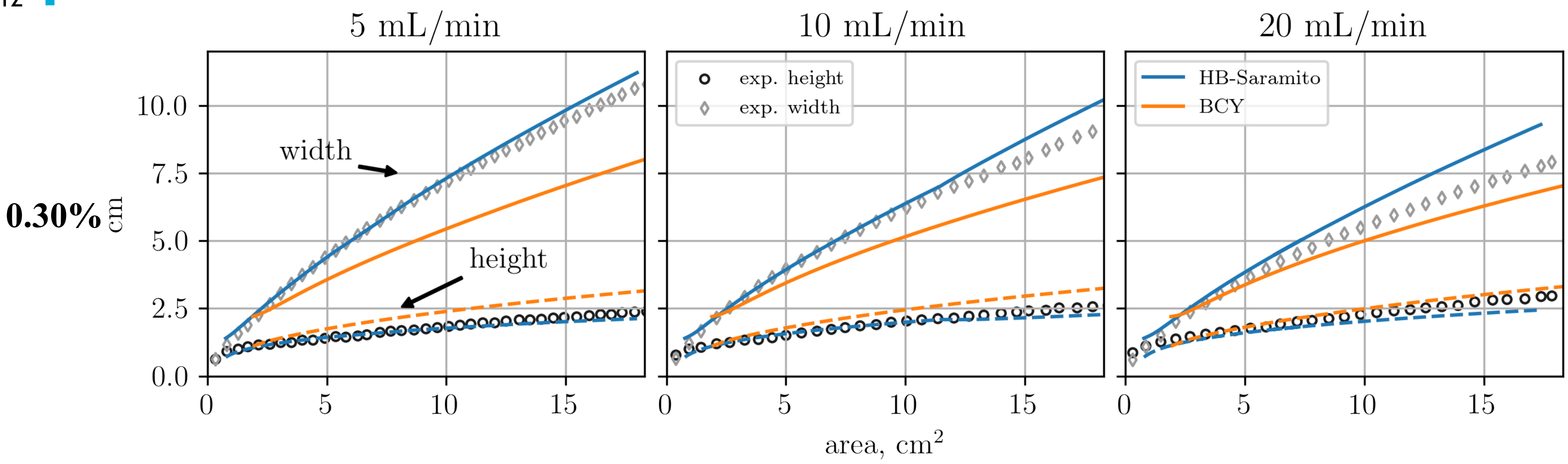


HB-Saramito drop height/width



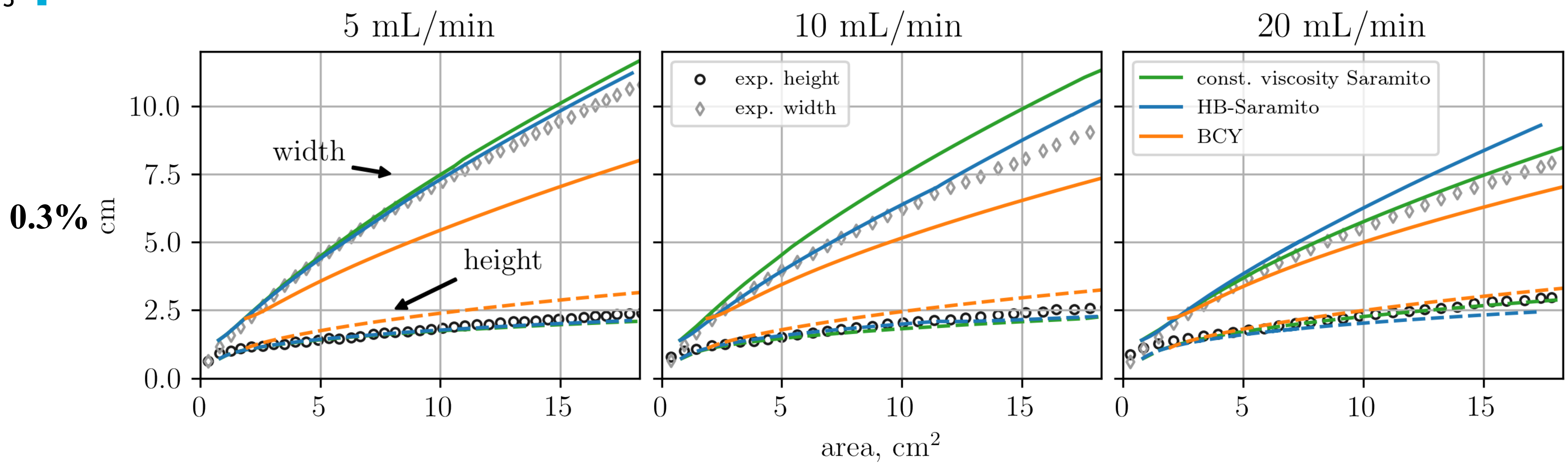
- HB-Saramito model is predictive of both height and width, esp. at the lowest inlet flow rate
  - width tends to be over-estimated with growing flow rate and cross-sectional area

Computed drop height/width

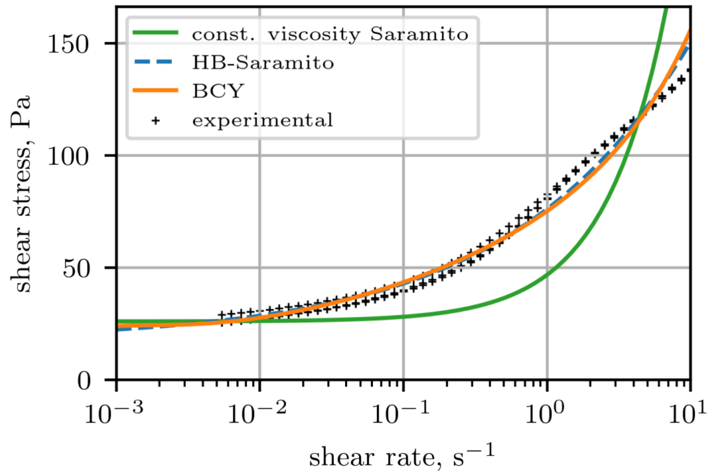


- Overall, BCY model is less predictive of droplet dimensions, but accuracy improves for the largest flow rate considered

Computed drop height/width

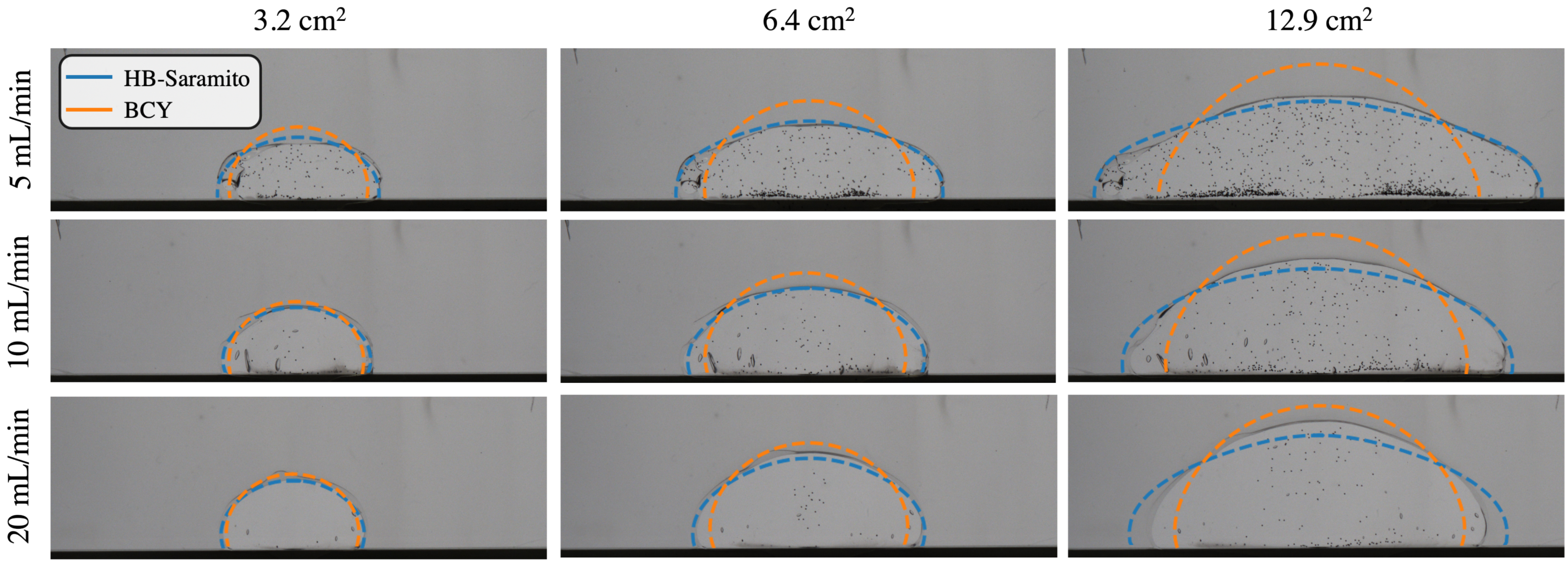


- Constant-viscosity Saramito model considered in previous work
  - Stress/shear rate curve agrees with experimental data for low (< 1 s^{-1}) shear rates
  - Generally less predictive than the HB-variant of the Saramito model
  - More accurate than BCY model for both height width predictions despite stress/shear rate fit



J. McConnell, W. Ortiz, J.C. Sutherland, P. Newell, A.M. Grillet, A.M. McMaster, R.B. Bhakta, R.R. Rao *Computational modeling and experiments of an elastoviscoplastic fluid in a thin mold-filling geometry*, Journal of Non-Newtonian Fluid Mechanics. 30 (2022), 104851

Computed drop shape for 0.3% Carbopol



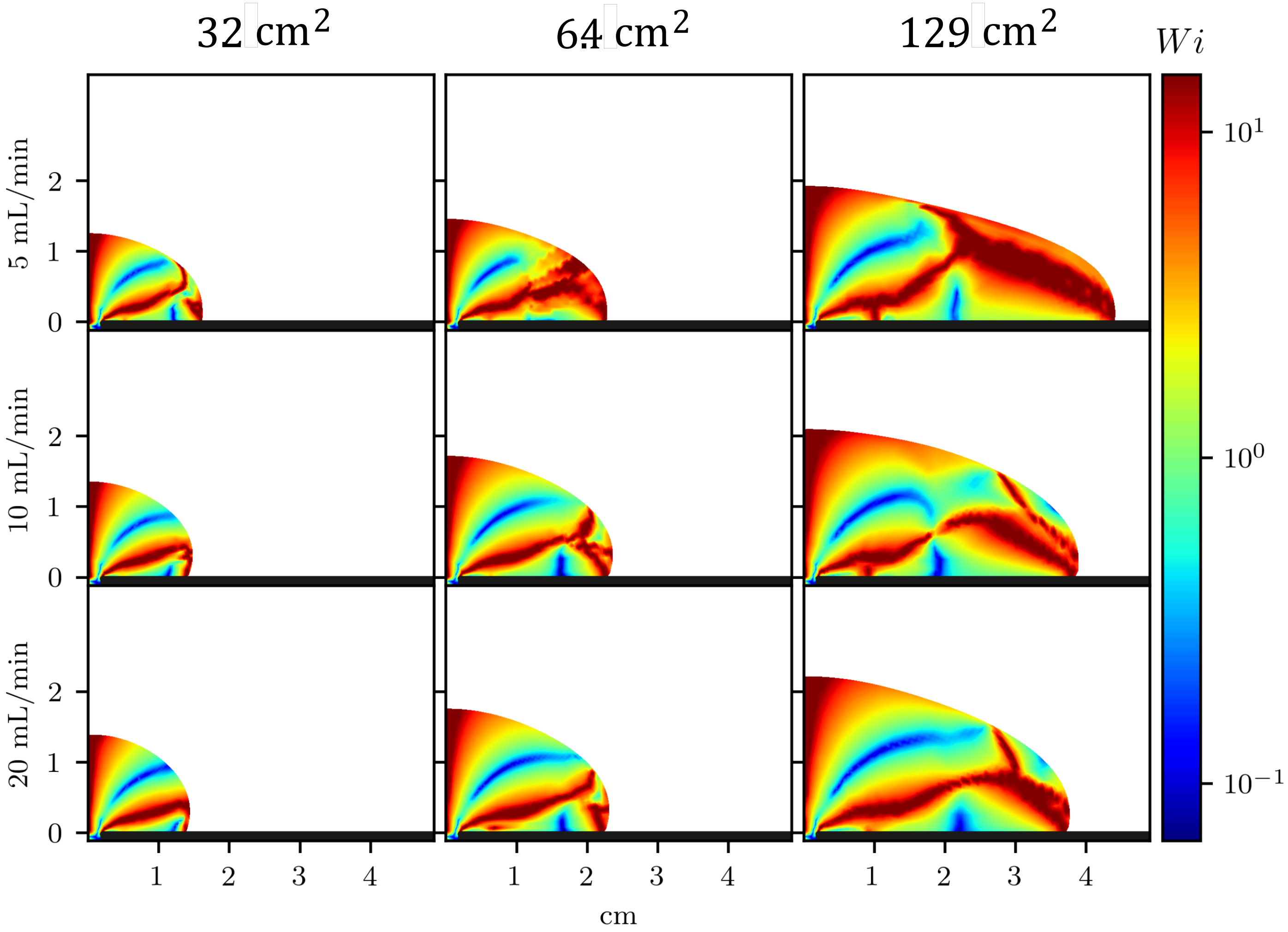
- Experimental drop transitions from round to triangular as volume is increased
  - For a fixed droplet volume, higher flow rate leads to a rounder droplet
- HB-Saramito model predicts this behavior (though imperfectly)
  - BCY model struggles to show transition to a triangular shape at larger volumes

Local Weissenberg number indicates normal stresses are non-negligible

$$Wi = \sqrt{\frac{(\boldsymbol{\sigma}_{xx} - \boldsymbol{\sigma}_{yy})^2 + (\boldsymbol{\sigma}_{yy} - \boldsymbol{\sigma}_{zz})^2 + (\boldsymbol{\sigma}_{zz} - \boldsymbol{\sigma}_{xx})^2}{\boldsymbol{\sigma}_{xy}^2 + \boldsymbol{\sigma}_{xz}^2 + \boldsymbol{\sigma}_{yz}^2}}$$

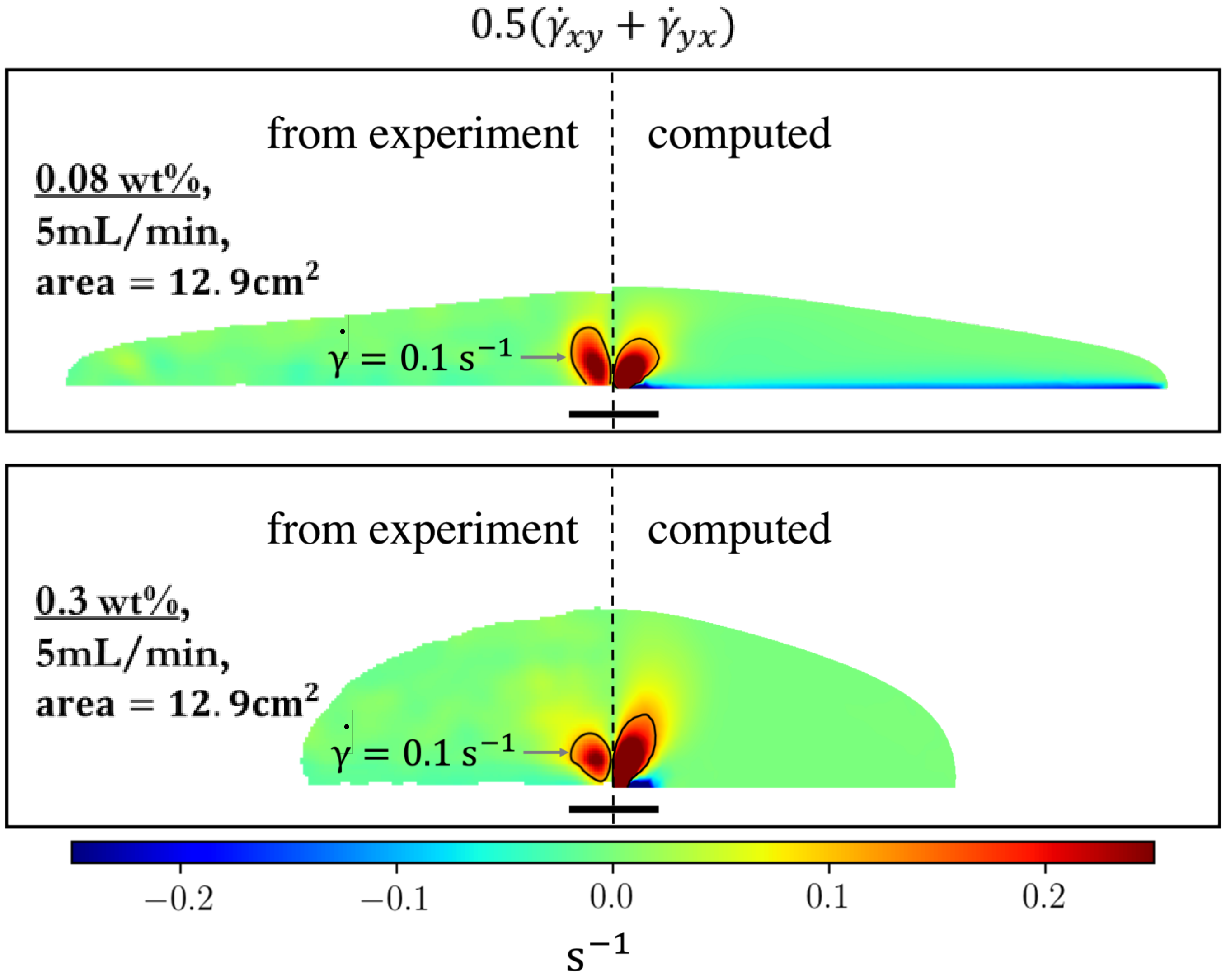
Pictured:
Wi computed from HB-Saramito model at z-plane of symmetry for 0.3% Carbopol

- Alternating zones of high and low Wi predicted to occur for the range of flow rates considered
- High Wi zones may explain the performance shortcomings of the BCY model



Comparison of experimental and HB-Saramito shear rate

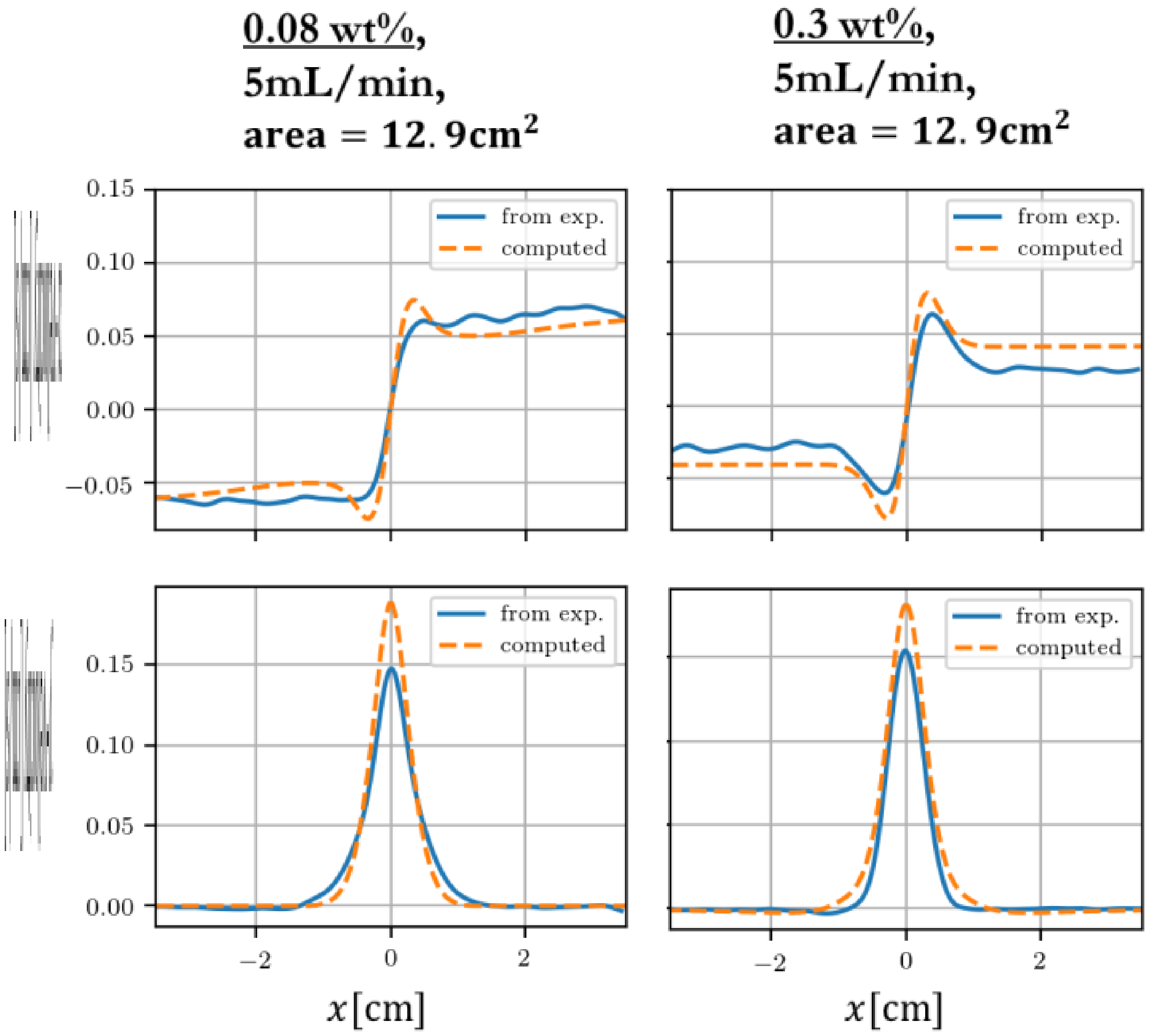
- For the available data, shear rate computed by the HB-Saramito model is generally in agreement with experimental values
- Largest differences manifest near the inlet region:
  - Magnitude of near-wall shear rate is overestimated – no slip BC near inlet doesn't reflect experimental observations
  - Experimental data pictured is smoothed – 8 pixel resolution over 10 images



Comparison of experimental velocity to HB-Saramito computations

Pictured: x- and y- velocities on a horizontal line 4mm above the bottom boundary ($y = 0.4$ cm)

- Computations match experimental velocities fairly well
  - Difference in x-velocity influenced by differences in computed and experimental droplet heights
  - Spatial averaging reduces the magnitude of y-velocity peaks



Work in progress: flow simulations using the Kamani-Donley-Rogers (KDR) EVP model

$$\lambda_1 \overset{\triangledown}{\boldsymbol{\sigma}} + \boldsymbol{\sigma} = \eta_f \dot{\boldsymbol{\gamma}} + \lambda_2 \overset{\triangledown}{\dot{\boldsymbol{\gamma}}} \qquad \lambda_1 = \lambda_2 + \lambda_3$$

$$\eta_f = \frac{\tau_y}{\dot{\gamma}} + k|\dot{\gamma}|^{n-1} \qquad \lambda_2 = \frac{\eta_s}{G}, \quad \lambda_3 = \frac{\eta_f}{G}$$

Target problem:

Steady flow of a 0.3% Carbopol solution over a sphere in a cylindrical vessel

cylinder radius: $R_c = 10$ cm,

sphere radius: $R_s = 1$ cm

Avg. inlet velocity : $v_{inlet} = 0.8$ cm/s

No-slip BCs imposed on all solid surfaces

$n = 0.5$ $\quad G = 525$ Pa

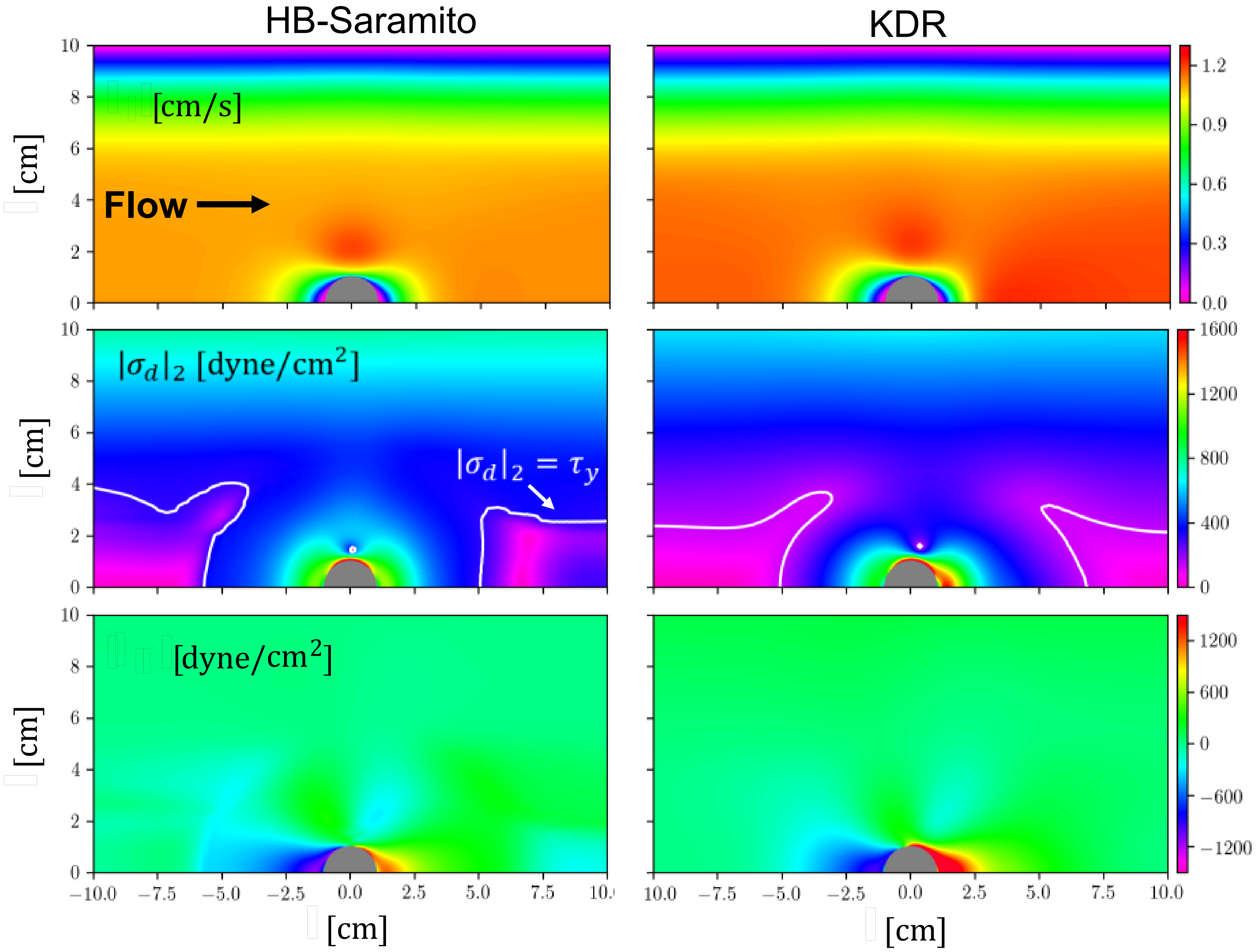
$k = 71.5\ \text{Pa} \cdot \text{s}^n$ $\quad \eta_s = 30\ \text{Pa} \cdot \text{s}$

$\tau_y = 14$ Pa

Kamani, Krutarth, Gavin J. Donley, and Simon A. Rogers. *Unification of the Rheological Physics of Yield Stress Fluids*. Phys. Rev. Lett. 126:21 (2021): 218002

Flow over a sphere: comparing the KDR and HB-Saramito models

- Both EVP models exhibit axial asymmetry of velocity field
  - This asymmetry is more apparent with the KDR model
- An unyielded ring around the sphere is predicted by both models
- Transition of the deviatoric stress norm, $|\sigma_d|_2$, is smoother for the KDR model
  - $|\sigma_d|_2 = \tau_y$ boundary for each model are similar
- Both models predict substantial normal stresses in the vicinity of the sphere



Summary and conclusion

The numerical and modeling framework developed for this work predicts morphological changes of growing EVP drops observed in flow visualizartion experiments

- Drop shape predicted by HB-Saramito model consistent with experimentally-observed drop shapes
- HB-Saramito model yields accurate predictions for fluid drop height over a range of flow rates.
- Predicting drop width is more difficult – the EVP model considered was generally more accurate than the BCY model.
- Shear rate and horizontal velocity computed from the HB-Saramito model mostly 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
  - Unsteady flow simulations using the KDR model
  - Confined free-surface flows over an obstruction

Acknowledgements

- Laboratory Directed Research and Development program at Sandia National Laboratories

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