High-Fidelity Numerical Modeling of Spray Droplet Formation
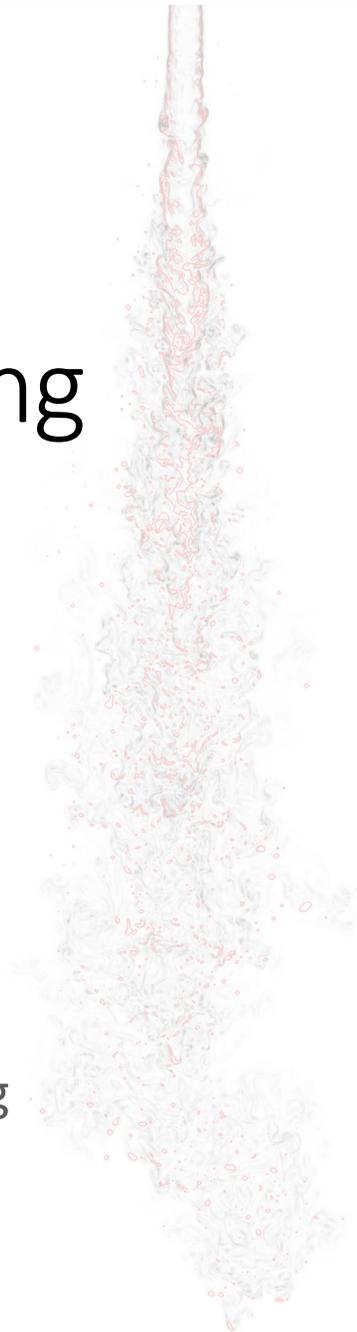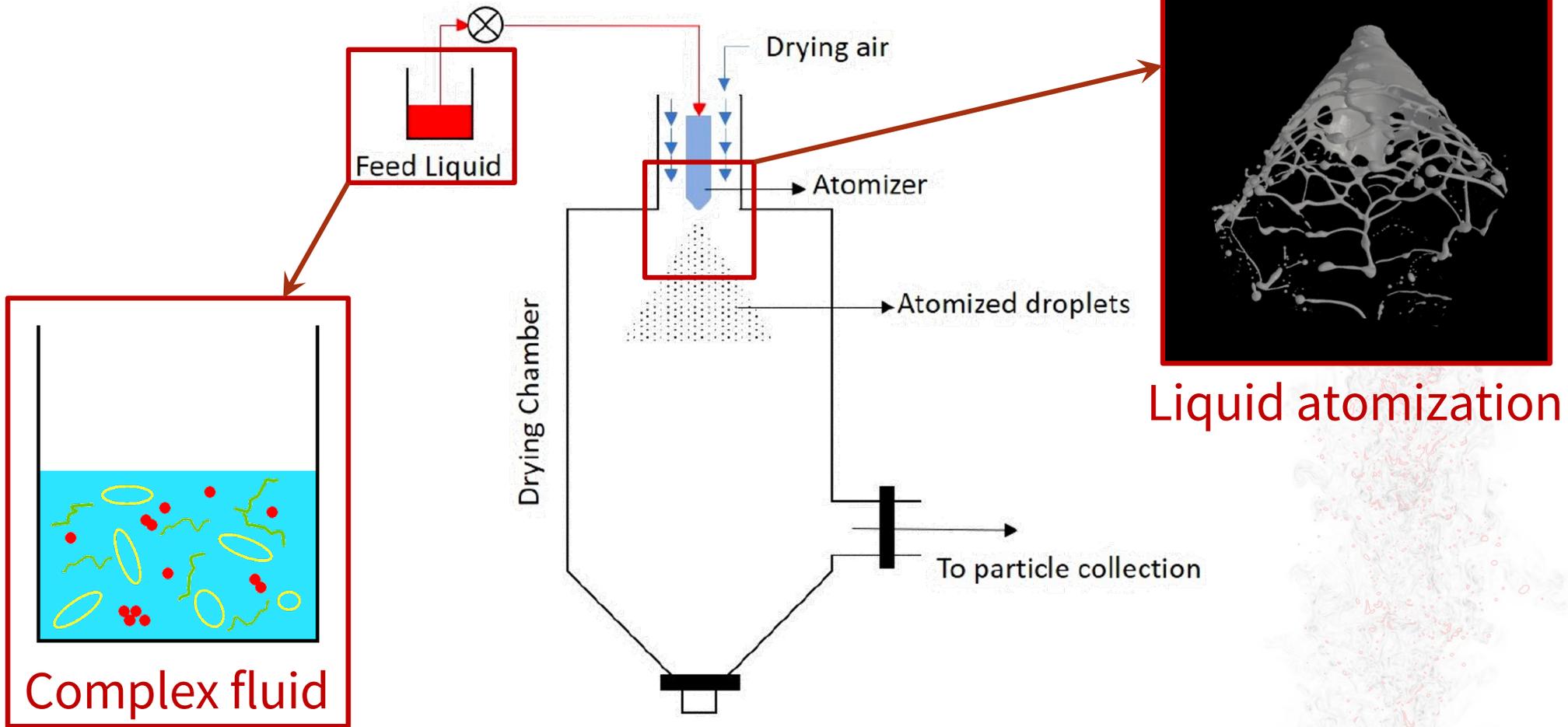
Olivier Desjardins and Joseph Giliberto
Sibley School of Mechanical and Aerospace Engineering
Cornell University

Cornell University
Computational Thermo-Fluids
Laboratory

Motivation – Atomizing complex fluids

Feed Liquid

Drying air

Atomizer

Atomized droplets

Drying Chamber

To particle collection

From Bhonsale et al., *Processes* (2019)

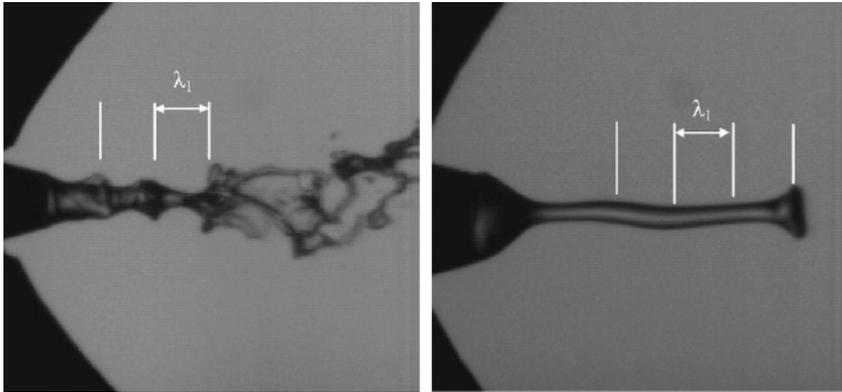**Liquid atomization**

Complex fluid

- Atomized liquid can exhibit high effective viscosity, shear-rate-dependent viscosity (e.g., shear-thinning behavior), viscoelasticity, viscoplasticity, etc…

Select experimental work

High viscosity atomization
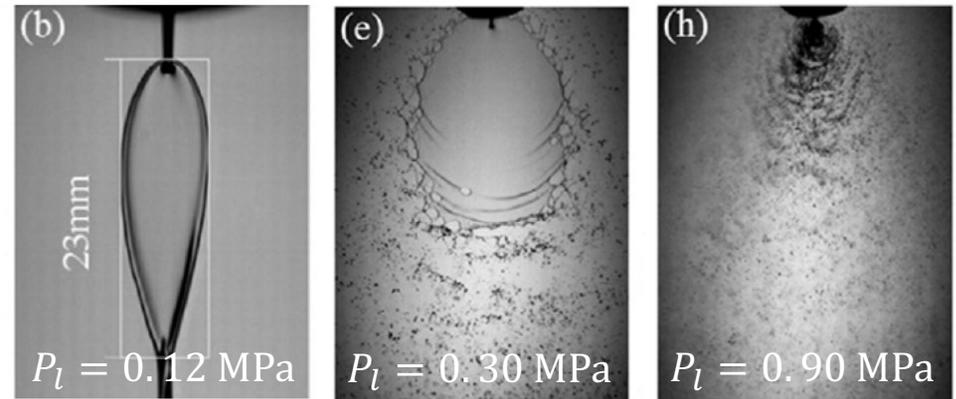Aliseda et al., *IJMF* (2008)

water
$\mu \approx 10^{-3}$ Pa · s

glycerol-water
$\mu \approx 10^{-1}$ Pa · s
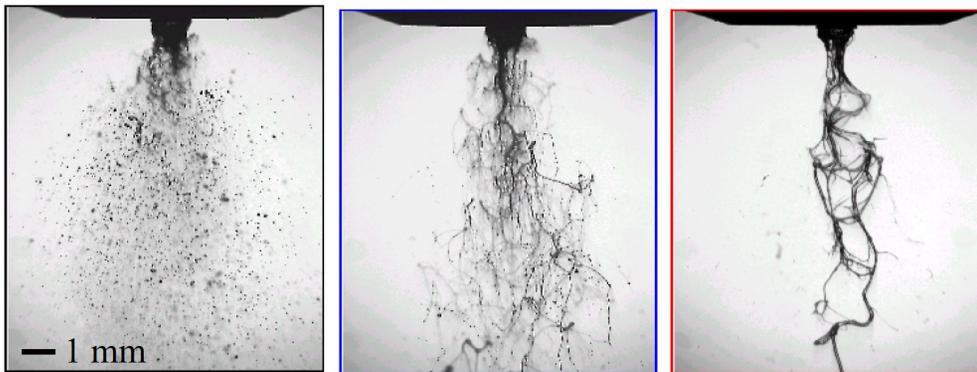
Atomization of shear-thinning fluids
Ma et al., *IJNNFM* (2015)

water + 0.35 wt.% Carbopol 934

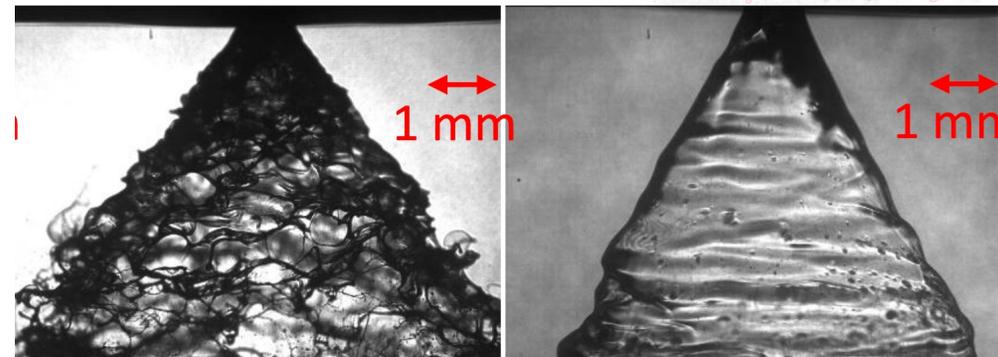## Impact of viscoelasticity
Christanti & Walker, *Atom. & Sprays* (2006)

— 1 mm

⟶ Increased polymer concentration ⟶

Multiple complex fluids and nozzle types
Ashgriz group, *IFPRI report* (2022)

1 mm   1 mm

⟶ Increased fluid viscosity ⟶

High-fidelity multiscale modeling of atomization

LES of spray atomization in two-fluid configuration

Drop size distribution
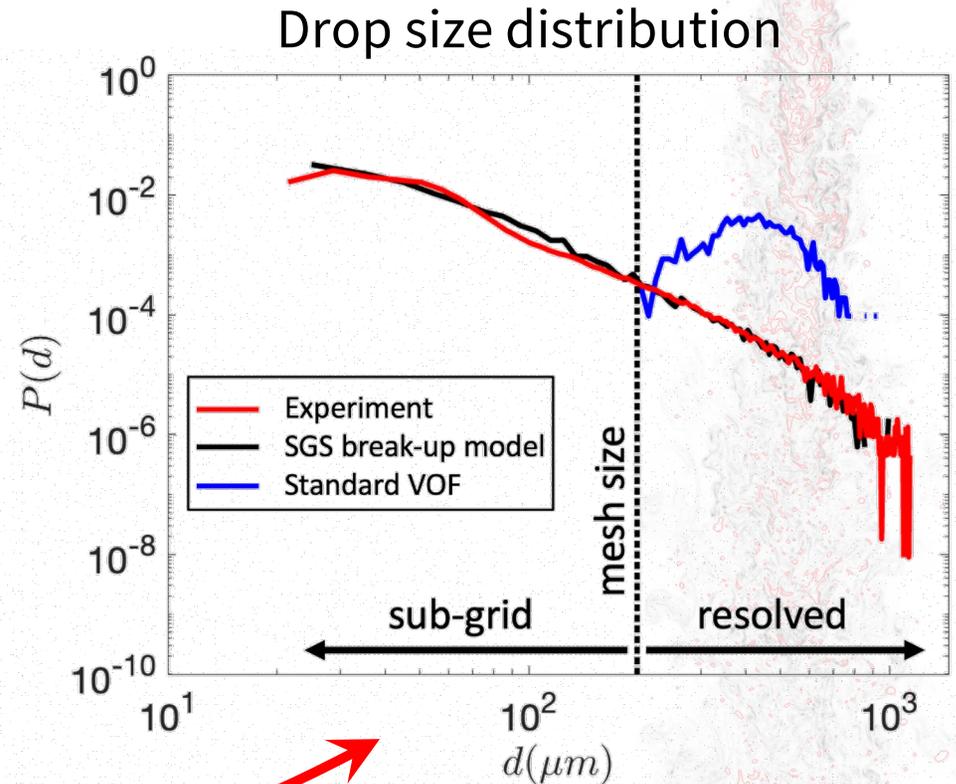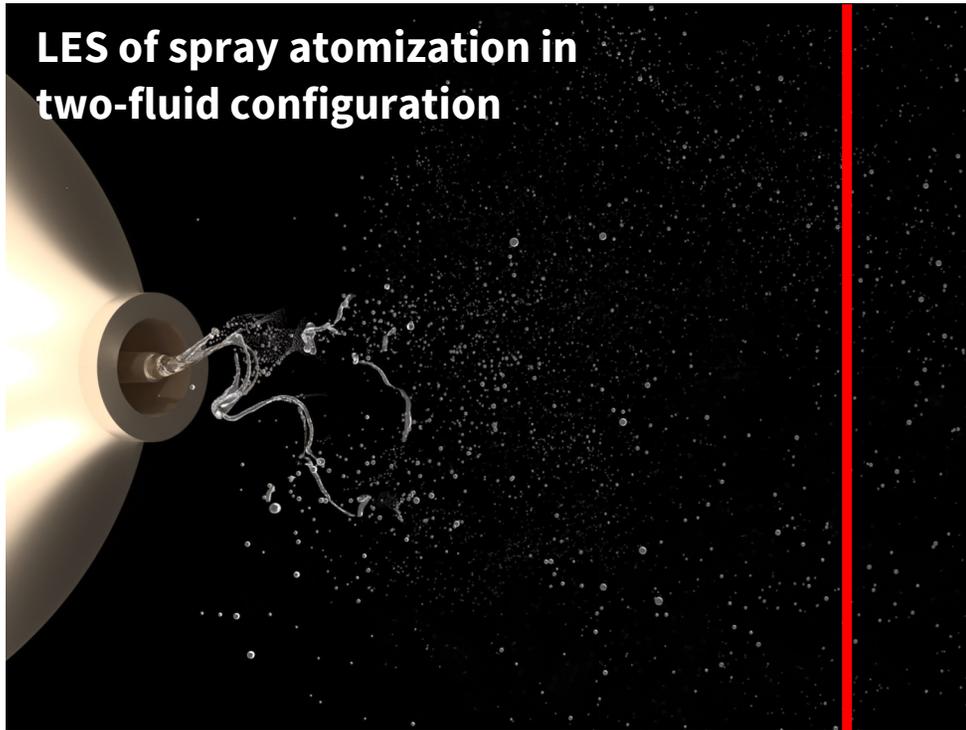
➢ **Recently developed multiscale modeling framework for spray atomization shows promise for mesh-independent drop size predictions**

Project objective and proposed workplan

- <u>Objective</u>

  Assess and enhance ability of our novel high-fidelity multiscale spray atomization model for complex fluids

- <u>Proposed work plan</u>

Year 1
- ➤ Assess influence of high viscosity fluid in air-blast configuration
- ➤ Identify experimental datasets for complex fluid atomization

Year 2
- ➤ Compare against experimental data
- ➤ Assess performance of our strategy

Year 3
- ➤ Implement non-Newtonian fluid model
- ➤ Improve modeling closures for complex fluids

Project objective and proposed workplan

- <u>Objective</u>

  Assess and enhance ability of our novel high-fidelity multiscale spray atomization model for complex fluids

- <u>Proposed work plan</u> **and accomplishments in Year 1**

Year 1   **in pressure-swirl configuration**
  - ➢ **Assess influence of high viscosity fluid** ~~in air-blast configuration~~
  - ➢ **Identify experimental datasets for complex fluid atomization**

Year 2
  - ➢ Compare against experimental data
  - ➢ Assess performance of our strategy

Year 3
  - ➢ **Implement non-Newtonian fluid model**
  - ➢ Improve modeling closures for complex fluids

Computational modeling of non-Newtonian fluids

- Various levels of complexity can be considered

1. <u>High constant viscosity</u>
   - No model needed
   - Implicit time integration might be necessary

2. <u>Shear-rate-dependent viscosity</u> [1]
   - Various models available: power-law, **Carreau**, Cross, Ellis, etc…
   - Variable viscosity flow solver necessary

3. <u>Viscoelasticity</u>
   - Active research area:
     - Oldroyd-B model [2]
     - Giesekus model
     - Finite Extensible Non-linear Elastic models: FENE-P [3], **FENE-CR** [4]
   - Multiple additional transport equations necessary

1. Chhabra & Richardson, Non-Newtonian Flow & Applied Rheology   2. J. Oldroyd *Proc. R. Soc. Lond. A* (1950)
3. Bird et al. *J. Non-Newt. Fluid Mech.* (1980)   4. Chilcott & Rallison *J. Non-Newt. Fluid Mech.* (1988)

Mathematical model

- Single velocity, two-phase, incompressible, Navier-Stokes

$$\nabla \cdot \boldsymbol{u} = 0 \qquad \text{Continuity}$$

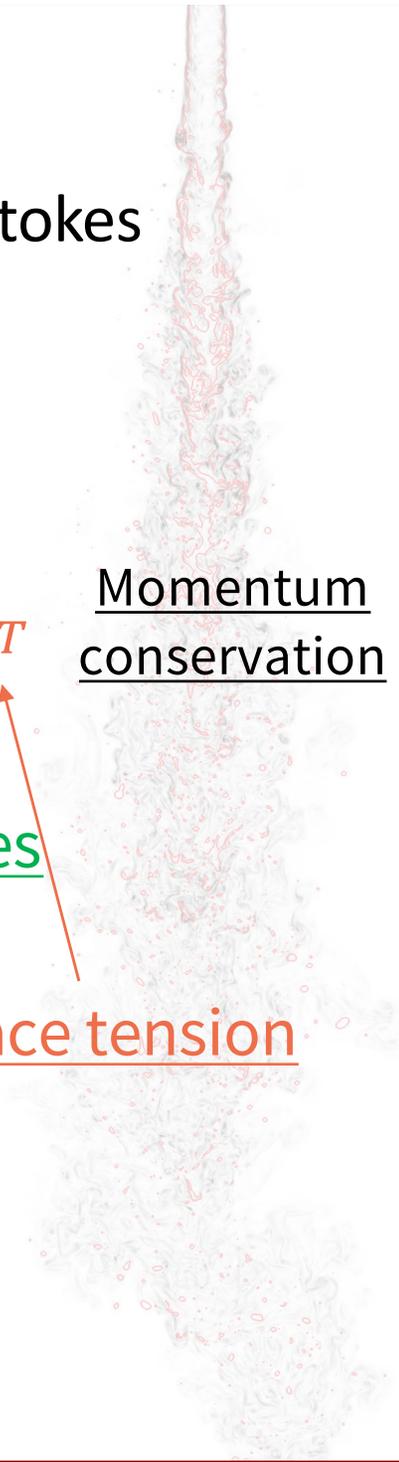$$\frac{\partial \alpha}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha = 0 \qquad \text{Liquid volume conservation}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \textcolor{red}{\nabla \cdot \boldsymbol{\tau}} + \textcolor{blue}{\nabla \cdot \boldsymbol{\tau}_p} + \textcolor{green}{\nabla \cdot \boldsymbol{\tau}_{\text{sgs}}} + \textcolor{orange}{\boldsymbol{F}_{ST}} \qquad \text{Momentum conservation}$$

Viscous stresses

Turbulent stresses

Elastic stresses
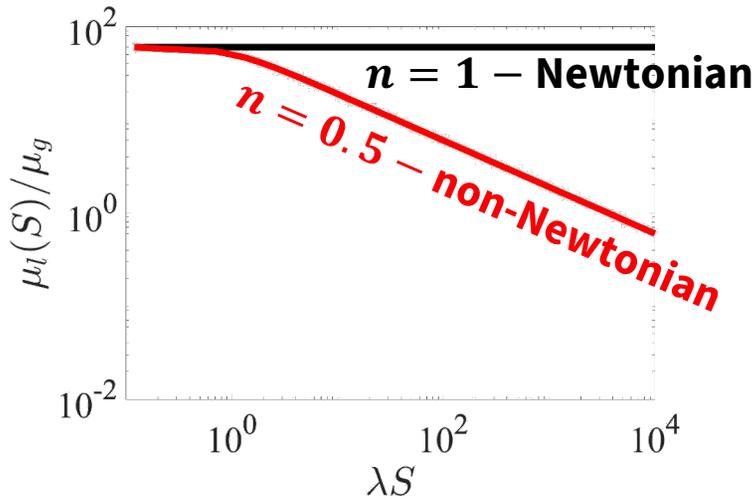
Surface tension

Mathematical model

- Single velocity, two-phase, incompressible, Navier-Stokes

$$\nabla \cdot \boldsymbol{u} = 0 \qquad \text{Continuity}$$

$$\frac{\partial \alpha}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha = 0 \qquad \text{Liquid volume conservation}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \nabla \cdot \boldsymbol{\tau}_p + \nabla \cdot \boldsymbol{\tau}_{\text{sgs}} + \boldsymbol{F}_{ST} \qquad \underline{\text{Momentum conservation}}$$

Viscous stresses – Carreau model

$$\boldsymbol{\tau} = 2\mu \boldsymbol{S} \text{ with } \boldsymbol{S} = \frac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\text{T}}\right)$$

$$\text{and } S = \sqrt{2\boldsymbol{S} : \boldsymbol{S}}$$

$$\rho = \alpha \rho_l + (1 - \alpha)\rho_g$$

$$\mu = \alpha \mu_l + (1 - \alpha)\mu_g$$

$$\mu_l = \mu_s + \mu_p \text{ with } \mu_p = \mu_{p,0}\left(1 + (\lambda S)^2\right)^{\frac{n-1}{2}}$$

Graph axes: $\mu_l(S)/\mu_g$ versus λS

$n = 1 - $ **Newtonian**

$n = 0.5 - $ non-Newtonian

Mathematical model

- Single velocity, two-phase, incompressible, Navier-Stokes

$$\nabla \cdot \boldsymbol{u} = 0 \qquad \text{Continuity}$$

$$\frac{\partial \alpha}{\partial t} + \boldsymbol{u} \cdot \nabla \alpha = 0 \qquad \text{Liquid volume conservation}$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \boldsymbol{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \nabla \cdot \boldsymbol{\tau}_p + \nabla \cdot \boldsymbol{\tau}_{\text{sgs}} + \boldsymbol{F}_{ST} \qquad \frac{\text{Momentum}}{\text{conservation}}$$

$$\boldsymbol{\tau}_p = \mu_p f \frac{\mathbf{C} - \mathbf{I}}{\lambda}$$

with $\mathbf{C} =$ conformation tensor

$\mathbf{I} =$ identity tensor

Elastic stresses – FENE-CR model
- ➤ Elastic dumbbells model of polymers
- ➤ Represents a Boger fluid

and $\mathbf{C}$ is solution of $\dfrac{\partial \mathbf{C}}{\partial t} + \boldsymbol{u} \cdot \nabla \mathbf{C} = \nabla \boldsymbol{u} \cdot \mathbf{C} + \mathbf{C} \cdot (\nabla \boldsymbol{u})^T - f \dfrac{\mathbf{C} - \mathbf{I}}{\lambda}$

Alves et al. *ARFM* (2021)   Ohta et al. *J. Non-Newt. Fluid Mech.* (2019)   Varchanis et al. *J. Non-Newt. Fluid Mech.* (2022)
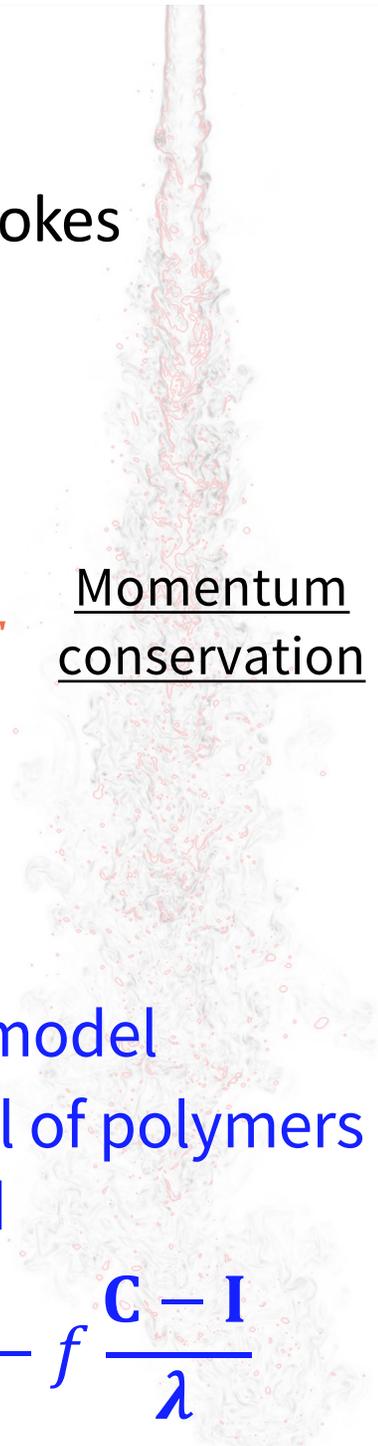
Demonstration – Pouring shampoo

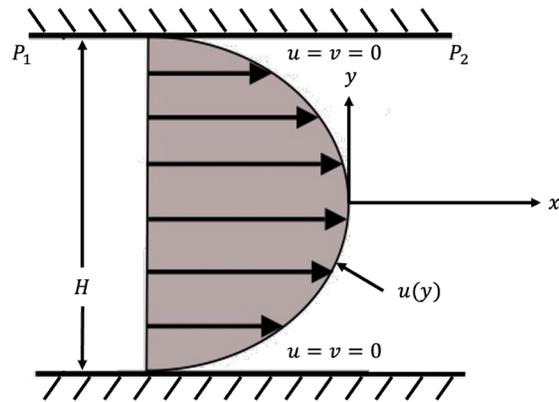water   high viscosity   shear-thinning   shear-thinning and viscoelastic
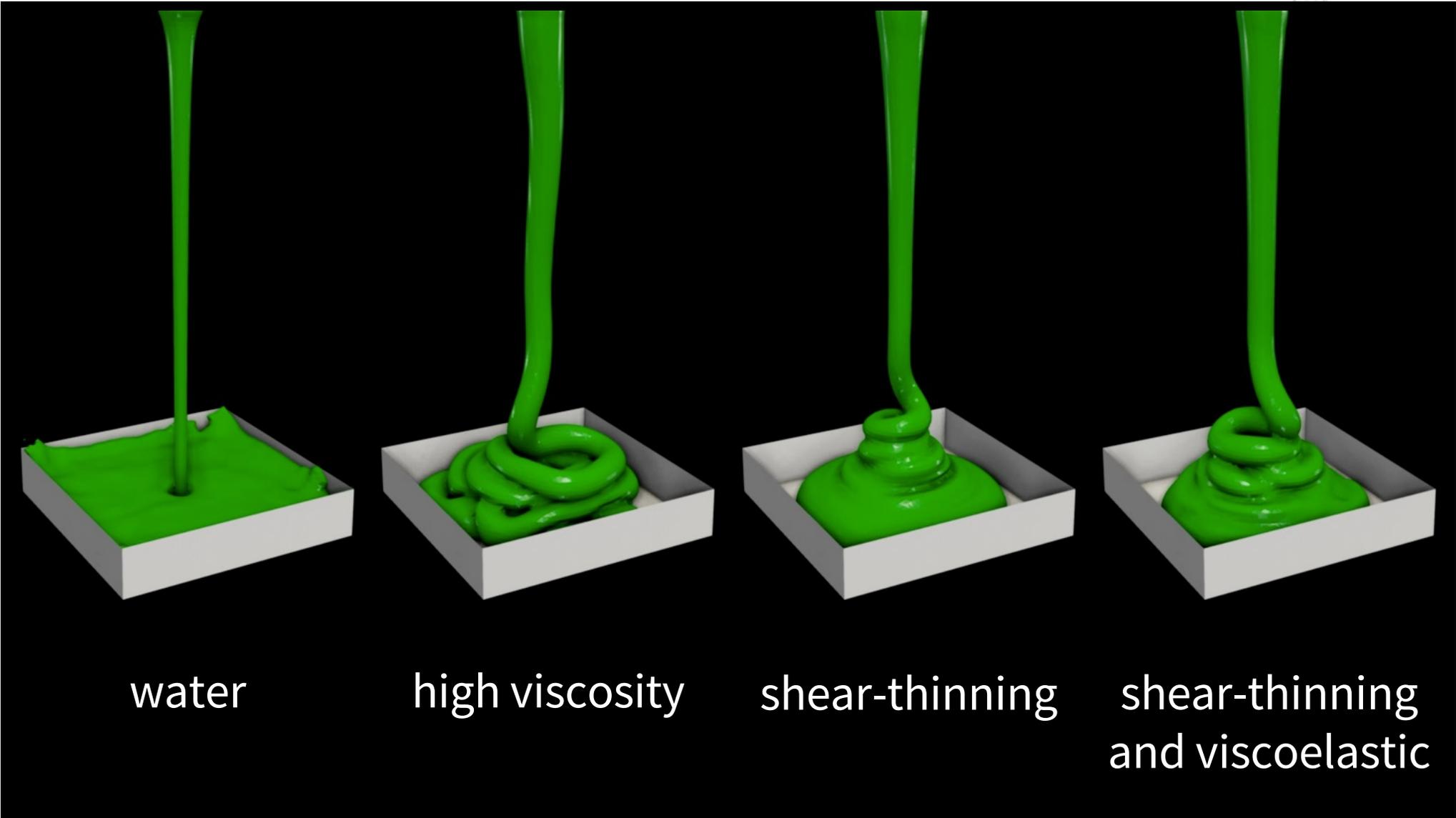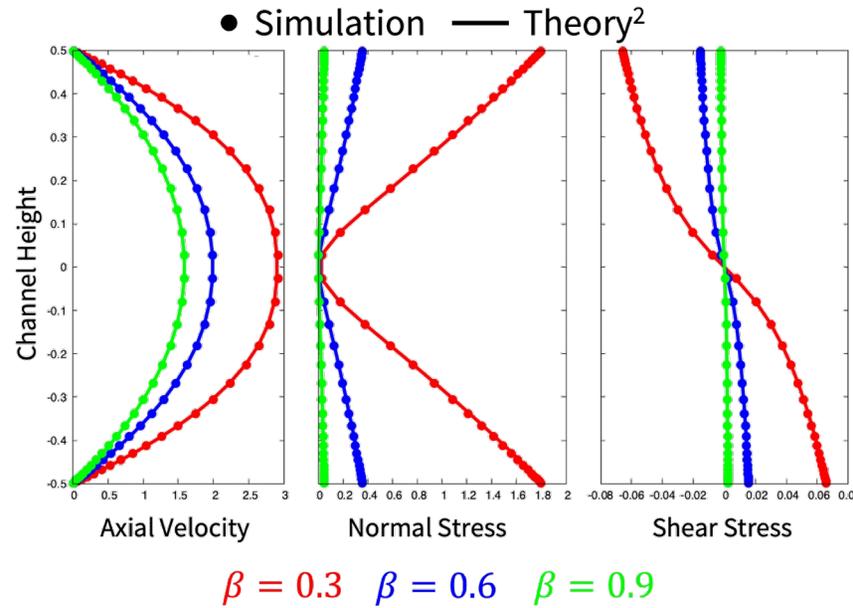
Verification and validation

1. Bird et al. *J. Non-Newt. Fluid Mech.* (1980)
2. Cruz, Pinho, Oliveira. *J. Non-Newt. Fluid Mech.* (2005)
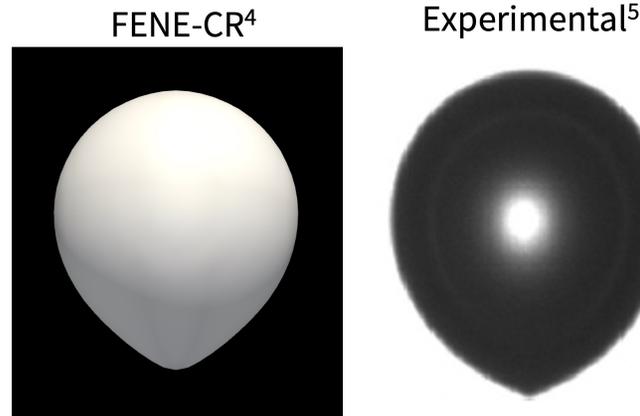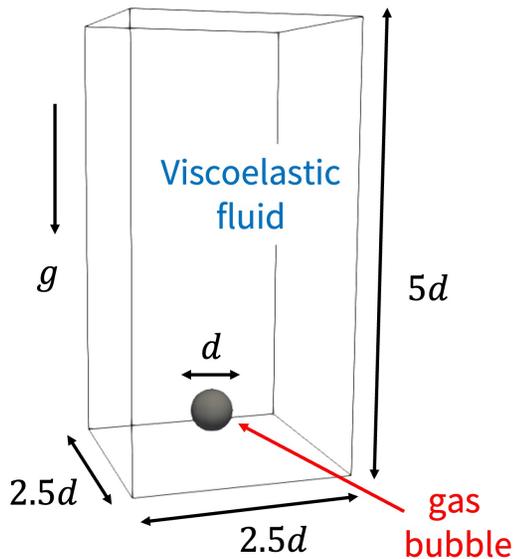
FENE-P[1] Channel Flow

Viscosity Ratio:

$$\beta = \frac{\mu_s}{\mu_s + \mu_p}$$

● Simulation —— Theory[2]

Axial Velocity   Normal Stress   Shear Stress

$\beta = 0.3$ $\beta = 0.6$ $\beta = 0.9$

Rising Bubble[3]

Viscoelastic fluid

g

H

$5d$

d

$2.5d$

$2.5d$

gas bubble

FENE-CR[4]

Experimental[5]

➢ Viscoelasticity induces cusp shape in bubble

3. Ohta et al. *J. Non-Newt. Fluid Mech.* (2019)
4. Chilcott & Rallison *J. Non-Newt. Fluid Mech.* (1988)
5. Pliz & Brenn *J. Non-Newt. Fluid Mech.* (2007)

Pressure-swirl atomization

Turbulent swirling
annular pipe

$$\frac{D}{\Delta} = 192$$

Swirl atomizer

$$\frac{D}{\Delta} = 32$$

$10D$

$12D$
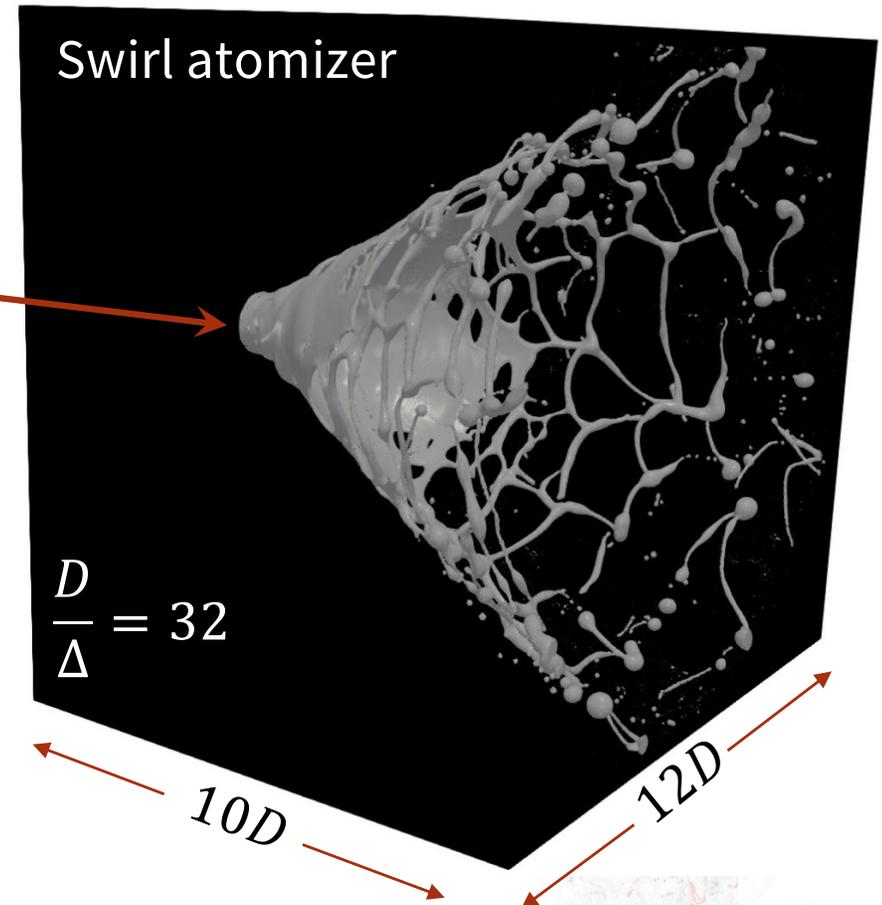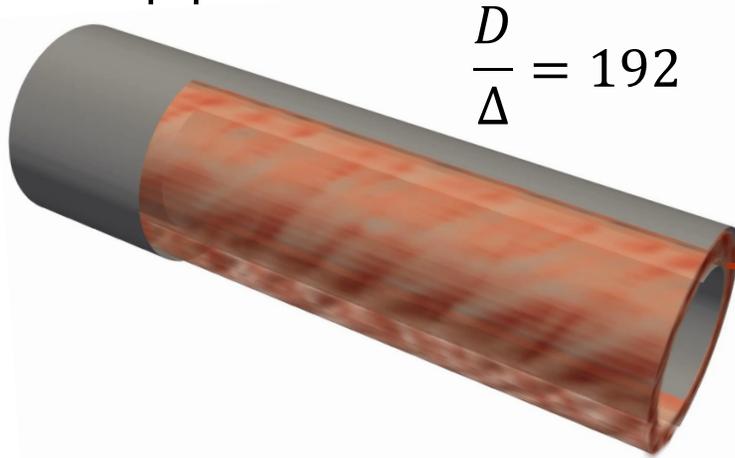
Dimensionless numbers

Re_l	We_l	μ_l/μ_g	ρ_l/ρ_g
100	**1000**	**1000**	**1000**
500	1000	200	1000
1000	1000	100	1000
5000	**1000**	**20**	**1000**

$$\text{Re}_l = \frac{\rho_l U D}{\mu_l} \qquad \text{We}_l = \frac{\rho_l U^2 D}{\sigma} \qquad \text{SN} = \frac{2 \int \overline{(\rho uw)} r^2 \,\mathrm{d}r\mathrm{d}\theta}{D \int \overline{(\rho u^2)} r \,\mathrm{d}r\mathrm{d}\theta} = \mathbf{1.2}$$

Pressure-swirl atomization
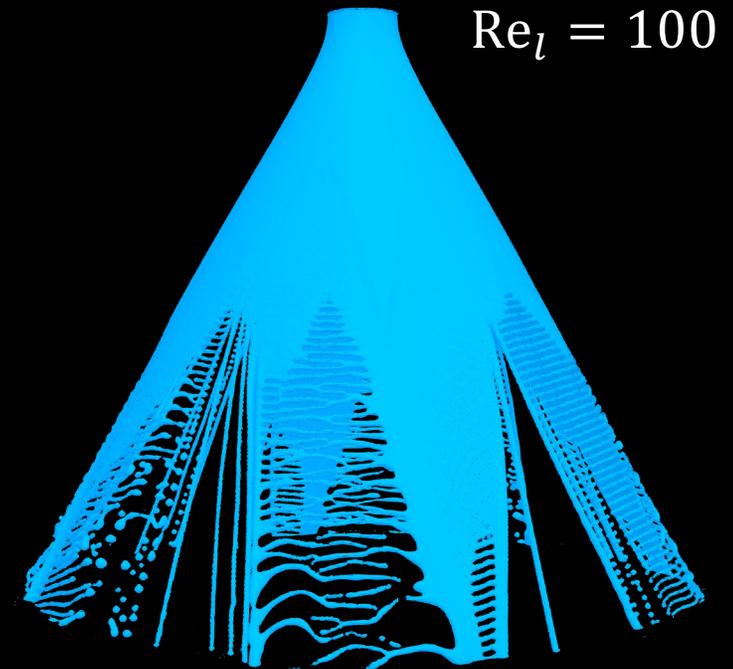
80% Glycerin, $Re_l \sim 850$[1]
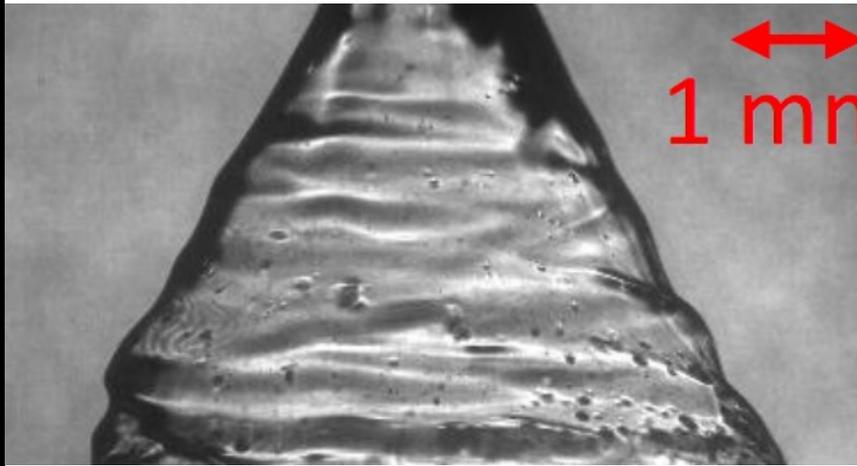
@ nozzle exit

60% Glycerin, $Re_l \sim 4500$[1]
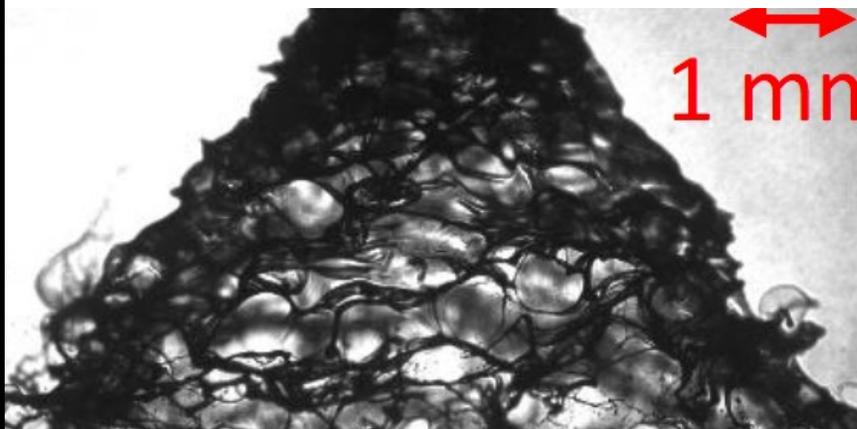
@ nozzle exit

$Re_l = 100$

$Re_l = 5000$

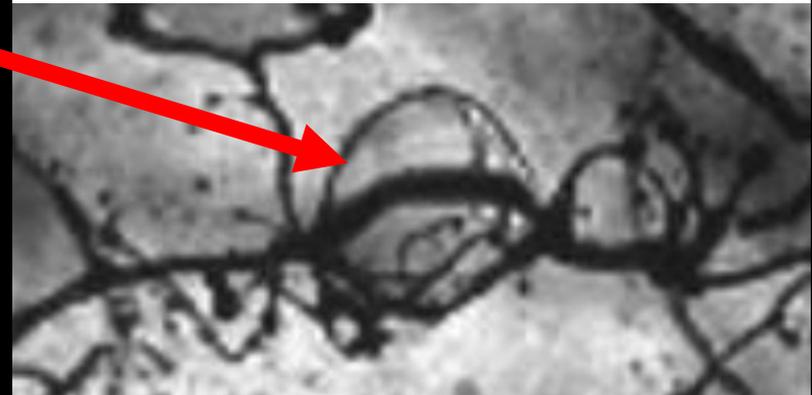1. Ashgriz *IFPRI Final Report FRR-96-05* (2022)
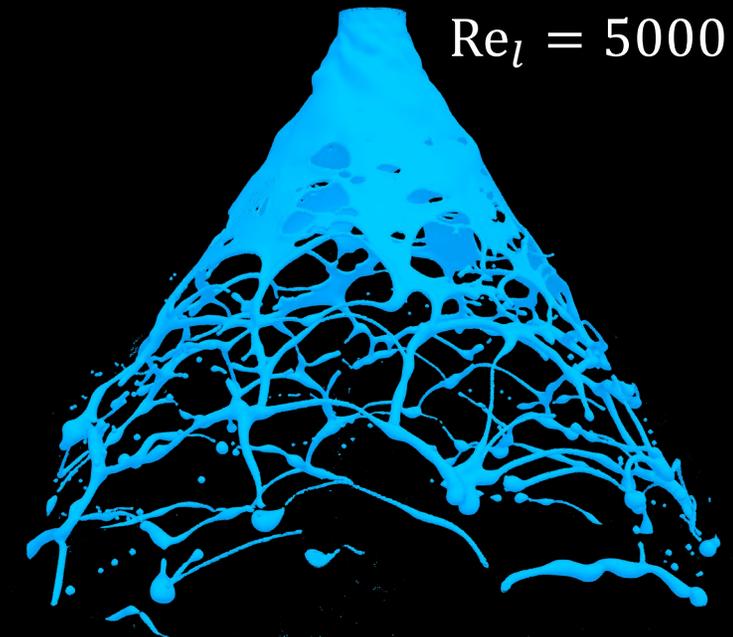
Pressure-swirl atomization

$$\text{We}_l^{\text{exp}} \approx 10\,\text{We}_l^{\text{sim}}$$
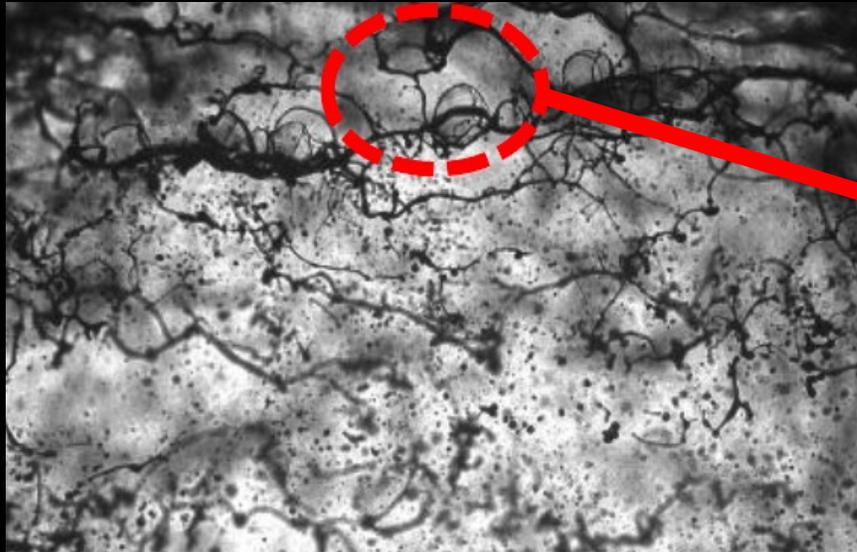
@ 5 mm downstream

Bag break-up of ligament

60% Glycerin, $\text{Re}_l \sim 4500$[1]

1 mm

@ nozzle exit

$\text{Re}_l = 5000$
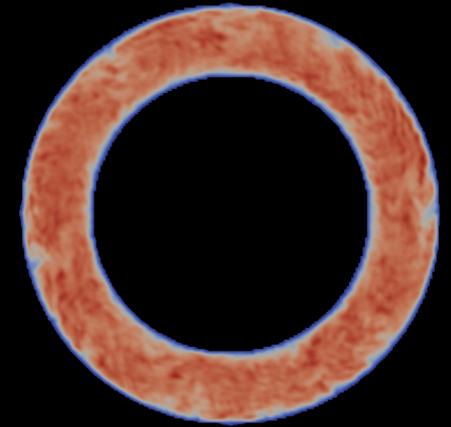
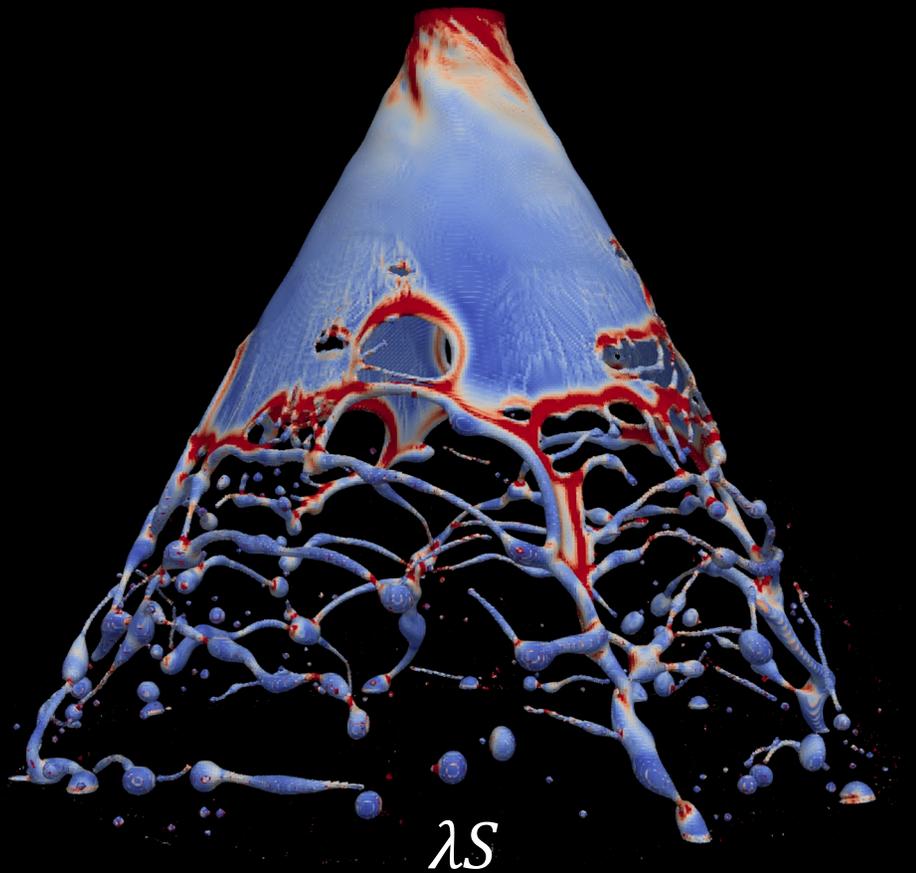1. Ashgriz *IFPRI Final Report FRR-96-05* (2022)
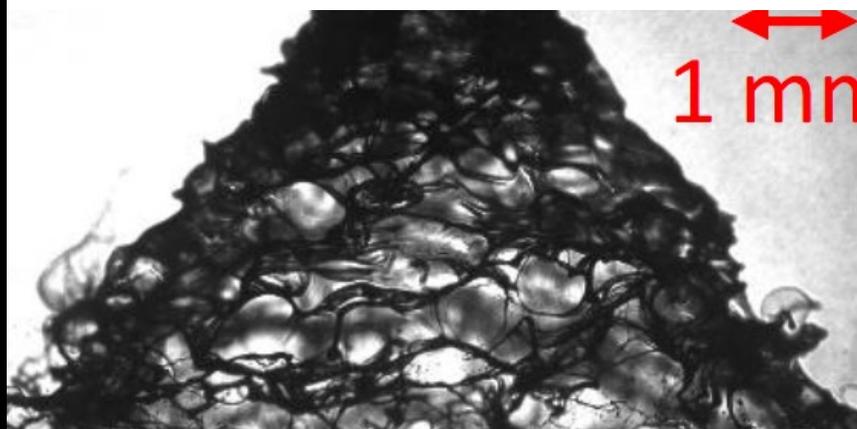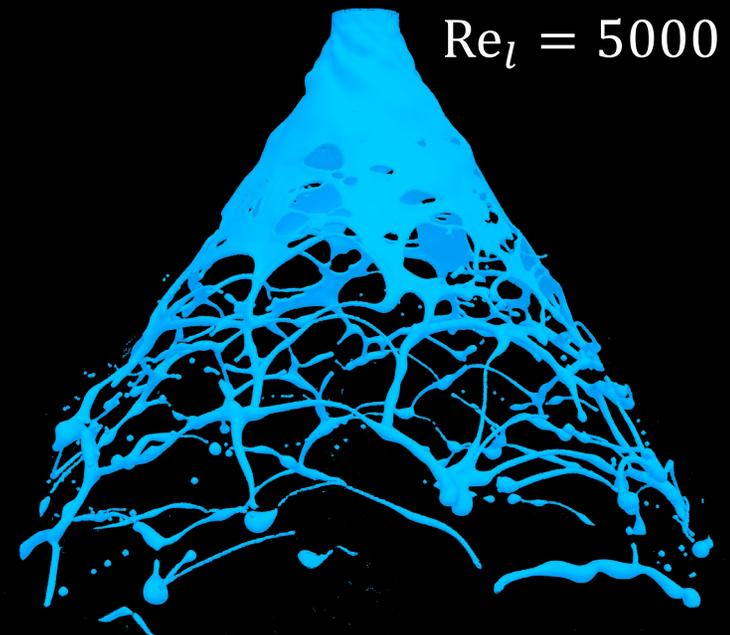
Pressure-swirl atomization

$\mathrm{Re}_l = 1000$
$\mathrm{We}_l = 500$

Shear-thinning properties:
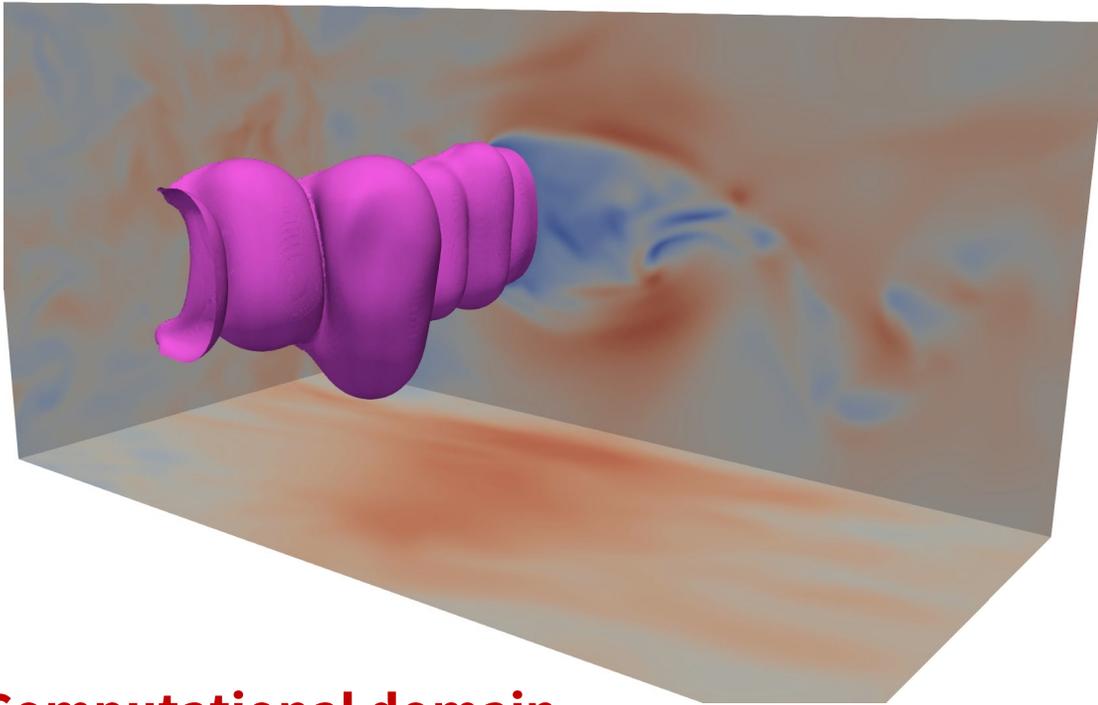$$\frac{\lambda D}{U} = 10 \quad n = \frac{1}{2}$$

Annular pipe is
fully turbulent

λS

0.0e+00 2   4   6   8   10   12   14   16   2.0e+01

Isolated ligament break-up in a cross-flow

D Ligament diameter
U Cross-flow bulk velocity

Dimensionless numbers

$$\mathrm{Re}_g = \frac{\rho_g U D}{\mu_g} = 100$$

$$\mathrm{We}_g = \frac{\rho_g U^2 D}{\sigma} = 10$$

Computational domain

- Inflow-outflow in streamwise direction
- Periodic in cross-streamwise directions
- Inlet flow includes homogeneous isotropic turbulence at $R_\lambda = 45$ and $\mathrm{TI} = 10\%$
- 30 million cells
- $40D \times 20D \times 20D$

Model	μ_l/μ_g	ρ_l/ρ_g
Newtonian	50	1000
Newtonian	**500**	**1000**
Shear-thinning	**500**	**1000**
Shear-thinning and viscoelastic	**500**	**1000**

Isolated ligament break-up in a cross-flow

Newtonian, high viscosity

4 bags are formed

Shear-thinning $\frac{\lambda D}{U} = 10$ $n = \frac{1}{2}$
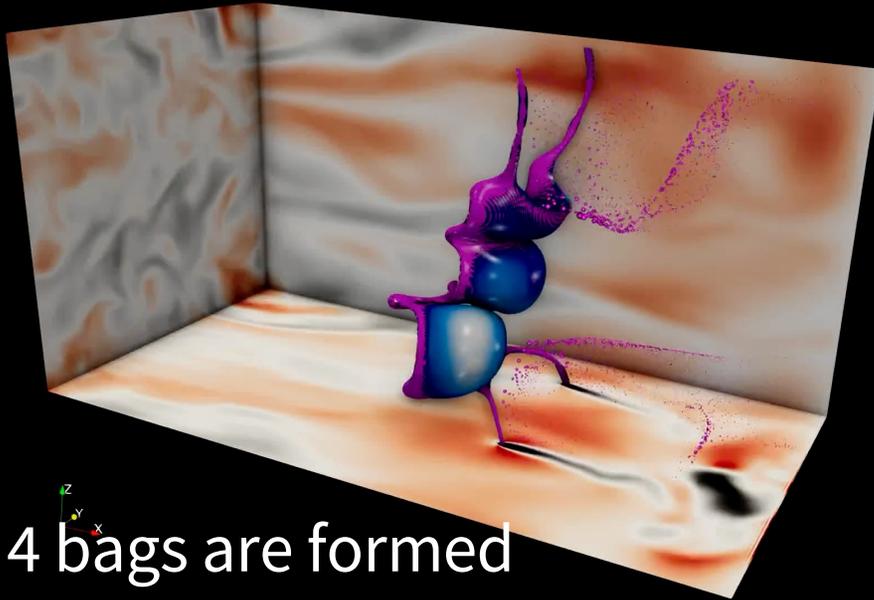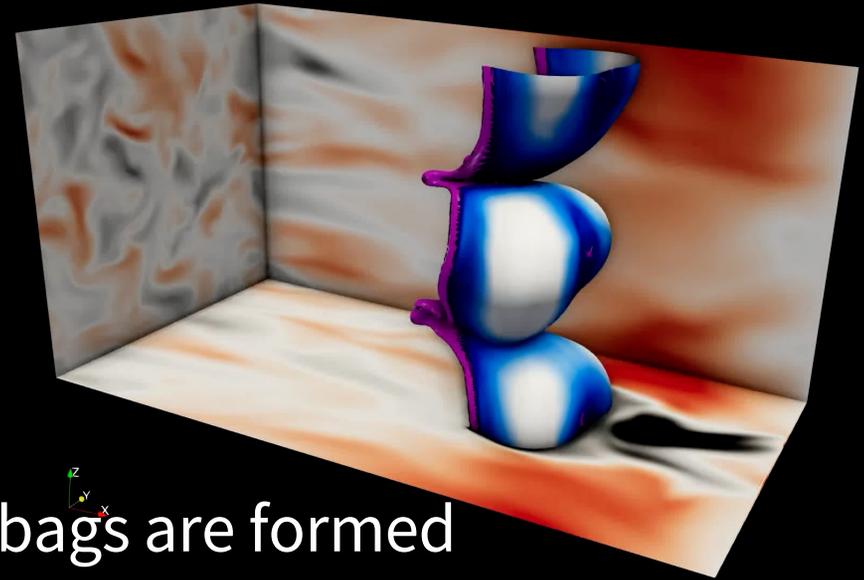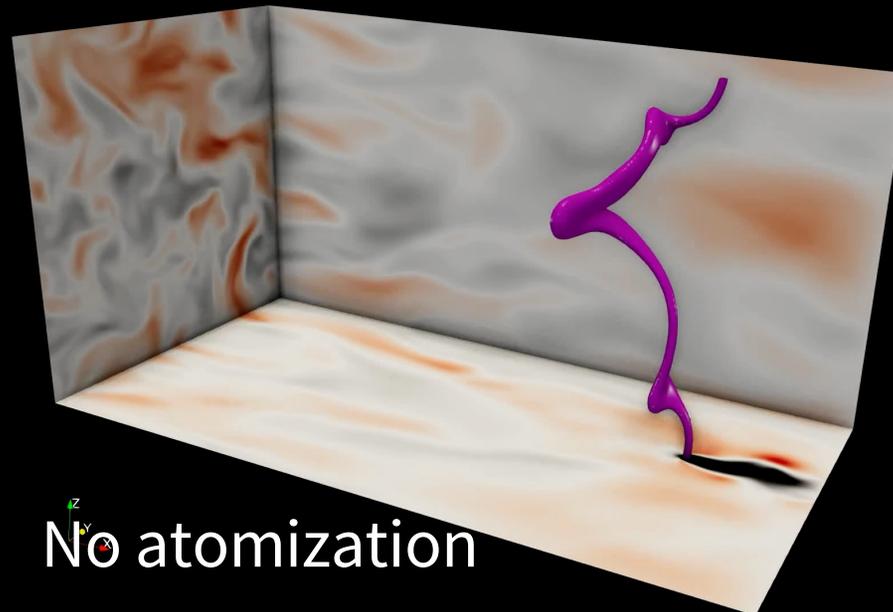

2 bags are formed

Shear-thinning and viscoelastic

$$\frac{\lambda D}{U} = 10 \quad n = \frac{1}{2}$$

No atomization

Conclusions and future steps

1. Complex fluid model implemented and tested

    - Further validation is ongoing

2. Effect of high viscosity and complex rheology on pressure swirl atomization

    - Qualitative agreement with experimental observations
    - Quantitative comparisons will be the focus of year 2

3. Effect of high viscosity and complex rheology on isolated ligament break-up in cross-flow

    - Configuration allows us to reach efficiently realistic conditions
    - Enhanced viscosity, shear-thinning, and viscoelasticity have significant effects on the development of bags on ligaments
    - Quantitative comparisons of resulting drop size predictions are ongoing
    - Viscous Rayleigh-Taylor theory will be considered