

HIGH-FIDELITY NUMERICAL MODELING OF SPRAY DROPLET FORMATION

An enhanced volume of fluid framework for multi-scale atomization modeling

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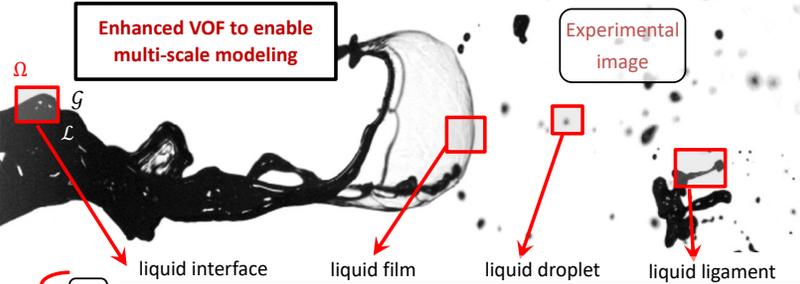
Problem: Unable to accurately predict drop size pdf in standard two-phase CFD methods

- Break-up is due to numerical errors instead of appropriate microscale physics
- Spurious numerical break-up happens at the limit of mesh resolution
- Enormous cost to run high resolution models → still not addressed via mesh refinement

Relevance to IFPRI: Modeling spray formation for high viscosity and complex liquids presents additional challenges due to increase (compared to low viscosity, Newtonian liquids) of thin films and ligaments during atomization

Enhanced VOF to enable multi-scale modeling

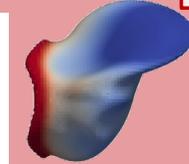
Experimental image



Closure methods

SGS Surface Tension in eVOF¹

- Standard implementation of surface tension (e.g., based on volume fraction gradient) term fails due to vanishing volume fraction



Experiment by Opfer et al., 2014

Standard VOF

eVOF with CSF surface tension

eVOF with new surface tension

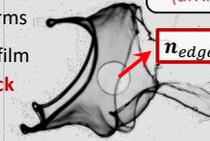
$$\overline{\sigma \kappa \mathbf{n}} \delta \neq \sigma \kappa \nabla \alpha$$

Film Retraction Modeling in eVOF: High Viscosity and Viscoelasticity

- Ignore temporal, convective, and viscous SGS terms
- Assume $\bar{\mathbf{u}} \approx \bar{\mathbf{u}}^l \approx \bar{\mathbf{u}}^g$ except at the edge of the film
- At edge of film, assume that viscous Taylor-Culick retraction is dominating

$$\bar{\mathbf{u}} \approx \bar{\mathbf{u}}^g \text{ and } \bar{\mathbf{u}}^l - \bar{\mathbf{u}}^g \approx \sqrt{2\sigma/\rho_l h} \mathbf{n}_{edge}$$

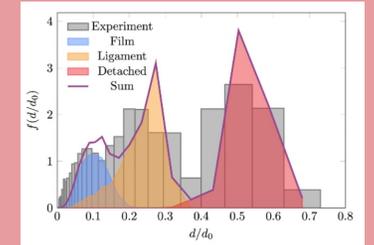
- Distribute velocity using a Stokeslet solution to conserve mass
- Hole nucleation based on local film thickness criterion



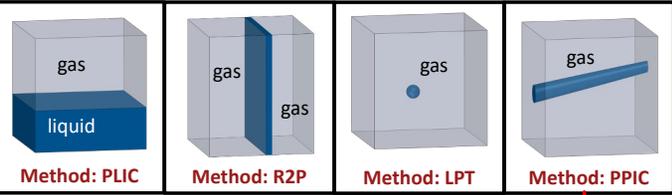
Chandra et al. (arXiv 2023)

Low Viscosity Break-up Modeling in eVOF³

- Ignore temporal, convective, and viscous SGS terms
- Assume $\bar{\mathbf{u}} \approx \bar{\mathbf{u}}^l \approx \bar{\mathbf{u}}^g$ except at the edge of films
- At edge of film, assume that break-up dynamics are dominating
 - Model droplet shedding from retracting rim
 - Based on theory of Wang and Bourouiba⁴
 - Hole nucleation based on local film thickness criterion



Modeling Method



Sub-grid scale film capturing

- Reconstruction with 2 Plane¹
- Two interfaces exist in each cell
- Effectively eliminates numerical topology change for films

Sub-grid scale topologies

- Piecewise-Parabolic Interface Calculation²
- Paraboloid interface in each cell
- Able to directly represent sub-grid scale films and ligaments

Volume-filtered framework for Enhanced VOF

- Systematically filter over the grid size
- \bar{f} : filtered quantity
- \bar{f}^l, \bar{f}^g : filtered liquid & gas quantities

Continuity equation

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

Phasic barycenter transport equation

$$\frac{\delta}{\delta t} \psi = 0$$

Liquid volume fraction transport equation

$$\frac{\delta}{\delta t} \bar{x}^l = \bar{\mathbf{u}}^l \quad \frac{\delta}{\delta t} \bar{x}^g = \bar{\mathbf{u}}^g$$

Liquid distribution function

$$\psi(\mathbf{x}, t) = \begin{cases} 1, & \text{if } \mathbf{x} \in \mathcal{L} \\ 0, & \text{if } \mathbf{x} \in \mathcal{G} \end{cases}$$

Navier-Stokes equation

$$\frac{\partial \bar{\rho} \bar{\mathbf{u}}}{\partial t} + \nabla \cdot (\bar{\rho} \bar{\mathbf{u}} \otimes \bar{\mathbf{u}}) = -\nabla \bar{p} + \overline{\sigma \kappa \mathbf{n} \delta}$$

$$\text{Non-trivial closed term } + \nabla \cdot [\bar{\mu} (\nabla \bar{\mathbf{u}} + \nabla \bar{\mathbf{u}}^T)]$$

$$\text{Unclosed terms } \tau_t + \nabla \cdot [\tau_c + \tau_v]$$

VOF	Enhanced VOF: SGS Interface Capturing	Enhanced VOF: SGS Interface Capturing + Film Retraction
Break-up due to numerical error	SGS film maintained, but no break-up	Hole nucleation criterion: $h_{min} = \Delta/2$ ligament break-up via Rayleigh-Plateau

⇒ Explicit modeling of hole nucleation and film retraction below the grid-size leads to ligament formation and break-up