High-Fidelity Numerical Modeling of Spray Droplet Formation

An enhanced volume of fluid framework for multiscale atomization modeling

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2025 IFPRI Annual General Meeting

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

Accomplishments:

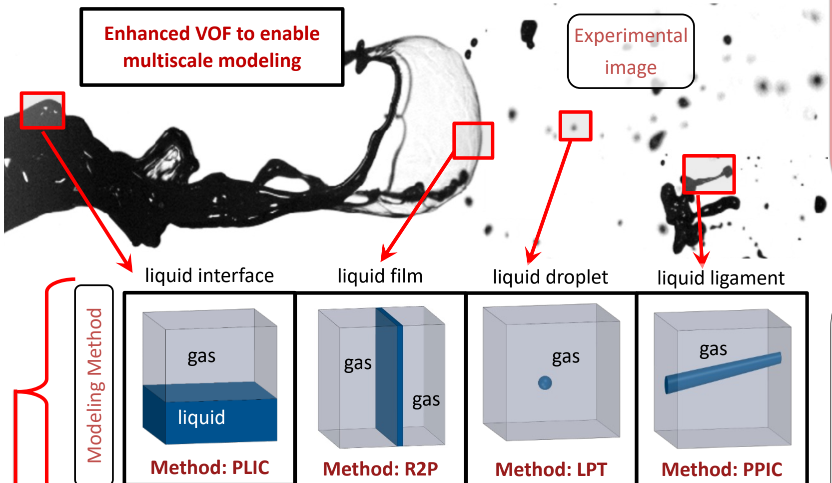
- Formalized a volume-filtered multiscale modeling framework for liquid-gas atomization
- Modeled pressure swirl atomization with sub-grid scale thin film tracking + sub-grid scale film retraction model + physics-based ligament break-up model
- Good qualitative & quantitative agreement with experimental measurements[3,4]
- Implemented and validated stress model for multiphase non-Newtonian fluid flows

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

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

Enhanced VOF to enable multiscale modeling



Sub-grid scale film capturing

- Reconstruction with 2 Planes[1]
- Two interfaces exist in each cell
- Effectively eliminates numerical topology change for films

Future: Sub-grid ligament capturing

- Piecewise-Parabolic Interface Calculation[2]
- Paraboloid interface in each cell
- Able to directly represent sub-grid scale films and ligaments

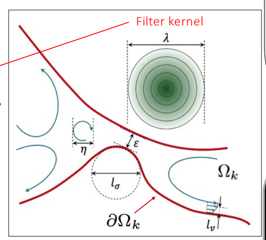
Volume-filtered framework for SGS Modeling

Indicator function for phase k

$$\phi_k(\boldsymbol{x},t) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \Omega_k(t) \\ 0 & \text{otherwise} \end{cases}$$

Volume-filtering operation

$$\boldsymbol{a}(\boldsymbol{x},t) = \int_\Omega \boldsymbol{a}(\boldsymbol{y},t)\, g(\boldsymbol{y}-\boldsymbol{x})\,\mathrm{d}\boldsymbol{y}$$



Volume-filtered flow equations

$$\int_\Omega \left(\frac{\partial \phi_k}{\partial t} + \widetilde{\boldsymbol{u}}_k^{\,k} \cdot \nabla \phi_k\right) g\,\mathrm{d}\boldsymbol{y} = 0$$

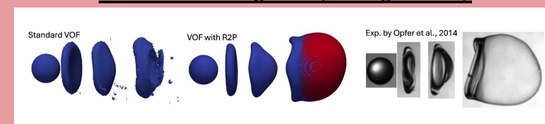
$$\frac{\partial \alpha_k \overline{\rho_k}^k \widetilde{\boldsymbol{u}}_k^{\,k}}{\partial t} + \nabla \cdot \left(\alpha_k\left(\overline{\rho_k}^k \widetilde{\boldsymbol{u}}_k^{\,k} \otimes \widetilde{\boldsymbol{u}}_k^{\,k} + \overline{p_k}^k \boldsymbol{I} - \overline{\boldsymbol{\tau}_k}^k\right)\right) = \boldsymbol{\mathcal{M}}_k^{\mathrm{sf}} + \boldsymbol{\mathcal{M}}_k^{\mathrm{s}}$$

with $\alpha_k = \overline{\phi_k}$, $\alpha_k \boldsymbol{a}^k = \overline{\phi_k \boldsymbol{a}}$, $\widetilde{\boldsymbol{a}}^k = \overline{\rho_k \boldsymbol{a}}^k / \overline{\rho_k}^k$

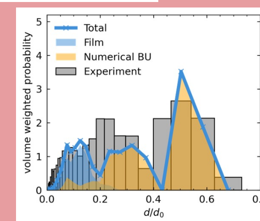
Standard LES model

Related to velocity equilibrium between phases

Sub-filter modeling of droplet bag break-up[5]



1. Assume that liquid and velocities are **in equilibrium** everywhere
2. Assume film break-up occurs when **minimum film thickness falls below $\mathcal{O}(1\ \mu m)$**[6]
3. Assume **instantaneous conversion of film into Lagrangian droplets** from Gamma distribution[6]
4. Let **ligament break-up occur automatically** due to PLIC numerical errors

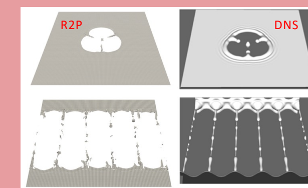


Sub-filter modeling of film retraction

A priori testing for sub-filter films shows:

1. Away from the rim $\boldsymbol{u}^l \approx \boldsymbol{u}^g$
2. At the rim $\boldsymbol{u}^l - \boldsymbol{u}^g \approx U_{TC}\boldsymbol{n}_{edge}$

with Taylor-Culick velocity $U_{TC} = \sqrt{2\sigma/\rho_l h}$ and h is film thickness



Retraction from multiple holes on flat film

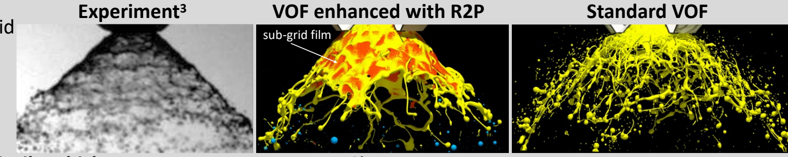
Application to Research Simplex Atomizer (RSA)

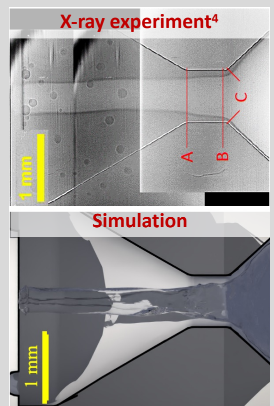
Experimental test conditions

- MIL-PRF-7024 Type II calibration fluid
- Injection pressure: 50 and 100 bar

Simulation information

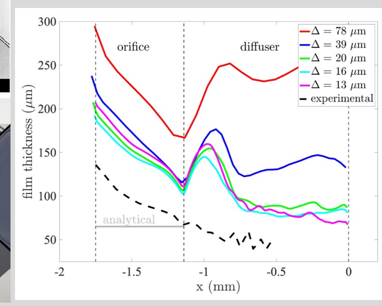
- Domain size: 1 cm^3
- Dirichlet inflow on pipes





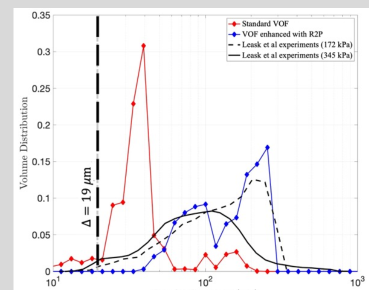
Air Core & Film Thickness

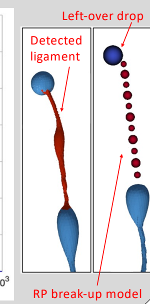
- Simulations **reproduce well experimentally observed gas core**, but film is too thick



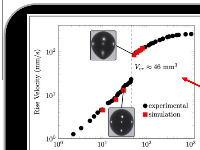
Drop Sizes

- Kim & Moin (2020) model from Rayleigh-Plateau theory
- VOF+R2P **captures well the drop size distribution**
- Standard VOF shows diameter ≈ mesh resolution

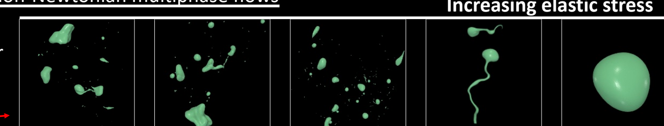




Simulating non-Newtonian multiphase flows



- Discontinuous semi-Lagrangian transport for conformation tensor
- Leads to cost savings
- Enables efficient simulation of atomization



Proposed Work: Extend SGS modeling framework to account for rheology and model non-Newtonian pressure-swirl atomization

1. Han, Chiodi, and Desjardins, *J. Comp. Phys.* (2024) 2. Evrard, Chiodi, van Wachem, Desjardins, *SIAM J. Sci. Comput.* (2023) 3. Leask et al. *J. Fluids Eng.* (2019) 4. Sforzo et al. *ICLASS* (2021) 5. Han and Desjardins *IJMF* (2024) 6. Jackiw and Ashgriz *J. Fluid Mech.* (2022)