

High-Fidelity Numerical Modeling of Spray Droplet Formation

Prof. O. Desjardins, Cornell University

Challenge: Eulerian interface capturing methods have become commonplace for two-phase flow CFD, in particular to predict multiphase flows with break-up that are of great importance in many engineering applications related to the production of powders. However, a long-standing limitation of these methods is their **inability to simulate topology change events accurately**. Even under extreme mesh refinement with the correspondingly enormous computational cost, break-up remains fundamentally numerical. As a result, the efficient and accurate prediction of droplet size distributions in spray formation has remained elusive so far, especially if the atomized fluid is **highly viscous and non-Newtonian**.

Enabling idea: In the vast majority of turbulent multiphase flows with break-up, surface tension dominates the small scale dynamics. The interface topology is then essentially **limited to simple shapes such as ligaments, films, and drops**, as illustrated in Fig. 1. Moreover, the surface tension-driven dynamics of these small-scale features is well understood. Very recently, the PI has introduced new Eulerian interface capturing methods that have the

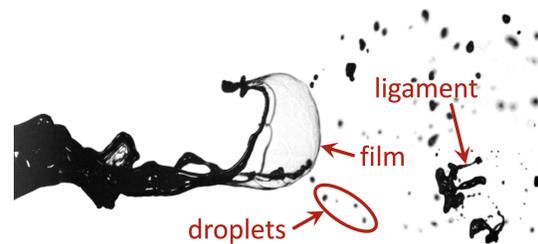


Fig. 1: Simple interface topologies in multiphase flows with break-up (image courtesy of Aliseda et al., U. Washington).

ability to represent simple interfacial shapes at the sub-grid scale (SGS). Specifically, these **methods can accurately and conservatively capture films and ligaments much smaller than the mesh size**, opening the door to SGS modeling of multiphase flows.

Overall objective: This project will enable efficient SGS modeling of surface tension-driven dynamics and break-up in non-Newtonian two-phase flows, thereby greatly reducing simulation costs and making accurate prediction of droplet size distributions possible.

Specific objectives: This project will pursue three main tasks:

1. In the first three years of IFPRI-funded research, our work has focused on modeling SGS films and their dynamics. This renewal project will focus on SGS ligaments, aiming to capture their dynamics reliably and to convert them into droplets with appropriate physics-informed models.
2. Using the non-Newtonian modeling framework developed in the current project, fully resolved simulations of non-Newtonian films and ligaments undergoing break-up will be performed and analyzed to develop improved SGS break-up models.
3. The pressure-swirl atomizer configuration currently studied will be used to demonstrate SGS modeling of spray formation with high viscosity non-Newtonian liquids.

1 Introduction

1.1 Limitations of interface capturing

Eulerian interface capturing methods such as the Volume Of Fluid (VOF) method have become ubiquitous in two-phase computational fluid dynamics, and are now routinely applied to predict spray formation [1–4]. In fact, a standard practice has emerged in recent years:

- The phase interface deformation and topology change is captured on a fixed mesh using an Eulerian interface capturing technique such as VOF (geometric [5] or algebraic [6]), level set [7], or diffuse interface [8].
- The detached droplets are then identified using a Connected Component Labeling (CCL) technique [9]. Once sufficiently spherical, the identified droplets are removed from the Eulerian mesh and transferred to a Lagrangian representation [2, 3, 10] for easy and efficient tracking.

While that approach appears sound and pragmatic, it has not led to significant successes when predicting droplet size distributions: direct comparisons of drop size probability distribution function (pdf) between simulations and experiments remain rare and tend to be unsuccessful, with the conclusion often being made that a finer mesh is needed [11]. Addressing the root cause of these difficulties when predicting drop size pdfs is the main goal of this project.

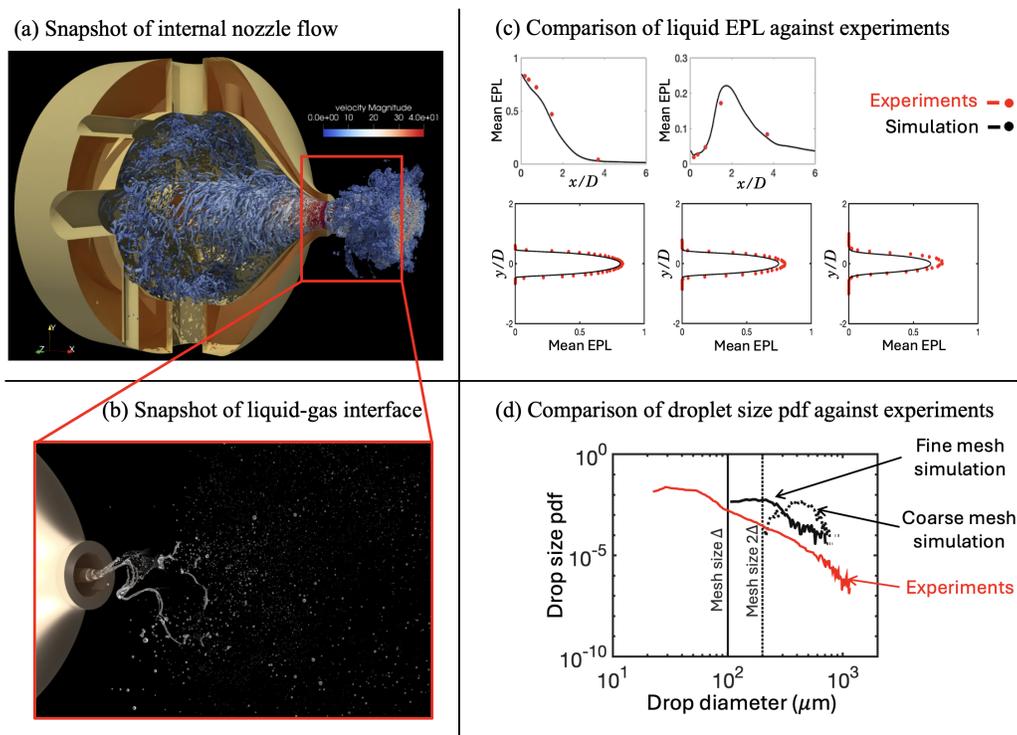


Fig. 2: High fidelity VOF simulation of air-blast atomization with comparison against experiments. An instantaneous snapshot of the Q-criterion inside the nozzle is shown in (a), illustrating the complex turbulent flow field. The resulting liquid-gas interface that develops outside the nozzle in the spray formation region is shown in (b). Excellent agreement between simulations and X-ray data for liquid equivalent path length (EPL) is demonstrated in (c), yet the drop size probability distribution function (pdf) is shown to be mesh-dependent and does not agree well with experimental PDPA measurements in (d).

Figure 2 presents a recent VOF simulation of air-blast atomization from Desjardins’ group [12]. We reported excellent agreement with experimental measurements over a wide range of statistics,

including mean and rms line-of-sight liquid depth profiles, jet flapping frequency, and pdf of intact liquid core length. However, drop size pdf results are disappointing: the drop size distribution is found to be directly controlled by the mesh size. Studies from other groups observe a similar behavior and often attempt to argue that the largest droplet sizes may be converging, even though the smaller ones are not [13–15]. We explain below the root causes of this lack of convergence.

Numerical challenge: Eulerian interface capturing methods are plagued by catastrophic numerical errors when two interfaces approach one another, as illustrated in Fig. 3. For VOF methods, these errors induce spurious topology changes on the scale of the mesh. For standard level set methods, they lead to significant mass loss. For diffuse interface methods, they often lead to effective mixing between the two immiscible phases. Irrespective of the choice of method, the outcome is that break-up is controlled by numerical errors once interfacial scales approach the mesh size, **preventing any Eulerian interface capturing method from correctly predicting topology changes**. Naturally, one might argue that Adaptive Mesh Refinement (AMR) [16] or dual-mesh techniques [17] address this issue by ensuring a mesh size smaller than all interfacial scales. However, during break-up events, the smallest interfacial scale eventually reaches zero, logically requiring the mesh size to then also reach zero. For example, recent simulations of droplet bag break-up by Ling and Mahmood [18] use AMR to achieve an effective resolution of 2000+ cells per droplet diameter at a computational cost of 4.3 million core-hours, yet the authors note that “*film break-up is due to numerical cut-off*”.

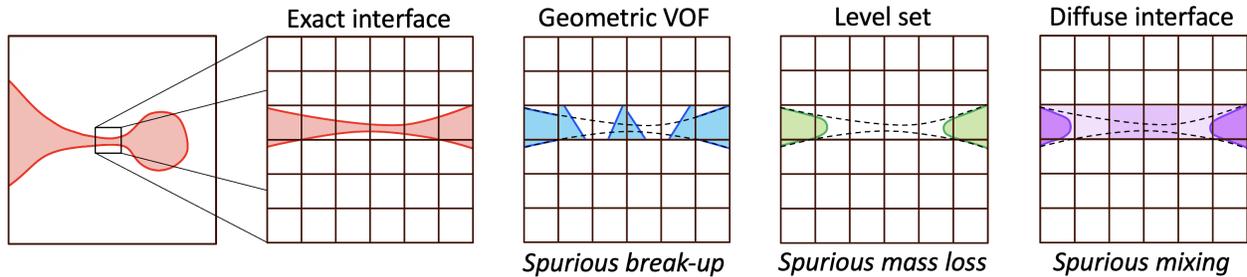


Fig. 3: Schematics illustrating the catastrophic numerical errors that develop when two interfaces approach one another in various Eulerian interface capturing schemes.

Physical modeling challenge: Even in the limit of infinite resolution, it should be noted that the Navier–Stokes equations that are commonly solved for two-phase flows do not account for the physical mechanisms leading to topology change in the first place. At the sub-micron scale, it has been observed that non-continuum effects control the pinch-off of viscous ligaments [19], and hole formation in sheets can “nucleate” from trapped bubbles, impurities, temperature fluctuations [20], and intermolecular forces such as Van der Waals [21]. Therefore, it is reasonable to expect that, for simulations of two-phase flows with break-up to be truly predictive, one needs to eventually account for these effects via appropriate sub-grid scale models.

Given the computational cost of mesh adaptation and the limitations of the continuum hypothesis, we argue that a new modeling strategy is needed to correctly and efficiently simulate two-phase flows with topology changes.*

*Which does not mean that AMR is not useful: the work proposed herein should be seen as complementary to AMR, and could greatly benefit from its use.

1.2 Recent advances in sub-grid scale interface capturing

As illustrated in Fig. 1, the smallest scales of turbulent multiphase flows are often surface-tension dominated, leading to simple interfacial topologies such as films, ligaments, and droplets. In addition, their surface-tension driven dynamics are well understood and described by theory. Therefore, there exists opportunities to capture these shapes and model their dynamics at the sub-grid scale.

SGS interface capturing: In recent work, Desjardins and his group introduced a novel reconstruction method for VOF called R2P (Reconstruction with 2 Planes), which enables the robust capture of films of thicknesses much less than the grid resolution [22, 23]. Section 2.1 provides more details on R2P, as well as evidence of its benefits for simulating spray formation in realistic scenarios. Other reconstruction methods have also been recently proposed by Desjardins and his group (including a piecewise-parabolic interface reconstruction method [24] and SciML-enabled interface reconstruction [25]) that have the potential to enable SGS ligament capturing, which is a focus of this renewal proposal (Task 1).

SGS modeling of surface tension-dominated flows: Detailed theories exist to describe the surface-tension driven dynamics of thin films. For instance, the retraction of a punctured thin film is analytically described by the self-similar Taylor–Culick solution, and the stability of a film in a cross-flow can be inferred from the Rayleigh–Taylor theory [26, 27]. Using such concepts, recent work in Desjardins’ group introduced a thin-film break-up model based on SGS film capturing with R2P combined with the film break-up theory of Wang and Bourouiba [28]. The success of this model at predicting the aero-breakup of a liquid droplet is described in Section 2.2, along with current effort on film retraction modeling. The development of improved SGS models for non-Newtonian films and ligaments is a focus of this renewal proposal (Task 2).

1.3 Relevance to IFPRI

Powder production often involves atomizing a liquid mixture into fine droplets that become solid particles upon drying, a process known as spray drying. Since the produced powder depends directly on the outcome of atomization, the droplet size distribution should be carefully controlled. Yet, a well-controlled and predictable droplet size distribution is very challenging to achieve in practical applications, especially when considering that the liquids used in spray drying applications are often highly viscous non-Newtonian slurries for which off-the-shelf correlations and phenomenological models are simply not available. Consequently, spray drying often requires an expensive trial-and-error optimization process. As such, IFPRI members can **benefit enormously from advancing predictive CFD of non-Newtonian spray formation.**

Typical fluids of interest to IFPRI members exhibit non-Newtonian effects, in particular shear-thinning and viscoelastic behaviors, which have been shown to suppress break-up and lead to a predominance of highly stable liquid films and ligaments, as illustrated in Fig. 4. Our proposed strategy of capturing thin films and ligaments at the sub-grid scale seems ideally suited for such flows, therefore simulating non-Newtonian spray formation in realistic conditions is a focus of this renewal proposal (Task 3).

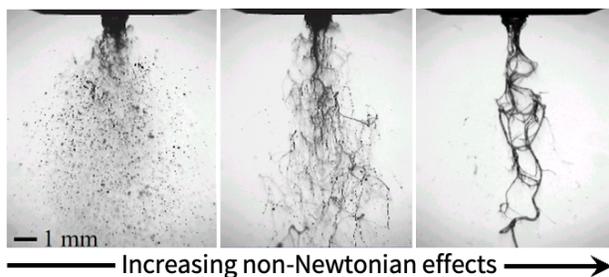


Fig. 4: Snapshots of an atomizing non-Newtonian jet break-up experiment [29]. Increasing viscoelasticity and shear-thinning effects suppresses atomization but promotes highly stable thin films and ligaments.

2 Prior work

2.1 Sub-grid scale film capturing with R2P

In Section 1, we argued that topology change events in Eulerian interface capturing methods are always mesh-dependent: this is due to the mesh size providing a minimal length scale for interface folding below which topology change is triggered. This is most obvious in the case of bag break-up, wherein a fast gas penetrates a liquid structure and inflates a thin liquid film into a large bag-like shape. From theory and experimental observations, the thin liquid film is expected to have a thickness close to or below a micron by the time the bag breaks. In simulations, however, the bag always ruptures when the film reaches the mesh resolution. To address this issue head on, Desjardins and his team introduced a new interface reconstruction method for geometric VOF called Reconstruction with 2 Planes (R2P) [22, 23]. As its name indicates, R2P represents the liquid-gas interface as two planes that co-exist within a single computational cell. In comparison to the widely used Piecewise Linear Interface Calculation (PLIC) [5], this new algorithm greatly improves the accuracy of the reconstruction, in particular when dealing with thin structures such as films. The placement of the two planes requires the solution of a non-linear optimization problem in six dimensions, which we solve efficiently thanks to an excellent initial guess formulated from transported surface data, and an efficient and mass-conserving distance-finding algorithm that accounts for two planes with arbitrary orientation. The ability of R2P to capture the formation and transport of SGS liquid films in a two-phase flow simulation is illustrated in Fig. 5: in that example, the droplet is discretized with about 20 cells per diameter, which means that **the film thickness is orders of magnitude smaller than the mesh**, yet no spurious break-up is seen with R2P. This new method opens the door to SGS modeling of film dynamics and break-up, and provides direct evidence that this proposed project is based on a sound concept.

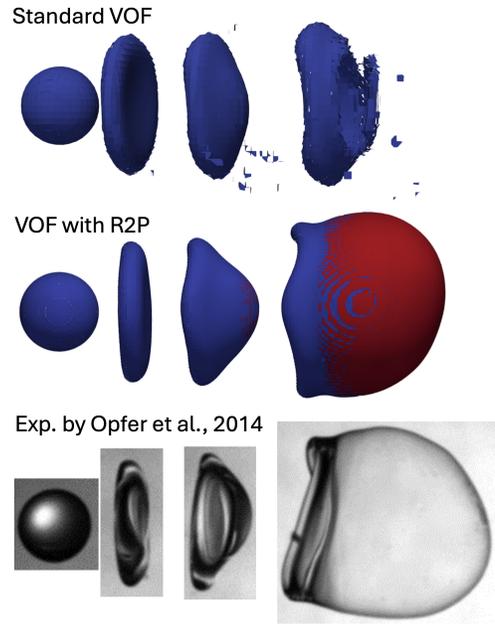


Fig. 5: Bag formation when a liquid droplet is exposed to a gas cross-flow at a Weber number of about 15: standard VOF with PLIC breaks up right away into meaningless droplets (top), while VOF with R2P preserves the thin liquid film without any spurious break-up as the film falls below the mesh resolution (middle), in agreement with experiments [30] (bottom).

2.2 Sub-grid scale modeling of film break-up with R2P

A first SGS film break-up model was recently proposed by Desjardins and his team [23, 31]. First, we assume that the film ruptures whenever its thickness falls below 2 microns, in accordance with experimental observations [20]. When rupture happens, the SGS film retracts from its rim according to Taylor–Culick theory and sheds droplets, as described in a recently proposed theory by Wang and Bourouiba [28]. In our simulations, this is modeled by progressively converting the SGS film into Lagrangian droplets in a mass-conserving manner, using a recently proposed model for the drop size pdf [20]. Finally, the ligament break-up model of Kim and Moin [32] is used to predict the outcome of the fragmentation of the left-over large rim. This strategy is demonstrated in Fig. 6 with the problem of a droplet at a Weber number of approximately 15 undergoing bag break-up in a cross-flow: a thin liquid sheet is formed, and bursts into $\mathcal{O}(10^4)$ droplets, while the rim

forms a ligament that survives longer and undergoes a slower Rayleigh–Plateau break-up process. The modeled break-up process is in excellent qualitative agreement with experimental images by Opfer et al. [30], and the resulting drop size pdf is found to be in excellent agreement with recent holographic measurements by Guildenbecher et al. [33]. Again, since the bag is entirely tracked at the sub-grid scale, a mesh size of only about 20 cells per drop diameter is sufficient to achieve convergence of the bag and drop statistics.

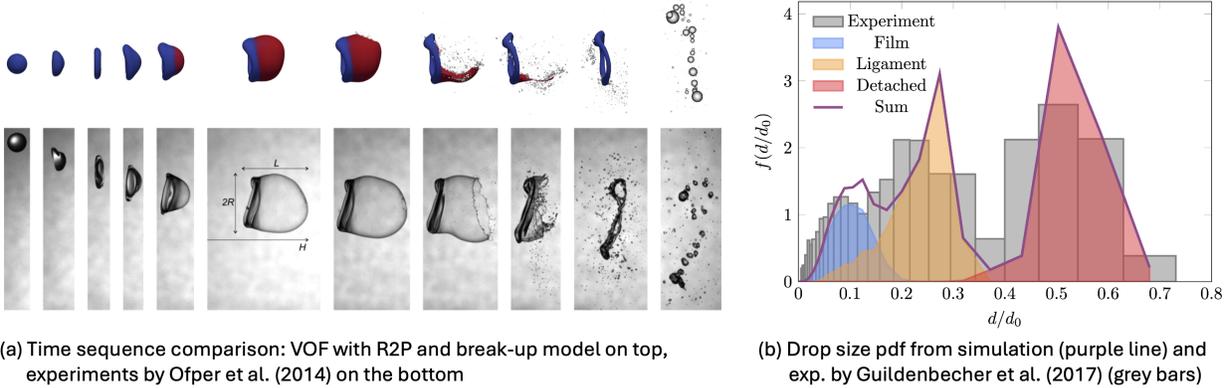


Fig. 6: Bag break-up model based on R2P: (a) compares qualitatively the simulated film break-up with experimental images by Opfer et al. [30], while (b) compares quantitatively the resulting droplet size distribution against measurements by Guildenbecher et al. [33].

2.3 Sub-grid scale modeling of film retraction

The film break-up model described above is well-suited for low-viscosity Newtonian liquids where droplets are shed as the film bursts and retracts. In contrast, high viscosity or non-Newtonian liquid films will retract fully without shedding droplets, as illustrated in Fig. 7, which requires a different modeling strategy. To that end, we introduce a SGS film retraction model based on the theoretical Taylor–Culick velocity defined by

$$U_{TC} = \sqrt{2\sigma/\rho_l h}, \quad (1)$$

which is the theoretical retraction velocity for the rim of a film of thickness h with a liquid of density ρ_l and surface tension coefficient σ . We explicitly add this velocity at the edge of SGS films when transporting the moments of the liquid distribution function, providing a simple algebraic closure for SGS film retraction dynamics.[†]

We demonstrate this framework in the same droplet break-up case as described in Section 2.2 and present successive snapshots of the deforming droplet in Fig. 8. Instead of droplets being shed as in Fig. 6, we find instead a stable film that retracts progressively from multiple holes as it is transported downstream, leaving behind a webbing of ligaments. Note that since no SGS ligament capturing is used in this test, the ligaments break into droplets due to lack of numerical resolution. SGS ligament capturing will be needed to achieve the full benefits of this work and match more closely the experimental snapshot in Fig. 7.

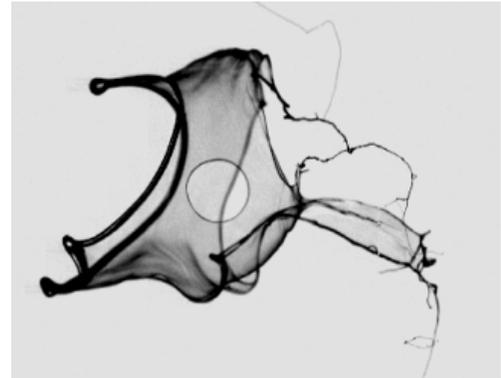


Fig. 7: Experimental snapshot of droplet bag break-up for a non-Newtonian liquid [34]. A circular hole growing via Taylor–Culick retraction is visible in the middle of the image, and a webbing of thin ligaments is left over from film retraction.

[†]More details are provided in our 2024 annual report.

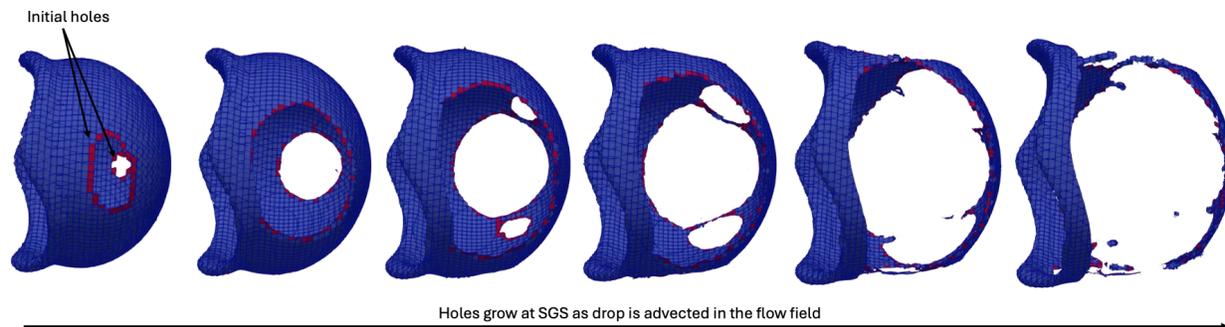


Fig. 8: SGS film retraction model deployed in droplet bag break-up. Cells colored in red correspond to the detected SGS film edge regions where the Taylor–Culick retraction model is applied.

2.4 Sub-grid scale ligament capturing with PPIC

With the intent to boost the accuracy of the interface reconstruction/transport problem and enable novel SGS reconstruction capabilities, the PI’s group has recently developed a VOF reconstruction method based on Piecewise Parabolic Interface Calculations (PPIC) [24, 35–37]. This was made possible by the derivation of exact closed-form expressions of the geometric moments generated by the clipping of a polyhedron with a paraboloid surface [35]. These solutions have been formulated and implemented in IRL [38] in a way that prevents round-off error singularities and robustly handles degenerate cases. In [35], we show that our PPIC algorithm is the first of its kind to be machine-accurate, robust, and fast (with a unit-cost only about 6 times larger than the fastest available open-source PLIC algorithm). While we have yet to test it in complex flow simulations, Figure 9 illustrates the potential of PPIC at representing SGS ligaments.

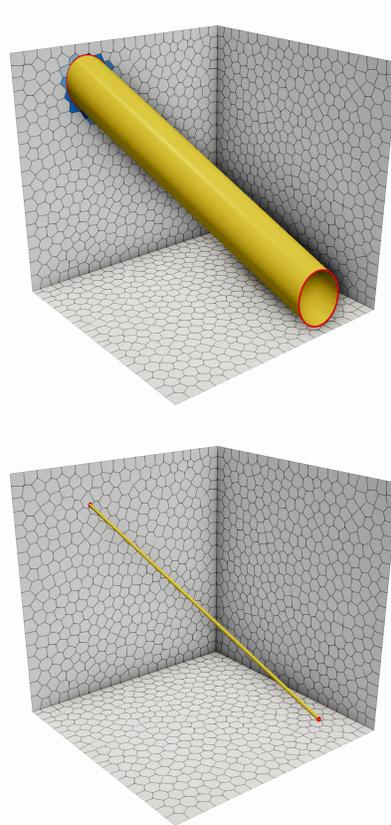


Fig. 9: A ligament is accurately represented by a piecewise-quadratic interface approximation even when its thickness decreases below the mesh size (bottom).

2.5 R2P-enabled film capturing in pressure-swirl atomization

Finally, we demonstrate the use of R2P to enable efficient SGS film capturing in the case of pressure swirl atomization. Using a canonical geometry for a simplex atomizer previously studied both experimentally [39] and computationally [40] (dubbed *Reference Simplex Atomizer*, or RSA [41]), we perform preliminary simulations of the near-injector liquid-gas flow using a standard VOF method and using a VOF method enhanced with R2P for SGS film capturing, and present them in Fig. 10 along with an experimental image of the same flow. The top-right image highlights that the R2P simulation successfully sustains a stable liquid film for nearly the same duration as observed experimentally. In contrast, the standard VOF simulation, shown in the top-left, prematurely breaks down into ligaments and droplets. Furthermore, the figure compares the spray cone angles from the experimental case, as reported in [39], with those obtained from the simulations. Although the spray angles for the simulations were measured manually and should be

interpreted cautiously, they show reasonable agreement with the experimental measurements.

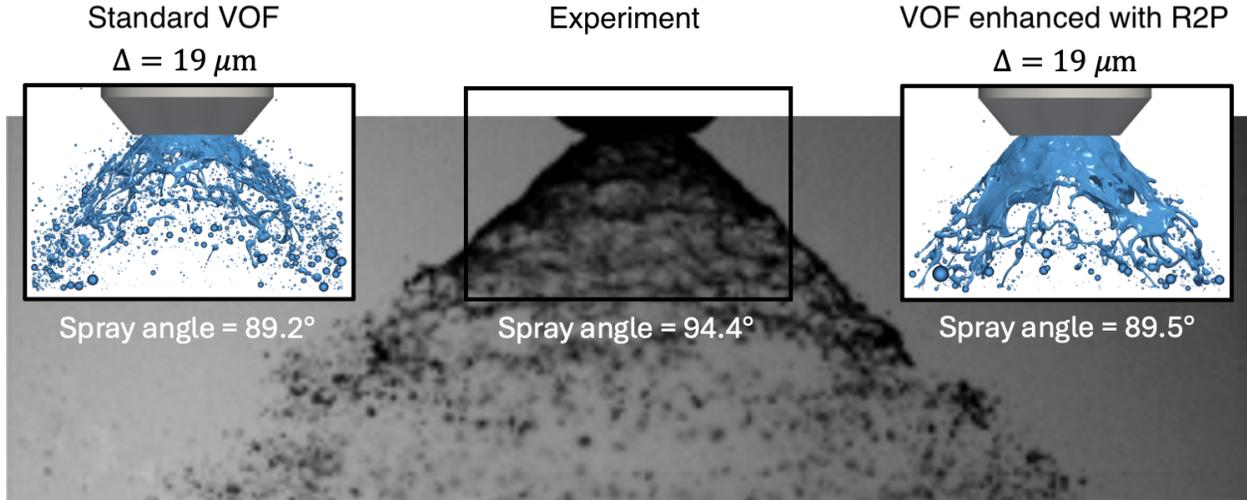


Fig. 10: Liquid issued from RSA pressure swirl nozzle: experiments are shown in the middle in greyscale [39], our calculation using standard VOF is on the top left, our calculation using enhanced VOF with R2P-based SGS film capturing is shown on the top right.

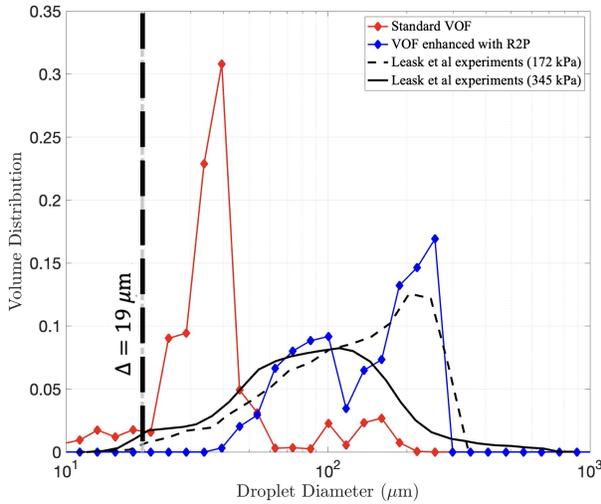


Fig. 11: Comparison of volume-weighted diameter distribution obtained from the R2P and standard VOF simulations and the experiments of Leask et al. [39].

We also provide a preliminary comparison of the volume-weighted drop diameter distribution with the experimental measurements from Leask et al. [39] in Fig. 11. The diameter distribution obtained using standard VOF methods exhibits a clear pile-up of droplets close to the mesh size and does not agree well with experimental measurements. In contrast, the R2P-enhanced VOF simulation shows excellent agreement with experimental data, confirming the usefulness of the proposed approach for complex atomizing flow problems.

2.6 Modeling of non-Newtonian two-phase flows

In our ongoing IFPRI project, we have implemented a non-Newtonian fluid model called ePTT (exponential Phan-Thien Tanner [42]) that is capable of modeling both shear-rate dependent viscosity and viscoelastic stresses, and combined it with a new hybrid advection scheme that is capable of handling the discontinuity that results from the conformation tensor existing only in the liquid phase. We validated this approach in the canonical case of a gas bubble rising in a quiescent viscoelastic liquid, where we demonstrated significant computational cost reductions compared to previously published numerical studies done on a similar rising bubble case.[‡]

[‡]More details are provided in our 2024 annual report.

3 Proposed work and timeline

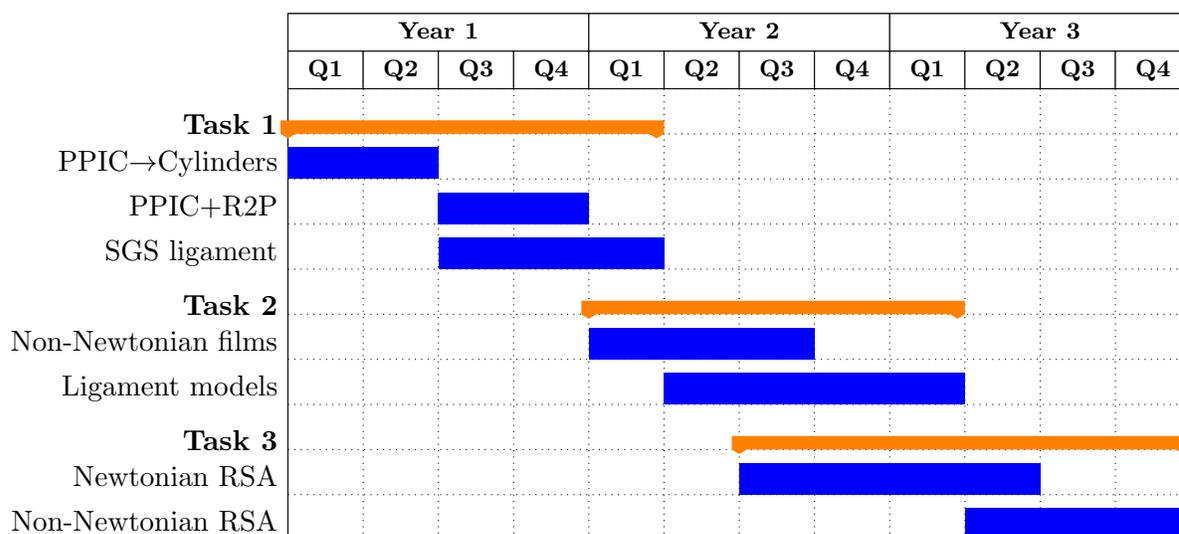
For several decades, the “automatic” [43] or “natural” [44] handling of topology changes in Eulerian interface capturing has been presented as a key advantage of these methods. Nevertheless, the multiphase flow modeling community is progressively coming to the realization that such automatic topology changes stem from catastrophic numerical errors and have little to do with the physical mechanisms of break-up and coalescence [15]. In fact, numerical topology changes may be **the most serious shortcoming** of Eulerian interface capturing methods, preventing accurate predictions of drop size distributions. So far, researchers have tried to circumvent the issue by increasing mesh resolution, often through heavy reliance on AMR [18]. In contrast, our work in this project relies on a different strategy, which aims at capturing simple but ubiquitous interfacial structures at the sub-grid scale, thereby eliminating automatic topology changes, and then models their break-up and subsequent surface tension-driven dynamics using physics-informed closures.

In this renewal project, our objective is to enable the SGS capture of ligaments, providing new break-up models that are applicable to non-Newtonian liquids, and demonstrate the resulting framework in a realistic pressure-swirl spray formation problem.

This three-year renewal project will be organized around three main research tasks described below.

- **Task 1 – *Enable SGS ligament capture using PPIC***: Section 2 demonstrates that R2P has reached maturity and can be used reliably to capture SGS films in complex atomizing flows such as shown in Fig. 10. In contrast, our ability to capture SGS ligaments is still lacking. While PPIC has shown promise for SGS ligament capturing, as shown in Section 2.4, it has yet to be deployed and tested in complex flows. Yet, Figs. 4 and 7 highlight well the importance of these ligaments: if highly viscous and non-Newtonian films do not shed droplets as they retract, then the main mechanism for droplet formation is the break-up of left-over ligaments. Therefore, SGS ligament capturing is the most important next step in this project.
 - **Task 1.1 – *Simplify PPIC for cylinder reconstruction***: PPIC approximates interfaces by optimally fitting general paraboloids, an expensive and delicate exercise. We propose to first modify PPIC in order to fit the interface by simple cylinders instead, a much lower complexity exercise which should be easier to use in realistic flows.
 - **Task 1.2 – *Integrate ligament and film reconstruction within the same framework***: With film capturing from R2P and ligament capturing from PPIC, we need on-the-fly selection of the most appropriate local interface reconstruction strategy. To that end, we will analyze the moments of inertia of the local liquid region to best determine whether it is well-resolved or not, and if not, whether R2P or PPIC is most appropriate.
 - **Task 1.3 – *Demonstrate SGS ligament capturing in a canonical Rayleigh–Plateau flow***: The canonical problem of the capillary destabilization of a cylindrical ligament will be considered in order to demonstrate our SGS capturing capabilities. In particular, we expect that using PPIC, a ligament should not break up even when it falls below mesh resolution.
- **Task 2 – *Develop physics-informed SGS models***: In Section 2, two closure models are presented for SGS film dynamics: a film bursting model and a film retraction model. This task focuses on further enhancing SGS models by including non-Newtonian effects for SGS films and developing appropriate models for SGS ligaments.

- **Task 2.1 – Develop non-Newtonian-aware SGS models for films:** The impact of non-Newtonian fluid properties on the Taylor–Culick retraction velocity can be readily obtained from fully-resolved 2D simulations using the ePTT viscoelastic model already developed. Using that data, we will modify our film retraction model to account for non-Newtonian effects. Moreover, elastic stresses within SGS films will lead to internal redistribution of the liquid volume, ultimately stabilizing films and delaying hole formation [34]. We will develop a simple algebraic model to capture that effect at the sub-grid scale.
- **Task 2.2 – Develop SGS models for ligaments:** Task 1 will enable the capture of SGS ligaments. These will require multiple new SGS models to accurately represent their dynamics, in particular capillary break-up and drag. For capillary break-up, we can adapt the already-existing ligament break-up model of Kim et al. [32], although it would require modifications if the fluid is viscoelastic. For drag, we may be able to assume that thin ligaments are inertialess, in which case they can simply be transported at the gas velocity. Otherwise, we can use slender body theory to approximate the drag on a cylinder.
- **Task 3 – Demonstrate full framework in a realistic non-Newtonian pressure swirl atomization case:** The final task will focus on demonstrating our complete modeling framework to predict a hollow cone simplex atomizer operating with a non-Newtonian liquid.
 - **Task 3.1 – Simulate the RSA nozzle with Newtonian liquid:** The first demonstration will use the full framework, including SGS film and ligament capturing, to predict the drop size distribution in the RSA case, for which extensive experimental data is available.
 - **Task 3.2 – Simulate the RSA nozzle with non-Newtonian liquid:** Then, we will use a non-Newtonian liquid chosen in collaboration with IFPRI liaisons to demonstrate our framework in fully realistic conditions. At the moment, no experimental data is available for non-Newtonian fluids for the RSA nozzle, however a new measurement campaign is ongoing at UC Irvine led by Prof. McDonell (with whom Prof. Desjardins collaborates) that includes non-Newtonian fluids. Impact of non-Newtonian properties will be explored and also compared to prior observations by Prof. Ashgriz in his IFPRI project.



4 Team Qualifications

Professor Desjardins is uniquely qualified to conduct this research. He has over twenty years of experience working on high fidelity computational modeling of turbulent multiphase flows. He develops numerical methods and modeling strategies to investigate turbulent liquid-gas flows and particle-laden flows using large-scale computing resources. Specifically, he has focused on the prediction of turbulent liquid atomization, as well as the dynamics of dense disperse two-phase flows. He is the recipient of the National Science Foundation CAREER Award and the International Conference on Multiphase Flow Junior Award, and he recently lead a \$9 million ONR MURI project on spray control.

5 Budget

For the proposed work, \$40,000 per year for three years is requested. This amount accounts for one semester per year for a Cornell graduate student, some time for Prof. Desjardins, travel once a year internationally to the IFPRI general meeting, and limited funds for minor equipment. A detailed budget is included, along with a budget justification.

6 Response to feedback from the IFPRI Winter meeting

We greatly appreciate the positive feedback provided after the Winter IPFRI meeting. Two specific questions are addressed here:

1. *Are suspensions in scope? If not, how would one think about adding particles to ligaments and/or films; does the proposed modeling framework offer opportunities and/or advantages to modeling droplet formation in atomized suspensions?*

While suspensions are not in scope, the flow solver used by the PI (NGA2) is readily capable of handling Lagrangian solid particles in addition to liquid-gas flows, so solid suspensions could be explored, should specific opportunities or questions arise.

2. *Are there plans to make these developments available in commercial CFD codes to facilitate adoption by industry?*

We appreciate the need for these methods to be made available via commercially available codes, and we have begun discussing specific opportunities for technology transfer with Siemens StarCCM+ stakeholders.

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