High-Fidelity Modeling of Atomization from Nozzle Flow to Fully Developed Spray

Executive Summary

The objective of this research project is to demonstrate the ability of a recently-advanced high-fidelity modeling framework for spray formation to predict drop size and velocity distributions in high viscosity liquid atomization systems, such as found in spray drying applications. This framework, which has been developed by the PI's research group as part of an ongoing ONR MURI project on fuel spray control, hinges on several enabling components: (1) the large eddy simulation (LES) of the two-phase flow field, including the internal nozzle flow, in order to capture directly the large-scale flow dynamics critical to the liquid destabilization and break-up, (2) a fully conservative Eulerian interface tracking technique with the ability to capture subgrid scale liquid features such as thin films and thin ligaments, known to be of critical importance in the break-up of viscous fluids, and (3) a simple break-up model to convert these thin liquid features into spray droplets that can be tracked in a Lagrangian fashion.

In contrast to most existing atomization models, this framework has several key advantages: it is based on first principles instead of an assumed break-up phenomenology, it models an atomizer end-to-end, i.e., from its inlet to a fully dispersed spray, and it benefits from a much lower cost than brute-force direct numerical simulation (DNS). However, it has only been demonstrated on a two-fluid atomizer configuration with water and air so far. This project will explore the influence of higher viscosity and non-Newtonian behavior on the prediction of drop sizes. It is expected that thin liquid sheets and ligaments will dominate the atomization of higher viscosity fluids (e.g., in contrast to water), for which the ability to track subgrid scale interfacial features will prove invaluable. The work will begin by exploring the effect of increasing liquid viscosity on the predicted spray generated by an academic two-fluid atomizer for which extensive water-air data is available, but will seek reference data from IFPRI members and collaborators in order to validate the performance of the framework with high viscosity/non-Newtonian liquids.

1 Introduction

The reliable formation of a spray is a critical component of many engineering systems. In particular, producing powders often involves atomizing a liquid mixture into fine droplets, then drying them into solid particles. In this process known as spray drying, the quality of the powder hinges on the quality of the liquid atomization process, and as such, the droplet size distribution needs to be 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 very viscous, potentially non-Newtonian slurries. Consequently, these systems are often designed and optimized through an expensive trial-and-error process instead of predictive modeling. **The main goal of this project is to bridge this gap by demonstrating that modern, high-fidelity CFD modeling of atomization can predict spray drop size and velocity distributions from first principles, thereby providing a critical modeling tool to engineers.**

Experimental studies of liquid atomization are needed to provide validation data for models and simulations. However, they present significant challenges: the liquid droplets effectively shield the liquid core and prevent optical access, making direct examination of the spray formation mechanisms difficult under realistic conditions. Velocity measurements in the gas phase cannot easily be obtained close to the liquid, so experiments are often limited to characterizing the size and velocity of droplets far downstream of the near-field spray formation region. Even when the atomizing flow is visible, light-scattering-based measurements require very careful analysis in order to extract quantitative data (e.g., see [1]). Recently, experimentalists have started using X-ray imaging techniques and other non-scattering methods in order to quantify liquid statistics in the near-field successfully [2]. For the first time, these new X-ray datasets are providing an opportunity to validate in details numerical simulations of atomization.

In a nutshell, all liquid atomizers follow the same principle: impart kinetic energy to the liquid-gas flow in such a way that as much of it as possible is converted into surface energy (i.e., more drops and smaller drops). The kinetic energy can be given to the liquid directly (using acoustic forcing for nebulizers, moving geometry for rotary disks, or pressurized tanks for pressure-driven atomizers), it may be given to the surrounding gas (using a pressurized gas in two-fluid atomizers), or a mixture of both (e.g., aerated injectors, jet-in-crossflow). Moreover, drop sizes can be selected by carefully choosing the topology of the liquid – in particular, the liquid is often flattened into a thin sheet (e.g., via prefilming or swirling flows). This wide range of atomization processes presents a fantastic challenge to modelers: they each display fundamentally different phenomenologies that, depending on operating conditions, can be dominated by turbulence, Kelvin–Helmholtz instabilities, Rayleigh–Taylor instabilities, flapping dynamics, ligament break-up, or bag bursting, to list just a few. Therefore, no single phenomenological reduced-order atomization model can be expected to capture accurately spray drop sizes over a range of injection strategies, flow conditions, and fluid properties. Nevertheless, the standard modeling strategy for atomization engineers today typically forgoes all details of the liquid injection process and break-up dynamics, instead representing the liquid stream as a series of large initial "blobs" that can be treated in a Lagrangian fashion and undergo break-up based on phenomenological processes such as surface instabilities [3–5], droplet shedding [6], and turbulence [7]. This approach is captured in the leftmost vignette in Fig. 1.

In contrast, first-principle higher-fidelity models based on the solution of the Navier-Stokes equations have the potential to capture all these phenomenologies appropriately, which is why they are the focus in this proposal. Of course, accurate simulations of multiphase turbulent systems in complex geometries are challenging to conduct, in part because of the wildly discontinuous densities and viscosities across the phases, as well as the singular surface tension force at the interface, and the wide range of length and time scales involved in these flows. Yet, numerical methods for complex atomizing multiphase flows have rapidly progressed in the recent years, and have reached a level of maturity that approaches that of single-phase flows. Given sufficient computational resources, it is possible to perform high-fidelity simulation of the early spray formation process, thereby providing direct access to droplet size and velocity in Eulerian frameworks such as level set and volume-of-fluid (VOF) methods. Note however that such simulations often require billions of degrees of freedom and thousands of computer cores over multiple weeks [8, 9], which limits their usefulness to purely academic studies in canonical configurations. This *full DNS strategy*, summarized in the rightmost vignette in Fig. 1, is not pursued in this project due to its inability to tackle atomization problems of industrial relevance.

Alternatively to DNS, **LES of two-phase atomizing flows is more promising for industrial applications**: instead of requiring all scales to be resolved, only the dynamically important

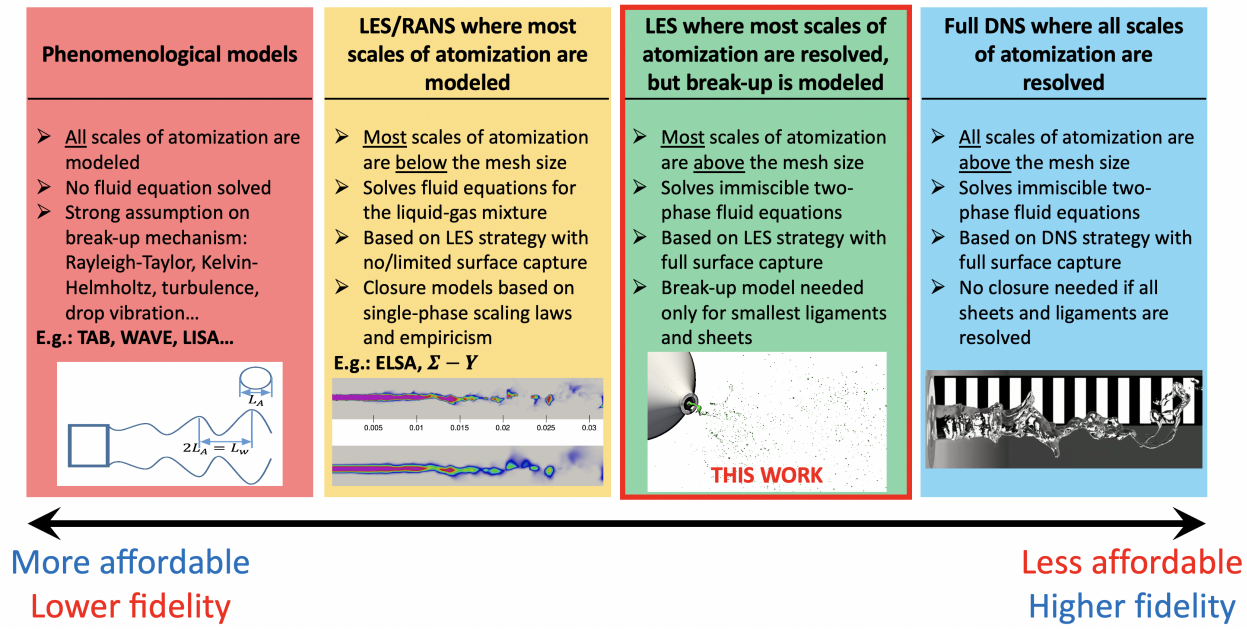

Figure 1: Overview of various modeling strategies for liquid atomization, ranging from ad-hoc, phenomenological models on the left which are cheap but non-predictive, to full DNS on the right which is accurate but overly expensive. The proposed work corresponds to the third box from the left, where only the final stage of ligament and sheet break-up is modeled.

large scales are resolved on the mesh, while the more universal small scales are modeled. One possible LES strategy is to choose a mesh size such that almost all interfacial dynamics happen at the subgrid scale, as summarized on the second vignette from the left in Fig. 1. Then, the liquid-gas interface does not need to be carefully tracked, but the entirety of the break-up process needs to be modeled: the $\Sigma - Y$ and ELSA models [10–12] are the most well-known examples of such a strategy. The subgrid scale closures needed are numerous, complex, and often based on empiricism and parameter fitting. In fact, recent results reported using this type of models still rely heavily on coefficient tuning and show that more work is needed to improve predictions (e.g., see [13]).

The third vignette from the left in Fig. 1 presents the alternative strategy pursued in this work. Still in the context of a two-phase flow LES, we propose to perform detailed interface tracking so that **most scales of interfacial deformation are captured on the mesh**. However, requiring that the mesh size is sufficiently small to resolve properly all topology-change events leads to an exorbitant cost, as mentioned earlier. This is especially true for high viscosity liquids for which very elongated ligaments and very thin sheets are know to abound. Therefore, we propose instead to model the break-up of thin liquid features at the subgrid scale by first tracking the geometry of these thin features as they fall below the mesh size, then using a simple closure to convert these thin features into Lagrangian droplets. This approach leads to several orders of magnitude of reduction in computational cost compared to full DNS, but only relies on models for the final, most universal step of break-up, thereby preserving high fidelity predictions.

2 Prior Research

Predictive high-fidelity modeling of atomization with application to spray control has been the focus of a ONR-funded Multidisciplinary University Research Initiative led by Prof. Desjardins at Cornell in the past five years. That project has led to significant advances in both numerical techniques and modeling framework for spray atomization. In particular, we demonstrated the first detailed validation of atomization simulations against X-ray data, and we proposed and demonstrated a novel modeling paradigm for spray formation simulations which explicitly addresses the mesh-dependent nature of break-up in interface capturing simulations.

2.1 High-Fidelity Multiphase Flow Simulations with Experimental Validation

The effort to perform high-fidelity modeling of spray formation has led to several advances of techniques for accurate multiphase flow simulations. In particular, a new multiphase-ready stabilized traction boundary condition was developed that allows for droplets to seamlessly leave the computational domain and also prevents interface wave reflection [14]. Additionally, a dynamic contact line model was developed that accounts for subgrid scale surface tension forces at the triple contact line [15]. This model allows the interface to meander along the edge of the nozzle's liquid needle, a phenomenon that was identified and quantified using X-rays, and found to influence the downstream dynamics. With these advances, we were able to carefully validate simulations of the early destabilization of a two-phase planar shear layer against linear stability analysis and experiments [14, 16], and simulations of a complete two-fluid annular airblast nozzle were validated against effective liquid path length (EPL) data obtained from X-ray measurements and against backlit imaging data (see Fig. 2).

2.2 Novel Modeling Framework for Mesh-Independent Break-up

Beyond improving the fidelity of the multiphase simulations of the very near-field region, we have focused on addressing head-on the issue of predictive break-up modeling. While level set and volume-of-fluid (VOF) methods provide visually pleasing interface topologies, it is important to understand that the droplet size distributions generated from classical interface capturing methods are *virtually always mesh-dependent*: this is due to the fact that the mesh size provides a minimal length scale for interface folding below which break-up 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 sheet into a large bag-like shape. From theory and experimental observations, the thin liquid sheet is expected to have a **sub-micron thickness** by the time the bag breaks. In contrast, in simulations, the bag always ruptures when the sheet reaches the mesh resolution. Simply put, it means that a true DNS of a flow with thin liquid bags would require a sub-micron mesh resolution, which is not affordable in most situations. To address this issue, we introduced a new approach that combines three elements: (i) the interface is reconstructed using R2P [17, 18], a new computational interface model that allows multiple interfaces per grid cells, thereby allowing for arbitrarily thin interfacial features to be tracked at the subgrid scale, (ii) regions that are likely to undergo break-up momentarily are identified and classified as Lagrangian objects, i.e., sheets and ligaments are identified as such using a specially-designed Connected Component Labeling (CCL) scheme [19, 20], and (iii) once a specified criterion has been reached, the sheet or ligament object is atomized through the use of a break-up model that creates droplets in a mass-conserving manner from physical arguments [21].

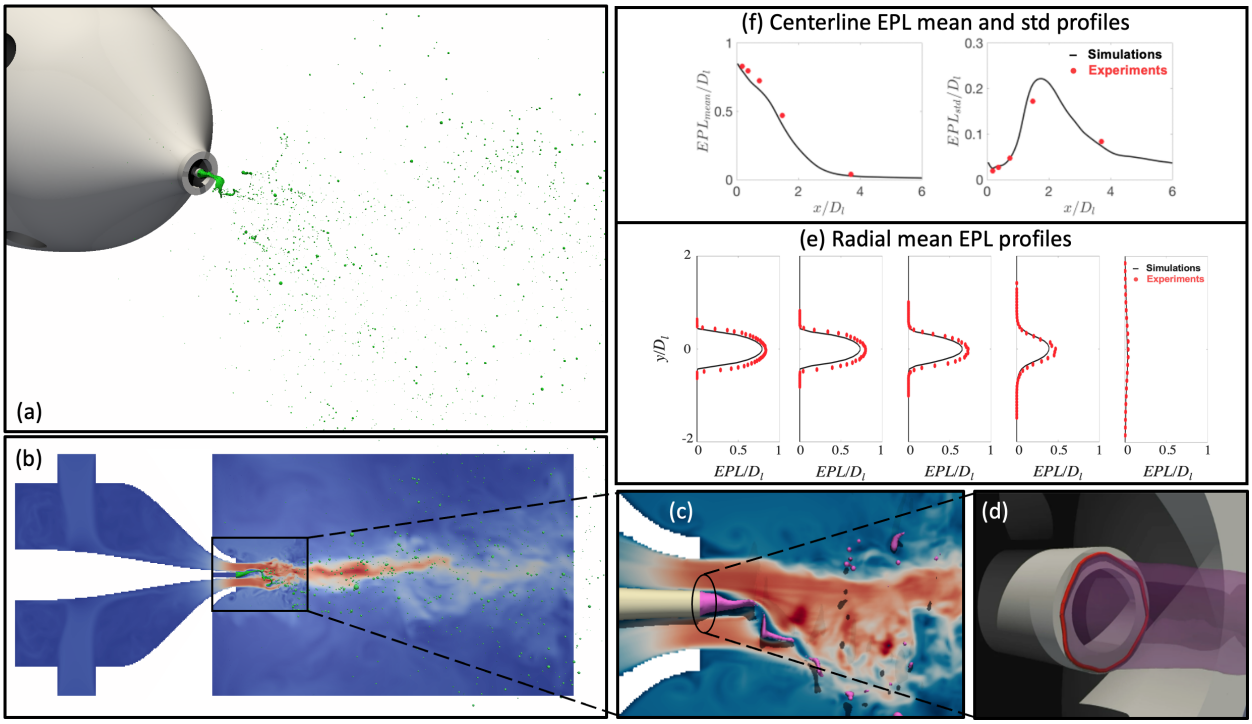

Figure 2: (a) Simulation of a complete annular airblast spray at a momentum flux ratio of 6, without swirl: the nozzle is visible on the top left in grey, and the liquid spray is shown in green. (b) Instantaneous velocity magnitude, showing the flow in the nozzle plenum, the near-field turbulence, and the turbulent spray dispersion downstream. (c) Zoom on the details of the liquid jet (shown in pink here) and the velocity field at the exit of the nozzle. (d) Zoom on the liquid needle, showing the dynamic anchoring of the liquid-gas interface. (e) and (f) show the comparison of the effective path length (i.e., line-of-sight integrated liquid length) obtained from X-ray measurements to the simulation data, along radial profiles and along the centerline.

This strategy is demonstrated in Fig. 3 with the classical problem of a droplet at a Weber number of approximately 20 undergoing bag break-up: a thin liquid sheet is formed, and bursts into $\mathcal{O}\left(10^4\right)$ droplets, while the rim forms a ligament that survives longer and undergoes a slower Rayleigh–Plateau break-up process. The classical VOF scheme, shown in green for a simulation with 13 cells across the droplet diameter, does not capture the formation of a bag and ultimately only generates a handful of large rim droplets. For such a VOF-based simulation to capture the correct drop size distribution via DNS, more than three orders of magnitude more grid cells would be needed. In contrast, the R2P+CCL+break-up model shown in pink at the same resolution of 13 cells per diameter generates a large bag which breaks into $\mathcal{O}\left(10^4\right)$ droplets as small as a few microns, in agreement with recent holographic measurements by Guildenbecher et al. [22]. Deployed in simulations of the canonical airblast nozzle studied mentioned above, this strategy enabled the end-to-end modeling of the atomization process shown in Fig. 2, a first of its kind. The drops generated by the break-up of the thin liquid structures are transferred to a Lagrangian representation, and their turbulent dispersion by the gas flow is computed downstream of the nozzle.

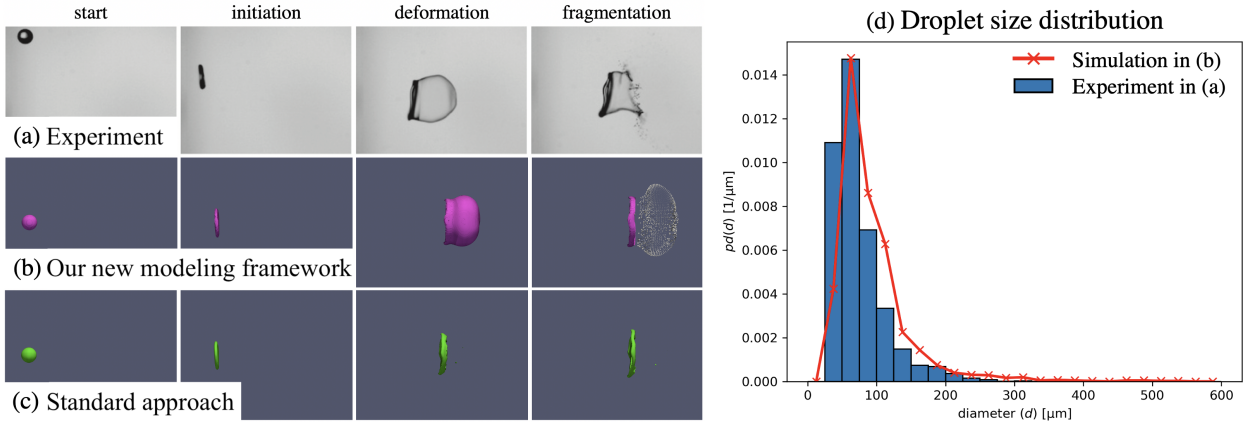

Figure 3: Bag break-up of a moderate Weber droplet: sequence of snapshots at four successive times from (a) experiments by Guildenbecher et al. [22], (b) a simulation using the new subgrid scale break-up model, and (c) a simulation using a standard volume of fluid strategy. The droplet size distributions generated by the bag break-up in (a) and (b) are compared in (d).

3 Proposed Work and Timeline

Several studies have elucidated the effect of increased viscosity on the performance of two-fluid airblast atomizers. For example, Mackrory [23] pointed out that ligaments that form during the primary break-up process are thinner and longer when the liquid is more viscous – and therefore more challenging to resolve numerically, which makes our approach that tracks these ligaments at the subgrid scale advantageous. Mackrory's study also reported a tendency of the more viscous liquids to pool at the nozzle lip, leading to large droplets being regularly released. Our ability to model accurately contact line physics will be important in capturing that effect. In general, the experimental consensus is that larger viscosities lead to larger droplets [24–27], although bimodal size distributions are not uncommon. These observations suggest that our spray modeling framework is already well-suited for predicting the atomization of high viscosity liquids without requiring significant changes, and as such we do not propose significant new development, instead focusing on assessing the performance of the framework, both in terms of computational cost and fidelity of predictions. Consequently, we propose the following work packages.

Work Package 1 – Exploring the Impact of Viscosity on Spray Formation

In WP1, we will investigate the impact of increasing liquid viscosity on the drop size and velocity distributions and on the atomization dynamics for the canonical two-fluid airblast atomizer that we developed as part of the ONR MURI project mentioned above. This atomizer, visible in Fig. 2 (a-c), captures the main features of externally mixed swirled two-fluid injectors, and has been extensively characterized using X-ray, backlit imaging, and PDPA for various swirl and momentum flux ratios using water and air, and as such it provides a validated starting point for our modeling effort. Increasing the viscosity presents no particular numerical challenge since our flow solver already treats the viscous terms fully implicitly, so we do not expect that we will have to drastically reduce the time step size to maintain stability, thereby keeping the cost of simulations low. We will compare the effect of increasing viscosity on the drop sizes to existing correlations, in particular the one proposed for high viscosity fluids by Aliseda et al. [27].

Timeline: Our ONR MURI airblast case will be studied with increasing liquid viscosity in year 1.

Work Package 2 – Detailed Validation of High Viscosity Liquid Spray Formation

In WP2, we will validate our detailed model predictions against experimental data. As a preliminary step during year 1, we will perform a review of the literature to identify the best reference data set for the purpose of validation. At the moment, we believe that the experimental work of Aliseda [27] might be optimal, especially given the close ongoing collaboration between the groups of Aliseda and Desjardins. We will also interact closely with IFPRI members and assess whether they can avail relevant pre-competitive data to augment our validation effort. Then, in year 2, we will study in details the experimental case (or potentially few cases) chosen in year 1 and compare our modeling predictions against spray measurements. We will draw conclusions regarding the computational performance of the method: in particular, we will characterize the impact of mesh resolution on the predictions, and the overall accuracy of our strategy.
Timeline: The best experimental dataset for validation will be identified in year 1, then the detailed comparison will be done in year 2.

Work Package 3 – Exploring the Atomization of Non-Newtonian Liquids

In WP3, we will first implement a simple non-Newtonian liquid model in our flow solver using a shear-dependent viscosity coefficient. While straightforward in an explicit flow solver, this will present some challenges in our time-implicit solver as the Jacobian of the viscous term will increase in complexity. We will test our implementation on well-known laminar flow solutions. We expect most of this work to be done within year 2, so we can then test the impact of non-Newtonian liquid dynamics on our model predictions in year 3. In particular, we expect that our current model closure for converting thin ligaments and sheets into droplets will need to be modified to reflect the non-Newtonian break-up dynamics of these simple topologies. The detailed study of the non-Newtonian Raleigh–Plateau instability for ligaments and of the Taylor–Culick instability for liquid sheets might be needed to elucidate how these fundamental break-up processes change for complex liquids.
Timeline: A simple non-Newtonian liquid with shear-dependent viscosity will be implemented in year 2, then will be used in atomization simulations in year 3 to better understand the capability of our approach for complex liquids. Subgrid scale modeling closures will be revisited for complex liquids.

4 Team Qualifications

Professor Desjardins is uniquely qualified to conduct this research. He has over fifteen 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 is currently leading 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.

References

[1] N. Machicoane, G. Ricard, R. Osuna-Orozco, P. Huck, and A. Aliseda. Influence of steady and oscillating swirl on the near-field spray characteristics in a two-fluid coaxial atomizer. *International Journal of Multiphase Flow*, 129:103318, 2020.

[2] N. Machicoane, J. K. Bothell, D. Li, T. B. Morgan, T. J. Heindel, A. L. Kastengren, and A. Aliseda. Synchrotron radiography characterization of the liquid core dynamics in a canonical two-fluid coaxial atomizer. *International Journal of Multiphase Flow*, 115:1–8, 2019.

[3] Rolf D. Reitz. Modeling atomization processes in high-pressure vaporizing sprays. *Atomisation Spray Technology*, 3(4):309–337, January 1987.

[4] P.J. O'Rourke and A. A. Amsden. The TAB Method for Numerical Calculation of Spray Droplet Breakup. *SAE* Paper 872089, 1987.

[5] Jennifer C. Beale and Rolf D. Reitz. Modeling spray atomization with the kelvin-helmholtz/rayleigh-taylor hybrid model. *Atomization and Sprays*, 9(6):623–650, 1999.

[6] Rolf D. Reitz. Modeling the primary breakup of high-speed jets. *Atomization and Sprays*, 14(1), 2004.

[7] K. Y. Huh. A phenomenological model of diesel spray atomization. *Proc. of The International Conf. on Multiphase Flows '91-Tsukuba*, 1991.

[8] Y. Ling, D. Fuster, S. Zaleski, and G. Tryggvason. Spray formation in a quasi-planar gas-liquid mixing layer at moderate density ratios: A numerical closeup. *Phys. Rev. Fluids*, 2:014005, 2017.

[9] J. Carmona, N. Odier, O. Desjardins, B. Cuenot, A. Misdariis, and A. Cayre. A comparative study of direct numerical simulation and experimental results on a prefilming airblast atomization configuration. *Atomization and Sprays*, 31:9–32, 2021.

[10] A. Vallet and R. Borghi. Modélisation Eulerienne de L'Atomisation d'un Jet Liquide. *C. R. Acad. Sci. Paris Sér. II b*, 327:11015–10208, 1999.

[11] R. Lebas, T. Menard, P. A. Beau, A. Berlemont, and F. X. Demoulin. Numerical simulation of primary break-up and atomization: DNS and modelling study. *International Journal of Multiphase Flow*, 35:247–260, 2009.

[12] J. Chesnel, J. Reveillon, T. Menard, and F. X. Demoulin. Large eddy simulation of liquid jet atomization. *Atomization and Sprays*, 21:711–736, 2011.

[13] B. Wang, M. J. Cleary, and A. R. Masri. Coupling explicit volume diffusion with $\Sigma - Y$ model for LES of airblast atomisation. In *ICLASS 2021, 15th Triennial International Conference on Liquid Atomization and Spray Systems*, Edinburgh, UK, August 29 - September 2, 2021, 2021.

[14] Cyril Bozonnet. Primary wave of an air-water mixing layer: a numerical study. *Doctoral Dissertation, Grenoble Alpes University*, 2021.

[15] Sheng Wang and Olivier Desjardins. 3D numerical study of large-scale two-phase flows with contact lines and application to drop detachment from a horizontal fiber. *International Journal of Multiphase Flows*, 101:35–46, 2018.

[16] C. Bozonnet, J.-P. Matas, G. Balarac, and O. Desjardins. Stability of an air-water mixing layer: focus on the confinement effect. *Journal of Fluid Mechanics*, accepted, 2022.

[17] Robert Chiodi. Advancement of numerical methods for simulating primary atomization. *Doctoral Dissertation, Cornell University*, 2020.

[18] Robert Chiodi and Olivier Desjardins. General, robust, and efficient polyhedron intersection in the interface reconstruction library. *Journal of Computational Physics*, 449:110787, 2022.

[19] Kelli Hendrickson, Gabriel D. Weymouth, and Dick K.P. Yue. Informed component label algorithm for robust identification of connected components with volume-of-fluid method. *Computers and Fluids Fluids*, 197:104373, jan 2020.

[20] Austin Han and Olivier Desjardins. Liquid structure classification towards topology change modeling. In *ICLASS 2021, 15th Triennial International Conference on Liquid Atomization and Spray Systems*, Edinburgh, UK, August 29 - September 2, 2021, 2021.

[21] Austin Han and Olivier Desjardins. Liquid structure classification towards breakup and coalescence modeling. In *ILASS-Americas 31st Annual Conference on Liquid Atomization and Spray Systems*, Madison, WI, May 16-19, 2021, 2021.

[22] Daniel R. Guildenbecher, Jian Gao, Jun Chen, and Paul E. Sojka. Characterization of drop aerodynamic fragmentation in the bag and sheet-thinning regimes by crossed-beam, two-view, digital in-line holography. *International Journal of Multiphase Flows*, 94:107–122, 2017.

[23] A. J. Mackrory. Characterization of black liquor sprays for application to entrained-flow processes. *Doctoral Dissertation, Brigham Young University*, 2006.

[24] G. Ferreira, J. A. García, F. Barreras, A. Lozano, and E. Lincheta. Design optimization of twin-fluid atomizers with an internal mixing chamber for heavy fuel oils. *Fuel Process. Technol.*, 90:270–278, 2009.

[25] Z. H. Li, Y. X. Wu, C. R. Cai, H. Zhang, Y. L. Gong, and K. Takeno. Mixing and atomization characteristics in an internal-mixing twin-fluid atomizer. *Fuel*, 97:306–314, 2012.

[26] Z. H. Li, Y. X. Wu, H. Yang, C. R. Cai, H. Zhang, K. Hashiguchi, K. Takeno, and J. Lu. Effect of liquid viscosity on atomization in an internal-mixing twin-fluid atomizer. *Fuel*, 103:486–494, 2013.

[27] A. Aliseda, E. J. Hopfinger, J. C. Lasheras, D. M. Kremer, A. Berchielli, and E. K. Connolly. Atomization of viscous and non-Newtonian liquids by a coaxial, high-speed gas jet. Experiments and droplet size modeling. *International Journal of Multiphase Flow*, 34(2):161–175, 2008.