SPECIAL ISSUE

ON SIMULATING PRIMARY ATOMIZATION

Guest Editors

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PREFACE

Understanding the physical details of the initial breakup of liquids to form sprays in engineering applications remains one of the outstanding problems in multi-phase flows (Gorokhovski and Herrmann, 2008). While progress has been made in recent years to study the so-called primary atomization region experimentally, using, for example, ballistic imaging (Linne et al., 2006) and X-ray techniques (Wang et al., 2006), such analysis cannot yet provide the full four-dimensional data with sufficient spatial and temporal resolution for a detailed analysis. In addition, there remains an ongoing discussion of how to correctly interpret the obtained data in the dense spray region at the injector, i.e., the primary atomization region, for some experimental techniques (Bachalo, 2013).

Numerical simulations, on the other hand, have the potential to generate the needed comprehensive data sets. However, to become a tool that can be used complimentary to or even instead of experimental analysis, numerical simulations have to be based not only on governing equations derived from first principles, but they must also use verifiable numerical methods and have sufficient numerical resources available for both solution verification and validation (Chigier et al., 2011). Fortunately, significant advances have been made in recent years, both in terms of numerical methods and available computational resources, to help researchers tackle the challenge of simulating primary atomization.

These simulations often have different underlying goals. On the one hand, large-scale simulations are performed to help understand the underlying physics of the initial breakup processes, with the goal of helping in the development of improved models that then can be used in an engineering context. These direct numerical simulations are typically performed in either canonical configurations, such as shear layers and isotropic turbulence, or simplified geometries such as liquid jets injected into quiescent environments. On the other hand, computational resources have progressed to the point that detailed simulations of the primary atomization process for actual engineering applications

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are becoming feasible, thereby aiming to replace lower fidelity models of the breakup process with higher fidelity detailed simulations.

Issues 11 and 12 of *Atomization and Sprays* are dedicated to providing an overview of the current state of the art in simulating primary atomization. Researchers from many of the groups at the forefront of simulation-based primary atomization research have been invited to contribute to these issues, providing the interested reader with a broad overview not only of the current state, but also the remaining challenges and required future work.

Issue 11 contains four contributions. The paper by Demoulin et al. (2013) summarizes efforts to use direct numerical simulations of the initial atomization process of turbulent liquid jets to improve their primary breakup modeling based on the Eulerian-Lagrangian spray atomization model. In addition, ways to develop large-eddy simulation formulations to mitigate the large cost associated with direct simulations and to move toward mesh-independent results are discussed. The required subgrid source terms for a surface density equation is determined using direct numerical simulations of liquid/gas flows in a canonical configuration, i.e., homogeneous isotropic turbulence.

The contribution by Berard et al. (2013) focuses on the breakup of underwater buoyant oil jets and plumes using both experiments and simulations. Motivated by the 2010 deep water oil spill in the Gulf of Mexico, the physics of the atomization process over a wide range of the relevant characteristic numbers is studied, albeit under conditions that are feasible both experimentally and numerically. Good agreement between experiments and simulations is reported for all cases, suggesting that simulations may be used to study flow conditions that may be outside the regime of achievable conditions in a laboratory experiment. The paper further demonstrates that although many numerical techniques for primary atomization have been developed with fuel injection atomization in mind, these can naturally be applied to other atomization scenarios, such as underwater petroleum spills.

The paper by Desjardins et al. (2013) presents a suite of computational tools that have been developed in an effort to simulate turbulent primary atomization from first principles. Complex geometries common in realistic injectors are accounted for using an immersed boundary approach. Simulations of air-assisted breakup of both planar and coaxial liquid layers are shown to agree well with theoretical and experimental results. The computational tool is then employed to simulate the turbulent breakup of a liquid jet under Diesel engine conditions and the turbulent breakup in a pressure swirl as well as dual-orifice atomizer, providing qualitative insight into the atomization processes for realistic injector geometries.

The final paper in this issue by Li and Soteriou (2013) aims to apply high-fidelity, first principle simulations to the geometric complexity of a realistic aerospace combustor multi-nozzle/swirler injector. The presented simulation framework combines interface capturing for the primary atomization region, adaptive mesh refinement to provide the necessary mesh resolution, Lagrangian droplet models to describe the large number of

resulting spray drops, and immersed boundary techniques to describe the geometric complexity of the injector. With the continued increase in available computational resources, this type of approach of incorporating first principle simulations of the initial breakup process into simulations of the entire injector may become more and more widespread in the future, since it has the potential of eliminating the modeling uncertainty of the primary breakup process.

Issue 12 contains four additional contributions. The paper by Chen et al. (2013) studies the formation and fragmentation of liquid sheets formed by two impinging jets. Their approach based on the Volume-of-Fluid method uses adaptive mesh refinement in order to efficiently satisfy the varying mesh resolution requirements due to the multi-scale nature of atomization. Their results shed light on the flow patterns of the impinging jets, the sheet formation and rupture processes and the subsequent atomization into ligaments and drops over a range of Reynolds and Weber numbers.

The contribution by Berlemont et al. (2013) reports on synergies between high-fidelity simulations of jet atomization and experimental measurements. Not only are methods for comparing simulated data sets to experimentally obtained data for validation purposes presented, but also ways of improving experimental techniques based on the insight gained from simulation data are discussed. Advances due to this synergistic use of simulations and experiments hold the potential of significantly advancing our understanding of primary breakup resulting in improved models of the process.

The paper by Chenadec and Pitsch (2013) presents a novel second order unsplit Volume-of-Fluid method coupled to a consistent conservative monotonicity preserving discretization of the Navier-Stokes equations, motivated by the goal to study turbulent primary atomization at arbitrary density ratios. The method is applied to the study of a temporal atomizing planar jet, discussing the impact of mesh resolution on overall conservation errors and atomized drop size distributions. The authors then study the impact of density ratio and injector geometry on the atomization of a turbulent liquid jet issuing from a simplified, yet realistic injector, demonstrating that their simulation framework is able to yield quantitative trends regarding the atomizer performance.

Numerous experimental as well as numerical studies of the atomization process have pointed to ligament formation and their subsequent breakup into drops as a key step in the droplet formation process during primary atomization. The Rayleigh-Plateau instability of a liquid cylinder, representing an idealized configuration of the ligament dynamics during primary atomization, is thus studied in detail in the contribution by Deshpande et al. (2013) using the open-source software OpenFOAM. Examining a variety of different fuels, including JP-5, Diesel, and their potential renewable substitutes, they find a notable sensitivity in breakup times and satellite drop sizes for fuels with an Ohnesorg number of approximately $\mathrm{Oh} = 0.1$, conjecturing that this represents a boundary between viscous and inviscid behavior. They further find that the influence of the gas phase on the ligament evolution is negligible for the fuels studied ($0.015 < \mathrm{Oh} < 0.25$).

As demonstrated in these two special issues, detailed numerical simulations of the primary atomization process not only in canonical but also realistic injector geometries have become a reality and it is thus conceivable that, provided sufficient computational resources are available, simulations can be established as a predictive complimentary tool to experiments in studying and designing novel atomizers.

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