Review of Atomization: Current Knowledge and Recent Trends for Propulsion Combustors

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Abstract

This survey paper reviews the current status of knowledge, understanding, theory and models for the physics of atomization, particularly as it applies to gas turbine and rocket applications. Three areas pertinent to atomization issues in gas turbine and rocket combustors are covered: 1) recent advances in primary atomization physics and simulation techniques, 2) state-of-the-art understanding of selected physical mechanisms in atomization and dense phase mixing for rocket combustors, 3) current modeling approaches for gas turbine combustors. This paper updates several atomization technologies discussed in, and serves as a companion to, a related paper presented at the Eighth International Conference on Liquid Atomization and Spray Systems (ICLASS-2000) at Pasadena, CA, July 16-20, 2000 [1].

Introduction

There is no question that there are wide deficiencies in the combustion community's ability to *a priori* predict the atomization and subsequent combustion of a vaporizing spray within a combustor. However, customer and regulatory agency requirements have continued to spur efforts to improve primary atomization simulation techniques. The discussion below covers some developments regarding the state-of-the-art physical understanding, simulation methods and sub-models for atomization as pertaining to gas turbine and rocket combustion. Before proceeding with an examination of primary atomization physics, it should be noted that Sirignano [2] is an excellent resource with respect to droplet and spray development, transport, vaporization and collisions.

Discussion

Primary Atomization. Primary atomization refers to the generation of liquid ligaments/droplets from the parent surface emanating from the atomizer. Classical approaches to this problem have been mainly restricted to linear stability analyses which presuppose a column of liquid or a liquid sheet that is initially undisturbed. These analyses reveal wavelengths of instabilities; one supposes that these wavelengths remain prominent in the nonlinear deformation of the column/sheet in order to predict ligament and droplet sizes.

Recent advances in multiphase computational codes, on the other hand, have led to primary atomization modeling efforts where the liquid surface is directly represented and updated in a time-accurate calculation. The relevance of these attempts of first-principles atomization simulations is still limited in industry, but the insight on the physical processes these calculations provide is invaluable, considering the difficulty of even sophisticated diagnostics to penetrate dense sprays. Multiphase numerical methods include front-tracking [3], immersed boundary [4], boundary-fitted/moving grids [5], boundary integral [6], volume-of-fluid [7,8,9] and level set [10,11] implementations. In the boundary-integral approach, the flow equations are mapped from the immiscible fluid domains to the sharp interfaces separating them, thus reducing the dimensionality of the problem (the computational mesh discretizes only the interface). As in boundary-integral methods, in boundary-fitted/moving grids methods the flow equations and the interface boundary conditions can be posed exactly, but the entire fluid domain deforms with the interface. Interpolation onto the volume mesh is needed instead in immersed-boundary methods since the interfacial forces are calcu-

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lated on a surface mesh distinct from the volume mesh where the flow equations are solved. The interface-tracking methods enumerated above require, especially in three dimensions, additional programming effort to allow for topological changes, such as in ligament breakup or droplet coalescence. They however tend to provide superior accuracy in evaluating surface forces when compared to interface capturing methods.

Interface-capturing methods, such as volume-of-fluid (VOF) and level set, implicitly discretize interface information as an advected scalar, and therefore do not require additional implementation for topological changes of the interface – they can, in fact, favor spurious breakup under certain conditions. The main disadvantage of level set methods is that an insufficient grid density compared to the liquid thickness can lead to a volume loss in the simulation. Conversely, the straightforward imposition of a volume preservation constraint in the VOF method replaces mass loss with inaccurate mass motion, leading to small pieces of fluid non-physically being ejected as floatsam or jetsam. Simple interface reconstruction schemes also tend to limit the accurate evaluation of geometric information, such as normals and curvature. These issues prompted the development of hybrid schemes, such as coupled level set and volume-of-fluid methods [12,13], coupled marker and level set methods [14], or discontinuous Galerkin level set [15]. They also led to volume fraction curvature calculation either from a ‘‘height fraction’’ or from a temporary level set function [16,17], even achieving second-order accuracy with the method proposed in [12]. Despite their promise of more consistent results and higher accuracy, and perhaps because of the higher implementation cost, hybrid schemes have not found their way yet into commercial CFD software, which mostly relies on simple VOF schemes for interface capturing.

Numerical schemes used in primary atomization simulations are further categorized by their underlying data structure: for instance block-structured [12] or oct-tree [18] with dynamic adaptive mesh refinement, unstructured grids with static [19] or dynamic [20] adaptive mesh refinement, and so on. Whatever the merits of the discretization technique, in the commonly used hydrodynamic description of the liquid-gas interface as a taut membrane of zero mass and thickness, the occurrence of a liquid thread pinch-off is a mathematical singularity of the fluid dynamic equations. Singular solutions are in practice avoided by “stable” implementations of the multiphase algorithms, but independence from the details of such implementations has been guaranteed only for breakup caused by capillary instability [21]. Discretization-independent spray statistics has still to be fully achieved in cases where gas-liquid interaction is relevant, as in most cases of fuel atomization. See Figure 1 and Refs. [22,23].

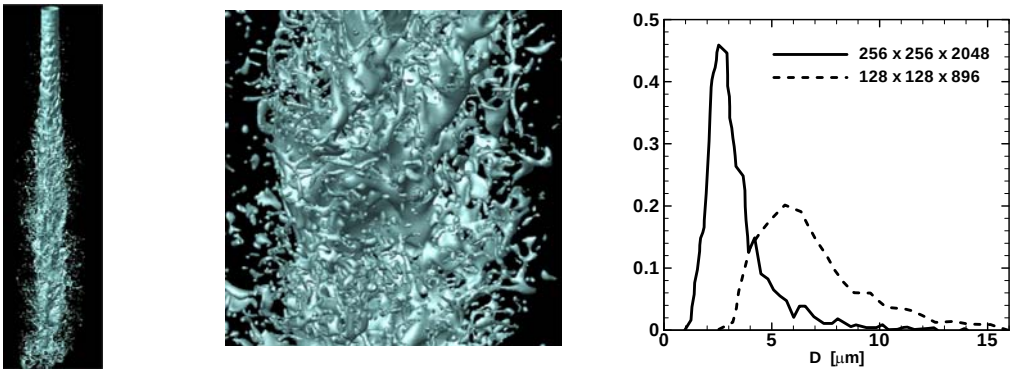

Figure 1. (a) Fuel injection calculation and (b) detail of ligament breakup from [13]. Frame (c) (normalized histogram of droplet sizes) shows that spurious breakup results in a droplet diameter distribution that is mesh-dependent [22].

State-of-the-Art Rocket Injector Atomization and Dense Phase Mixing. Injector types for liquid rocket engines are relatively unique in comparison with many ground-based combustors and most air-breathing aircraft engines. Since rocket vehicles travel outside of the atmosphere, these injectors typically do not operate with gaseous oxidizer in excess of stoichiometric proportions (e.g. excess air) in the thrust chamber. Propellants are stored in the launch vehicle in liquid phase, sometimes at cryogenic temperatures, leading to significantly higher injected mass fluxes than air-breathing engines and the need to atomize the oxidizer. Three types of injectors characterize most rocket

engines: shear coaxial, impinging and swirl coaxial injection elements. Some recent developments regarding each type are discussed below.

Three-dimensional computational simulations of a non-reacting shear coaxial element at subcritical conditions (that is, a round liquid jet surrounded by a coaxial gas stream) have been conducted by Kim, et. al. [24]. The modeling approach is to use level set for the primary atomization and a Lagrangian stochastic spray model for the secondary atomization processes. The primary breakup appears to be first dictated by Kelvin-Helmholtz axisymmetric disturbance of the liquid jet and secondarily by Rayleigh-Taylor azimuthal disturbances. A similar early Kelvin-Helmholtz instability is also observed by Hosangadi, et. al. [25] for an isolated liquid nitrogen jet flowing into a stagnant medium. Kim, et. al. compare their results to experimental data and similar conclusions of Marmottant and Villermaux [26]. The data of the latter authors indicate a final primary atomization zone drop size proportional to the wavelength of the azimuthal waves. Lasheras and Hopfinger [27] indicate that the far field droplet size decreases as the velocity difference increases, consistent with the observations of Marmottant and Villermaux.

While the previous coaxial injector data sets have been for subcritical conditions, data are available at various reduced pressures with cryogenic fluids. At subcritical pressure conditions, Leyva, et. al. [28] have found that liquid nitrogen intact (dark) liquid core lengths and droplet sizes appear to decrease with velocity ratio and momentum ratio. At transcritical (just above critical pressure) and supercritical conditions, the droplets disappear, although a dark, dense core remains visible at least for low velocity and momentum ratios. A summary of dark and potential core length behavior with momentum ratio (M), phase and pressure is shown in Figure 2 from Davis, et. al. [29]. The data show a tendency for two basic trends: a grouping of data which includes single phase shear coaxial jets and near and supercritical coaxial jets which scale as $M^{-0.5}$, and a grouping for dark core lengths for two-phase subcritical coaxial jets which scale as $M^{-0.2}$. Reacting flows at supercritical conditions appear to have similar behaviors. Meyer, et. al, [30], showed that at supercritical conditions the flowfield immediately downstream of the injector appears to be dominated by a fluid-fluid mixing process rather than spray formation processes characteristic of subcritical liquid injectors both for non-reacting and reacting coaxial injector flowfields. Leyva, et. al. also show that transverse acoustic disturbances produce significant transverse displacements of the dark core for a range momentum ratios $2<M<10$ for subcritical conditions.

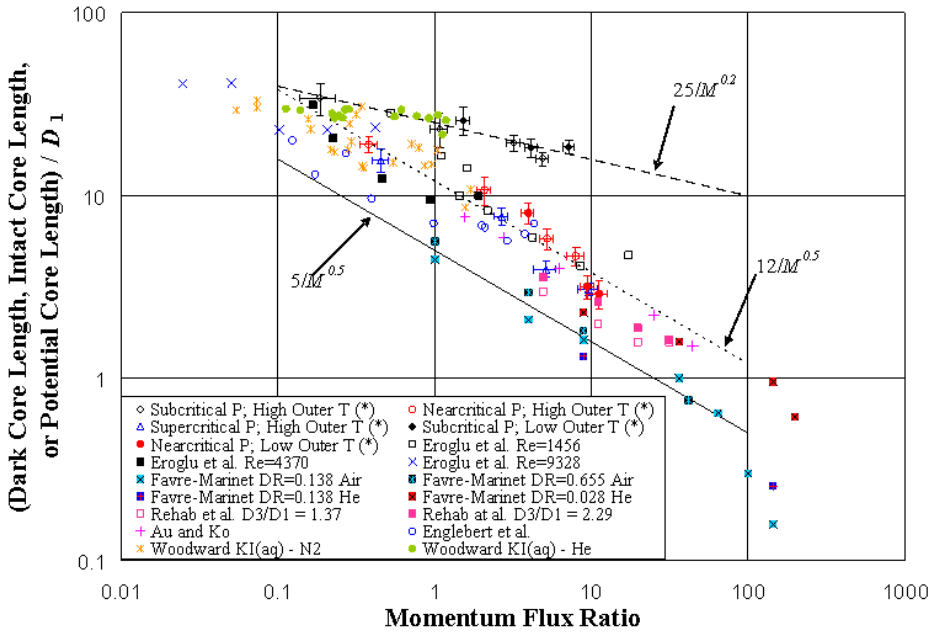

Figure 2. Dark core or potential core length for non-reacting jets correlated with momentum flux ratio (from [29]).

With respect to cold flow simulations of impinging jets, Inoue, et. al. [31], use a cubic-interpolated propagation level set method (CIP-LSM) and a multi-interface advection and reconstruction solver (MARS) technique for analyzing the atomization process and a hybrid level set method for the convection. Their results for two non-reacting impinging jets show formation of a sheet downstream of the impingement point which rapidly breaks up in a flapping mode, dominated by a Kelvin-Helmholtz instability owing to the stagnant gas phase.

Nusca [32] has undertaken a full simulation of liquid impinging injector combustors, albeit using monodisperse droplets of specified droplet size, and is able to show sustained combustion oscillations to pressure perturbations and He bubbles.

Using an LES scheme, Zong and Yang [33] show that various unsteady flow modes control swirl injector dynamics. These modes include hydrodynamic and Kelvin-Helmholtz instabilities and vortical wave structures of various scales. This simulation is limited to an azimuthal sector with periodic boundary conditions due to the large computational demand. Bazarov and Yang [34] discuss how such mechanisms can lead to injector flow sensitivity and response to combustion oscillations.

Current Industrial Gas Turbine Computation Modeling Practice. In current industrial CFD applications, liquid sprays are often modeled as packets of droplets with common properties (size, velocity, temperature, etc.). These packets are tracked in a Lagrangian reference, coupled to the CFD flow field, and possibly subject to secondary breakup [35-36]. Primary breakup models that define the initial droplet size distribution, the position relative to the injector exit, and the velocity distribution, are often based on linear instability analysis [37]. The alternative to this approach in CFD practice is to estimate spray characteristics based on flow conditions and atomizer features using empirical data [38]. Recently, however, modelers have established heuristic approaches that prescribe the droplets release rate and size distribution from "blobs" that are injected directly at the orifice [39,40,41]. In liquid jet in crossflow (LJIC) atomization, for instance, the size distribution is obtained from Reitz's model [35], whereas the flattening of the liquid column, due to gas flow accelerating at the column sides is taken into account by adding a spanwise acceleration component to the drops that mimics the observed far field droplet mass flux distribution.

With sufficient calibration data, blob models can capture the far field spray characteristics quite accurately. For the situation where the near-field gas-liquid interaction needs to be captured more closely, a physics-based, CPU-effective approach has been recently proposed that blends interface tracking and physics-based relations describing primary atomization [42,43]. With this approach, the characteristics of shear-dominated primary atomization are not computed directly, but rather derived at execution time from subgrid phenomenological atomization models. Further insights in the atomization process are expected from the first (partially validated) direct calculations of jet in crossflow atomization, see Fig. 3 and [11,44,45], but there is a long way ahead for these calculations to routinely enter into the engineering design process.

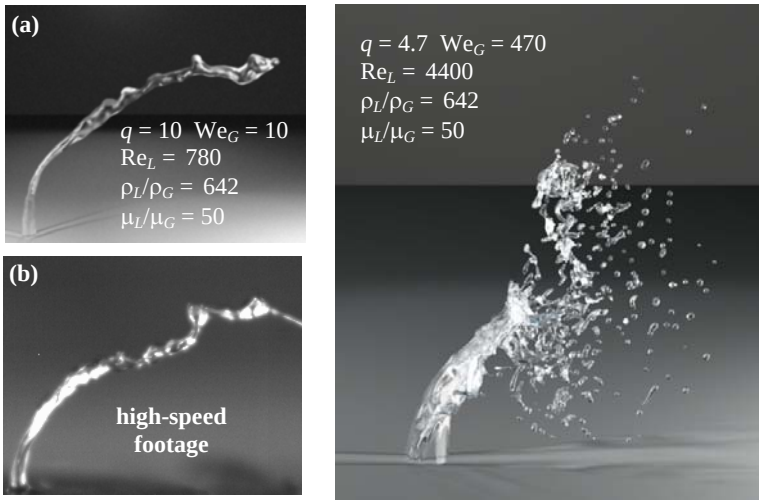

Figure 3. A snapshot from direct numerical simulation of liquid jet in crossflow (a) compared to high-speed footage from an experiment at the same injection conditions (b); simulation of jet start-up at high-Weber number (c) (from [45]).

Limited studies exist on the topic of jet atomization under time-dependent forcing. Because of the resulting time-dependent gas-liquid interaction, mass flow rate and diameter distribution of the spray may change substantially on time scales comparable to the flame response. For instance, changes in LJIC penetration can affect the proportion between smaller droplets stripped from the jet surface and the more penetrating larger ligaments from the column top. Existing models implicitly assume a time separation between jet forcing and primary atomization [43], but the limits of such hypothesis have not been probed yet.

At the present time, the simplest approach that correctly predicts dispersion of droplets in engineering simulations of combustors is the Large Eddy Simulation (LES) technique. See for example, Menon and Patel [46]. The later work indicates that a linear eddy mixing LES approach yields a more realistic flame anchoring, occurring downstream of the dump plane. An alternative approach, boundary element methods, shows that swirl injector response to perturbations follows linear theory for low frequencies but reaches a diminished response at larger frequencies [47]. A practice that will likely become more popular as more computational power becomes cheaply available is to extend the LES approach used in spray simulations to include the primary atomization region. The tacit assumption is that properties of homogeneity and isotropy the LES methods depend upon still hold there. A gas-liquid interface is however more akin (from the gas side) to a wall boundary, where typically LES methods require strong correction terms. An attempt of including wavy-wall-like effects on a gas-liquid interface can be found in [48,49], but it is fair to say that the research topic of interfacial LES remains entirely open.

Conclusions

Computational advancements, augmented by detailed experimental measurements, in primary atomization and injector simulation tools have reduced the amount of modeling needed to predict spray combustion characteristics of practical engines, at least on a research basis. These developments, paced by emissions reduction and performance requirements of production combustors, have occurred primarily over the last decade. Over the next decade, the authors expect that computational speed enhancements, numerical and modeling advances, and most importantly, implementation in commercial CFD codes will enable such methods to be used for parametric design studies and reduce development costs of advanced combustors. However, in the near-term, further work remains to implement high fidelity (e.g. LES family) techniques to primary atomization and to demonstrate accurate, discretization-independent spray statistics.

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