

A Novel Approach to Assess Diesel Spray Models using Joint Visible and X-Ray Liquid Extinction Measurements

Gina M. Magnotti and Caroline L. Genzale
Georgia Institute of Technology

ABSTRACT

Spray processes, such as primary breakup, play an important role for subsequent combustion processes and emissions formation. Accurate modeling of these spray physics is therefore key to ensure faithful representation of both the global and local characteristics of the spray. However, the governing physical mechanisms underlying primary breakup in fuel sprays are still not known. Several theories have been proposed and incorporated into different engineering models for the primary breakup of fuel sprays, with the most widely employed models following an approach based on aerodynamically-induced breakup, or more recently, based on liquid turbulence-induced breakup. However, a complete validation of these breakup models and theories is lacking since no existing measurements have yielded the joint liquid mass and drop size distribution needed to fully define the spray, especially in the near-nozzle region.

In this work, we compare physical models of aerodynamically-induced and turbulence-induced spray breakup and assess their influence on predictions of local spray behavior using 3D CFD simulations in CONVERGE. Motivated by these results, we propose a new spray model validation methodology, using a combination of quantitative measurements and light-scatter modeling, to help fully validate the joint liquid mass and mean drop size distribution in predicted sprays. In particular, we demonstrate that employing joint x-ray and visible liquid extinction measurements, in combination with light extinction modeling within the predicted spray, can provide unique evaluation of the predicted spray morphology and ensure a more accurate representation of the experimentally measured spray.

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INTRODUCTION

Atomization and spray breakup are known to significantly influence combustion and emissions formation in diesel engines [1,2,3], but the primary breakup process is not well understood currently. This gap in fundamental knowledge is largely due to the challenges associated with measuring this process since spray breakup is characterized by a large span of length and time scales [1] that are difficult to simultaneously resolve ($O[\mu\text{m}]$ and $O[\text{ns}]$, respectively). In addition, the optical density of fuel sprays is high, making it difficult for light to penetrate or "see into" the spray [4]. Current imaging technology is not able to provide the necessary simultaneous spatial and temporal resolution to directly view and study spray breakup phenomenon, while laser-based measurements are unable to probe spray characteristics in optically thick regions such as the near-nozzle region [5,6,7].

Even though direct measurement of primary spray breakup at diesel relevant conditions has not been possible, several theories and underlying mechanisms have been proposed and tested qualitatively. Disturbances at the liquid-gas interface induced by aerodynamic instabilities have been largely accepted as the mechanisms governing spray breakup at diesel engine conditions [8,9,10]. Indeed, linear stability analysis of an annular liquid jet convecting into a quiescent

gaseous ambient environment has shown that Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) instabilities can form on the surface of the liquid jet [11]. The growth of these instabilities is believed to cause breakup of the jet into droplets [10]. However turbulence generated inside the injector has also been shown to be an important phenomenon governing spray breakup [12,13,14,15,16,17,18]. Turbulent fluctuations in the injector are also believed to contribute to the initial disturbances on the liquid-gas interphase that result in droplet formation.

While there have been attempts to validate these phenomenological models against varying types of experimental data, studies have been inconclusive in determining the relative importance, or physical appropriateness, of these mechanisms under engine-relevant conditions. Validation of the aerodynamic theory underlying KH primary breakup models has been demonstrated primarily through its ability to qualitatively predict experimentally observed changes in breakup behavior for transitions through different breakup regimes (e.g. Rayleigh breakup, 1st wind-induced breakup, 2nd-wind induced breakup, and atomization) [9], or by the ability of spray models employing this theory to adequately capture liquid penetration velocities [10, 18]. Quantitative validation attempts of this theory have only been attempted through time-resolved imaging of

near-nozzle spray spreading behavior [12], or against sparse drop size measurements conducted far downstream of the nozzle (typically over 1000 nozzle diameters downstream) [10, 19]. Quantitative experimental validation of the aerodynamically-driven instability scales is still missing. This is of key significance since nearly all spray combustion computational fluid dynamics (CFD) codes employ this theory as the main mechanism for primary spray breakup. The theory of turbulence-driven atomization for high-pressure liquid jets has more recently developed, primarily based on high-magnification holographic imaging experiments [13-14]. This imaging technique has been applied to sprays to quantify the breakup size scales of many liquid jet configurations, providing quantitative validation to their turbulence-based scaling for jets under atmospheric conditions where density ratios of liquid fuel to ambient gas (ρ_l/ρ_g) are less than 500.

Limited experiments under higher ambient densities (up to ρ_l/ρ_g of around 100) showed some evidence of aerodynamic forces assisting the breakup process, but breakup still scaled with liquid turbulence properties [13], suggesting that the mechanism responsible for inducing initial jet instabilities was still turbulence at moderate ambient densities. Validation of turbulent breakup scaling for engine-relevant gas density conditions (ρ_l/ρ_g less than 60) is still needed to understand its relative contribution to spray breakup.

There is also the question of the appropriate experimental diagnostics to employ in order to characterize local spray behavior and probe spray breakup phenomenon. For example, PDPA measurements [20], which utilize a pair of crossed laser beams to probe local droplet characteristics such as size and velocity at the crossed beam point, can provide detailed spray structure measurements that are quite valuable for spray model validation, but measurements are limited to optically-thin regions of the spray and provide only the local drop size distribution [21-22]. Optical imaging diagnostics have also been used to visualize sprays [12, 23, 24, 25]. As previously mentioned, these techniques fail to capture the details of spray breakup due to length and time scale resolution limits.

Therefore, global spray imaging measurements based on edge detection, such as the liquid and vapor penetration, are typically used by modelers to calibrate their models for engine simulations [10, 26-27]. Validation against penetration measurements ensures accurate representation of momentum and energy exchange between the liquid spray and carrier gas. However, the authors have demonstrated that robust validation of both global and local spray behavior cannot be ensured through validation of liquid and vapor penetration alone [28]. In this work, two different spray models were shown to exhibit similar penetration behavior, yet predicted different spray morphologies. The challenge, therefore, still exists for the development of a diagnostic that can fully quantify fuel spray breakup, including the joint drop size and liquid mass distribution, under engine relevant conditions.

Recently, x-ray radiography data has enabled the quantification of the 2D projected distribution of liquid mass in fuel sprays [23, 29-30], including the optically-thick near-nozzle region. However, uncertainties remain on the interpretation of the data. Overall, the experimental images portray a much narrower spray than what has

been visualized via optical microscopy, suggesting inconsistencies with the detected liquid mass. Additionally, the technique measures a projected mass distribution and cannot distinguish the relative contributions of the droplet size and number density distributions within the probed volume. As will be shown later in this work, several droplet size and number density distributions can yield the same mass-distribution at a given point.

While x-ray radiography measurements can provide valuable quantitative liquid measurements, especially in the near-nozzle regions, a full validation of predicted local spray characteristics requires a different, or perhaps complementary, measurement technique that can further quantify the coupled droplet size and number density distributions. An attractive option is laser extinction or single line-of-sight (LOS) liquid extinction [28, 31, 32, 33] with visible light wavelengths. Measurements of visible light extinction quantify the path-integrated distribution of droplet size and number density (or liquid mass under isothermal conditions), which results in a measured optical depth [34-35]. In combining both x-ray and visible light measurements in the same local spray region under isothermal conditions, it is therefore possible to decouple the joint drop size and liquid mass distribution. Thus, x-ray radiography and visible light extinction measurements may provide complementary measurements of the joint drop size and liquid mass distribution, allowing for full spray morphology validation.

The use of light-scatter modeling can further provide a method for quantitative comparison between model predictions and visible light extinction data. Indeed, a light-scatter model for visible LOS extinction measurements in diesel sprays proposed by Magnotti and Genzale [28] demonstrated that direct comparison of modeled and measured extinction levels allowed for a more robust assessment of local spray morphology predictions than provided by conventional validation methods, which only validate global spray behavior, such as liquid and vapor penetration.

In this work, we evaluate spray models employing two different physical mechanisms for breakup of a non-cavitating diesel-like spray, namely aerodynamically-induced and liquid turbulence-induced breakup. We compare global and local spray predictions at a single diesel relevant condition. We show the limitations of validation solely against x-ray radiography data. When x-ray data is used jointly with visible liquid extinction data to validate model predictions, we demonstrate the promise of this methodology to quantitatively assess the physical basis of spray breakup models.

EXPERIMENTAL DATA

The x-ray radiography [23] and vapor penetration [36] data from Argonne National Laboratories and Sandia National Labs, respectively, are employed for model validation and assessment. Details regarding the two data sets are discussed below.

X-Ray Radiography Data

The x-ray radiography measurements, shown in Figure 1, were obtained from the Advanced Photon Source (APS) at Argonne National Laboratory [23]. The x-ray radiography measurements are an absorption-based

extinction measurement that quantifies the 2D projected distribution of liquid mass throughout the spray, defined as projected mass density (*PMD*). The time-averaged 2D distribution of *PMD* is displayed, where the axial distance is defined as the distance along the spray axis from the injector nozzle orifice, and the transverse distance is perpendicular to the spray axis. With increasing axial distance, the spray becomes more diffuse and *PMD* along the centerline of the spray decreases. The experiments were conducted under the Engine Combustion Network non-vaporizing, non-combusting Spray “A” condition, as defined in Table 1. Further details regarding the experimental set-up and data post-processing are detailed in the previous works from the Argonne Advanced Photon Source [37]. This type of measurement provides valuable information to spray modelers looking to validate their model predictions, particularly in the near nozzle region where optical-based measurements have been unable to yield quantitative measurements.

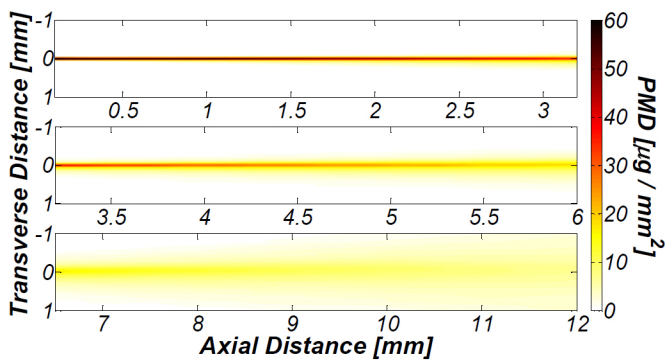


Figure 1. X-ray radiography measurements under the ECN non-vaporizing Spray “A” condition from the Advanced Photon Source at Argonne National Labs [23].

Table 1. Ambient and injection conditions for the nominal and non-vaporizing Engine Combustion Network non-combusting Spray “A” condition [36].

Experimental Parameter	Nominal Spray “A”	Non-Vaporizing Spray “A”
Fuel	n-dodecane	
Ambient Temperature [K]	900	303
Ambient Composition for Non-Combusting Condition	0% O ₂ , 89.71% N ₂ , 6.52% CO ₂ , 3.77% H ₂ O	100% N ₂
Ambient Density [kg/m³]	22.8	
Fuel Injection Pressure [MPa]	150	
Fuel Temperature [K]	343	
Injection Duration [ms]	1.5	
Total Injected Mass [mg]	3.6	
Nozzle diameter [μm]	90.0	
Nozzle C_d	0.86	
Nozzle K-factor	1.5	

Liquid Penetration Data

The liquid penetration data, shown in Figure 2, was conducted under the non-vaporizing, non-combusting Spray “A” condition, as detailed in Table 1. The liquid penetration data was obtained using Schlieren technique at Sandia National Labs in their constant volume spray vessel [36]. Further details regarding the experimental set-up and

spray vessel are detailed in the previous works from Sandia National Labs [38]. The accuracy of the predicted momentum exchange between the liquid phase fuel and ambient gases can then be assessed by comparing model predictions of liquid penetration for non-vaporizing Spray “A” with this experimental data.

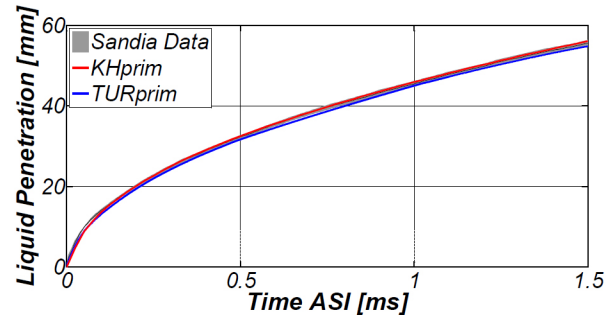


Figure 2. Comparison of liquid penetration data from Sandia National Labs [36] with model predictions of liquid penetration. Liquid penetration predictions from both aerodynamic (*KHprim*) and turbulent (*TURprim*) primary breakup models are shown to have good agreement with the experimental data, particularly during the steady portion of injection (0.5 to 1.4 ms).

COMPUTATIONAL MODELING

Two different physical mechanisms for primary spray breakup, aerodynamically-induced (*KHprim*) and turbulence-induced (*TURprim*) are modeled and compared against the x-ray radiography and vapor penetration data. The CFD model set-up is described below.

CFD Code

The commercial CFD code, CONVERGE, was utilized to simulate the injection of an n-dodecane spray into a constant volume chamber at ECN Spray A conditions [39]. The measured rate-of-injection (ROI) profile from Sandia is shown in Figure 3. The measured ROI along with the measured nozzle discharge coefficient ($C_d=0.86$) was used to calculate the injection velocities at the nozzle exit. Liquid mass is injected within a circle instead of at a point source to yield better mass distribution in the near-nozzle region [40]. The radius of the circle is equal to the nozzle radius. Using the “blob” injection model [41], 1 million computational parcels were injected to represent the dense spray. Other implemented sub-models include a hybrid Kelvin-Helmholtz Aerodynamics-Cavitation-Turbulence (KH-ACT) primary breakup model [17-18], a Rayleigh-Taylor (RT) secondary breakup model [10], O'Rourke droplet collision model, and a standard k-e turbulence model [42] with a turbulent round-jet correction [43] to simulate spray atomization and breakup. Two physical mechanisms for primary breakup are isolated and compared within the KH-ACT framework - aerodynamic (*KHprim*) and turbulence-induced (*TURprim*) breakup. These two models are therefore identical in set-up except for the employed primary breakup sub-model.

As shown later, the *KHprim* and *TURprim* models predict unique droplet sizes and spray morphologies because of the different characteristic length and time scales governing the physical

mechanisms. The characteristic length (r_c) and time (τ_{KH}) scales for aerodynamically-induced breakup, as proposed by Beale and Reitz [10], are:

$$\frac{da}{dt} = -\frac{a - r_c}{\tau_{KH}} \quad (1)$$

$$\tau_{KH} = \frac{3.726 B_1 a}{\Lambda \Omega} \quad (2)$$

$$r_c = B_0 \Lambda \quad (3)$$

where, a and r_c are the radius of the “parent” and “child” droplets, respectively, Ω is the maximum growth rate of the most unstable liquid surface wave, with corresponding wavelength, Λ , and B_0 is a break-up constant with a value of 0.61. The primary empirical constant employed in the KH break-up model is the time constant, B_1 , which is typically calibrated to a number approximately between 5 and 60 [10, 18]. A larger B_1 serves to increase the time required for injected droplets to decay to the primary breakup or child droplet size, r_c . The characteristic length (L_t) and time (τ_t) scales for turbulence-induced breakup are proposed by Huh and Gosman:

$$L_t = C_\mu \left(\frac{K^{1.5}}{\varepsilon} \right) \quad (4)$$

$$\tau_t = C_\mu \left(\frac{K}{\varepsilon} \right) \quad (5)$$

where K is the turbulent kinetic energy, ε is the turbulent dissipation rate, and C_μ is one of the model constants employed in the k - ε turbulence model [15,16,17,18]. Turbulence levels at the nozzle exit can be determined either by a force balance between the pressure force exerted on the fluid at the nozzle exit and turbulent stress within the nozzle [15,16,17,18] or by predictions of turbulence levels at the nozzle exit from high-fidelity internal nozzle flow simulations [44-45]. It should be noted that cavitation-induced primary breakup was not modeled in this computational study since the Spray “A” injector has been shown to suppress cavitation phenomenon [46].

Spray model constants, listed in Table 2, were tuned to match the predicted and measured liquid penetration, as shown in Figure 2. Ideally, as proposed in [28] for the vaporizing Spray “A” condition, a physically-based metric, such as the local liquid volume fraction, should be employed to define the computational liquid boundary for comparison against liquid penetration measurements. However, in absence of well-defined modeling practices for non-vaporizing sprays, the predicted liquid penetration was defined as the downstream axial location where 97% of the total injected mass has been encompassed.

The model predictions of liquid penetration are within the experimental uncertainty of the vapor penetration during the steady portion of injection, from 0.5 to 1.4 ms after start-of-injection (ASI). Since the parameters of interest in this work are evaluated and time-averaged during the steady portion of injection from 0.5 to 1.4ms, as evident in Figure 3, the selected model set-up demonstrates that the momentum exchange between the liquid phase fuel and ambient gases is adequately represented during this injection period.

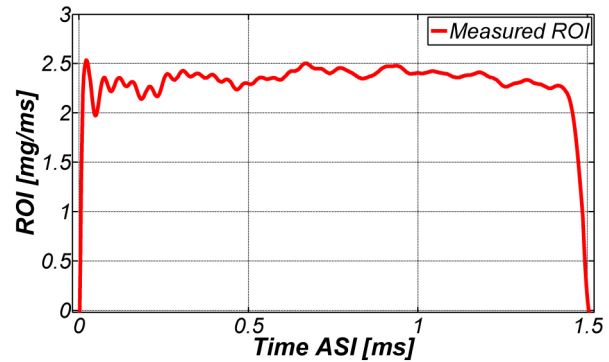


Figure 3. Measured rate of injection profile from Sandia National Laboratories for Spray A. The steady portion of injection is from 0.5 to 1.4 ms. The total injected mass is 3.6 mg.

Table 2. Key spray model constants and model set-up.

Model Parameters	Model Set-Up
B_1	8.0
C_{RT}	1.0
Breakup Length [mm]	0.0
$C_{T,CAV}$	1.0
K_0 [m^2/s^2] [44, 45]	3×10^3
ε_0 [m^2/s^3] [44, 45]	3×10^{10}

Computational Mesh and Initial Conditions

The combustion chamber was modeled using a 3-dimensional hexahedral structured mesh, as depicted in Figure 4. A large domain was selected in order to model a free fuel jet where the wall effects are insignificant within the timescales of interest. Fixed embedding was employed in the near-nozzle region to resolve the flow near the injector. Using two levels of Adaptive Mesh Refinement (AMR), the grid can be further refined outside of this region for both the velocity and temperature fields. A grid convergence study is presented to justify the selected grid. For the selected grid, the maximum number of cells during the simulation was 1.7 million, with a minimum cell size of 62.5 μm . Computations were initialized with a uniform ambient quiescent charge in the combustion chamber. Initialized values for the liquid turbulence levels at the nozzle exit are listed in Table 2 and are based on high-fidelity internal nozzle flow simulations [44-45].