

Computational and Experimental Investigation of Interfacial Area in Near-Field Diesel Spray Simulation

Adrian Pandal
Universidad de Oviedo

Jose M. Pastor and Raul Payri
Universitat Politecnica de Valencia

Alan Kastengren, Daniel Duke, Katarzyna Matusik, Jhoan S. Giraldo, and Christopher Powell
Argonne National Laboratory

David Schmidt
University of Massachusetts

ABSTRACT

The dense spray region in the near-field of diesel fuel injection remains an enigma. This region is difficult to interrogate with light in the visible range and difficult to model due to the rapid interaction between liquid and gas. In particular, modeling strategies that rely on Lagrangian particle tracking of droplets have struggled in this area. To better represent the strong interaction between phases, Eulerian modeling has proven particularly useful. Models built on the concept of surface area density are advantageous where primary and secondary atomization have not yet produced droplets, but rather form more complicated liquid structures. Surface area density, a more general concept than Lagrangian droplets, naturally represents liquid structures, no matter how complex. These surface area density models, however, have not been directly experimentally validated in the past due to the inability of optical methods to elucidate such a quantity. Optical diagnostics traditionally measure near-spherical droplet size far downstream, where the spray is optically thin. Using ultra-small-angle x-ray scattering (USAXS) measurements to measure the surface area and x-ray radiography to measure the density, we have been able to test one of the more speculative parts of Eulerian spray modeling. The modeling and experimental results have been combined to provide insight into near-field spray dynamics.

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INTRODUCTION

Fuel injection transforms a high-speed liquid jet into a spray of fine droplets that quickly evaporate. Because of the extremely small length scales and high speeds, the details of the atomization process remain obscure. Both experimental and modeling investigations have suggested that the turbulent interfacial dynamics create a convoluted surface composed of a short jet core, with many wrinkles, ligaments, and droplets [1, 2].

Because the interface between the fuel and surrounding gas is so complex, it is an over-simplification to think of the dense spray core as being comprised of isolated droplets. Instead, we use the "more general notion" of interfacial area density [3]. This metric, with dimensions of reciprocal length, represents how much interfacial area is present per unit of volume.

With extreme levels of computational effort [4] the interface details can potentially be resolved through interface tracking. However, in a typical engineering calculation, the mesh resolution is considerably coarser than in these high fidelity computations. If one presumes that these interfacial details are far smaller than the mesh size, smoothing features over at least one cell, the end result is a diffuse-interface treatment in an Eulerian framework [5]. This framework is naturally extensible to near critical or super-critical regimes [6]. Rather than directly tracking the unresolved interface features, they are modeled in an Eulerian framework. Other Eulerian approaches such as multifluid 'size-of-classes' [7] have been also applied for Diesel spray simulations [8, 9], but still rely on the assumption of nearly spherical droplets.

Diffuse-interface Eulerian spray models can be used to predict the evolution of the interfacial density within the context of diesel fuel injection [10]. These models have two common elements: a model for

the transport of liquid (or gas) and a model for the evolution of the interfacial surface area. The density of interfacial area is typically denoted by Sigma (Σ) while the liquid fraction is denoted by Y. Hence, we refer to the strictly Eulerian model as a Sigma-Y approach, in contrast to ELSA (Eulerian-Lagrangian Spray Atomization), which includes a transition to Lagrangian particle tracking.

The transport of the liquid employs mass-averaged convection along with turbulent mixing. This model is derived from basic Favre averaging or LES filtering [11]. Thus, the accuracy of the liquid fraction transport is largely dependent on the accuracy of the two-phase turbulent modeling. Despite the challenges of such modeling, there is at least an extensive theoretical basis to deal with the unclosed terms, putting the Y transport equation on a much firmer foundation than the interfacial evolution.

The interfacial evolution model, by predicting the amount of interfacial area per volume, can be used to predict drop size, once the primary atomization process is complete. This information is required if one wishes to employ a downstream transition to Lagrangian particle tracking, such as in the ELSA approach. However, the model for the interface evolution is somewhat more speculative, with several unclosed terms [12]. There are several interface modeling approaches that have been applied to sprays as researchers have explored competing ideas of how these terms should be treated [3, 11, 14].

In recent years, models of the dense spray evolution have begun to favor Eulerian interfacial transport equations over Lagrangian particle tracking [13, 14]. The advantages of Eulerian spray modeling in this region are as follows:

1. Closer coupling between the transport of liquid mass and the other transport equations [15]
2. No need to assume discrete droplets in the densest parts of the spray [11]
3. With adequate mesh resolution, the Eulerian approach is less likely to be mesh dependent than Lagrangian modeling [13, 16]
4. Good parallel scalability, without the necessity of handling load-balancing of Lagrangian particles [15]

For the present, Lagrangian particle tracking is the favored approach for in-cylinder simulations due to reasons of computational cost. However, with the diminishing cost of computational resources, Eulerian spray modeling has potential for applied engine development in the near future. Meanwhile, it offers valuable insights for studies of the near-field spray behavior and injector/spray coupling.

This paper uses a combined experimental and modeling approach to address the evolution of the interface in diesel fuel injection. The paper has several specific aims. The first is to validate the predictions of interfacial density more directly than previously possible. The interfacial density predictions have rarely been validated, and these validations have been in the context of downstream drop size. Using drop size for validation is not ideal, since we wish to avoid the assumption that the liquid is in the form of droplets. A few prior examples used DNS simulations [17] for validation. Others have

emphasized the location of the mass, but not the interfacial density [10]. If possible, we wish to validate directly versus experiments without resorting to the assumption of spherical droplets. This can be done via USAXS measurements, as explained in the next section.

It has been postulated that diesel spray evolution is dominated by turbulent dispersion rather than interfacial dynamics [18]. This mixing-limited hypothesis asserts that the details of the interface are irrelevant under diesel-relevant conditions, such as high ambient gas density and high injection velocity. In support of this hypothesis Garcia-Oliver et al. [10] noted successful prediction of numerous spray metrics at high ambient gas density conditions, with diminishing accuracy at lower gas densities.

There is no feedback mechanism in the typical Eulerian model by which the interfacial dynamics can impact the transport of the liquid fraction. Hence, by its current structure, the Sigma-Y model assumes that the mixing-limited conditions apply. In the current work, we study the spray under high ambient pressure conditions but low ambient temperature, unlike the evaporating conditions studied previously. We thus further investigate the range of applicability of this modeling framework.

In summary, we wish to (1) validate the transport of liquid mass and (2) assess when the model for interfacial evolution is accurate.

EXPERIMENTAL METHODOLOGY

The goal was to measure interfacial surface area in the dense spray core, near the injector exit, where the assumption of individual droplets may not be valid. Ultra-small angle x-ray scattering (USAXS) was chosen as a diagnostic technique due to its ability to interrogate the dense region and provide quantitative information about the complex interface without resorting to the assumption that the liquid is in the form of droplets [16].

USAXS measurements were performed at the 9-ID beamline of the Advanced Photon Source at Argonne National Laboratory. A solenoid diesel injection nozzle provided by the Engine Combustion Network (ECN) was investigated; the single-hole Spray A 210675 nozzle with a nominal hole diameter of 90 μm . The injector was mounted horizontally in a 0.5 L vessel pressurized with N_2 gas, which also supplied a purge flow of approximately 4 standard L min^{-1} in order to inhibit droplet accumulation within the domain during measurements. Table 1 summarizes the measured rail and chamber pressure combinations for the injection nozzle.

Table 1. List of investigated USAXS pressure conditions for each diesel injection nozzle.

Injector	Rail Pressure (bar)			Chamber Pressure (bar)
Spray A 210675	1500			6.7
Spray A 210675	1500	1000	500	20

A diesel common-rail injection system was used to pressurize n-dodecane fuel to the desired rail pressure. Table 2 lists the fuel properties at room temperature and pressure conditions.

Table 2. Properties of n-dodecane at 25°C and 1 bar.

Fuel Property	Value	Units
Density (ρ)	746	kg m ⁻³
Viscosity (μ)	1.8×10^{-6}	m ² s ⁻¹
Surface Tension (σ)	0.025	N m ⁻¹

The injection temperature was approximately 60, 40, and 30°C at 1500, 1000, and 500 bar, respectively. Each injector was fired at 3 Hz with an injection duration of approximately 2.5 ms. USAXS data were recorded in a 1 ms interval during the steady-state portion of the spray. Background measurements were also recorded over 80 ms before each scan to account for any changes within the measurement domain caused by previous spray events.

The Bonse-Hart instrument at the 9-IDbeamline measures the scattering intensity, $I_{\text{scat}}(q)$, for a wide range of scattering vectors, q [20]. A beam of x-rays at 17.9 keV is first shaped into a 100×500 μm H $\times$ V spot with a set of high precision 2D slits. The incoming beam is collimated with a pair of Si (220) crystals before impinging on the spray, from which the incident x-rays scatter at small angles. The scattered x-rays are filtered downstream with a pair of Si (220) analyzer crystals, and the scattered photons are measured with a detector. The pair of analyzer crystals is rotated to measure the transmitted beam intensity as a function of scattering vector. The scattering vector was varied between $1 \times 10^{-4} \text{ \AA}^{-1} < q < 1 \times 10^{-2} \text{ \AA}^{-1}$ with a step size of $1 \times 10^{-5} \text{ \AA}^{-1}$ at low q , with increasing step size for larger q . The scattering intensity as a function of q was measured at axial distances ranging from 1 to 20 mm downstream of the injection nozzle, at the centerline of the spray. Once $I_{\text{scat}}(q)$ is known, the differential cross-section may be calculated, and related to the total shape and surface area per volume of fuel droplets, with post-processing performed using the Irena data analysis package [21].

MODELING APPROACH

The Sigma-Y model considers the liquid/gas mixture as a pseudo-fluid with a single velocity field. Considering that the flow exiting the injector is operating at large Reynolds and Weber numbers, it is possible to assume a separation of the large scale flow features, such as mass transport, from the atomization process occurring at smaller scales. This allows the direct simulation of the large scale bulk transport of the liquid while unresolved turbulent transport is modeled using standard closures such as those used in Reynolds-averaged turbulence models.

To track the dispersion of the liquid phase an indicator function is used, taking a value of unity in the liquid phase and zero in the gas phase. The mean liquid volume fraction is denoted ($\bar{Y}$) and the mean mass averaged fraction is defined as ($\bar{Y} = \bar{\rho Y} / \bar{\rho}$). Favre averaging the transport equation for the liquid mass fraction yields Eq. (1)

$$\frac{\partial \bar{\rho} \bar{Y}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{Y}}{\partial x_i} = - \frac{\partial \bar{\rho} \bar{u}_i \bar{Y}'}{\partial x_i} \quad (1)$$

Where $\bar{u}'$ denotes the density weighted turbulent fluctuations in velocity and $\bar{Y}'$ denotes turbulent fluctuations in liquid mass fraction. The turbulent diffusion liquid flux term, $\bar{\rho} \bar{u}_i \bar{Y}'$, captures the effect of the relative velocity between the two phases [22]. This term is modeled using a standard turbulent gradient flux model, which successfully worked for Diesel spray compared to DNS results, as indicated in [12].

$$\bar{\rho} \bar{u}_i \bar{Y}' = - \frac{\mu_t}{Sc} \frac{\partial \bar{Y}}{\partial x_i} \quad (2)$$

Where μ_t is the turbulent viscosity and Sc the Schmidt number.

While the approach used here assumes that the resolved momentum of the liquid/gas mixture can be characterized by a single bulk velocity, the slip velocity can be expressed explicitly as derived by [11] and seen in Eq. (3)

$$\mathbf{u}_{il} - \mathbf{u}_{ig} = \frac{1}{\bar{Y}(1 - \bar{Y})} \bar{\mathbf{u}}_i \bar{Y}' \quad (3)$$

Under the assumption that the two phases form an immiscible mixture, the mass-averaged value of the indicator function is related to the density by:

$$\frac{1}{\bar{\rho}} = \frac{\bar{Y}}{\rho_l} + \frac{1 - \bar{Y}}{\rho_g} \quad (4)$$

An equation of state is then assigned to each phase. The gas phase obeys an ideal gas law, while the liquid phase is estimated following the Hankinson-Brost-Thomson (HBT) correlation [23], in which the liquid density is a function of temperature (T) and pressure (p).

To close the above system of equations, the temperature is obtained from a bulk mixture enthalpy equation expressed in the following terms:

$$\mathbf{h}(T) = \bar{Y} \cdot \mathbf{h}_l(T) + (1 - \bar{Y}) \cdot \mathbf{h}_g(T) \quad (5)$$

Here $\mathbf{h}_l$ and $\mathbf{h}_g$ denote the enthalpy of the liquid and gas phases respectively, and are calculated as the integrals of

$$d\mathbf{h}_l(T) = c_{p,l} dT \quad (6)$$

$$d\mathbf{h}_g(T) = c_{p,g} dT \quad (7)$$

Where $c_{p,i}$ is the specific heat capacity at constant pressure. This is obtained as a function of temperature (T) from a set of coefficients taken from JANAF tables of thermodynamics. This can be directly applied to the ambient gas, but not for the fuel. In this case, upon the principle of corresponding states, the Rowlinson-Bondi equation [23] that makes use of the departure heat capacity function is applied.