Application of Interface Area Density Modeling to Define Spray Plume Boundary

Y. Wang*,1, R. O. Grover2, D. P. Schmidt1, R. Diwakar2, T.-W. Kuo2

1 Department of Mechanical and Industrial Engineering
University of Massachusetts-Amherst
Amherst, MA 01003, USA

2 Propulsion System Research Lab
General Motors Global R&D
Warren, MI 48092, USA

Abstract

This study is devoted to the application of a predicted flow quantity called “interface area density” for Eulerian CFD simulation of two-phase flows. The interface area density (denoted as “Σ”) is defined as the liquid-gas interface area per unit volume in order to describe local sub-grid distribution of the two phases in any CFD cell. Transport equation for Σ is discussed. It is shown that a line-of-sight integration of Σ through the simulated spray plume offers a reasonable estimate of the optical thickness, which is a measure of the light intensity reduction due to light scattering on the interface. A procedure to define spray plume boundary based on the CFD results of Σ is proposed. Simulation results using the new definition are compared with experimental results of a gasoline spray injected from a single-hole nozzle.

* Corresponding author: wang46@uwalumni.com (Currently affiliated with ANSYS, Inc.)
Introduction

Many modern reciprocating internal combustion engines inject fuel directly into the combustion chamber. These engines allow control of load conditions by varying the amount of fuel injected. Also, the cylinder pressure rise rate and the peak combustion temperature can be controlled by generating inhomogeneity of the fuel-air mixture, which is achieved by optimizing the number of multiple injections and the amount and timing of each injection. The liquid fuel used in these engines, either gasoline or diesel, is injected into the combustion chamber with high pressure gradient in order to be atomized and vaporized quickly.

Two important parameters to assess the outcomes of fuel injection and atomization are spray penetration and spray spreading angle. They affect fuel distribution and utilization of space in the combustion chamber. Spray penetration measures the travel distance of liquid fuel from the injector nozzle exit along the axis of injection. Longer penetration indicates better utilization of space but increases the possibility of wall-wetting and incomplete combustion. Spray spreading angle measures diffusion of liquid fuel from the axis of injection. Larger spreading angle indicates better turbulent mixing but raises concern of plume-to-plume interaction when multi-hole injector is used, especially in gasoline-direct-injection (GDI) engines. Both parameters are affected by injector designs and engine operating conditions. Recent years have seen a growing interest of quantifying these effects and understanding the underlying physics by collaborative diagnostics and simulation efforts [1]. In this study, we focus on the spray spreading angle of gasoline sprays.

From the diagnostic side, the experiment of Zhang et al. [2] showed that the spray spreading angle is influenced by back pressure and fuel temperature, which determine whether the spray is “flashing” or “non-flashing”. In their experiment, fuel was injected from a single-hole injector into a high pressure optical accessible chamber. Fuel spray was illuminated using a high-intensity continuous Xenon lamp and imaged using a high speed CMOS camera. A long distance microscopic lens was mounted in front of the camera in order to obtain the magnified view of the near-nozzle spray structure. The image covers a spatial area of 8mm by 6mm in the near-nozzle region (Figure 1). The spray injection direction has a $30^\circ$ degree tilt relative to the injector’s centerline.

In order to quantify the spreading angle, spray plume boundary must be identified. The color lightness on the spray image indicates the light intensity received by the camera. Light color indicates strong light intensity received and dark color indicates weak light intensity received. It is fair to assume that the ambient air inside the spray chamber has refractive index of 1.0, and any light ray passing through the air without interfering
with any spray droplet is fully received by the camera. If the light ray intercepts a liquid droplet, it scatters in all the directions, and the light intensity received by the camera is reduced. Therefore, the location where transition from light to dark color occurs is determined as the spray boundary. The procedure to calculate the spreading angle is shown in Figure 2.

From the simulation side, prediction of spray plume angle is very challenging because a consistent definition of spray boundary is yet to be found. Zhang et al. [2] used a single-fluid Eulerian CFD code and simulated fuel injection as a submerged liquid jet. Mass fraction of a tracer function of the injected liquid was used to determine the spray spreading angle. Spray plume boundary was identified at the location where a certain percentage amount of liquid mass is enclosed within the plume. Despite its easy implementation, this definition carries little optical information and is inconsistent with the physics meaning of the spray plume boundary shown on the experiment images. Recently, Magnotti and Genzale [3] proposed a new definition of spray boundary by predicting extinction signals due to elastic light scattering on the spray. They applied this method to calculate liquid spray penetration using Lagrangian CFD spray model that offers more direct comparison against the experimental data. Enlightened by their work, in this paper we apply this method to an Eulerian two-phase flow CFD model for a new definition of the spray spreading angle.

Eulerian two-phase flow model assumes both liquid and gas phases as continuum. For fuel injection simulations, this is a suitable assumption for internal nozzle flows and near-nozzle flows when the local liquid phase is continuous relative to the CFD grid size. However, atomization must be accounted for as the intact liquid breaks up into spray droplets.

A quantity called “interface area density” was introduced for this purpose [4]. The interface area density, denoted as \( \Sigma \), is defined as liquid-gas interface area per unit volume (unit: length\(^{-2}\)). The value of \( \Sigma \) indicates how the two phases are locally distributed. Consider a CFD cell containing 30% liquid and 70% gas in volume. If the two phases are separated by a well-defined laminar interface, the interface area size is expected to be small. If the liquid phase is atomized into droplets and ligaments that are turbulently diffused into the gas phase, the total interface area inside the cell is expected to be significantly increased. Note that the liquid volume fraction (\( \Psi_{\text{liq}} = 30\% \)) is the same in both cases, but the way that the liquid phase is distributed is different. Assuming all the liquid phase in a cell can be modeled with spherical droplets, an equivalent Sauter Mean Diameter (SMD) can be uniquely defined as:

\[
SMD = \frac{6 \Psi_{\text{liq}}}{\Sigma}
\]  

The concept of “droplet” is good only when the liquid phase is dilute. In the case of dense liquid, an equivalent SMD for bubbles should be defined as \( 6 \Psi_{\text{gas}}/\Sigma \). The \( \Sigma \) modeling together with the Eulerian two-phase flow approach is termed as “Eulerian-Spray-and-Atomization (ESA)” approach [4, 5].

In this study, the \( \Sigma \) modeling in Eulerian two-phase flow CFD simulations is used to define the boundary of a spray plume and measure its spreading angle. In the following, we first describe the numerical model for \( \Sigma \), and then introduce the assumptions and procedures to define the spray plume angle. Data from Zhang et al.’s gasoline spray experiment [2] is used as validation.

**CFD Model**

An Eulerian two-phase flow CFD solver implemented into the OpenFOAM C++ library [6] is used for this study. The solver considers two fluid, one being the injected fuel and the other being non-condensable air as the ambient fluid. The fuel can be either liquid or vapor or a mixture of both. Each CFD cell is filled with either pure liquid or pure gas or a mixture of both. The gas phase can contain both the fuel vapor and the non-condensable air. Mixing of liquid and gas phase in a CFD cell is assumed to be homogeneous, and the sub-grid status of the two phases is modeled by the interface area density \( \Sigma \). In each CFD cell, pressure and momentum relaxation and heat transfer between the two phases are assumed to be very fast such that they always have the same velocity, pressure and temperature. Vaporization and condensation of the fuel are calculated by a Homogeneous Relaxation Model (HRM). More details of the flow solver can be found in [7, 8]. Modeling of \( \Sigma \) is based on a transport equation [4]:

\[
\frac{\partial \Sigma}{\partial t} + \frac{\partial}{\partial x_j} (u_j \Sigma) = \frac{\partial}{\partial x_j} \left( D_t \frac{\partial \Sigma}{\partial x_j} \right) + a_{eq} \Sigma \left( 1 - \frac{\Sigma}{\Sigma_{eq}} \right) + \frac{\Delta \Sigma}{\Sigma_{\text{init}}} + \frac{\Sigma}{\Sigma_{\text{init}}} \text{ initialization}
\]

In which \( D_t \) is a turbulent diffusivity coefficient defined as \( v_t/S_c \), where \( v_t \) is the kinematic turbulent viscosity and \( S_c \) is a dimensionless Schmidt number. The turbulent diffusion term accounts for the fact that interface area is diffused by the turbulent flow motion, just as other flow quantities are. Turbulence is modeled with a RANS (Reynolds-Averaged-Navier-Stokes) approach with a standard \( k-\epsilon \) model [9], where \( k \) is the turbulent kinetic energy (TKE) and \( \epsilon \) is its dissipation rate.
The equilibrium source term indicates that if the local turbulent flow is homogeneous and isotropic such that the spatial derivative terms in the equation can be neglected, the interface area density should evolve into a local equilibrium value as $\Sigma_{eq}$. The relaxation time required to reach the equilibrium, defined as $\tau_{eq}$, is related to the speed coefficient $a_{eq} = 1/\tau_{eq}$. The equilibrium is thought to be based on a balance between local TKE and “surface energy” [4, 10]. With the interface considered as a stretched elastic membrane, surface energy is proportional to the surface tension coefficient of the liquid fuel, $\sigma$, and the interface area size. Existence of the equilibrium was supported by the numerical experiment of Duret et al. [10]. Their formulation of $\Sigma_{eq}$ writes as:

$$\Sigma_{eq} = C_{eq} \frac{(\rho_{liq} + \rho_{gas}) \bar{Y}_{liq} (1 - \bar{Y}_{liq}) k}{\sigma}$$  \hspace{1cm} (3)

Where $C_{eq}$ is a parameter that varies from 1.0 to 2.0. The equilibrium interface area density is zero for pure liquid and pure gas. This is consistent with the physics meaning of $\Sigma$. Vallet et al.’s [4] and Beau’s [11] formulations are based on similar arguments about the equilibrium but they are not proper to be applied for dense liquid flows.

The speed coefficient, $a_{eq}$, determines how fast the balance between TKE and surface energy is achieved. Since the balance is a result of turbulent interaction between the two phases, the time required to reach the balance is determined by the local turbulence activity. If turbulence is very active, we expect very fast interaction and redistribution of energy between the two phases. The simplest way to model $a_{eq}$ was proposed by Vallet et al. [4]:

$$a_{eq} = C_{a} \frac{e}{k}$$  \hspace{1cm} (4)

In which $C_{a}$ is a modeling constant taken as 1.0. More sophisticated models that consider interaction of any two droplets in a computational cell were proposed by Beau [11]. These models generally introduce non-linearity by making $a_{eq}$ dependent on $\Sigma$ itself. In this study, the simple model (4) is adopted.

The third term on the right-hand-side of Eq. (2) is a production source term for $\Sigma$. The speed coefficient $A$ is modeled as [4]:

$$A = C_{A} \frac{-\bar{u}_{i}' \bar{u}_{j}'}{k} \frac{\partial \bar{u}_{i}}{\partial x_{j}}$$  \hspace{1cm} (5)

It scales with a turbulent production term for the TKE ($k$). Under the RANS turbulent viscosity assumption, the Reynolds stress term is proportional to the mean flow velocity gradient: $-\bar{u}_{i}' \bar{u}_{j}' = \nu_{t} \frac{\partial \bar{u}_{i}}{\partial x_{j}}$. Therefore, $A$ can be written as:

$$A = C_{A} \frac{\nu_{t} \partial \bar{u}_{i}}{k} \frac{\partial \bar{u}_{i}}{\partial x_{j}}$$

in which $C_{A}$ is a modeling constant taken as 1.0. This term accounts for the production of interface area density ($\Sigma$) due to mean flow shear force or so-called “stretching”, which is an important mechanism for TKE production. Due to the assumption of the balance between TKE and surface energy, it is expected that TKE production results in production of $\Sigma$. The previously-mentioned equilibrium source term only accounts for the scenario of locally homogeneous and isotropic turbulence, in which the $A$ term vanishes. The $A$ term, on the other hand, accounts for inhomogeneous and non-isotropic turbulence effects.

Both the equilibrium and the turbulent mean flow stretching term are proportional to the interface area density $\Sigma$. If $\Sigma$ is zero, both terms are deactivated. This is saying that there will be no production if there is no interface. Therefore, proper initialization of $\Sigma$ is important. The last source term in the transport equation (2), $\dot{\Sigma}_{init}$, is for this purpose. We consider the physics meaning of the minimum value of $\Sigma$ in any computational cell. If the cell is filled with pure liquid or gas, $\Sigma$ should be zero because there is no interface. If the cell contains both phases, $\Sigma$ must be positive. When the two phases have a laminar interface in between, the interface area size is smallest. Indeed, any disturbance to the interface that generates curvature would increase the area size. Based on the definition of $\Sigma$, it is fair to estimate this minimum value as $V^{-1/3}$ where $V$ is the volume of the CFD cell. The source term is written as:

$$\dot{\Sigma}_{init} = \frac{\Sigma_{min} - \Sigma}{\Delta t} \text{pos}(\Sigma_{min} - \Sigma)$$

$$\text{pos}(x) = \begin{cases} 
1 & \text{if } x > 0 \\
0 & \text{if } x \leq 0
\end{cases}$$

$\Sigma_{min} = 0$, when $Y_{liq} < \varepsilon$ or $Y_{liq} > 1 - \varepsilon$

$\Sigma_{min} = V^{-1/3}$, when $\varepsilon < Y_{liq} < 1 - \varepsilon$

where $\varepsilon$ is a small number taken as 1.0e-3. Using $\Sigma_{min}$ to define the initial interface area density, we assume that the initial interface is laminar. It is noted that the minimum value calculated as $V^{-1/3}$ is dependent on the CFD grid size. In a DNS simulation where the grid size is extremely refined, $V^{-1/3}$ becomes a Dirac function.
going to infinity [12]. To avoid this trouble, the concept of Σ modeling should be applied only when the grid size is larger than the characteristic droplet or bubble size. Indeed, this is exactly the purpose of introducing the Σ modeling.

**Prediction of Gasoline Spray Spreading Angle**

In order to define spray plume boundary, Magnotti and Genzale [3] started by using the Beer-Lambert Law to quantify how much percent of light intensity is received after the light passes through the plume:

\[
\frac{I}{I_0} = e^{-\tau}
\]  

(6)

in which \(I_0\) is the incident illumination intensity and \(I\) is the received intensity. \(\tau\) is called optical thickness or extinction. \(\tau = 0\) indicates no interference with the droplet. Given the connection between the color lightness on the spray image and the received light intensity, it is feasible to use the quantity \(I/I_0\) to represent a “digitized” color lightness. However, it is challenging to model \(I/I_0\) because light generated by the Xenon lamp has multiple wavelengths. For simplicity, we assume that the light source has a single illumination wavelength. Also assumed is that spray is composed of spherical droplets; all fluid (fuel and air) have real refractive index; the light-scattering events occurring when light intercepts droplets are independent to each other [3]. For a specific light ray penetrating through the spray, the optical thickness \(\tau\) can be modeled as:

\[
\tau = \int_{-\infty}^{+\infty} c_{ext} n/V d\eta
\]

In which \(n/V = \Sigma/(\pi d^2)\) is the droplet number density (recall Eq. (1)), and \(c_{ext}\) is the extinction cross-section which is proportional to the light intensity scattered away from the light ray’s original travel direction \(\eta\). It was shown [3] that \(c_{ext}\) is proportional to the square of drop diameter \(d\) if \(d\) is larger than 0.3 \(\mu m\) (“Mie regime”). This critical value is close to the wavelength of the incident light (0.68 \(\mu m\) in [3]). The gasoline spray of interest in this study has averaged droplet size in the range of 10 to 30 \(\mu m\) which is much larger than the critical value. The Mie regime is assumed to apply and we have:

\[
\tau \propto \int_{-\infty}^{+\infty} \Sigma d\eta
\]

Substitute into Eq. (6):

\[
\frac{I}{I_0} \propto \exp \left( -\int_{-\infty}^{+\infty} \Sigma d\eta \right)
\]

(7)

This formulation predicts the normalized light intensity received by the camera. The line-of-sight integration of the surface area density \(\Sigma\) is used as a metric for the optical thickness. Indeed, more interaction with droplet surface indicates more light scattered as the light ray penetrates through the spray and consequently weaker light intensity received. The only drawback at this point is that we have simplified the light source by assuming single-wavelength light, which could be improved in future work.

CFD simulations of internal-nozzle and near-nozzle flows were conducted on a setup that mimics Zhang et al.’s experiment. A polyhedral computational mesh was generated to discretize the flow domain. The mesh consisted of roughly 445,000 cells. An extrusion layer of 2 cells length was used to resolve the near-wall region, as shown in Figure 3 (Top). The cylindrical nozzle hole contained a coaxial counterbore that is connected to the plenum-shaped spray chamber. The plenum was used to save computational cost as it is unnecessary to simulate the full spray chamber. The plenum’s diameter was 9mm, allowing flow to fully develop after exiting the nozzle. Zero-gradient outflow boundary conditions were applied on the hemispherical boundary of the plenum chamber. The sphere-shaped needle inside the injector was held static. Figure 3 (Bottom) shows a cut plane at the middle of the simulation domain which is colored by the contour of the predicted \(\Sigma\). Significant increase of \(\Sigma\) is observed near the counterbore walls. This indicates occurrence of atomization right after the fuel enters the counterbore region and before it enters the spray chamber. This is very different compared to the common diesel injector nozzle without any counterbore, in which atomization occurs after the fuel enters the spray chamber.

The test conditions are listed in Table 1. Under each condition, CFD simulation was first run to the steady state. Then, a line-of-sight integration of \(\Sigma\) was conducted within a rectangular region that is 6.0mm wide and 2.8mm tall, shown by the dash line in Figure 3 (Bottom). Hypothetical light rays penetrate the simulation domain in the perpendicular direction with respect to the screen. The “light rays” have 0.05 mm spacing between each other, and a total number of 6720 integrations were performed. Each integration resulted in one normalized light intensity based on Eq. (7).
Table 1: Test matrix of the gasoline spray cases using pressure ratio $p_{\text{amb}}/p_s$ to characterize whether the spray is non-flashing or flashing, in which $p_s$ is the saturation pressure of the fuel at temperature $T_f$. Fuel temperature ($T_f$) varies from 45 to 85 degree C and ambient pressure ($p_{\text{amb}}$) varies from 40 to 200 KPa. According to Zhang et al. [2], $p_{\text{amb}}/p_s > 1$ is considered as non-flashing, $0.4 < p_{\text{amb}}/p_s < 1$ as transition, $p_{\text{amb}}/p_s < 0.4$ as flashing.

<table>
<thead>
<tr>
<th>$T_f (\degree C)$</th>
<th>45</th>
<th>55</th>
<th>65</th>
<th>75</th>
<th>85</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_{\text{amb}}$ (KPa)</td>
<td>30</td>
<td>0.67</td>
<td>0.46</td>
<td>0.33</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>40</td>
<td>0.89</td>
<td>0.62</td>
<td>0.44</td>
<td>0.33</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>2.22</td>
<td>1.54</td>
<td>1.11</td>
<td>0.82</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>4.44</td>
<td>3.08</td>
<td>2.22</td>
<td>1.64</td>
</tr>
</tbody>
</table>

Figure 3: Computational setup of the single-hole gasoline spray simulation. (Top) Zoom-in view of the nozzle region. The nozzle has a length-to-diameter ratio of 1.5 and the diameter (D) is 200 µm. (Bottom) A cut-plane at the middle of the simulation domain. Note that the computational domain extends 5mm upstream of the injector tip which is not fully displayed in this figure.

Figure 4: Predicted normalized light intensity $I/I_0$ based on Eq. (7). In this test case, fuel temperature was 45 degree C and ambient pressure was 200 KPa. The raw contour plot (Top) was converted to the binary plot (Bottom) using a threshold value $I/I_0 = 0.2$. 
A two-dimensional plot of the normalized light intensity is shown in Figure 4 (Top). The light intensity is zero in the near-nozzle liquid core which indicates no light received by the “camera”. It is 1.0 out of the spray plume where light penetrates fully through the ambient air without any scattering. Within most parts of the spray plume, it varies from zero to 1.0. A threshold value must be determined in order to define the plume boundary. In this study we chose the value as 0.2. Based on this threshold value, the contour plot was converted to a binary plot shown in Figure 4 (Bottom). We then used the same image-processing procedure for the experimental images (Figure 2) to calculate the predicted spray spreading angle.

![Figure 5: CFD prediction of spray plume angle as a function of the pressure ratio p_{amb}/p_s compared against the measurement.](image)

Figure 5 shows comparison between the predicted spray plume angle and the measurement. The prediction captures the trend of increasing plume angle with decreasing pressure ratio $p_{amb}/p_s$. Specifically, the prediction captures the trend of increasing plume angle with $p_{amb}/p_s$ below 1.0 where transition from non-flashing to flashing occurs.

**Summary**

This study explores a new definition of spray plume boundary in an Eulerian two-phase flow CFD simulation. This definition uses a line-of-sight integration of the interface area density ($\Sigma$) to simulate the reduction of light intensity due to light scattering. Spray spreading angle derived from this definition of plume boundary is more consistent with its counterpart used by the experimentalists. The predicted trend of spray plume angle variation with respect to the pressure ratio is encouraging compared to the data.

Future work will focus on extending the simulation conditions to lower back pressures (20 KPa) for more validations in the flashing regime. The proposed method will be improved by considering multiple wavelengths from the light source and more validations of the $\Sigma$ transport equation calculation.

**Acknowledgement**

Funding support from the Propulsion System Research Lab of General Motors Global R&D is greatly appreciated. We thank Mr. Eli Baldwin and Ms. Mar-yam Moulai at University of Massachusetts Amherst for their great help with the CFD flow solver and programming. We also thank Prof. Francois-Xavier Demoulin at CORIA-Université de Rouen who made enlightening comments on the interface area density modeling.

**Nomenclature**

- $a$: speed coefficient for equilibrium
- $A$: speed coefficient for turbulent stretching
- $C$: modeling constant
- $D$: diffusivity, or nozzle diameter
- $d$: droplet diameter
- $\Delta t$: simulation time step
- $\varepsilon$: turbulent kinetic energy dissipation rate, or a small number
- $\eta$: line-of-sight direction
- $I$: light intensity
- $k$: turbulent kinetic energy
- $L$: nozzle length
- $\nu$: kinematic viscosity
- $n$: droplet number
- $P$: pressure
- $p$: density
- $\Sigma$: interface area density
- $Sc$: Schmidt number
- $\sigma$: surface tension coefficient
- $t$: time
- $\tau$: optical thickness, or time scale
- $u$: flow velocity (vector)
- $V$: CFD control volume size
- $x$: spatial coordinate
- $\bar{Y}$: volume fraction

**Subscripts**

- $0$: incident light
- $amb$: ambient
- $eq$: equilibrium
- $ext$: extinction of light
- $f$: fuel
- $gas$: gas
- $j$: index of a vector
- $liq$: liquid
- $min$: minimum
- $init$: initialization
\( s \) saturation  
\( t \) turbulence  

Superscripts  
' ' fluctuating component of a turbulent flow quantity  

References  