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Effects of primary breakup modeling on spray and combustion characteristics of compression ignition engines

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ABSTRACT

Injector flow dynamics and primary breakup processes are known to play a pivotal role in determining combustion and emissions in diesel engines. In the present study, we examine the effects of primary breakup modeling on the spray and combustion characteristics under diesel engine conditions. The commonly used KH model, which considers the aerodynamically induced breakup based on the Kelvin–Helmholtz instability, is modified to include the effects of cavitation and turbulence generated inside the injector. The KH model and the new (KH-ACT) model are extensively evaluated by performing 3-D time-dependent simulations with detailed chemistry under diesel engine conditions. Results indicate that the inclusion of cavitation and turbulence enhances primary breakup, leading to smaller droplet sizes, decrease in liquid penetration, and increase in the radial dispersion of spray. Predictions are compared with measurements for non-evaporating and evaporating sprays, as well as with flame measurements. While both the models are able to reproduce the experimentally observed global spray and combustion characteristics, predictions using the KH-ACT model exhibit closer agreement with measurements in terms of liquid penetration, cone angle, spray axial velocity, and liquid mass distribution for non-evaporating sprays. Similarly, the KH-ACT model leads to better agreement with respect to the liquid length and vapor penetration distance for evaporating sprays, and with respect to the flame lift-off location for combusting sprays. The improved agreement is attributed to the ability of the new model to account for the effects of turbulence and cavitation generated inside the injector, which enhance the primary breakup. Results further indicate that the combustion under diesel engine conditions is characterized by a double-flame structure with a rich premixed reaction zone near the flame stabilization region and a non-premixed reaction zone further downstream. This flame structure is consistent with the Dec's model for diesel engine combustion (Dec, 1997) [1], and well captured by a newly developed flame index based on the scalar product of CO and O_2 mass fraction gradients.

1. Introduction

The diesel engine has been the preferred power train for heavy-duty applications due to high energy density and efficiency. Moreover, there has been noticeable reduction in pollutants and noise emissions as a result of many innovations, especially in direct injection systems combined with turbo charging. However, engine manufacturers continue to face new challenges to improve engine efficiency and meet increasingly stringent emission regulations with respect to NO_x and particulate matter. For instance, the US EPA's current requirements for heavy duty truck engines manufactured after 1st January 2008 are set at 0.01 g/bhp-h for particulates and 0.2 g/bhp-h for NO_x, both an order of magnitude lower than those a decade ago. This provides a clear motivation for engine manufacturers to make enhancements in fuel injection system and combustion processes, based on fundamental understanding, and further reduce engine's raw emissions and improve fuel consumption.

In a diesel engine the liquid fuel is injected into the combustion chamber near the end of the compression stroke. Following injection, the fuel undergoes atomization and vaporization processes, followed by fuel–air mixing, ignition, and establishment of a lifted flame in the chamber. The dominant combustion processes associated with this flame are illustrated in Fig. 1, which is based on experimentally obtained laser sheet images of diesel combustion [2]. The figure shows a cold fuel jet (dark brown[1] region) and a fuel vapor rich region (light brown region) preceding a fuel-rich premixed flame (represented by the thin blue region), and a diffusion

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[1] For interpretation of color in Figs. 1, 3–17 the reader is referred to the web version of this article.

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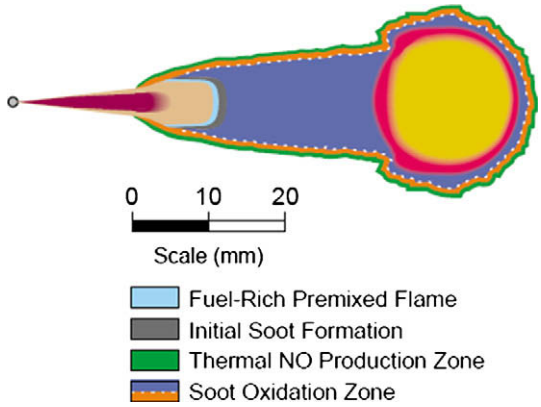

Fig. 1. Schematic of "conceptual" combustion model of Dec [1].

flame that surrounds the burning plume. Thus the combustion is characterized by a partially premixed or dual flame mode involving a rich premixed zone and a diffusion reaction zone. The dark blue region between these two reaction zones contains the products of incomplete oxidation due to rich combustion, which behave as intermediate fuels (CO, H_2, C_2H_2, etc.) and subsequently burn in the diffusion reaction zone. This region also represents the dominant soot initiation and formation zone, while most of the NO_x formation occurs in the diffusion flame, since it has the highest temperatures. The detailed structure of this dual flame and its emission characteristics strongly depend upon the location at which the flame is stabilized, i.e., the flame lift-off length, defined as the farthest upstream location of combustion on the spray axis. Thus the combustion and emission characteristics of a diesel engine are strongly coupled with the flame lift-off behavior, as demonstrated by several previous studies [1,3–6]. Since the flame lift-off characteristics are largely determined by the fuel atomization, vaporization, subsequent fuel–air mixing, and air entrainment upstream of the lift-off location, it is clear that these processes play a critical role in determining the engine combustion and emission characteristics.

The coupling between the spray and fuel–air mixing processes and the engine combustion and emissions has been investigated in previous studies [3–5,7–11]. Reitz and co-workers [9–11] performed experiments and simulations using KIVA, and examined the effects of injection, atomization and spray characteristics on the diesel engine combustion and emissions. Arcoumanis et al. [8] and Arcoumanis and Gavaises [12] numerically investigated the effects of nozzle flow and injection processes on the structure of diesel sprays. Siebers and co-workers [3–5] reported a series of experimental studies using an optically accessible, constant-volume vessel under diesel engine conditions, and investigated the effects of various injection and ambient parameters, including nozzle orifice diameter, injection pressure, ambient temperature, and density, on the combustion and emission characteristics. The effects were characterized in terms of the liquid length (L_l) and flame lift-off length (L_f). The liquid length is defined as the farthest penetration of liquid fuel in terms of the axial location [6], and is established where total fuel evaporation rate equals the injection rate. It represents a global parameter for characterizing the atomization and vaporization behavior, whereas the lift-off length is used to represent the combustion behavior. Siebers and Higgins [4] also examined interactions between these two parameters. For instance, $L_f > L_l$ implies that fuel evaporation is completed before combustion process begins, and the flame is established in a relatively rich mixture. On the other hand, for $L_f < L_l$, there is two-way coupling between combustion and spray processes, with the combustion process enhancing fuel evaporation and the relatively cooler spray decreasing the flame temperature.

The fuel injection and atomization processes are extremely complex involving transient two-phase, turbulent flows at high pressures, with a wide range of temporal and spatial scales. Consequently, the theoretical and computational studies of these flows have been very challenging. Various approaches used to model these flows can be broadly grouped into two categories. One approach follows an Eulerian–Lagrangian methodology [13], whereby the gas-phase equations are solved using Reynolds Averaged Navier Stokes (RANS) or Large Eddy Simulation (LES) methods, while the dispersed phase is solved using a Lagrangian formulation, tracking individual droplet parcels. Appropriate algorithms are employed to interpolate the gas-phase properties at the Lagrangian locations, and to distribute the interphase source terms at the Eulerian grid. One limitation of this approach is the insufficient grid resolution in the near injector region and the grid-independence of simulations, due to the basic assumption of Eulerian cell volume being sufficiently larger than the dispersed phase volume within the cell [14]. The second approach follows the Eulerian–Eulerian two-fluid methodology [15], treating different size classes of droplets as separate and inter-penetrating phases and solving conservation equations for each one of them. A major disadvantage of this approach is the excessive computational effort required as the droplet size distribution becomes wider. Some recent studies [11,16] have employed a hybrid approach, using an Eulerian method in the dense spray region, and switching to a Lagrangian method in the dilute region. It is important to note that for any of these approaches, the accuracy of simulations critically depends upon the sub-models used to represent the various dispersed phase processes, such as atomization, droplet collision, deformation, and vaporization. In particular, the modeling of atomization, especially in the near nozzle region, has been shown to be pivotal in determining the spray and combustion characteristics in diesel engines [8,11,12,17,18]. A realistic atomization model in the primary breakup region should include the essential physics associated with the two-phase flow both inside and outside the injector.

While there have been extensive studies of the primary and secondary atomization phenomena, fundamental processes associated with these phenomena are still not well understood. The liquid jet breakup is known to be caused by the Kelvin–Helmholtz (KH) and Rayleigh Taylor (RT) instabilities at the interface of the two fluids. The KH instability is due to high shear at the interface, while the RT instability is related to density difference between the two fluids. Accordingly, the most commonly used atomization models, namely the KH and RT models, are based on a linear analysis of these instabilities [19–21]. The literature review indicates that the Eulerian–Lagrangian approach using the KH–RT atomization models has been widely employed for diesel engine simulations. Most CFD-based engine simulation codes employ this methodology, using KH model for the primary breakup and a combination of KH–RT models for the secondary breakup. This approach has been found to be computationally efficient and reproduce the global spray behavior reasonably well. However, several studies have shown that fuel atomization in the region close to the injector nozzle is also strongly influenced by cavitation and turbulence in the liquid jet [12,22]. The cavitation structures developed inside the nozzle orifice can reach the exit, implode, and cause jet integration. Similarly turbulent eddies emerging from the nozzle can cause further jet disintegration. While the effects of cavitation and turbulence on the primary breakup are well established, most of the atomization models used in CFD-based engine simulations only consider aerodynamic jet breakup based on the KH instability.

The present study aims to investigate the effects of modeling the primary breakup processes on the spray and combustion characteristics under diesel engine conditions. In our previous study [23,24], the KH model was modified to include the effects of cavi-