Applied Energy 129 (2014) 123–134

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy

Effect of internal nozzle flow and thermo-physical properties on spray characteristics of methyl esters

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HIGHLIGHTS

- Nozzle flow and spray characteristics of methyl esters have been studied.
- A new hybrid spray model was implemented into KIVA4 CFD code.
- Nozzle flow simulation shows methyl stearate has less cavitation.
- Methyl linoleate atomization is comparable with diesel atomization.
- Methyl stearate has poor atomization compared to other methyl esters.

ARTICLE INFO

Article history:
Received 3 February 2014
Received in revised form 10 April 2014
Accepted 30 April 2014
Available online 23 May 2014

Keywords:
Spray characteristics
Cavitation
Methyl esters
Hybrid spray model

ABSTRACT

In compression ignition engines, the quality of the spray atomization significantly affects the performance and emissions of the engine. The differences in thermo-physical properties of biodiesel have significant effect on both the internal nozzle flow and spray characteristics. In this study, the internal nozzle flow and spray characteristics of three major methyl esters found in various biodiesels, namely methyl oleate, methyl stearate, and methyl linoleate were studied as a representative of different biodiesels. A new hybrid spray model developed by coupling cavitation induced spray model with KHRT model in KIVA4 CFD code was used in this study. The model was validated against diesel spray characteristics obtained from the experiments conducted in house using constant volume spray chamber and good agreement was found. The internal flow simulations shows that methyl stearate cavitates the least followed by methyl oleate and linoleate. The spray simulations shows that spray tip penetration of methyl stearate is higher than other methyl esters and diesel because of its high viscosity and large droplet diameter. Methyl linoleate was found to atomize better than other esters and comparable to diesel. However at high ambient temperature, liquid length is highly dominated by both latent heat of vaporization and viscosity.

1. Introduction

Currently researches are focused on improving the compression ignition engine operation in attempt to reduce pollutant emissions without sacrificing the fuel economy. Also demanding energy security concerns triggers the search for alternative, renewable and bio-derived fuels throughout the world [1]. Researchers are coming up with new biodiesel fuels from different feedstock based on the local availability and cost [2,3]. The combustion process of different fuels is significantly affected by the fuel spray atomization process and cetane number, etc. The computational fluid dynamic (CFD) tools become valuable in reducing number of experiments in optimizing the engine performances. However, the predicted levels of pollutant concentration and power output are comprehensively dependent on the description of the spray breakup process. The difference in thermo-physical properties of biodiesel derived from different feedstock have significant effect on the fuel spray atomization, combustion and emission formation. In order to improve the performance of different biodiesel in terms of emissions and power output, various injection strategies have been implemented, after all, the combustion process is governed by the spray breakup process [4]. The spray break-up process controls the fuel–air mixing by better atomization followed by evaporation of fuel which eventually allows the combustion process to reach high efficiencies. In addition, the fuel injected at high pressures creates turbulence in interaction with the swirl flow inside the combustion chamber and affects the combustion speed.

Usually biodiesel have methyl esters with as many as 17–19 carbon atoms. Different biodiesel has different composition of methyl

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http://dx.doi.org/10.1016/j.apenergy.2014.04.109
0306-2619/

esters; however, the major constituent governs the chemical and physical properties of the biodiesel fuel. Generally, for modeling purpose, the properties of major composition of the methyl esters are used to depict the properties of biodiesel fuel [5] or properties of mixture composition are considered [6,7]. According to literature [8,9], biodiesels generally have higher composition of methyl stearate (C18:0), methyl oleate (C18:1) and methyl linoleate (C18:2) (refer Table 3 in [8] and Table 6 in [9]). Though there are many experimental study related to biodiesel spray development [10–13], discovery of new feedstock makes it difficult to generalize the phenomenon. Nevertheless, there are some simulations on spray behavior found in literature related to specific biodiesel like soy bean [14,15] and rape seed based biodiesel [5], but their results cannot be further extended in interpreting the behavior of other biodiesels.

The spray breakup process also depends on the internal flow in the nozzle orifice of the injectors [16–18]. Many studies have shown that cavitation inception inside the injector nozzle holes substantially affects the primary break-up of the exiting liquid jet and spray characteristics [19–25]. Generally, it was reported that fuel spray tip penetration decreases and spray cone angle increases with formation of vapor inside the nozzle holes [18,26–28]. Although the cavitation inception in nozzle holes significantly contributes to spray break-up process, only very few literature were found which coupled them together to model the spray development process [29–31]. Moreover, the KHRT spray model which is widely used in engine application does not include the cavitation and turbulence effect into break-up mechanism. Thus a hybrid spray model which accounts for cavitation and turbulence inside the injector nozzle holes along with aerodynamic and deceleration instabilities on the droplet surfaces is necessary to better capture the spray development mechanism. The study on spray characteristics of biodiesel taking into account of cavitation in the nozzle holes is very limited and it should be noted that the simulations were only done for soy bean based methyl esters [32,33]. The differences in thermo-physical properties are also expected to significantly affect the nozzle flow characterization and eventually the spray breakup of biodiesel fuels. Thus the spray breakup process of biodiesel should include the cavitation phenomenon that influences the atomization process. Availability of very few studies on modeling spray atomization of biodiesel taking into account the nozzle flow characterization and absence of extension of work to different biodiesels provided motivation for the present work.

In this study, the spray atomization of three major methyl esters present in biodiesels: methyl oleate, methyl stearate and methyl linoleate were studied in order to generalize the spray behavior of different biodiesels. A new hybrid spray model which includes cavitation induced breakup model coupled with KHRT model was used in this study. In order to account for the cavitation into the spray model, internal flow simulations were done in prior for all three methyl esters and compared with diesel. The new spray model was validated with non-vaporizing spray results obtained in-house using constant volume spray chamber for diesel fuel at different injection pressure and ambient pressure. Then the spray behavior of different methyl esters were compared with diesel in terms of spray tip penetration, Sauter Mean Diameter (SMD), liquid length at different injection pressure and ambient conditions. Finally, conclusions were drawn based on the results obtained.

2. Methodology

2.1. Experimental set-up

The experimental set-up is shown in Fig. 1. The macroscopic spray characterization has been performed in constant volume high pressure chamber to reproduce the high gas density inside the diesel engine combustion chamber during the compression stroke. The chamber was designed to operate up to 6 MPa at room temperature. The chamber was pressurized using nitrogen (N_2) gas. For visualization purpose, optically polished quartz glass window of size Φ150 mm was provided on one side of the chamber. The fuel injection system used consists of Denso common rail pump run by 2.24 kW electric motor controlled electronically, a Denso common rail injector and a digital electronic control unit to precisely control quantity and duration of injection. The common rail injector used to investigate the spray characteristics of diesel fuel is a 7 hole micro-sac type injector. The dimensions of the nozzle hole were determined by using a silicone mold of Polydimethylsiloxane (PDMS) material by approach similar to Macián et al. [34]. The scanning electron microscope (SEM) image and dimensions of the nozzle hole is shown in Fig. 2. The measured dimensions shows that the orifice diameter is 175 ± 3 μm and length of orifice is 1000 ± 50 μm, radius of curvature at the inlet is 15 μm and the cone angle of the spray is 150 ± 2°. The spray visualization was carried out using Photron Fastcam SA5 high speed camera. The camera sensor is 12 bit monochrome with a spatial resolution of 20 μm pixel and with a minimum exposure time of 1 μs. The images were captured at 20 k fps with a resolution of 832 × 448 pixels and at exposure time of 1/20,000 s. Illumination was created using a 400 W Hydrargyrum medium-arc Iodide (HMI) lamp with electronic ballast. The image processing was done using custom written code in Matlab. The spray tip penetration and cone angle measurements were performed using ImageJ code. The image processing sequence is shown in Fig. 3. The experiment was done for diesel fuel at different injection pressures and ambient densities and the results were used for further validation of the spray modeling.

2.2. Numerical approach

In this study, the simulation is done in two steps. In the first step, simulation of cavitation inside the injector nozzle hole is done in Fluent 12.1 using the two-fluid Schnerr and Sauer model [35–38]. Then in the second stage, simulation of spray break-up process is done using new hybrid spray break-up model in KIVA4 CFD code taking into account, the results obtained from nozzle flow simulation. The new hybrid spray break-up model was developed by coupling KHRT model with the cavitation induced spray sub model. The results of local distribution of flow field variables in the nozzle orifice exit obtained from the cavitating flow simulations are introduced into the spray break-up model to capture the turbulence and cavitation effects. The new model is implemented into KIVA4 in the way such that the dominant break-up process is determined by the maximum of length to time scale ratio since the droplet size decreases with this ratio and also this ratio determines the rate at which the breakup takes place. The mathematical form of the implementation of the new hybrid model is shown in equation below

$$\frac{L_B}{\tau_B} = \max\left\{\frac{L_{KH}}{\tau_{KH}}; \frac{L_{RT}}{\tau_{RT}}; \frac{L_{cav}}{\tau_{cav}}\right\} \quad (1)$$

where L is the characteristic length and τ is the characteristic time and the subscripts B, KH, RT, cav represent dominant break-up process, Kelvin–Helmholtz (KH) model, Rayleigh–Taylor (RT) model, and cavitation model respectively. In this model, the droplets are subjected to break-up by competition between the three sub models based on the maximum of length to time scale ratios for each parcels at each time step. The mathematical description of spray sub models is given in Table 1. This new model is implemented into KIVA4 using a separate sub-routine written in FORTRAN language. In addition to the new spray model, the standard turbulence model,