
DOI link
https://doi.org/10.1016/j.egypro.2017.12.074

ePrints link
http://eprint.ncl.ac.uk/pub_details2.aspx?pub_id=245909

Date deposited
09/02/2018

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Experimental and Numerical Investigation on the Macroscopic Characteristics of Hydrotreated Vegetable Oil (HVO) Spray

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Abstract

The macroscopic characteristics of Hydrotreated vegetable oil (HVO), a renewable biodiesel, were investigated by both experimental and numerical approaches in this paper. The experiment on spray of 0.6ms injection duration was conducted in a constant volume vessel (CVV) at 1800 bar common rail pressure, 70 bar ambient pressure and 100°C ambient temperature, and the numerical work with the Wave breakup model and RNG k-ε turbulence model was done on a corresponding 2D geometric model at the same condition. The results indicated that the spray tip penetration grew with a decreasing tip velocity and the cone angle increased gradually after a dramatic growth and slight drop. Moreover, the prediction of numerical method, when used in conjunction with experimental studies, was proven effective in elucidating the macroscopic characteristics of HVO spray. The error between the predicted spray tip penetration and the experimental one was no more than 4\% except that within 0.2ms flow time after SOI. In addition, the predicted cone angle was in similar trend to the experimental one and the error was within 10\% after 0.2 ms.

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Peer-review under responsibility of the scientific committee of the 9th International Conference on Applied Energy.

Keywords: Biodiesel, spray, numerical calculation, constant volume vessel

1. Introduction

Hydrotreated vegetable oil (HVO) is the mixture of paraffinic hydrocarbons with high cetane number and absence of aromatics, sulphur and oxygenates benefiting to better engine performance and reduction of emissions. Meanwhile, unlike ester-based biodiesel fuels, it also has no problems such as deposition, poor storage stability and poor cold properties, which makes it a superior sustainable biodiesel fuel [1, 2]. Therefore, some researches have
been done on the application of HVO [3] as a renewable energy source for vehicles. Lehto et al. [4] compared the NO\textsubscript{x} and smoke emissions of HVO with diesel fuel EN590 in a single-cylinder engine with 30% EGR and found that HVO produced lower smoke emissions and enabled higher EGR than diesel fuel. Liu et al. [5] investigated HVO blends with diesel fuel at high EGR rate and reported increased soot emissions caused by the higher combustion temperature of HVO blends. Singh et al. [6] also studied the emissions and fuel consumption of a heavy duty diesel engine fuelled with HVO and found the particulate matter, carbon monoxide, unburnt hydrocarbon and brake specific fuel consumption (BSFC) were all lower than diesel fuel. Nevertheless, these investigations of HVO were about the engine performance, and no detailed spray characteristics were mentioned.

As known, spray characteristics of liquid fuels influence the performance of combustion in engines, and finally determine the level of pollutant emissions. Therefore, the spray characteristics are important factors to evaluate the quality of a renewable fuel for engine application. Accordingly, Thomas et al. [7] did experiments on the spray of several biofuels including HVO in a constant volume vessel (CVV) and found HVO had shortest penetration and largest cone angle. Besides, a modified empirical equation was also developed for the prediction of the length of spray penetration. To explore a more detailed numerical approach on liquid fuel spray, Battistoni and Grimaldi [8] adopted the Wave breakup model in a CFD simulation to predict the macroscopic spray characteristics of several biofuels. The result proved good prediction of Wave breakup model [9] for spray tip penetration, but HVO was not studied in this work. Meanwhile, Gong et al. [2] tested the spray properties of HVO at both non-evaporating (room temperature) and the evaporating (high temperature) conditions via RANS and large eddy simulation (LES), and found HVO produced similar droplet size and spray tip penetration to diesel fuel at room temperature but slightly smaller ones than diesel at high temperature. However, both RANS and LES strongly depend on high-performance hardware and are too time consuming, and the spray cone angle was not mentioned in this study.

As a promising renewable energy source for diesel engines, HVO has not been fully studied on its spray properties. Meanwhile, the spray characteristics of HVO also need cheaper and more convenient numerical methods to investigate. Therefore, the main macroscopic spray characteristics of HVO would be studied by a numerical approach with the Wave breakup model and the corresponding experiment would also be done in a CVV to validate it in this paper.

2. Experiments

2.1. Apparatus

The experimental system consists of a fuel delivery system, a constant volume vessel (CVV), a monitor and control system and optical diagnostic devices, as shown in Fig. 1. The common rail in the fuel delivery system can provide up to 1800 bar fuel pressure. The CVV has an internal volume of 5.65 litres and four 90 mm viewing size silica windows 90° apart from each other. With an external 4.5 kW ceramic band heater on the wall and an external LAUDA Integral XT 150 chiller to cool down the windows and pressure
transducer, the CVV can work at as high as 600K internal air temperature at 70 bar internal air pressure. A single-hole solenoid injector with 0.16mm orifice diameter is installed at the top of the CVV and triggered by a LabVIEW program to produce injection of fuels.

To observe the macroscopic features of spray, a high speed PHANTOM V710 monochrome CCD camera was mounted to one of the windows with a maximum 1280 × 800 pixels resolution at up to 75,000 fps sampling rate and a 100 W xenon lamp on the opposite window was installed to provide constant background light for the camera. The monitor and control system was mainly written by a LabVIEW program, which can display the temperature and pressure of the internal air and the temperature of the heater and windows on the front panel, and control the temperature of the chiller and the switch of the heater automatically. The Hydrotreated vegetable oil (HVO) was selected as the tested fuel, whose properties are shown in Table 1.

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>Density (kg/m³) at 15 °C</th>
<th>Viscosity (mm²/s) at 40 °C</th>
<th>Surface tension (N/m)</th>
<th>Aromatics content</th>
<th>Cetane Number</th>
<th>LHV (kJ/kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HVO</td>
<td>780.1</td>
<td>3.02</td>
<td>0.028</td>
<td>0</td>
<td>78</td>
<td>43902</td>
</tr>
</tbody>
</table>

### 2.2. Experimental procedures

In the experiment, the HVO was heated to 80 °C according to the engine conditions and then was injected at 1800 bar rail pressure, 70 bar ambient pressure and 100°C ambient temperature. The duration of each injection was 0.6ms. The injection duration was defined from the time when the injected fuel was visible to the time when the tail of the spray left the tip of the injector. The start time of the injection duration can also be called the start of injection (SOI). The injection rate of the injector is shown in Fig. 2. The high speed CCD camera was triggered by the same signal as the injector, and its resolution was set to 256 × 256 pixels at 50,000 fps sampling rate to capture the spray pattern every 0.02ms. The penetration and cone angle at each time can be obtained to validate the numerical model. The total flow time in the experiment was 1ms for data acquisition. The spray tip penetration in this research is the length between the head and the tail of spray field. The cone angle is a vague value and is defined as the angle formed by two lines touching most outer boundaries of spray field on both sides and joining together at the tail of spray.

### 3. Numerical calculations

#### 3.1. Numerical models

As atomization in the vessel was turbulent flow, the RNG k-ε model was selected for the modelling, which is more accurate and reliable for rapidly strained flows than the standard k-ε model. And the Standard Wall Functions was selected for the near-wall treatment as almost no flow-wall interaction occurred in the near wall zone.
For the discrete phase, the Reitz Wave model was selected as the breakup model because it is appropriate for high speed fuel injections when the Weber number (We) is larger than 100, which considers the breakup of the droplets to be induced by the relative velocity between the gas and liquid phases. In this model, we assume that the Kelvin-Helmholtz instability dominates droplet breakup, and the size of child droplets is proportional to the wavelength of the unstable surface wave on the parent droplet, as shown in Eq. (1).

Where \( r \) is the radius of the child droplet, \( B_0 \) is a constant set to 0.61 according to Reitz’s work [9]. Moreover, the changing rate of the droplet radius is defined as Eq. (2), where \( a \) is the radius before breakup and \( \tau \) is the breakup time determined by Eq. (3).

The breakup time constant \( B_1 \) can be in the range of 1 to 60 depending on the injector calibration and it determines how quickly the parcel will lose mass [10]. The \( \Omega \) is the maximum growth rate and \( \Lambda \) is the corresponding wavelength of parent droplet, which are obtained from Eq. (4) and (5), where \( Oh = \sqrt{We}/Re \) is the Ohnesorge number, \( Ta = Oh\sqrt{We} \) is the Taylor number and \( Re = \rho U^2 a/\sigma \) is the Reynolds number. The footnote 1 and 2 refer to the liquid phase and gas phase respectively.

In the Wave model, Eq. (3) gives a rate to calculate the accumulated shed mass from the parent droplet until it reaches 5% of the initial parcel mass, when Eq. (1) creates a radius for a new parcel with the same properties as the parent one. The newly-formed parcel is given a velocity randomly selected in the plane orthogonal to the direction vector of the parent parcel at this time and the momentum of parent parcel is also adjusted to keep the conservation of momentum.

\[
\frac{\Lambda}{a} = 9.02 \left( \frac{1+0.45Oh^{0.5}(1+0.4Ta^{0.7})}{(1+0.87We^{1.67})^{0.6}} \right)
\]

\[
\Omega \sqrt{\frac{a^3}{\sigma}} = \frac{0.34+0.38We^{1.5}}{(1+Oh)(1+1.4Ta^{0.6})} r
\]

### 3.2. Numerical setup

In order to simulate the process of atomization in the CVV, a 2D geometric axisymmetric model of the CVV was built with the size of 273mm \( \times \) 75mm, whose diagram was shown in Fig. 3. And 180628 structural cells was drawn whose minimum size was 0.02mm \( \times \) 0.02 mm in the fluid domain. The wall of the vessel was set to no-slip adiabatic wall. The surface injection type was selected for the fuel inlet and the mass flow rate at the inlet was set according to the regulation of injection rate in Fig. 2. The materials in the domain are the air (ideal gas, 100°C and 70 bar), the air-HVO vapour mixture and the droplet particles (liquid discrete phase fluid). The Wave breakup model was selected in the discrete phase model (DPM) as the both primary and secondary breakup models and the constants \( B_0 \) and \( B_1 \) were 0.61 and 10 respectively. The initial droplet diameter at the inlet was set to 0.16mm, which was the same as the orifice diameter of the injector. The drag law of droplets was dynamic-drag. For the solution methods, the implicit transient formulation and the pressure-velocity coupled scheme was selected. The flow courant number was 50 and the relaxation factors for all variables were 0.1. The time step size was \( 1 \times 10^{-5} \) s and the number of time steps was 100, thus the total flow time after SOI was 1 ms.

### 4. Results and discussion

Fig. 3. Diagram of the numerical domain

An example of spray field obtained by experimental and numerical methods was shown in Fig. 4 at 0.6ms after the start of injection (SOI). As shown in Fig. 5, the spray tip penetrations after SOI were obtained by experimental
and numerical methods at 1800 bar rail pressure, 70 bar ambient pressure and 100°C ambient temperature. Both experimental and numerical data indicated that the tip penetration kept growing even after 0.6ms, when the injection stopped, but the velocity at the spray tip dropped with the penetration proceeding downstream. In the injection duration, the fuel was driven by the rail pressure and diffused in the air once injected, thus the droplets at the tip and edge zones broke up and mixed with the air, which slowed down the velocity of the spray tip. After the injection stopped at 0.6ms, the spray penetrated in the air only by inertia, which made the velocity of the tip reduced more.

Fig. 5 also showed a good agreement between the experimental data and numerical data on spray tip penetration from 0.2ms to 1ms (less than 4% bias), which proved the performance of the Wave breakup model was of high accuracy in this range.

However, the prediction of the numerical model was significantly lower than the experimental spray tip penetration before 0.2ms. It was probably because the Wave breakup model is designed for high speed flow but the velocity of the fuel near the outlet of the injector at the beginning was in fact not high enough according to Fig. 2.

As shown in Fig. 6, the experimental cone angle increased dramatically to about 20° before 0.2ms after SOI and then experienced a slight drop at 0.3ms, after which it grew gradually to nearly 25° with the flow time. The large cone angles indicate good spray quality and thus contribute to high combustion efficiency when applied in engines. The numerical cone angle had a similar overall tendency and the error was within 10% at most flow time except for that before 0.2ms. The trends of both experimental and numerical spray cone angle indicated that the spray before about 0.3ms was not stable and thus resulted in fluctuations, which was the reason that the cone angle
experienced sharply growth and drop during this period. After 0.3ms, the spray became fully developed so the cone angle started slight increase gradually. The regulation of injection rate indicated that the mass flow rate of the injector increased significantly before 0.3ms, because the injection pressure in the injector was still quite lower than the rail pressure when the needle inside the injector just started to move up. According to previous research [11], the cone angle is not sensitive to injection pressure, whilst the Wave model assumes the size of child droplets are determined by the wavelengths the Kelvin-Helmholtz waves on parent droplets, which are likely to be impacted by the injection pressure. Consequently, the cone angle, associated with the size of droplets, viewed rapid increase with the increasing injection pressure before 0.2ms, after which the injection pressure became stable.

5. Conclusions

The experiment on the spray of HVO, a newly developed sustainable biodiesel fuel, was conducted in a constant volume vessel (CVV) at 1800 bar rail pressure, 70 bar ambient pressure and 100℃ ambient temperature. The numerical work was also done on the same process in a corresponding 2D geometric model at the same condition using the Wave breakup model. The conclusions are following:

- Both the experimental and numerical spray tip penetrations increased after the start of injection (SOI) but the velocity of the tip kept dropping as the spray proceeded downstream.
- The Wave model showed high accuracy in predicting the spray tip penetration, especially from 0.2ms to 1ms after SOI, where the bias with experimental data was within 4%, despite a larger bias before 0.2ms.
- Both the experimental and numerical spray cone angle experienced a dramatic increase and drop at first and then a gradual growth with the flow time proceeding.
- The predicted cone angle by the Wave breakup model agreed well with the experimental one with the error no more than 10% after 0.2ms.

Therefore, the numerical model employed in this paper has a good performance in predicting the macroscopic characteristics of HVO spray and thus bring an economical way to estimate the performance of any renewable fuels on combustion and pollutant emissions.

Acknowledgements

The authors would like to thank the supports by EPSRC through (EP/K503885/1) for the project Study of engine waste heat technologies, from NSFC-RS Joint Project under the grant number No. 5151101443 and IE/151256. The first author also would like to thank for sponsorship towards the PhD study from the SAgE doctoral Training Award under grant number NH/140671210 and financial support from Chinese Scholarship Council under No. 201508060054.

Biography

Dr Yiji Lu, born in June 1989, is currently a research associate in Newcastle University. He graduated from Shanghai Jiao Tong University in 2011 for his bachelor degree, he conducted his M.Phil. and Ph.D. in Newcastle University in 2012 and 2016. His Ph.D. program was fully sponsored by EPSRC and was awarded the ‘2015 Chinese Government Award for Outstanding Self-financed Students Abroad’ from China Scholarship Council. His research interests include but not limited to advanced waste heat recovery technologies, engine thermal management, advanced engine development, engine emission technologies, chemisorption cycles and expansion machines for power generation system. He has been regularly invited to review the manuscripts for the scientific journals including Applied Energy, Applied Thermal Engineering, Energy (the International Journal), and Energy for Sustainable Development.
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