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# Sensitivity analyses of biodiesel thermo-physical properties under diesel engine conditions

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ABSTRACT

This reported work investigates the sensitivities of spray and soot developments to the change of thermo-physical properties for coconut and soybean methyl esters, using two-dimensional computational fluid dynamics fuel spray modelling. The choice of test fuels made was due to their contrasting saturation-unsaturation compositions. The sensitivity analyses for non-reacting and reacting sprays were carried out against a total of 12 thermo-physical properties, at an ambient temperature of 900 K and density of 22.8 kg/m$^3$. For the sensitivity analyses, all the thermo-physical properties were set as the baseline case and each property was individually replaced by that of diesel. The significance of individual thermo-physical property was determined based on the deviations found in predictions such as liquid penetration, ignition delay period and peak soot concentration when compared to those of baseline case. Among all the properties, latent heat of vaporisation produced the greatest effect on the spray and soot developments under the tested conditions, as evidenced by a longer liquid penetration of 35.0% and a reduced peak soot concentration of 22.8%. Besides, coupled effects among the thermo-physical properties were also determined. Meanwhile, the effects of thermo-physical properties were found to vary with the addition of unsaturation levels and chemical kinetics in the simulation.



## 1. Introduction

The rise of biodiesel as a reliable alternative fuel has stimulated extensive interest and research to further exploit this fuel for power generation in ground transportation sector. Therefore, numerous studies have been conducted either on experimental or numerical fronts to understand the combustion characteristics of biodiesel under engine environment. Many apparent benefits are reported when biodiesel is utilised in diesel engine, such as low levels of carbon monoxide [1], soot formation [1] and particulate matter emissions [2,3]. However, several drawbacks are also found when biodiesel is directly fuelled into diesel engine, without any modification to the engine. For example, the lower heating value of biodiesel as compared to that of diesel contributes to the increased fuel consumption and lower engine power output [1]. Furthermore, higher levels of nitrogen oxides emission [1,4] are also detected when biodiesel replaces diesel.

One main reason that contributes to the distinct combustion characteristics between diesel and biodiesel is the fuel compositions. The majority components contained within diesel are hydrocarbons, while biodiesel comprises largely alkyl esters. For this reason, the chemical structures of these two fuels are dissimilar as biodiesel contains additional oxygen atom and double bonds in comparisons to the pure hydrocarbons in diesel. As such, the thermo-physical properties of biodiesel, which are developed based on the fuel compositions, are distinguishable from those of diesel. Several experimental works have discovered that the spray characteristics of biodiesel are contributed by the fuel thermo-physical properties. For example, Genzale et al. [5] suggested that the higher values of liquid density and liquid viscosity of biodiesel contributed to longer LPL (liquid penetration length) than that of diesel. On the other hand, Nerva et al. [6] noticed that the higher mass flow rate for SME (soybean methyl ester) was due to the higher liquid density and liquid viscosity. Apart from these experiment findings, the

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significance of thermo-physical properties is also noticeable in numerical modelling. For example, Kuti et al. [7] detected that the extended LPL of PME (palm methyl ester) as compared to that of diesel was caused by the higher boiling point of the biodiesel. Besides, Lee and Huh [8] also pointed out that the larger SMD (Sauter Mean Diameter) and slower mixing rate of SME are induced by the higher liquid viscosity and liquid surface tension of biodiesel as compared to those of diesel. These studies have thus proven the key role of thermo-physical properties in the development of spray.

As such, many studies have since been conducted to develop accurate thermo-physical properties for biodiesel [9–14]. For example, several key thermo-physical properties for SME such as critical properties, liquid density and latent heat of vaporisation were evaluated by Yuan et al. [9] using different correlations found in the literature. In their reported work, Yuan et al. [9] observed that the evaluated thermo-physical properties was influenced by the unsaturation levels of biodiesel although the evaluated properties were not validated. Besides, precise estimations of boiling points for the FAME (fatty acid methyl ester) components and biodiesel mixtures are also emphasized because the boiling point values are further adopted into the calculations of other thermo-physical properties [15].

Despite the increasing awareness of the need to formulate more precise thermo-physical properties, only a handful of works have been conducted to evaluate the effects of thermo-physical properties of biodiesel. Ra et al. [13] were one of the earliest groups who analysed the effects of thermo-physical properties of biodiesel. Based on their single drop and diesel engine simulations, they identified the importance of liquid density and vapour pressure on single drop vaporisation, retardation in injection timing, ID (ignition delay) period and in-cylinder peak pressure. Nevertheless, the possibility of coupled effects in diesel engine simulation was suggested by Ra et al. [13] because no distinct changes in combustion characteristics were observed when the individual thermo-physical property of SME was substituted. In another separate study by Mohamed Ismail et al. [14], an analysis on the sensitivities of thermo-physical properties specifically for PME was carried out based on the simulations of spray and diesel engine combustion. Mohamed Ismail et al. [14] concluded that liquid density, liquid surface tension, vapour diffusivity and vapour pressure were the most sensitive fuel properties. Besides, collective effects from all the thermo-physical properties were also identified because increased errors were detected in the predicted ID period and vaporised fuel mass when all the thermo-physical properties of PME were substituted by those of diesel. These works however did not focus on the sensitivities of the fuel spray development to the thermo-physical properties for biodiesel fuels which are derived from different feedstocks. Additionally, the analyses carried out by Ra et al. [13] and Mohamed Ismail et al. [14] did not consider the subsequent impacts on the soot development during quasi-steady period.

Based on these, this work aims to understand how do the thermo-physical properties affect the quasi-steady spray and soot while retaining similar numerical case settings and chemical kinetics throughout the analyses. Here, these issues are addressed by conducting sensitivity analyses under quasi-steady non-reacting spray and reacting spray conditions. The sensitivity analyses are performed with an open-source CFD (computational fluid dynamics) code, OpenFOAM (Open Field Operation and Manipulation) version 2.0.x for CME (coconut methyl ester) and SME, where both fuels represent low and high levels of unsaturation, respectively. The predicted spray and soot results for CME are compared against those of SME such that the significance of unsaturation levels can be identified. Besides, selected individual thermo-physical property is coupled together in order to determine the coupled effects among the thermo-physical properties for CME and SME, respectively. Furthermore, the influence of chemical kinetics on the effects of thermo-physical properties is also assessed by comparing the predictions between the non-reacting and reacting sprays. For all the sensitivity analyses, the baseline case is defined as the case where all the thermo-physical properties are specified. In the non-reacting sensitivity analyses for individual and coupled thermo-physical properties, the identification of significant fuel properties is based on the deviations found in the predictions of LPL, VPL (vapour penetration length), SMD, radial mixture fraction and fuel evaporation ratio when compared to those of baseline case. Meanwhile, the predicted LPL, ID period, LOL (lift-off length) and SVF (soot volume fraction) in the reacting spray are the parameters used to appraise the effects of individual thermo-physical property. Here, the analysis on coupled properties is excluded because the coupled effect can be combined from the effect of individual thermo-physical property, as identified from the non-reacting spray analysis.

## 2. Methodology of sensitivity analysis

### 2.1. Development of thermo-physical properties

Two types of biodiesel fuels namely, CME and SME were selected here because of their contrasting saturation and unsaturation levels, as shown in Table 1. The thermo-physical properties for CME and SME, which were plotted against a temperature range of 280 K up to the critical temperature of each fuel as shown in Fig. 1(a)–(l), were calculated based on the actual fuel compositions in Table 1. Similar methods of evaluation to those of Mohamed Ismail et al.'s work [14] as listed in Table 2 were employed here. Improvement was made to the evaluation of vapour diffusivity by taking into account of the binary interaction between fuel and air as proposed in the Lennard-Jones potential [16], instead of the binary interactions among FAME components considered by Mohamed Ismail et al. [14]. The newly evaluated vapour diffusivities for CME and SME in Fig. 1(h) correspond similarly to those published by Ra et al. [13], for which the vapour diffusivities of biodiesel are higher than those of diesel. On the other hand, the thermo-physical properties for diesel were calculated using the correlations of n-tetradecane ($C_{14}H_{30}$) obtained from the OpenFOAM fuel properties library. n-tetradecane was selected here to represent diesel because the thermo-physical properties of this component deviated by only 8% when compared to those of diesel, among the fuel range of cyclohexane ($C_6H_{12}$) to heneicosane ($C_{21}H_{44}$) examined by Lin and Tavlarides [17]. The calculated thermo-physical properties for CME, SME and diesel were then integrated as specific fuel libraries into OpenFOAM.

### 2.2. Experimental setup

The simulations of non-reacting and reacting sprays for SME were modelled based on the experiment carried out by Nerva et al.

**Table 1**
Compositions for CME and SME based on measured FAME mole fractions.

| FAMEs | Fuel types | |
|---|---|---|
| | CME wt. (%) | SME wt. (%) |
| Saturated | | |
| Methyl laurate ($C_{13}H_{26}O_2$) | 47.0 | – |
| Methyl myristate ($C_{15}H_{30}O_2$) | 19.0 | – |
| Methyl palmitate ($C_{17}H_{34}O_2$) | 10.0 | 8.0 |
| Methyl stearate ($C_{19}H_{38}O_2$) | 3.0 | 4.0 |
| Unsaturated | | |
| Methyl oleate ($C_{19}H_{36}O_2$) | 7.0 | 25.0 |
| Methyl linoleate ($C_{19}H_{34}O_2$) | 2.0 | 55.0 |
| Methyl linolenate ($C_{19}H_{32}O_2$) | – | 8.0 |