

Effects of Fuel Physical Properties on Diesel Engine Combustion using Diesel and Bio-diesel Fuels

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ABSTRACT

A computational study using multi-dimensional CFD modeling was performed to investigate the effects of physical properties on diesel engine combustion characteristics with bio-diesel fuels. Properties of typical bio-diesel fuels that were either calculated or measured are used in the study and the simulation results are compared with those of conventional diesel fuels. The sensitivity of the computational results to individual physical properties is also investigated, and the results provide information about the desirable characteristics of the blended fuels. The properties considered in the study include liquid density, vapor pressure, surface tension, liquid viscosity, liquid thermal conductivity, liquid specific heat, latent heat, vapor specific heat, vapor diffusion coefficient, vapor viscosity and vapor thermal conductivity. The results show significant effects of the fuel physical properties on ignition delay and burning rates at various engine operating conditions. It is seen that there is no single physical property that dominates differences of ignition delay between diesel and bio-diesel fuels. However, among the 11 properties considered in the study, the simulation results were found to be most sensitive to the liquid fuel density, vapor pressure and surface tension through their effects on the mixture preparation processes.

INTRODUCTION

Biodiesel fuel is seen as a promising alternative to conventional diesel for use in compression-ignition (CI) engines. As a plant-based fuel, it can be produced domestically, is a renewable energy source, and essentially has a closed carbon cycle over its lifetime [1]. In terms of emissions, it has been reported that biodiesel tends to reduce unburned hydrocarbons, carbon monoxide, and particulate matter compared to its petroleum counterpart, while the NO_x level is likely to increase with increasing biodiesel fraction in blended fuels [2, 3]. Although it has been suggested through experimental research [2-7] that the difference of combustion between biodiesel and regular diesel can be attributed to differences in both the physical properties

and the chemical oxidation mechanisms between the two fuels, biodiesel combustion is not as well understood as the combustion of regular diesel.

While the effects of the physical and chemical properties of the fuel on combustion can be investigated experimentally, a computational study is an effective approach for investigating parametric effects of physical properties on mixture preparation, ignition and combustion, and subsequent pollutant formation. In recent evolution of computational methods of diesel engine operation, more effort has been made in modeling the in-cylinder processes. As spray injection, which is a critical physical process in mixture preparation, affects the subsequent combustion process, the accuracy of physical models is of significant importance. The performance of physical models also strongly depends on the accurate estimation of physical and chemical properties of the fuel.

Following a review of the literature concerning the physical properties of alternative fuels, Chakravarthy et al. [8] compiled and presented a complete set of bio-diesel properties required for detailed engine simulations. Based on that research, in this paper, a study of the effects of physical property differences between biodiesel and diesel fuels on CI engine operation is presented. The sensitivity of computations of engine combustion to the individual properties is also investigated. In order to decouple the effect of differences in reaction chemistry between biodiesel and diesel, the simulations were performed by replacing the physical properties of diesel with those of biodiesel, while keeping the same reaction mechanism as that used for diesel engine simulations [9].

BIODIESEL PROPERTIES

The physical properties of mixtures of hydrocarbons and biodiesel can be determined by calculating the physical properties of each individual component, and then imposing mixing rules to derive the properties of the mixtures. This method is feasible for biodiesel, which consists of a relatively simple formulation of fatty acid

esters. Properties of biodiesel and their methods of estimation have been described by Chakravarthy et al. [8]. Table 1 lists various physical properties that are required for spray and combustion simulations and how these are commonly derived. In the present study, the same strategy as that used by Chakravarthy et al. was employed to obtain the necessary properties of biodiesel surrogate fuel. 11 physical properties (p1 to p11) were considered in the study of biodiesel engine operation and its sensitivity to physical properties.

The assumed composition of biodiesel for the calculation of physical properties, which is based on Gas-Chromatography analysis of Soy-biodiesel, is listed in Table 2.

Table 1. Methods of estimation of physical properties.

No.	Physical property	Method of analysis/references
p1	Liquid density	Orrick & Ebar Group contribution [10], Rackett equation [11], Araújo and Meireles [40]
p2	Vapor pressure	Pitzer method[10,11], Araújo and Meireles [40]
p3	Surface tension	Weighted average of individual surface tensions [10]
p4	Liquid viscosity	Group contribution method [10], empirical correlations [12], Logarithmic equation [13], weighted average of individual components [14]
p5	Liquid thermal conductivity	GC TCD experimental analysis [15], numerical analysis [16], empirical correlations [17]
p6	Heat of vaporization	Pitzer method[10,11], Araújo and Meireles [40]
p7	Vapor heat capacity	GC TCD experimental analysis [15], numerical analysis [16], empirical correlations [17]
p8	Vapor diffusivity	Chapman-Enskog kinetic theory (Skelland [18])
p9	Vapor viscosity	Correlation from Chung and coworkers [19,20]
p10	Vapor thermal conductivity	Correlation from Chung and coworkers [19,20]
p11	Liquid Heat capacity	Interpolation of Lagrange polynomials [21], group contribution [22]
p12	Critical properties	Group contribution [10], correlation based on 400 fuels [11]
p13	Mixing rules for critical properties of mixtures	Lee-Kesler equation [10], Lumped parameter continuous thermodynamics [23]

Table 2. Assumed composition of biodiesel.

component	amount [mol %]
Hexadecanoic acid, methyl ester	17.0
Octadecanoic acid, methyl ester	9.0
9-Octadecenoic acid, methyl ester	30.0
9,12-Octadecadienoic acid, methyl ester	44.0

THERMODYNAMIC PROPERTIES

The critical properties of biodiesel are needed for thermodynamic calculations. Although it is difficult to obtain critical properties of prototypical biodiesel experimentally because the compounds decompose at temperatures below the critical point, they were estimated using group additivity and empirical formulations taken from Yuan et al. [10] following Reid et al. [11]. Mixture properties were determined using Lee-Kesler mixing rules. An equation of state model was used as suggested by Araújo and Meireles [40]. In the present study, the molecular weight and critical temperature of the considered biodiesel-surrogate were set to 292 g/mole and 775 K, respectively.

The density of the biodiesel-surrogate was obtained from data predicted by the Rackett equation [11], which matches the available experimental value, $\rho_{ref} = 0.8976 \text{ g/cm}^3$, at T_{ref} of 273.15K [24]. The densities are plotted in Fig. 1. Liquid density variation is considered in the present spray models, as well as in the mass and momentum balance equations in the gas and liquid phase interactions. Note that, the density of the diesel-surrogate is somewhat underestimated since diesel is represented by $C_{14}H_{30}$ in this study.

The vapor pressure of the biodiesel-surrogate was computed using a Peng-Robinson equation of state (PR-EOS) based on lumped parameter critical properties, which closely matches the literature formulation [25]. Figure 2 shows the vapor pressure variation of the two fuels as a function of liquid temperature. Compared to that of the diesel-surrogate, the vapor pressure of the biodiesel-surrogate is much lower, which is expected to influence the spray evaporation process significantly.

The heat of vaporization of the biodiesel-surrogate was also calculated up to the critical point, and is plotted along with that of the diesel-surrogate in Fig. 3. Compared to the diesel-surrogate, the heat of vaporization of the biodiesel-surrogate is lower at low temperatures, while it becomes higher at high temperatures. Since spray droplets are heated up quickly during the vaporization process in the combustion chamber, it is expected that the evaporation of the biodiesel-surrogate will be more affected by the high temperature characteristics of the heat of vaporization.

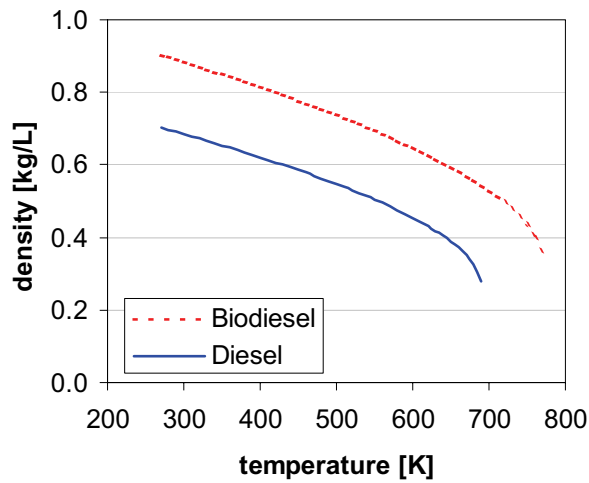


Figure 2. Liquid density profiles for biodiesel and diesel surrogate fuels. The density of biodiesel-surrogate was calculated as in Ref. [8].

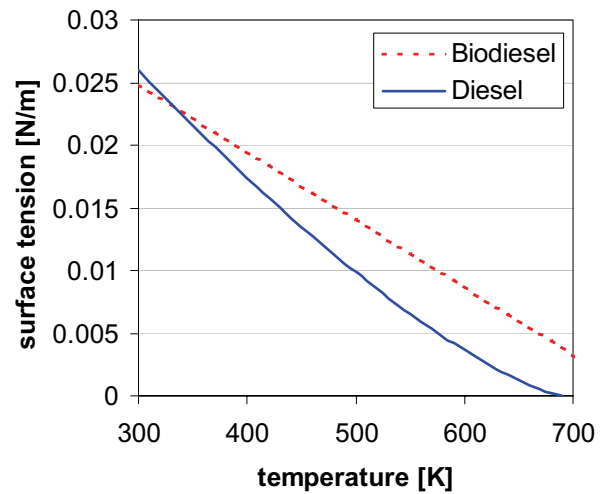


Figure 4. Surface tension profiles of biodiesel and diesel surrogate fuels.

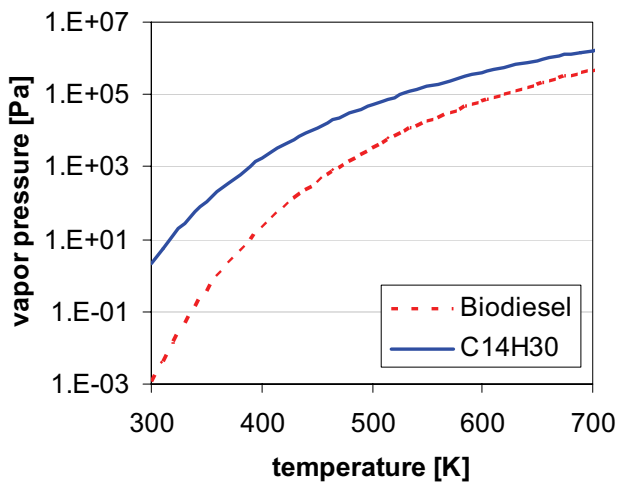


Figure 2. Vapor pressure profiles for biodiesel and diesel surrogate fuels.

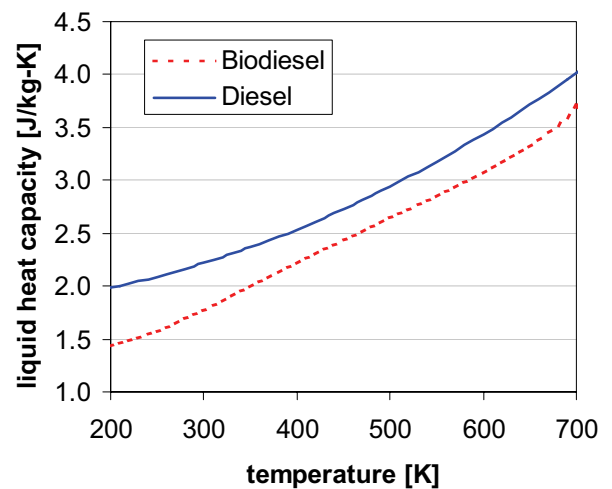


Figure 5. Profiles of liquid heat capacity for biodiesel and diesel surrogate fuels.

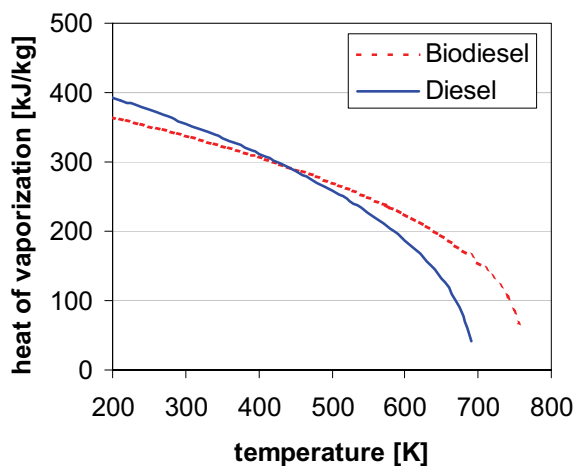


Figure 3. Profiles of heat of vaporization for biodiesel and diesel surrogate fuels.

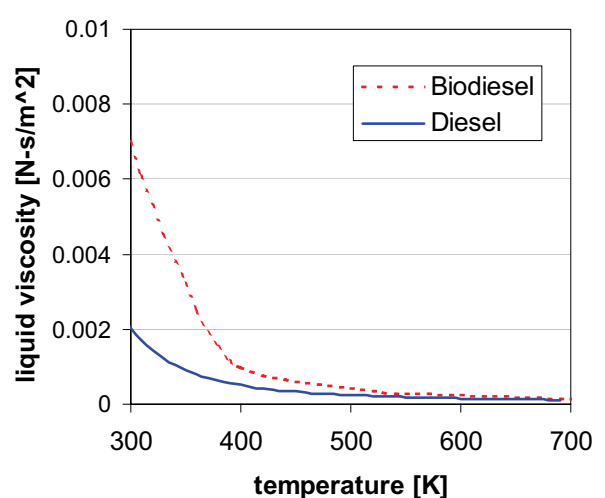


Figure 6. Profiles of liquid viscosity for biodiesel and diesel surrogate fuels.

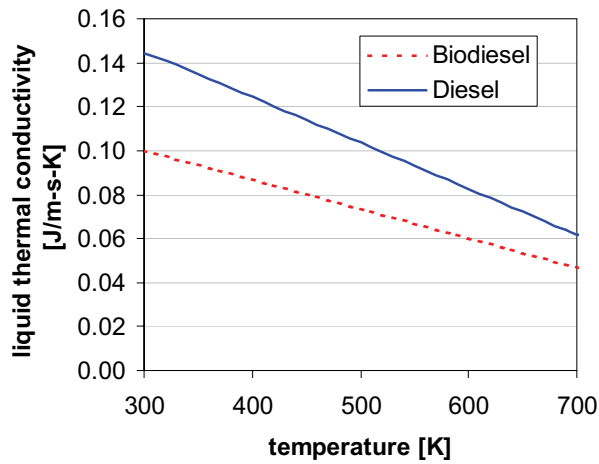


Figure 7. Profiles of liquid thermal conductivity for biodiesel and diesel surrogate fuels.

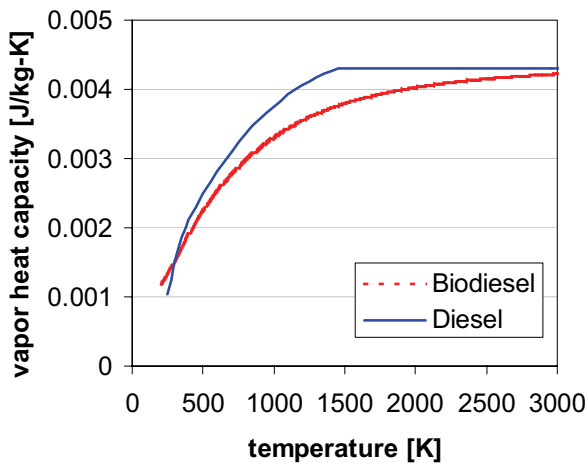


Figure 8. Profiles of vapor heat capacity for biodiesel and diesel surrogate fuels.

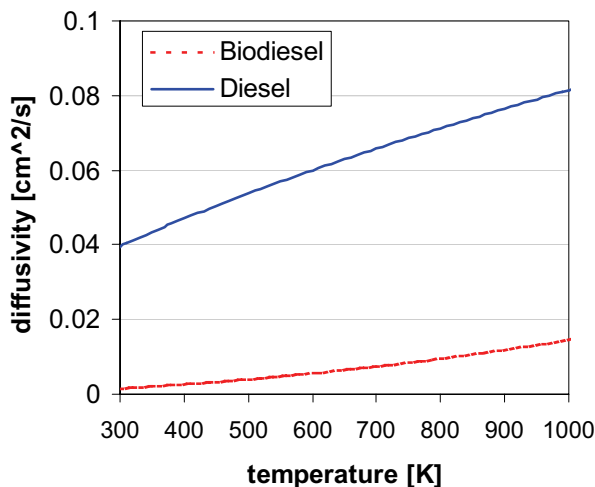


Figure 9. Profiles of diffusivity in air for biodiesel and diesel surrogate fuels at ambient pressure.

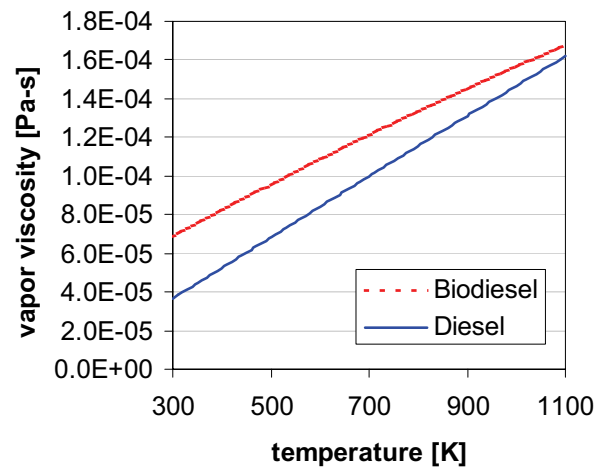


Figure 10. Profiles of vapor viscosity for biodiesel and diesel surrogate fuels.

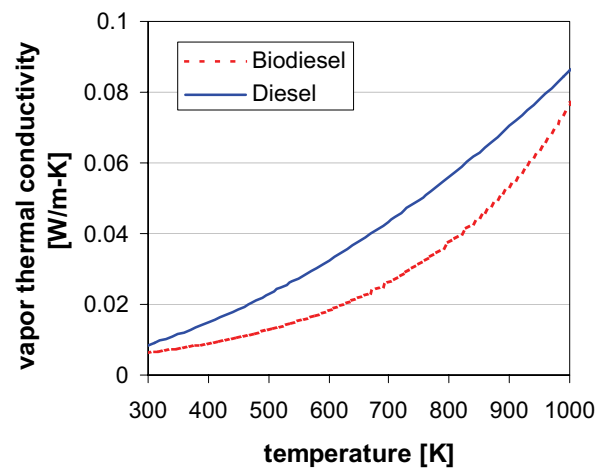


Figure 11. Profiles of vapor thermal conductivity for biodiesel and diesel surrogate fuels.

Surface tension is one of the key properties considered in spray breakup and collision/coalescence models. Empirical correlations were used to obtain surface tension of the biodiesel-surrogate. The surface tension is a linear function of temperature, with little change with the weighting factors of the different methyl esters. The surface tension of the biodiesel-surrogate is about the same as that for the diesel-surrogate at room temperature, but it decreases slower with temperature. In Fig. 4, the biodiesel-surrogate surface tension is compared with that of the diesel-surrogate as a function of temperature.

The heat capacity for methyl esters can be correlated as a function of the number of carbon atoms in the parent carboxylic acid moiety [26]. Compared to diesel, biodiesel's heat capacity per unit mole is nearly 50% higher at temperatures near boiling point. However, when it is compared per unit mass, as used in the energy equation, the heat capacity of the biodiesel-surrogate is lower than that of the diesel surrogate. This

implies that the biodiesel-surrogate droplets may be heated faster than the diesel-surrogate droplets. The liquid heat capacities of the two fuels are compared in Fig. 5.

Liquid viscosity is considered in modeling drop internal flow, drop breakup and wall film motion. The liquid viscosity of the biodiesel-surrogate is higher than that of the diesel-surrogate, especially at low temperatures where most of the breakup processes take place in the cylinder. Therefore, it is expected that the breakup process is most affected by the viscosity difference. Comparison of the viscosities of the two fuels is shown in Fig. 6.

Liquid thermal conductivity is used in the present drop interior model to calculate the heat transfer between the drop interior and the surface where a transient temperature distribution is assumed. The thermal conductivity of the biodiesel-surrogate is slightly lower than that of the diesel-surrogate, as shown in Fig. 7.

The vapor heat capacity of the fuel is important in calculating the internal energy and temperature distribution of gas mixtures surrounding the spray drops, which substantially affects the transient heat transfer from the surrounding gas mixture to the drop surface. This is especially true where the fuel drops vaporize rapidly so that the fuel/air mixtures become rich. The vapor heat capacity of biodiesel was surrogated with that for Methyl Oleate, which is available in the literature [27]. Its vapor heat capacity is slightly lower than that of the diesel-surrogate over the temperature range of interest, as shown in Fig. 8.

TRANSPORT PROPERTIES

The transport properties of the vapor phase, i.e., diffusivity, viscosity, and thermal conductivity, were estimated for the soy biodiesel mixture at a number of elevated temperatures and pressures, including above the critical point [8].

The diffusivity for biodiesel vapor is much lower than that for diesel. Note that, in the present study, the pressure dependency of vapor diffusivity is taken into account through the density variation in the mass diffusivity. The viscosity of biodiesel vapor is slightly higher than that of diesel while its thermal conductivity is lower than that of diesel. Viscosity and thermal conductivity show little dependency on pressure, thus only the temperature dependency was considered in the present study. Figures 9 to 11 show comparisons of the diffusivity, viscosity and thermal conductivity of the two surrogate fuels, respectively.

SENSITIVITY TO PHYSICAL PROPERTIES

As mentioned above, 11 physical properties were considered to study the sensitivity of numerical simulations of engine operation to the individual physical properties of the biodiesel-surrogate. In order to

estimate the sensitivity to each property, only one property was varied from the value of the base fuel to that of the other fuel while all other properties were fixed at those of the base fuel. Two ways of sensitivity checking were considered; one considered the diesel-surrogate as the reference and the properties were changed individually from the diesel-surrogate (base) to the biodiesel-surrogate and the other is from the biodiesel-surrogate (base fuel) to the diesel-surrogate.

The energy conservation equation between the liquid and vapor phases in the evaporation process is given as

$$e_{liq} = e_{vap} + RT/W - P_v/\rho_l - h_{vap}$$

where e_{liq} is the liquid internal energy, e_{vap} is the vapor internal energy, R is the gas constant, T is the temperature, W is the molecular weight, P_v is the vapor pressure at temperature T , ρ_l is the liquid density, and h_{vap} is the heat of vaporization.

However, it should be noted that the vapor heat capacity (involved through the vapor internal energy), heat of vaporization, vapor pressure and liquid heat capacity (involved through the liquid internal energy) are also coupled through the Clausius-Clapeyron equation, i.e.,

$$\left(\frac{dP_{vap}}{dT} \right)_{sat} = \frac{h_{vap}}{T(1/\rho_g - 1/\rho_l)}$$

When any one of the properties considered in the Clausius-Clapeyron equation is changed, the equality of the energy equation is inevitably violated. Therefore, adjustment must be made to one of the other properties to maintain equality of the equation, as listed in Table 3.

Table 3. Properties adjusted with sensitivity variable.

Sensitivity property	Adjusted property
Liquid heat capacity	Heat of vaporization
Vapor heat capacity	Heat of vaporization
Heat of vaporization	Liquid heat capacity
Vapor pressure	Liquid heat capacity

PHYSICAL SUB-MODELS

For simulating the spray processes and the mixing and combustion of fuel/air mixtures in the cylinder, various physical sub-models were employed in the KIVA-ERC-CHEMKIN code which is based on KIVA3V Release 2 [28] coupled with the CHEMKIN II library [29]. The sub models include ones related drop breakup, collision and coalescence, drop deformation, drop evaporation, wall impingement and vaporization, etc.

A hybrid primary break-up model [30] that is computationally effective as well as comprehensive enough to account for the effects of aerodynamic and properties and nozzle flow was employed. In this