Improvements to a Biodiesel-fueled Engine Model using Realistic Chemistry and Physical Properties

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Abstract
Biodiesel-fueled engine simulations were performed using an updated version of the KIVA3v-Release 2 code coupled with Chemkin-II for detailed chemistry. A discrete multi-component approach was applied to account for the five common components of soy-based biodiesel fuel. Each of the biodiesel components was represented by accurate physical and thermodynamic properties. Biodiesel chemistry was represented by a mechanism that was previously reduced from a detailed methyl decanoate/methyl-9-decenoate mechanism developed at the Lawrence Livermore National Laboratory. A mixture of methyl decanoate and methyl-9-decenoate was used as the biodiesel chemistry surrogate to account for both the saturated and unsaturated components found in real biodiesel fuels. Non-reacting biodiesel spray experiments were reproduced using the KIVA model, and the KH-RT spray break-up model constants were adjusted to improve the liquid penetration trend under varying density and temperature conditions. The complete biodiesel engine model was shown to adequately reproduce the pressure and heat release rate predictions of diesel engine combustion experiments fueled with a soy methyl ester biodiesel. These results show that the model gives accurate predictions of biofuel spray vaporization and combustion for these conditions. The current biodiesel model was also compared to a previous model and found to improve the magnitude of the NOx emissions predictions, as well as capture the trend of decreasing NOx with increasing load.

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Introduction

An increased interest in biodiesel combustion in the past decade highlights the need for engine models that can accurately predict effects due to varying fuel characteristics. Such models offer the promise of reducing or even eliminating much of the time and expense associated with engine testing in the laboratory over a wide range of operating conditions.

An accurate engine model requires that both the combustion chemistry and the physical processes (spray break-up, atomization, vaporization, etc.) are well represented. These two aspects of the model depend on the fuel’s composition. Biodiesel is made from the transesterification of fatty acids with an alcohol [1]. In the United States, soy is the most common feedstock, which is processed with methanol, resulting in a biodiesel fuel that is mainly composed of five methyl esters: methyl palmitate $(\text{C}_{16}\text{H}_{34}\text{O}_{2})$, methyl stearate $(\text{C}_{17}\text{H}_{36}\text{O}_{2})$, methyl oleate $(\text{C}_{18}\text{H}_{36}\text{O}_{2})$, methyl linoleate $(\text{C}_{18}\text{H}_{32}\text{O}_{2})$, and methyl linolenate $(\text{C}_{18}\text{H}_{30}\text{O}_{3})$. As seen in Figure 1, methyl palmitate and methyl stearate are saturated, while methyl oleate, methyl linoleate, and methyl linolenate contain one, two, and three double-bonds, respectively. A common short-hand notation for these methyl esters is simply $\text{C}_{x}y$, where ‘$x$’ represents the number of carbon atoms in the alkyl chain and ‘$y$’ represents the number of carbon-carbon double-bonds (e.g., C16:0 for methyl palmitate).

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure1}
\caption{Five common components of biodiesel: (a) methyl palmitate, (b) methyl stearate, (c) methyl oleate, (d) methyl linoleate, and (e) methyl linolenate.}
\end{figure}

Previous biodiesel [2, 3] models focused on single-component fuels, coupling a single species with representative physical properties (i.e., methyl oleate) to the kinetic reaction mechanism of a representative chemistry surrogate. As computer capabilities improve, it becomes possible to include a more realistic representation of the fuel, both in terms of physical properties and chemistry. This paper provides an overview of the multi-component engine model implemented in KIVA3v-Release 2 and highlights improvements to both the physical properties and fuel chemistry for biodiesel combustion. Property information was obtained for each of the five main components of soy biodiesel and added to the KIVA fuel library. Kinetic reaction mechanisms for the biodiesel fuel surrogates methyl decanoate and methyl-9-decenoate were used to represent the fuel chemistry of the saturated and unsaturated components, respectively.

Simulation Model

Engine simulations were conducted using KIVA3v-Release 2 coupled with the Chemkin II library for chemistry [4-7]. The IVC temperature, pressure and species concentrations are supplied to the chemistry model, which considers each cell as a well-stirred reactor. In subsequent time-steps, species concentrations and thermodynamic conditions are passed to the chemistry solver and the rate of change of each species is calculated based on the mass fraction, density, production rate and molecular mass of each species. Turbulence was accounted for using the RNG $\kappa$-$\varepsilon$ model. However, turbulence-chemistry interactions were not considered in this work. Previous researchers [8-10] have found that energy release is dominated by chemistry effects and not by sub-grid-scale turbulent transport. NOx formation was modeled with the addition of four species and 12 reactions to the mechanism [11, 12] and soot was not considered in this work.

An improved spray model that uses gas-jet theory was applied to reduce grid dependencies, and improve both the relative velocity of the droplets and gas, and the entrainment rate [13]. Spray break-up was modeled using the hybrid Kelvin-Helmholtz (KH)/Rayleigh-Taylor (RT) spray model [14]. The KH model predicts the primary break-up stage by evaluating the break-up time, $\tau_{\text{KH}}$, using Equation 1, in which $B_1$ is an adjustable constant, and $\Omega_{\text{KH}}$ and $\Lambda_{\text{KH}}$ are the calculated frequency and wavelength of the fastest growing wave, respectively (in KIVA, $B_1$ is termed “cnst22” and given a value 40). As seen in the equation, a larger $B_1$ results in a longer break-up time and larger droplets.

\begin{equation}
\tau_{\text{KH}} = \frac{3.726B_1 r}{\Omega_{\text{KH}} \Lambda_{\text{KH}}} \tag{1}
\end{equation}

The radius of a child droplet in the KH model is calculated using Equation 2, where $B_0$ is an adjustable constant (in the KIVA model, $B_0$ is termed “balpha” and is assigned a value of 0.6).

\begin{equation}
r_c = B_0 \Lambda_{\text{KH}} \tag{2}
\end{equation}

A break-up length, $L_b$, is calculated using Equation 3,

\begin{equation}
L_b = C_b d_0 \sqrt{\frac{\rho_f}{\rho_a}} \tag{3}
\end{equation}
where $\rho_f$ and $\rho_a$ are the fluid and air densities, respectively, and $d_0$ is the parent droplet diameter. $C_{\text{RT}}$ (known as “distant” in KIVA) is an adjustable constant with a value of 1.9. Beyond this break-up length, the RT model is utilized in modeling secondary break-up of the individual drops.

When the wavelength of the fastest growing wave on a given droplet is smaller than the droplet diameter, RT waves grow on the droplet surface. When the waves grow for a time greater than the break-up time, the droplet breaks up into child droplets. The radius of each child droplet is given in Equation 4, where $C_{\text{RT}}$ is an adjustable constant (“cnst3rt” in KIVA with a value of 0.10) and $K_{\text{RT}}$ is the calculated wave number. In general, a smaller $C_{\text{RT}}$ value will produce smaller child droplets.

$$r_c = \frac{\pi C_{\text{RT}}}{K_{\text{RT}}}$$

Ra and Reitz [15, 16] expanded the KIVA3v-Release 2 package to include discrete multi-component (DMC) fuel considerations. Unlike a single-component model, the DMC code allows preferential evaporation based on the specific properties of each component. In addition, these individual components can be coupled with representative species in the reaction mechanism to account for component-specific chemistry. Properties of interest for the DMC model are listed in Table 1.

**Properties for DMC Model**

<table>
<thead>
<tr>
<th>Property</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Molecular mass</td>
<td>[6]</td>
</tr>
<tr>
<td>Liquid density</td>
<td>[17]</td>
</tr>
<tr>
<td>Heat of formation</td>
<td>[17][18]*</td>
</tr>
<tr>
<td>Critical temperature</td>
<td>[17][18]*</td>
</tr>
<tr>
<td>Latent heat of vaporization</td>
<td>[19][20]*</td>
</tr>
<tr>
<td>Vapor pressure</td>
<td>[19][20]*</td>
</tr>
<tr>
<td>Liquid specific heat</td>
<td>[19][20]*</td>
</tr>
<tr>
<td>Surface tension</td>
<td>[19][20]*</td>
</tr>
<tr>
<td>Liquid viscosity</td>
<td>[19][20]*</td>
</tr>
<tr>
<td>Vapor thermal conductivity</td>
<td>[19]</td>
</tr>
<tr>
<td>Liquid thermal conductivity</td>
<td>[19]</td>
</tr>
<tr>
<td>Vapor diffusivity</td>
<td>[19]</td>
</tr>
</tbody>
</table>

* methyl linoleate and methyl linolenate only

**Table 1.** Physical properties required by the KIVA-DMC model

The spray and engine simulations were run on a computer cluster that consists of an array of Intel® Pentium™4 and Core™2 processors. The spray simulations finished in about 1 hour on a single processor. The engine simulations were run in parallel and took about 40 hours on two processors (about 80 CPU hours total).

**Fuel Chemistry**

In order to adequately represent the combustion chemistry of biodiesel fuel, an accurate chemical kinetic mechanism must be available. Previous work used a combination of methyl butanoate ($\text{C}_4\text{H}_{10}\text{O}_2$) and n-heptane ($\text{C}_7\text{H}_{16}$) to represent biodiesel chemistry with some success [2, 3]. More recently, researchers at the Lawrence Livermore National Laboratory (LLNL) have proposed methyl decanoate ($\text{C}_{11}\text{H}_{22}\text{O}_2$) as a biodiesel fuel surrogate, arguing that its longer carbon chain provides a better prediction of the ignition and species history [21]. Since biodiesel is typically composed of several unsaturated methyl esters, the methyl decanoate mechanism was expanded to include methyl-9-decanoate ($\text{C}_{11}\text{H}_{22}\text{O}_2$), which has a double-bond at the ninth position on the carbon chain [22].

In the current study, fuel chemistry for the two saturated biodiesel species was represented by the saturated chemistry surrogate, methyl decanoate (MD), and the unsaturated species were represented by methyl-9-decanoate (MD9D). As a result of their long carbon chains, the detailed MD/MD9D mechanism from LLNL contains 3299 species and 10806 reactions, which is too large to be directly applied in engine computational fluid dynamics (CFD) models.

The theory of directed relation graph (DRG) is a widely-used reduction technique that was first proposed by Lu and Law [23] to identify unimportant species by considering how they are coupled to other species in the mechanism. The method was later improved by considering error-propagation (DRGEP) in the work of PerpIot-Desjardins and Pitsch [24].

Shi, et al. [26] developed a model that uses the DRGEP method to reduce mechanisms and test the results in a single-zone HCCI engine simulation using the Senkin library [27]. Performance parameters (CA50, peak pressure and peak heat release) of the reduced mechanism are compared to those of the detailed mechanism and the reduction process is automatically repeated until the performance parameter errors between the two mechanisms exceed a specified tolerance.

In a recent study [25], the automatic reduction code of Shi, et al. [26] was modified to include a constant volume reactor model and used, along with chemical lumping of isomers, to reduce the detailed MD/MD9D mechanism. The reduced MD/MD9D mechanism was combined with a multi-chemistry mechanism that contains oxidation reactions for a variety of fuel species [16]. This was done anticipating that the present reduced biofuel mechanisms will be used to model biodiesel fuel blends in the future. Limited reaction rate tuning was required to account for pathways removed in the reduction. The resulting model contained 77 species and 216 reactions, including those for n-heptane oxidation and NOx formation. The mechanism was
validated against the ignition delay times of the detailed mechanism for a pressure of 60 bar, equivalence ratios of 0.5, 1.0, and 2.0, and temperatures from 700 K to 1300 K. Figure 2 shows the final ignition delay results for the stoichiometric cases. Additional details of the reduction strategy and code can be found in Ref. [25].

**Figure 2.** Ignition delay time predicted for (a) methyl decanoate and (b) methyl-9-methyl decanoate fueling under stoichiometric conditions. Reduction and analysis performed in Ref. [25].

**Physical Properties**

The current KIVA code uses a discrete multicomponent approach to modeling the physical properties of the fuel components. Molecular mass was supplied by Chemkin based on the chemical structure of each species. Liquid density and heat of formation for each component were found in the Knovel Critical Tables online database [17]. Critical temperature and the remaining temperature-dependent property values for methyl palmitate, methyl stearate, and methyl oleate were found in the database maintained by the Design Institute for Physical Property Research (DIPPR) [19]. However, much of the data for methyl linoleate and methyl linolenate were unavailable. Critical temperature values were found from Ref. [18] and the BDProp program developed at the University of Illinois at Urbana-Champaign [20] was used to calculate vapor pressure, density, heat of vaporization, and viscosity for these two fuels. This program estimates biodiesel fuel properties based on its methyl ester composition. For the present study, the composition was set to 100% for the component of interest. Until more information becomes available, the thermal conductivity, specific heat, and diffusivity of methyl oleate were used for methyl linoleate and methyl linolenate. However, it was anticipated that the oleate properties are adequate to represent those of the missing data.

In addition to the physical properties, it is also important to provide accurate thermodynamic data for each component to ensure proper estimates of enthalpy, entropy and specific heat. This data has been conveniently tabulated in NASA format for use in models such as Chemkin [28]. The enthalpy was used to calculate the lower heating value (LHV) of the fuel surrogate using the composition reported in Ref. [29]. The paper reported a value of 37.4 MJ/kg and the model predicted a similar value of 37.7 MJ/kg.

Most of the physical properties of the five components were similar in comparison to each other. However, some of the key properties of the biodiesel components are drastically different from those of diesel. Figure 3 compares the vapor pressure, viscosity, and density of methyl oleate and tetradecane (C\textsubscript{14}H\textsubscript{30}), a component commonly used to represent single-component diesel fuel properties. It is seen that biodiesel’s vapor pressure is much lower, which can lead to poor evaporation. Also, viscosity is much higher. This, coupled with the high density of the fuel components, is expected to produce long liquid spray tip penetrations and potentially a significant amount of wall wetting in engine cases.
Fuel Distillation

A single droplet model [30] was used to create the distillation curve seen in Figure 4. The boiling point temperatures of the five biodiesel fuel components are shown as dashed lines with their respective molar contribution to the overall fuel composition. It should be noted that the boiling temperatures of the most significant components are within 25 K, which results in a nearly horizontal curve. The simulation results are shown compared to three commercial soy biodiesel fuels from Ref. [31]. The specific composition of the commercial biodiesel fuels was not reported and the slight discrepancy between the model and literature is attributed to high molecular mass hydrocarbon species (i.e., higher boiling points) that may be present in the real fuel. Currently the biodiesel model only considers the five methyl esters mentioned previously. Additional species may be included in the fuel surrogate in future studies.

Spray Simulations

The next step in the model development was to assess the spray characteristics of the fuel. Higgins et al. [32] studied the effect of physical properties on the liquid-phase penetration of several fuels. Liquid length was measured and a correlation was developed for each fuel. The experimental apparatus was the constant volume spray chamber at Sandia National Laboratories that is described in Ref. [33]. Biodiesel fuel was tested at four density (7.3, 14.8, 30.0, and 45.0 kg/m$^3$), and four temperature (800, 900, 1000, 1100 K) conditions that are representative of conditions seen in diesel engine operation. These were non-reacting experiments with an inert gas mixture of 89.7% N$_2$, 6.5% CO$_2$, and 3.8% H$_2$O present in the cylinder prior to fuel injection.

Figure 3. Comparison of physical properties, (a) vapor pressure, (b) liquid viscosity, and (c) liquid density, for tetradecane (a common diesel surrogate) and the five biodiesel components.
The injector orifice diameter, discharge coefficient, and the injection duration were given as 246 µm, 0.78, and 5.0 ms, respectively. The fuel distribution for their correlation was assumed to be: 12% C16:0, 5% C18:0, 25% C18:1, 52% C18:2, and 6% C18:3 (by mass).

The sprays were assumed to be axisymmetric, and the constant volume spray chamber was reproduced for the simulations using a 2-D sector representing half of the spray chamber. Two grids were tested. The first consisted of about 14000 cells that gradually increase in size from 0.67 mm at the injector to 1.5 mm at the edges. The second grid consisted of about 5000 cells of about 2 mm in size. Figure 5 compares the liquid penetration prediction for the two grids [13, 34]. It can be seen that the gasjet model predicts liquid lengths that are nearly independent of grid size. Hence, the gasjet model was used throughout the study and a coarse grid was chosen for computational efficiency.

Assuming an ideal gas, the known density and gas temperature were used to calculate the initial pressure for the constant volume simulations. The injector characteristics and duration were used with the fuel density to determine the mass of fuel injected. The initial biodiesel spray simulations used the KH-RT spray constants originally applied in diesel spray cases. It was found that the original spray constants under-predicted liquid length and did not capture the appropriate trend with varying temperature and density. A trial and error method was used to find a combination of spray constant values that gave the most improvement to the liquid penetration predictions over the range of temperatures and densities. Figure 6 compares the liquid length of the experiments to those predicted using the original (dashed lines) and improved (solid lines) spray constants.

Table 3 shows the original and improved spray constant values. The primary break-up stage was found to be the most influential for biodiesel. The increased cnst22 increases the break-up time in the KH model, which results in less disturbance in the liquid droplets in the primary break-up stage (see Equation 1). Once a child droplet is formed, the radius is smaller due to the decreased balpha value (Equation 2). Increasing the distant constant increases the break-up length (Equation 3), which causes the fuel to remain in the KH regime longer. The secondary breakup constant, cnst3rt, had an inconsistent effect on the liquid length and the original value was maintained (Equation 4).
Table 2. Comparison of original and improved KH-RT spray constants for biodiesel fuel

<table>
<thead>
<tr>
<th>KH-RT Name</th>
<th>KIVA Name</th>
<th>Original Values</th>
<th>Improved Values</th>
</tr>
</thead>
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<tr>
<td>$B_0$ (eqn 2)</td>
<td>balpha</td>
<td>0.6</td>
<td>0.3</td>
</tr>
<tr>
<td>$B_1$ (eqn 1)</td>
<td>cst22</td>
<td>40</td>
<td>80</td>
</tr>
<tr>
<td>$C_{RT}$ (eqn 4)</td>
<td>cst3rt</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>$C_0$ (eqn 3)</td>
<td>distant</td>
<td>1.9</td>
<td>2.2</td>
</tr>
</tbody>
</table>

Table 2. Comparison of original and improved KH-RT spray constants for biodiesel fuel

Engine Simulations

Finally the biodiesel model was applied to engine simulations and compared to experimental data. The experiment chosen for this work [29] was the same used to validate previous biodiesel combustion models [2, 3]. The experiments were performed on the Sandia compression-ignition optical research engine (SCORE) operating under a conventional diesel combustion strategy, with injection near top dead center (TDC) and zero exhaust gas recirculation (EGR). Four low-speed, high-load conditions were tested. The grid used in the simulation contained about 13200 cells that were 3 mm in the radial direction. Table 3 shows the operating conditions and relevant engine parameters. An injection rate profile from Ref. [35] was used to estimate profiles for the given injection durations.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Engine type</td>
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</tr>
<tr>
<td>Bore x stroke</td>
<td>125mm x 140 mm</td>
</tr>
<tr>
<td>IVC</td>
<td>-153° aTDC</td>
</tr>
<tr>
<td>EVO</td>
<td>116° aTDC</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>225 mm</td>
</tr>
<tr>
<td>Piston bowl diameter</td>
<td>90 mm</td>
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<tr>
<td>Piston bowl depth</td>
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</tr>
<tr>
<td>Swirl ratio</td>
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</tr>
<tr>
<td>Displacement</td>
<td>1.72 L</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>11.3 : 1</td>
</tr>
<tr>
<td>Engine speed</td>
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</tr>
<tr>
<td>Time of injection</td>
<td>-1.1° aTDC</td>
</tr>
<tr>
<td>Intake air pressure</td>
<td>2.3 bar</td>
</tr>
<tr>
<td>Engine loads</td>
<td>10-16 bar gIMEP</td>
</tr>
<tr>
<td>EGR</td>
<td>None</td>
</tr>
</tbody>
</table>

Table 3. Experimental operating conditions and engine parameters [29]

Pressure and heat release rate we compared to the experiments for the four load conditions and the profiles can be found in the Appendix. The simulation and experiment were well matched for all the cases, which indicates a good representation of biodiesel spray and combustion for these conditions.

NOx was also measured at each load condition. Here, NOx is the combination of the NO and NO$_2$ species. Figure 7 compares the experimental NOx measurement and the NOx predicted by two KIVA models. The triangles represent the previous single-component biodiesel model [2], which used a mixture of methyl butanoate and n-heptane to represent the fuel chemistry. The circles represent the current multi-component model described in this work. The current model improves the magnitude of the NOx prediction and more effectively captures the trend of decreasing NOx with increased load.

Figure 7. NOx (as NO+NO$_2$) comparison between the experiment, the previous KIVA biodiesel model (triangles) [2], and the current KIVA biodiesel model (circles)

In order to gain a better understanding of the NOx trend observed with increasing load, the temperature and NOx histories were investigated using the current model. Figure 8 shows that the average in-cylinder temperature was highest for the highest load condition, and the peak temperatures remained high as a result of the high fueling and long fuel injection duration adding energy later in the cycle. One would expect the higher temperatures to lead to higher NOx. However, NOx is lowest for that condition due to the late end-of-injection timing and its effect on the local oxygen concentrations, as described next.
Figure 8. Temperature and NOx histories for each load in the KIVA simulation

In-cylinder images were generated to compare the NOx and oxygen mole fractions for each of the conditions. Figure 9 shows that at 10° aTDC the oxygen and NOx distributions look very similar for each load condition.

Figure 9. In-cylinder (a) oxygen and (b) NOx distributions for each load condition at 10° aTDC

Figure 10 shows that near 20° aTDC, the low load condition finishes injecting and the energy release and NOx predictions of the four load cases begin to diverge. Injections for the higher load conditions continue, and the fuel oxidation releases more energy and decreases the amount of oxygen available for NOx formation.

Figure 10. Comparison of (a) accumulated heat release and (b) oxygen mass for each load condition

By 30° aTDC, the oxygen and NOx distributions for each load are distinctly different. In Figure 11, it can be seen that the areas of low oxygen correspond to the region of the spray where fuel oxidation occurs. NOx formation also occurs in this region due to the high temperatures. These images confirm that in the later crank angles, the higher load cases have less oxygen available in this region and therefore, lower NOx.

Figure 11. Comparison of NOx and oxygen mole fraction for each load condition at (a) 10° and (b) 30° aTDC
Figure 11. In-cylinder (a) oxygen and (b) NOx distributions for each load condition at 30° aTDC

The improved NOx trend observed with the current KIVA biodiesel model indicates that it provides a more realistic distribution of in-cylinder O\textsubscript{2} for each load condition. This improvement is likely the combined result of more realistic spray and vaporization, as well as more representative fuel chemistry. This model will play an important role in future work, which will investigate the role of fuel properties and chemistry in the formation of emissions in varying operating conditions and combustion strategies.

Conclusions

A practical biodiesel fuel model was created from detailed chemical kinetic and realistic physical property data. A reduced reaction mechanism for methyl decanoate and methyl-9-decenoate oxidation was applied, using methyl decanoate as the chemistry surrogate for the saturated biodiesel species, and methyl-9-decenoate to represent the unsaturated species. Physical properties for the five main components of soy biodiesel were added to the KIVA multi-component model to simulate realistic vaporization of the fuel species.

Liquid spray penetration predictions of the model were compared to constant volume spray experiments, and improvements were made to the KH-RT spray constants for use with biodiesel fuel. The improved spray constants were applied in biodiesel-fueled engine simulations using the KIVA3v-Release 2 code and compared to low speed, high load engine experiments. Ignition, pressure, and heat release rate were well predicted. NOx was slightly over-predicted, but the trend of increased NOx with decreased load was well captured. The simulations show that the in-cylinder NOx levels are correlated with the available O\textsubscript{2} levels, and the availability of O\textsubscript{2} decreases as the load is increased, leading to decreased NOx. The present results suggest that the biodiesel model developed in this work provides an adequate representation of biodiesel combustion under the conditions tested and improves the NOx predictions compared to the previous KIVA biodiesel model. Future simulations will assess the model under varying operating conditions and combustion regimes.

Acknowledgement

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References


Appendix

Figure A1. Pressure and heat release rate validation for the 10 bar IMEP load case

Figure A2. Pressure and heat release rate validation for the 12 bar IMEP load case

Figure A3. Pressure and heat release rate validation for the 14 bar IMEP load case

Figure A4. Pressure and heat release rate validation for the 16 bar IMEP load case