COMPUTATIONAL OPTIMIZATION OF BIODIESEL COMBUSTION USING RESPONSE SURFACE METHODOLOGY

by

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Original scientific paper
DOI: 10.2298/TSCI161229031G

The present work focuses on optimization of biodiesel combustion phenomena through parametric approach using response surface methodology. Physical properties of biodiesel play a vital role for accurate simulations of the fuel spray, atomization, combustion, and emission formation processes. Typically methyl based biodiesel consists of five main types of esters: methyl palmitate, methyl oleate, methyl stearate, methyl linoleate, and methyl linolenate in its composition. Based on the amount of methyl esters present the properties of pongamia biodiesel and its blends were estimated. CONVERGE™ computational fluid dynamics software was used to simulate the fuel spray, turbulence and combustion phenomena. The simulation responses such as indicated specific fuel consumption, NOx, and soot were analyzed using design of experiments. Regression equations were developed for each of these responses. The optimum parameters were found out to be compression ratio – 16.75, start of injection – 21.9° before top dead center, and exhaust gas re-circulation – 10.94%. Results have been compared with baseline case.

Key words: CONVERGE™, optimization, response surface methodology, pongamia biodiesel, variable compression ratio engine

Introduction

Biodiesels are attractive sources of energy to replace fossil fuels used in IC engines. This is because of their desirable attributes such as being sustainable, biodegradable, and carbon neutral. Biodiesels can also be used in existing CI engines with small or no modifications. Many researchers found that the use of biodiesels can reduce emissions such as unburned hydrocarbons (UHC), soot, and CO, but a slight increase in NOx was observed. Typically biodiesels can be assumed to be methyl or ethyl esters but methyl esters were widely used because they show better performance and emission characteristics [1-5].

Simulation of IC engines has gained popularity in recent days due to availability of sophisticated computational facilities and CFD codes for the accurate prediction of spray and combustion phenomena. A suitable 3-D computational model with proper reaction mechanism and spray model can accurately predict the combustion characteristics. Physical and chemical properties of biodiesel such as normal boiling point, critical properties, vapor pressure, latent heat of vaporization, density, viscosity, thermal conductivity, and surface tension have great impact on the spray and combustion modelling whose accuracy also redefines the

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accuracy of numerical predictions. An et al. [6] presented correlations to predict the properties for 5 methyl esters namely methyl palmitate, methyl oleate, methyl stearate, methyl linoleate, and methyl linolenate.

Brakora et al. [7] described a reduced reaction mechanism for biodiesel combustion which consists of 41 species and 150 reactions. The mechanism predicted well as that of the comprehensive mechanism which consists of 264 species and 1219 reactions. They have also developed a reduced reaction mechanism for biodiesel blends which consists of 53 species and 156 reactions. The reduced mechanism gave the advantage of lesser computational time with reasonable accuracy. Brakora and Reitz [8] performed a reduction in the chemical mechanism which suits to the multi fuel component species like biodiesel and its blends; the reaction mechanism contains 69 species and 192 reactions.

A review of pongamia biodiesel combustion from the open literature by Murugesan et al. [9] reveals the following salient features. Pure pongamia biodiesel can be directly used in diesel engines without any alterations with slightly inferior performance than that of diesel. Addition of little amounts of biodiesel to mineral diesel is a worthy strategy for increasing alternative fuel consumption and B20 is the best alternative fuel. Brake thermal efficiency of biodiesel (B20) is slightly increased and brake-specific energy consumption is reduced slightly when compared with B100. But in comparison with mineral diesel, the BSFC of B20 could not improve at baseline configuration whereas emission characteristics were reduced and at par with diesel in most of the literature available.

Qi et al. [10] analyzed the effect of start of injection timing and exhaust gas re-circulation (EGR) rate on the combustion and emissions of a direct injection CI engine using split injection strategy with neat soybean biodiesel. The results show that the increase of EGR rate increases the brake specific fuel combustion (BSFC) and soot emission whereas NOx emissions were decreased. Results also reveal that BSFC was slightly increased, NOx emissions were evidently decreased, and soot emissions remained almost same with the retarded main injection timing.

Gopal and Kanupparaj [11] conducted experiments on CI engine with blends of pongamia biodiesel and diesel without any modification of existing engine design. The PME 20 (pongamia 20% and diesel 80%) allows for better performance and lower emissions over the various blends and it is also on a par with petro diesel. Wilson [12] optimized diesel engine control parameters such as clearance volume, fuel injection pressure (FIP), nozzle-hole diameter, start of injection (SOI), and load using Taguchi design of experiments (DOE) in order to get the best performance in terms of NOx and BSFC. They also derived relations between operating parameters and responses and identified that the results of experimental data had a good agreement with the predicted results. It was also analyzed that among all the parameters FIP has a great influence on NOx. They concluded that the DOE is an effective and efficient way to develop a robust design in order to get optimum performance and emissions.

The complexity of the in-cylinder combustion phenomena can be modeled using CONVERGE™ [13] CFD software, in which turbulence modeling, combustion modeling, and spray modeling are used simultaneously to predict the performance and emission characteristics precisely. Response surface methodology (RSM) is also a proven technique which reduces the number of experiments to be conducted and saves time and human effort. It can also predict the model with reasonable accuracy [14].

There is plenty of literature available on each of these individual effects on performance and emissions. But the interaction effects of these parameters were not discussed much on the performance and emissions. The present work focuses on CFD simulations of ponga-
nia biodiesel combustion in a variable compression ratio (VCR) engine and to analyze the effect of parameters such as CR, SOI, and EGR on performance and emissions. The present study also uses output responses from the CFD study and analyzed using a systematic approach RSM [15]. These effects are studied in the present simulation study and also aimed to optimize the operating parameters in order to obtain minimum emissions and improved performance.

The CFD simulation

The engine sector model shown in fig. 1, with the dimensions given in tab. 1, is considered for the present study. The fuel properties are given in tab. 2. The simulations are carried out using CONVERGE™ CFD software. The models used in CFD package for different physical phenomena are shown in tab. 3. The numerical simulation is validated with experimental data and also compared with literature [11] with PB 20 (pongamia methyl ester 20% and 80% diesel) as a fuel. The properties of the selected biodiesel (PB 20) are estimated using MATLAB code based on the correlations developed by An et al. [6]. These properties are given as input to numerical simulations.

Validation of model

Comparison of pressure with respect to crank angle for baseline configuration of experimental and simulation model are shown in fig. 2. It can be observed that simulation results are in good agreement with the experimental. The difference in peak pressure for the experimental and simulation is observed to be around 7%. The emissions are also compared for the experimental and simulation models in tab. 4. The difference between experimental and simulation is found to be 2% and 8%, respectively, for NOx and soot emissions.

Results and discussion

Three parameters, CR, SOI, and EGR were chosen to optimize the engine configuration with a view to attaining better performance and emissions. A total of 17 experiments
were conducted and their responses tabulated in tab. 5. The CR is varied from 14 to 18, SOI is varied from 17° bTDC to 26° bTDC and EGR percentage is varied from 0 to 20 in three levels. The RSM was used in the current work for analyzing the output responses to obtain the regression equations.

### Evaluation of the regression model

The regression models are analyzed based on analysis of variance (ANOVA) which gives the $p$ value for different response parameters such as ISFC, NO$_x$, and soot emissions. The $p$ values for output responses are given in tab. 6. These $p$ values tell us whether the particular parameter is significantly affecting the output responses or not. The reference limit for $p$ value was chosen as 0.05. The models are significant as their $p$ values are less than 0.05 [25, 26].

It can be observed from tab. 6 that the individual parameters (CR, SOI, and EGR) have significant effect on all the responses since their $p$ value is less than 0.05. Interaction effects of (CR·SOI) and (SOI·EGR) also have significant effect on all the responses. The CR·EGR has no significant effect on the output responses since their $p$ value is greater than 0.05. So the interaction effects that are significant are only discussed in the present section. The regression statistics goodness of fit, $R^2$, adjusted $R^2$, and predicted $R^2$ for all the responses is shown in tab. 7. For a model to fit the data well, the difference between predicted and adjusted $R^2$ should be less than 0.2.

The quadratic models have been developed for ISFC, NO$_x$, and soot in terms of input parameters in eqs. (1), (2), and (3), respectively.

$$\text{ISFC} = 312.5 + 5.72 \cdot \text{CR} - 4.33 \cdot \text{SOI} + 1.720 \cdot \text{EGR} + 0.114 \cdot \text{CR}^2 - 0.0236 \cdot \text{SOI}^2 - 0.0318 \cdot \text{EGR}^2 - 0.2650 \cdot \text{CR} \cdot \text{SOI} - 0.0366 \cdot \text{CR} \cdot \text{EGR} - 0.0031 \cdot \text{SOI} \cdot \text{EGR}$$

(1)
\[ \text{NO}_x = 410.68 - 51.27 \cdot \text{CR} - 2.94 \cdot \text{SOI} - 0.417 \cdot \text{EGR} + 0.198 \cdot \text{CR} \cdot \text{SOI} - \]
\[ - 0.033 \cdot \text{CR} \cdot \text{SOI} - 0.002 \cdot \text{SOI} \cdot \text{EGR} + 1.72 \cdot \text{CR}^2 + 0.0047 \cdot \text{SOI}^2 + 0.0213 \cdot \text{EGR}^2 \]  
(2)

\[ \text{Soot} = 35.34 - 3.61 \cdot \text{CR} - 0.174 \cdot \text{SOI} - 0.044 \cdot \text{EGR} - 0.0163 \cdot \text{CR} \cdot \text{SOI} - \]
\[ - 0.0011 \cdot \text{CR} \cdot \text{EGR} - 0.0038 \cdot \text{SOI} \cdot \text{EGR} + 0.11 \cdot \text{CR}^2 + \]
\[ + 0.0047 \cdot \text{SOI}^2 + 0.00154 \cdot \text{EGR}^2 \]  
(3)

Table 5. Experimental design and their responses

<table>
<thead>
<tr>
<th>S. No.</th>
<th>Parameter</th>
<th>ISFC [gkW(^{-1})h(^{-1})]</th>
<th>NO(_x) [gkg(^{-1}) of fuel]</th>
<th>Soot [gkg(^{-1}) of fuel]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>16 26 0</td>
<td>235.00</td>
<td>40.01</td>
<td>0.81</td>
</tr>
<tr>
<td>2</td>
<td>18 17 10</td>
<td>239.48</td>
<td>48.72</td>
<td>0.98</td>
</tr>
<tr>
<td>3</td>
<td>18 21.5 20</td>
<td>231.23</td>
<td>51.12</td>
<td>0.64</td>
</tr>
<tr>
<td>4</td>
<td>18 26 10</td>
<td>225.12</td>
<td>56.52</td>
<td>0.42</td>
</tr>
<tr>
<td>5</td>
<td>16 21.5 10</td>
<td>248.12</td>
<td>32.52</td>
<td>0.95</td>
</tr>
<tr>
<td>6</td>
<td>14 17 10</td>
<td>265.27</td>
<td>22.84</td>
<td>2.45</td>
</tr>
<tr>
<td>7</td>
<td>14 26 10</td>
<td>260.45</td>
<td>23.52</td>
<td>2.48</td>
</tr>
<tr>
<td>8</td>
<td>14 21.5 0</td>
<td>257.15</td>
<td>27.45</td>
<td>2.12</td>
</tr>
<tr>
<td>9</td>
<td>16 21.5 10</td>
<td>247.15</td>
<td>32.52</td>
<td>0.95</td>
</tr>
<tr>
<td>10</td>
<td>16 21.5 10</td>
<td>248.12</td>
<td>32.52</td>
<td>0.95</td>
</tr>
<tr>
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<td>14 21.5 20</td>
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<td>2.53</td>
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<td>16 21.5 10</td>
<td>247.18</td>
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<tr>
<td>14</td>
<td>16 17 20</td>
<td>253.15</td>
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<td>1.54</td>
</tr>
<tr>
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<td>18 21.5 0</td>
<td>224.15</td>
<td>61.15</td>
<td>0.32</td>
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<tr>
<td>16</td>
<td>16 26 20</td>
<td>243.45</td>
<td>30.0</td>
<td>1.25</td>
</tr>
<tr>
<td>17</td>
<td>16 17 0</td>
<td>244.15</td>
<td>36.45</td>
<td>1.03</td>
</tr>
</tbody>
</table>

Table 6. The \(p\) values for model terms of ANOVA analysis

<table>
<thead>
<tr>
<th></th>
<th>ISFC</th>
<th>NO(_x)</th>
<th>Soot</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regression model</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>SOI</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>CR</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
<td>&lt;0.001</td>
</tr>
<tr>
<td>EGR</td>
<td>&lt;0.001</td>
<td>&lt;0.0001</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>CR-SOI</td>
<td>0.019</td>
<td>0.005</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>CR-EGR</td>
<td>0.381</td>
<td>0.187</td>
<td>0.255</td>
</tr>
<tr>
<td>SOI-EGR</td>
<td>0.001</td>
<td>0.002</td>
<td>0.02</td>
</tr>
</tbody>
</table>
Table 7. The RSM model evaluation

<table>
<thead>
<tr>
<th>Model</th>
<th>ISFC</th>
<th>NO$_x$</th>
<th>Soot</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R^2$</td>
<td>0.9923</td>
<td>0.9976</td>
<td>0.9989</td>
</tr>
<tr>
<td>Adjusted $R^2$</td>
<td>0.9823</td>
<td>0.9945</td>
<td>0.9975</td>
</tr>
<tr>
<td>Predicted $R^2$</td>
<td>0.9267</td>
<td>0.9617</td>
<td>0.9823</td>
</tr>
</tbody>
</table>

**Interaction effect of SOI and CR**

It can be observed from fig. 3 that at lower CR, the interaction of SOI and CR is significant, but not fruitful in reducing ISFC. But at higher CR, the interaction is beneficial in reducing ISFC. Advancing the injection timing to 26° bTDC increased NO$_x$ emissions and reduced the soot emissions. This is due to the fact that in-cylinder temperature and pressures were low at the time of fuel injection, which increases the ignition delay. At the same time increase in compression ratio resulted in increased in-cylinder temperature and thus NO$_x$ emissions were increased, whereas soot emissions are decreased due to efficient combustion. From figs. 4 and 5 it can be interpreted that the combination of high compression ratios and early fuel injection timings resulted high NO$_x$ emissions but less soot emissions. Soot emissions were high and NO$_x$ emissions were low at retarded injection timings and low compression ratios.

**Effects of SOI and EGR**

Figure 6 shows the interactive effects of injection timing and exhaust gas recirculation on ISFC. As the start of injection is advanced from 17° to 26° bTDC, ISFC is decreased. Also, as the EGR is increased from 0% to 25%, ISFC increased. But this phenomenon is dominant at lower EGR. This is due to fact that the EGR reduces the oxygen concentration while also increasing the specific heat of the charge and thus drops the in cylinder temperature which results in inefficient combustion.
From the results shown in figs. 7 and 8, it can be interpreted that the combination of low EGR and early fuel injection timings resulted in high NO\textsubscript{x} emissions but very little soot emissions. Soot emissions were high and NO\textsubscript{x} emissions were low at retarded SOI and higher EGR.

**Optimization**

The previous discussions on the effects of SOI, CR, and EGR on the performance and emission characteristics revealed that the smallest CR of 14 and retarded SOI of 17° bTDC resulted in lower NO\textsubscript{x}, higher ISFC, and higher soot emission. On the other hand, higher CR and advanced SOI resulted in higher NO\textsubscript{x}, reduced ISFC and decrease in soot values. There is an absolute trade-off observed between NO\textsubscript{x} and soot. So parameters must be optimized in order to get lower emissions without any cost of its performance. In desirability based approach, different solutions were obtained. The solution with highest desirability is preferred. The lowest from the experimental data (in case of emissions/minimization objective) is taken as desirability of 1. The value of desirability tells us how close the optimum is to the lowest value. Desirability of 0.97 was obtained at the following parameters CR – 16.75, SOI – 21.9° bTDC, and EGR – 10.94%. Table 8 shows the comparison of optimized and baseline cases and it is observed that simultaneous reduction in soot and NO\textsubscript{x} is attained with some improvement in ISFC. Optimum configuration reduced ISFC, NO\textsubscript{x} and soot by 2%, 31%, and 34%, respectively.
Conclusions

The following conclusions were drawn based on the numerical simulations using CONVERGETM software. The DOE RSM methodology was employed for designing the minimum number of simulations and their levels.

- The DOE is very useful in analyzing the simulation results in a statistical approach and eventually help us to determine the most influential parameters that affect the performance and emissions.
- The NOx emissions were evidently decreased and soot emissions increased with increasing rate of EGR.
- Increase in SOI increases NOx and reduces soot and ISFC.
- Decrease in CR increases soot emissions and ISFC whereas NOx is reduced.
- The interaction effects of CR and SOI were dominant for the responses of NOx and soot.
- The interaction effects EGR and SOI were dominant for the responses ISFC and NOx.
- The interaction effects CR and EGR were very less significant as compared to other two combinations.
- The optimum set of parameters was found out to be CR – 16.75, SOI – 21.9° bTDC, and EGR – 10.94%.

Acknowledgment

This work was supported by Center of Excellence (COE), Center for sustainable energy studies of Technical Education Quality Improvement Programme (TEQIP-II), India.

Nomenclature

- aTDC – after top dead center
- bTDC – before top dead center
- BSFC – brake specific fuel consumption
- CFD – computational fluid dynamics
- CI – compression ignition
- CR – compression ratio
- DOE – design of experiments
- EGR – exhaust gas recirculation
- FIP – fuel injection pressure
- IC – internal combustion
- ISFC – indicated specific fuel consumption
- RPM – rotations per minute
- RSM – response surface methodology
- SOI – start of injection
- VCR – variable compression ratio

References


