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Performance simulation of a reactivity-controlled compression ignition (RCCI) engine fueled with waste cooking oil biodiesel (WCO) with a focus on consumption trends of fuel constituents

S. Talesh Amiri[1], R. Shafaghat[2,*], O. Jahanian[3], R. Alamian[4]

[1] Ph.D. Student, Mech. Eng., Babol Noshirvani University of technology, Babol, Iran
[2] Prof., Mech. Eng., Babol Noshirvani University of technology, Babol, Iran
[3] Assoc. Prof., Mech. Eng., Babol Noshirvani University of technology, Babol, Iran
[4] Postdoctoral Research Fellowsheep, CORIA Lab, INSA Rouen Normandie

*Corresponding author: rshafaghat@nit.ac.ir

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Abstract

Using the low-temperature combustion strategy is one of the effective solutions to reduce NOx emission; In the present study, a single-zone code was developed considering the detailed chemical kinetic mechanism to investigate the performance of an RCCI engine with gasoline-diesel/WCO biodiesel hybrid fuel. First, the numerical results were compared with the experimental results to check the validation, and then the functional parameters and the production and consumption rates of each specific species were checked at different loads. The study of the consumption of chemical species showed that unsaturated fatty acids are consumed more quickly in the combustion process. Diesel consumption speed is also lower than WCO in all loads.

Keywords: waste cooking oil biodiesel fuel; saturated fatty acid; Zero-dimensional simulation RCCI engine.

1. Introduction

The review of past studies shows that using WCO biodiesel can increase engine operating temperature and NOx emissions. Various methods including EGR [1], fuel blending with additives such as ethanol and gasoline [2], and adding water inside the combustion chamber [3] have been proposed to reduce NOx emissions [4]. However, one of the most suitable methods for NOx emission reduction is using the low-temperature combustion engine strategy. In LTC engines, the combustion temperature, NOx, and soot emissions are simultaneously reduced due to the increased homogenization of the air-fuel mixture. Among the LTC strategies, the RCCI engine is more popular due to the acceptable control of the ignition start moment [5, 6]. For this reason, the use of biodiesel fuel in the RCCI engine can reduce NOx emissions in addition to CO, HC, and soot emissions [7]. Also, many experimental studies were carried out on the effect of the types of biodiesel fuel; The results show that the fatty acids that make up biodiesel fuel have a significant effect on the combustion phasing. In this regard, in order to accurately evaluate the performance of all types of waste oil biodiesel fuels in RCCI engines, it is very important to check the consumption rate of the constituent species of this fuel; Therefore, the present study aims to numerically investigate the use of biodiesel fuel from waste oil on the performance of a low-temperature combustion engine with RCCI strategy with a combination of diesel and gasoline; So that the process of production and consumption of different types such as saturated and unsaturated fatty acids and its effect on engine performance can be seen. It is worth noting that due to the high importance of investigating different types of fuel, the kinetic mechanism of the chemical joint was used in this study; Also, due to the high number of species and reactions in this mechanism, due to the high speed of solving the single-zone code to increase the speed of calculations, a one-dimensional single-zone code for simulating the RCCI engine with diesel-WCO/gasoline mixed fuel in the MATLAB software environment It was developed based on the specifications of the target engine. Also, in order to define the kinetic mechanism of the chemical joint and implement the combustion equations on the geometry of the problem, Cantera plugin was used as a couple with MATLAB software.

In the present study, a single-zone code was developed in the MATLAB software environment with the Cantera plugin for zero-dimensional investigation of species consumption rates. To

validate the numerical results, the study of Chidambaram and Krishnasamy was used. In an experimental study, they investigated the performance of WCO fuel in an RCCI engine. Engine performance was evaluated at four different times; So that the range of BMEP changes was from 1.06 to 4.24 times (Table 1). According to Table 1, the ratio of PFI to DI at 20% of the applied load was 47.08 and this ratio increased with the increase of engine load; Therefore, with an increase in the applied load on the engine, despite the increase in the fuel-air ratio, less WCO fuel entered the combustion chamber.
In the current numerical study to investigate the rate of production and consumption of WCO fuel constituents, the target engine was simulated in these four states according to Table 1, and the production and consumption process of waste oil biodiesel fuel constituents was also investigated in these four states.

Table 1. Experimental test cases specification

Parameter	Optimized values			
Case number	1	2	3	4
Rated load (%)	20	40	60	80
BMEP (bar)	1.06	2.12	3.19	4.24
Premixed port fuel energy (%)	47.08	57.87	82.21	94.11
DI timing (CAD bTDC)	30	30	30	30
Air fuel ratio	61.57	48.37	38.11	30.14

The process of WCO fuel preparation and transesterification is shown in Figure 1. The specifications of the used fuels are presented in Table 2 and the constituent species of biodiesel fuel (from the GC identification test) are presented in Table 3. In this work, a light, air-cooled, naturally aspirated single-cylinder diesel engine was used for agricultural water pumping (Table 4). It is worth noting that gasoline fuel was defined as PFI fuel and a mixture of diesel fuel and WCO as DI fuel; In such a way that the gasoline fuel mixed with air entered the combustion chamber from the intake manifold, the diesel/biodiesel combined fuel was injected directly into the combustion chamber.

Figure 1. trance esterification proses

A single-zone code was developed according to the governing equations and considering the kinetics of the chemical joint to approximate the ignition start time and quantitatively and qualitatively investigate the behavior of the variables in an RCCI engine. The logic of the code operation is that first, the molar ratio of fuel and air along with the boundary conditions are received as input data. The differential equation of volume changes is solved by ODE method and with the ode15 command in each time step in MATLAB software, the volume of the cylinder is determined. After calculating the volume, pressure and temperature of the chamber is checked by solving the thermodynamic equations at every moment. The molar ratio of the species changes as soon as the time step reaches the moment of HRF fuel injection, and the volume change process continues. At each time step, the temperature data are matched to the chemical mechanism. As soon as the temperature and pressure of the cylinder chamber reach the combustion conditions, the kinetic mechanism of the chemical joint starts to solve the equations related to the chain chemical reactions, taking into account the speed of the reaction rate; In this regard, in addition to calculating the rate of production and consumption of species, the amount of released heat is also calculated. The algorithm of the developed code is presented in Figure 3. According to the species of the fuel, in the present simulation, the kinetic mechanism of the chemical composition of methyl linolenate fuel including 582 species and 21174 reactions was used.
In the single-zone model, the following assumptions are considered:

- Simulation is done for closed cycle of the engine.
- The whole system at the first moment is considered as a region with the same temperature, pressure and concentration of compounds.
- The fluid inside the chamber before and after combustion is assumed to be an ideal gas.
- Direct injection fuel is added to the assembly in gaseous form at the desired moment.
- The mass of the system is constant, the leakage of gases from the gap of the rims is neglected.
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The most important results of the present numerical study are as follows:

- The ignition start moment, with increasing load, gets closer to the fuel injection start moment. Also, with the increase in fuel mass, due to the high proportion of LR fuel, the period of formation of cold ignition becomes shorter (figure 2).

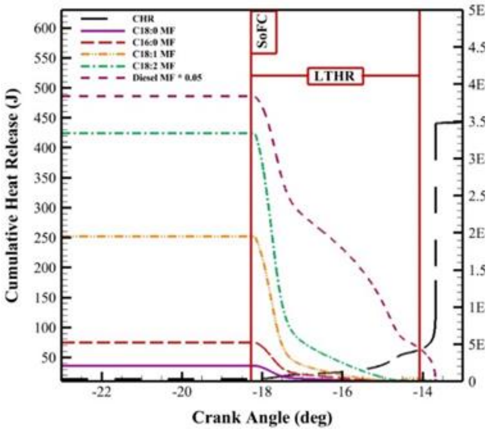

Figure 2. The ignition start moment

- The ignition start moment does not change significantly at maximum load, because the energy ratio of FPI is much higher than that of DI.
- The start of formaldehyde production in all cases is at the same time as the release of low temperature heat, during the process of low temperature heat release, formaldehyde is produced and consumed. Also, the beginning of the production of hydroxyl species is at the same time as the beginning of the high temperature heat release process, its consumption process continues until the end of the combustion process. The molar ratio of formaldehyde produced to hydroxyl decreases with the increase of the engine load and due to the decrease in the ratio of DI to FPI fuel, and leads to a decrease in the cold ignition interval.
- The moment of starting the consumption of saturated and unsaturated species is not much different and the process of consuming diesel and biodiesel species starts almost at the same time; If the rate of consumption of chemical species of unsaturated fatty acid is much higher than that of unsaturated species (figure 3).
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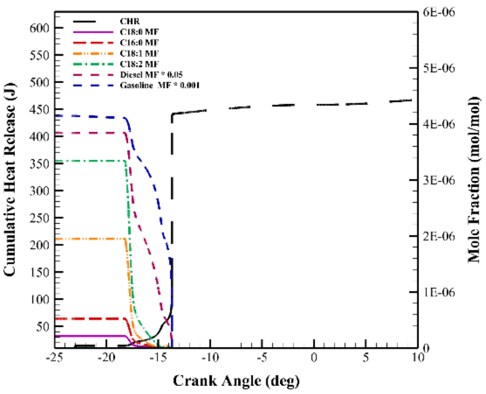

Figure 3. The consumption rate of fuel constituents

3. Conclusion

In the present study, the performance of a compression combustion engine in RCCI mode with the combination of diesel-biodiesel WCO and gasoline was numerically investigated. A single-zone code was developed in MATLAB-Cantera software to simulate the target engine. The detailed kinetic mechanism of the desired combined fuel was applied to accurately investigate the rate of consumption of the constituent species of biodiesel fuel in a single-zone simulation. The results of the present study showed that with the increase in fuel mass (due to the high proportion of LR fuel), the period of formation of cold ignition becomes shorter. Also, the moment of starting the consumption of saturated and unsaturated species is not much different and the process of consuming diesel and biodiesel species starts almost at the same time; If the rate of consumption of chemical species of unsaturated fatty acid is much higher than that of unsaturated species.

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