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Numerical investigation of exhaust gas emissions for a dual fuel engine configuration using diesel and pongamia oil

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ABSTRACT

The investigation presented in this paper focuses on determination of gaseous exhaust emissions by computational simulation during combustion in compression ignition engine with pongamia oil substitution. Combustion is modeled using Equilibrium Constants Method (ECM) with MATLAB program to calculate the mole fraction of 10 combustion products when pongamia oil is burnt along with diesel at variable equivalence ratio and blend ratio. It had been observed that pongamia oil substitution causes decrease in the CO emission and increase in the NO_x emission as the blend ratio as well as equivalence ratio increases.

1. Introduction

Environmental concerns and the possible role of alternative renewable fuels are leading the first actions towards the production of sustainable fuel supply. Biofuels for diesel engine comprise vegetable oils and biodiesel, neat or blended with mineral diesel fuels (Pischinger et al., 1982). The concept of using biodiesel in diesel engine originated from the demonstration of first diesel engine by the inventor "Rudolf Diesel" at the world exhibition in Paris in 1900 by using peanut oil as a fuel. Due to abundant supply of petrol diesel, R&D activities on vegetable oils were not seriously pursued till 1970s (Last, 2012). Since the petroleum fuels are dwindling fast alternative and environmental friendly renewable substitute must be identified. Apart from the fuel depletion aspects diesel engines are the major sources of urban air pollution and particulate emission. Using alcohol fuels in diesel engine substantially increase the aldehyde emission and these could cause a significant pollutant when these fuels are used in large quantities compared to gasoline and diesel (Kumar et al., 2003). Hence biodiesel is good fuel substitute because biodiesels are free from carcinogenic, mutagenic, which decreases certain emissions like CO, unburned HC and particulate matters. Here pongamia oil blends with diesel is used as an alternative fuel. The oil is extracted from seed of legume tree *Pongamia pinnata*. The constituent of these seed is 3.8% of ash, 9.7% of sugar, 7.07% of protein, 24% of oil, 10.7% of free amino acids and 0.27% of fatty acids. Significant experimental research work has been done by Venkataraman (2008) for investigating the performance and emission characteristic of pongamia biodiesel in DICI and HCCI engine.

In the present study, an effort is made by developing a combustion mathematical model to determine exhaust gas that causes serious effects on environment by using pongamia-diesel blend fuels. Based on Equilibrium Constant Method (ECM) (Turns, 2013), a computer program using MATLAB has been developed for the blended fuels to calculate the mole fractions of various emitted gases. ECM is based on thermodynamic measurements and empirical calculations. It is very accurate and precise in solving most of chemical kinetics problems. Thermodynamic data for elements, combustion products and many pollutants are available in a complication published by the National Bureau of Standards, called the JANAF (Joint Army–Navy–Air Force) tables.

2. Combustion model

Governing equation for the reaction combustion equations were performed based on following assumption (Heywood, 2011)

1. All the gases are assumed to be perfect and homogenous.
2. Range of equivalence ratio is 0.5–1.5.
3. There is no delay time.
4. Effect of convection, conduction and radiation is neglected.

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Nomenclature

CO_2	Carbon dioxide
H_2O	Water
N_2	Nitrogen gas
O_2	Oxygen
CO	Carbon monoxide
H_2	Hydrogen gas
H	Hydrogen atom
O	Oxygen atom
OH	Hydroxide
NO	Nitrogen oxide
ECM	Equilibrium Constant Method
DICI	Direct Injection Compression Ignition
HCCI	Homogenous Charge Compression Ignition
HC	Hydrocarbon
JANAF	Joint Army–Navy Force
Φ	Equivalence ratio

5. No chemical changes in diesel, biodiesel and are prior to the combustion.
6. All the properties are time dependent.

The governing equations are prepared by assuming 10 combustion products and a system of equation appears and this can be solved by Newton–Raphson method prior to its implementation into MATLAB program. The combustion reaction is given by

$$B(C_aH_bO_c)+D(C_\alpha H_\beta O_\chi N_\delta)+(a_s/\Phi)(O_2+3.76N_2) \rightarrow n_1CO_2+n_2H_2O+n_3N_2+n_4O_2+n_5CO+n_6H_2+n_7H+n_8O+n_9OH+n_{10}NO \quad (1)$$

where
- B-mole fraction of pongamia biodiesel.
- D-mole fraction of diesel.
- a_s-stoichiometric air–fuel ratio.
- Φ-equivalence ratio.
- $n_i=(i=1–10)$ no. of moles of each combustion emission product.

Atomic balance of C, H, O and N leads to

$$C: B(a) + D(\alpha) = n_t(x_1 + x_5) \quad (2)$$

$$H: B(b) + D(\beta) = n_t(2x_2 + 2x_6 + x_7 + x_9) \quad (3)$$

$$O: B(c) + D(\chi) + (2a_s/\Phi) = n_t(2x_1 + x_2 + 2x_4 + x_5 + x_8 + x_9 + x_{10}) \quad (4)$$

$$N: D(\delta) + 3.76(2a_s/\Phi) = n_t(2x_3 + x_{10}) \quad (5)$$

Addition of all mole is given by

$$\Sigma x_i = 1 (i = 1–10) \quad (6)$$

where x_i is the mole fraction of ith species of various combustion emission product and n_t represents the total number of moles after combustion where $x_i=n_i/n_t$ and $n_t=\Sigma n_i$ $(i=1–10)$.

The dissociation reactions and the equilibrium constants associated are Stull and Prophets (1971)

$$1/2H_2 \leftarrow\rightarrow H,\ K_1 = \left(x_7\sqrt{p}\right)/\sqrt{x_6} \quad (7)$$

$$1/2O_2 \leftarrow\rightarrow O,\ K_2 = \left(x_8\sqrt{p}\right)/\sqrt{x_4} \quad (8)$$

$$1/2H_2 + 1/2O_2 \leftarrow\rightarrow OH,\ K_3 = x_9/\left(\sqrt{x_6}\sqrt{x_4}\right) \quad (9)$$

$$1/2O_2 + 1/2N_2 \leftarrow\rightarrow NO,\ K_4 = x_{10}/\left(\sqrt{x_3}\sqrt{x_4}\right) \quad (10)$$

$$H_2 + 1/2O_2 \leftarrow\rightarrow H_2O,\ K_5 = x_2/\left(x_6\sqrt{x_4}\sqrt{p}\right) \quad (11)$$

$$CO + 1/2O_2 \leftarrow\rightarrow CO_2,\ K_6 = x_1/\left(x_5\sqrt{x_4}\sqrt{p}\right) \quad (12)$$

here K_i $(i=1–6)$ represents the equilibrium constants for the respective reactions and p represents the combustion pressure. The value of the equilibrium constant can be calculated using the formula

$$K_i = e^{(-\Delta G^{\circ}{}_{Ti}/RT_{comb})} \quad (13)$$

where $\bar{}_{Ti}^{\Delta G^\circ}$, T_{comb}, R represents Gibbs free energy, combustion temperature and gas constant respectively and these values are taken from JANAF table corresponds to combustion temperature.

The equilibrium constants from the equation (7–12) are rearranged to express the mole fraction of emission product in terms of X_i

$$X_1 = K_6X_5\sqrt{p}\sqrt{X_4} = S_6X_5\sqrt{X_4},\ \left(\text{where} S_6 = K_6\sqrt{p}\right) \quad (14)$$

$$X_2 = K_5X_6\sqrt{p}\sqrt{X_4}, = S_5X_6\sqrt{X_4},\ \left(\text{where} S_5 = K_5\sqrt{p}\right) \quad (15)$$

$$X_7 = K_1\sqrt{X_6}/\sqrt{p} = S_1\sqrt{X_6},\ \left(\text{where} S_1 = K_1/\sqrt{p}\right) \quad (16)$$

$$X_8 = K_2\sqrt{X_4}/\sqrt{p} = S_2\sqrt{p},\ \left(\text{where} S_2 = K_2/\sqrt{p}\right) \quad (17)$$

$$X_8 = K_2\sqrt{X_4}/\sqrt{p} = S_2\sqrt{p},\ \left(\text{where} S_2 = K_2/\sqrt{p}\right) \quad (18)$$

$$X_{10} = K_4\sqrt{X_4}\sqrt{X_3} = S_4\sqrt{X_4}\sqrt{X_6},\ (\text{where} S_4 = K_4) \quad (19)$$

To obtain the value of X_3, X_4, X_5, and X_6 Eqs. (3–6) is divided by equation and rearranged so that the equation we obtain contains four equation with four unknowns as follows:

$$2S_5X_6\sqrt{X_6} + 2X_6 + S_1\sqrt{X_6} + S_3\sqrt{X_4}\sqrt{X_6} – Z_1\left(S_1X_5\sqrt{X_4} + X_5\right) = 0 \quad (20)$$

$$2S_6X_5\sqrt{X_4} + S_5X_6\sqrt{X_4} + 2X_4 + X_5 + S_2\sqrt{X_4} + S_3\sqrt{X_4}\sqrt{X_6} + S_4\sqrt{X_4}\sqrt{X_3} – Z_2\left(S_6X_5\sqrt{X_4} + \sqrt{X_5}\right) = 0 \quad (21)$$

$$2X_3 + S_4\sqrt{X_3}\sqrt{X_4} – Z_3\left(S_6X_5\sqrt{X_4} + \sqrt{X_5}\right) = 0 \quad (22)$$

$$S_6X_5\sqrt{X_4} + S_5X_6\sqrt{X_4} + X_3 + X_4 + X_5 + X_6 + S_1\sqrt{X_6} + S_2\sqrt{X_6} + S_3\sqrt{X_4}\sqrt{X_6} + S_4\sqrt{X_4}\sqrt{X_3} – 1 = 0 \quad (23)$$

where

$$Z_1 = (Bb + D\beta)/(B\alpha + D\alpha)$$

$$Z_2 = \left(Bc + D\chi + 2(a_s/\Phi)\right)/(B\alpha + D\alpha)$$

$$Z_3 = \left(D\delta + (7.52a_s/\Phi)\right)/(B\alpha + D\alpha)$$

On solving above equation (20–23) we will get X_3 X_4 X_5 X_6 by substituting these values in the above mentioned equation (14–19) we will get the remaining mole fraction of combustion species.