Prediction of Cetane Number of Biodiesel Fuel from Fatty Acid Ethyl Ester (FAEE) Composition

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Abstract
In this paper, we predict the Cetane Number of the fatty acid ethyl ester according to weight percentage of fatty acids available in the fuel. The biodiesel fuel is produced with the transesterification method using ethanol and sodium hydroxide as catalyst from seven types of vegetable oils (sunflower, soybeans, canola, olive, corn, grape seed and rice bran). The weight percentage of fatty acid ethyl esters available in fuel was performed using the GC-Mass device according to ASTM standards. The CFR engine was used for measuring the Cetane Number in motoring method. The results of the tests were presented as a regression model between four independent and dependent variables. The four independent variables are palmitic acid, linoleic acid, oleic acid, stearic acid, and the dependent variable is Cetane Number. For evaluation of this model, other model presented were compared based on relation between Cetane number as dependent variable with density and aniline point of biodiesel fuel as independent variable that used from nonlinear regression analysis. Comparison of results showed that the linear regression according to the fatty acid ethyl ester composition has a higher coefficient of determination and prediction accuracy.

Keywords: Biodiesel, Cetane Number, Fatty Acid Ethyl Ester

1. Introduction
Emissions of air contaminants as CO, sulfur dioxide, nitrogen oxides, unburned hydrocarbons and aerosols of vehicles increase tremendously every year. One of the reasons that cause air pollution and climate changes is distribution of these materials. In addition, efforts is also considered to reduce dependence on oil products due to rapid decrease in oil resource and price instability¹.

Pure vegetable oils have been considered as an alternative for diesel fuel, but the high viscosity at room temperature made them unsuitable for diesel engines. However, Fatty Acid Methyl Ester (FAME) derived from them have lower viscosity than the pure oils. So research about the use of fatty acid ester as an alternative of diesel fuel is justifiable².

Biodiesel is a non-toxic, renewable fuel and has no sulfur and aromatic compounds. It consist alkyl esters fatty acids with long chain that is prepared from renewable resources such vegetable oils or animal fats. It has the general chemical formula 3C19H35COOR. Also it is only used as a fuel in internal combustion engines and heating systems³.

The fuel properties of biodiesel are strongly influenced by the properties of the fatty acid esters that are formed. Identification of these acids can be very effective on obtaining the properties of biodiesel fuels. More Attempts have been performed by various researchers to determine the composition of biodiesel in order to improve the combustion process. It was observed that the fuel properties of biodiesel play a significant role in the combustion process. The fuel Cetane Number is one of the most important factors in the combustion process⁴.

The Cetane Number is expressed as a rate of Fuel Preparation for the auto-ignition temperature and pressure conditions inside the combustion chamber. Fuel
injected into the cylinder should be ignited before reaching the maximum density and in the range of a few thousandths of a second. The Cetane Number indicates the natural tendency of the fuel to ignite. This means that higher Cetane Number causes the better performance of the engine and shorter ignition delay (the interval between injection and ignition) and finally the combustion performs quieter and more uniform. So the Cetane Number is an important parameter in the quality of biodiesel fuel.

The use of vegetable oils directly in diesel engines, due to the high oil viscosity and inappropriate atomization, cause problems such as low quality ignition and incomplete combustion of fuel. On the other hand, the formation of a layer of non-combustible fuel on the cylinder wall disrupts lubrication system. Also low Cetane Number of vegetable oils causes knock at low engine loads and low temperatures. In general, vegetable oils have high ignition delay and slower combustion than the diesel fuel. In result, maximum pressure in their combustion is also lower than diesel fuel. On the other hand, the engines that work with vegetable oils, due to blockage of the injector in high pressure, cannot have direct injection.

It is necessary to extend the relationship between weight percent of biodiesel fuel components and the Cetane Number. It can be obtained as a regression analysis. Regression analysis includes the relationship between a dependent variable and one or more predictor variables (or independent variables). In this research, the independent variable is percentage of fatty acids and dependent variable is Cetane Number.

2. Materials and Methods

In this research, the biodiesel fuel is produced with the trans-esterification method by using ethanol and sodium hydroxide as catalyst from seven types of vegetable oils (sunflower, soybeans, canola, olive, corn, grape seed and rice bran). Specific molar ratio of alcohol to oil (6 to 1) under certain temperature (70°C) and a certain specific weight of sodium hydroxide catalyst ratio (A percent weight of oil) was considered in accordance with optimum conditions for producing biodiesel fuel intensity mixer (600 rpm min). In this case, the fatty acids chain will be converted to impure fatty acid ethyl esters. But due to use of sodium hydroxide catalyst, pH of fuel got in the bases range that Chloride acid was used to neutralize it. Considering the fact that alcohol is evaporated and glycerin is solved in the water, in order to remove the existing glycerin and alcohol in fuel, water leaching process is performed by using distilled water in three stages. In this position the fuel is made pure. The determination of the weight rate percent (wt%) of the existing ethyl ester of fatty acids in these kinds of fuels is performed via GC-mass based on ASTM standard and using polar columns.

Measurement of Cetane Number of unknown fuel is possible by two methods, chemical method or air throttling. At the chemical method of Cetane Number measurement, the volume percentage of normal Cetane of unknown fuel is measured. At air throttling method, Cetane Number of fuel is measured by the CFR engine and the ignition delay time according to ASTM-D613 or din 51773 standard. The CFR engine is shown at Figure 1.

The Cetane Number has inverse relationship with the fuel ignition delay time. On the other hand, the ignition delay for a diesel engine is proportional with the Air to Fuel Ratio (AFR) or rate of fuel consumption to air.

This relationship is used for calculate of the Cetane Number. In the CFR engine, fuel consumption rate is constant and air consumption rate is variable so Cetane Number can be determined by measurement of fuel consumption rate a standard diagram (Cetane-Air consumption rate) that provided by the CFR engine manufacturer. For experiment performance, the CFR engine are calibrated by the normal Cetane base fuel. After engine calibration, the unknown fuel is poured into the engine. In CFR engine, fuel consumption rate is constant and for

Figure 1. CFR engine in University of Tabriz.
achieving a constant ignition delay time, only variable parameter is air consumption rate that ignition delay time remains the same as the previous standard by changing the air consumption. In the engine standard conditions, Cetane Number of fuel is determined from gage of air consumption measurement and diagram (Getane – Air consumption) that is provided by the CFR manufacturer. In the study, regression analysis was used for establishing the relationship between the Cetane Number and compounds of biodiesel fuel. Regression analysis established simple model between fatty acids as independent variable and Cetane Number as dependent variable.

3. Results and Discussion

Compounds present in biodiesel fuels.

In the study, the GC-mass set was used for detecting the biodiesel fuel compound. The results are shown in Table 1.

3.1 The Cetane Number is Measured by CFR Engine

Air meter gage was obtained by CFR engine according to DIN51773 standard. The results are shown in Table 2.

| Biodiesel   | Ethyl Stearate | Ethyl Palmitate | Ethyl oleate | Ethyl linoleate |
|-------------|----------------|-----------------|--------------|----------------|
| Soybean     | 9.393          | 4.807           | 32.133       | 53.666         |
| Rice bran   | 9.12           | 11.63           | 27.93        | 51.32          |
| Sunflower   | 12.395         | 5.112           | 25.873       | 54.694         |
| Olive       | 4.644          | 11.033          | 68.537       | 15.78          |
| grape seed  | 8.613          | 5.681           | 30.88        | 54.826         |
| Canola      | 9.473          | 6.25            | 32.933       | 51.344         |
| Corn        | 8.61           | 10.31           | 30.38        | 50.7           |

3.2 Modeling to Predict Cetane Number

Five types of biodiesel fuel (soybean – sunflower – olive – grape seed – rice bran) was used to determine a relationship between the CN and FAAE compounds. A linear regression analysis was performed by SPSS 17 software. A five matrix was formed with CN as the dependent variable and the pure (FAAE) compounds as the independent variables. The results are shown as Equation (1).

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CN = 1448.29 - 721.377 X_1 + 13.347 X_2 + 13.818 X_3 + 13.014 X_4
\]

CN: Cetane Number.
X_1: Ethyl Stearate.
X_2: Ethyl Palmitate.
X_3: Ethyl oleate.
X_4: Ethyl linoleate.

3.3 Validation for CN Prediction Model

As mentioned five types of biodiesel fuel was used in this model. Data from two types of biodiesel fuel, corn and canola, was used to validate the model. The average measured values of CN obtained from CFR engine in compare to the predicted values from equation, showed that the regression model can predict the Cetane Number with maximum error of 5% (Table 4).

| Biodiesel   | CN measured | CN predicted | Error % |
|-------------|-------------|--------------|---------|
| Soybean     | 41.2        | 46.38        | 11.68%  |
| Canola      | 44.25       | 46.38        | 4.81%   |
| Corn        | 49.35       | 46.38        | 5.68%   |
| Grape seed  | 48.1        | 46.38        | 3.71%   |
| Olive       | 44.81       | 46.38        | 3.43%   |
| Sunflower   | 45.75       | 46.38        | 1.28%   |
| Rice Bran   | 44.25       | 46.38        | 5.12%   |
| Corn        | 46.38       | 46.38        | 0.00%   |

Table 1. The Fatty Acid Ethyl Ester (FAAE) composition

Table 2. Air meter gage data for biodiesel fuels

| Biodiesel   | Repeat 1 | Repeat 2 | Repeat 3 | Average |
|-------------|----------|----------|----------|---------|
| Soybean     | 33.5     | 33       | 33       | 33      |
| Canola      | 33       | 33.5     | 33.5     | 33.5    |
| Sunflower   | 29       | 28       | 28       | 28      |
| Rice bran   | 29       | 29.5     | 29.5     | 29.5    |
| Grape seed  | 27       | 26       | 26       | 26      |
| Olive       | 25       | 25       | 25       | 25      |
| Corn        | 26.5     | 26.5     | 27       | 27      |

Table 3. CN measured

Table 4. Evaluation of Error
The predicted values of CN in compared to the measured values from CFR engine is shown in Figure 2.

Presented regression model can predict Cetane Number of biodiesel fuel with an error of less than 5 percent and correlation coefficient of 96.62%.

4. Conclusions

In this study, an equation established that the Cetane Number can be predicted by the FAAE composition of ethyl ester with 96.62% accuracy. Experimental results showed that the Cetane Number depends on fatty acid mono-esters in biodiesel fuel. Stearate saturated fatty acid (C16 = 0) with short hydrocarbon chains decrease fuel Cetane Number but linoleate unsaturated fatty acid (c18=0) with long hydrocarbon chains increases the biodiesel Cetane Number. So, the production of biodiesel fuel from vegetable oils, which have a high degree of saturation, can increase the Cetane Number of the fuel.

5. Reference

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