Biofuel Research Journal 2 (2014) 55-57

BRTeam BIOFUEL RESEARCH TEAM

Biofuel Research Journal

Journal homepage: www.biofueljournal.com

Short Communication

BiodieselAnalyzer©: a user-friendly software for predicting the properties of prospective biodiesel

Ahmad Farhad Talebi[1,2], Meisam Tabatabaei[1,3]* and Yusuf Chisti[4]

[1] *Biofuel Research Team (BRTeam), Karaj, Iran*

[2] *Semnan University, Semnan, Iran*

[3] *Microbial Biotechnology & Biosafety Department, Agricultural Biotechnology Research Institute of Iran (ABRII), Karaj, Iran*

[4] *School of Engineering, Massey University, Private Bag 11 222, Palmerston North, New Zealand*

HIGHLIGHTS

- Efficient and user-friendly software for estimating biodiesel properties.
- Estimating 16 different quality parameters of biodiesel based on fatty acid profile of oil feedstock.
- Especially a useful tool when a small sample of oil is available for analysis.

GRAPHICAL ABSTRACT

ARTICLE INFO

Article history:
Received 1 May 2014
Received in revised form 25 May 2014
Accepted 26 May 2014
Available online 31 May 2014

Keywords:
Biodiesel properties prediction
Biodiesel quality parameters
BiodieselAnalyzer©
Software
Fatty acids profile
Algal biodiesel

ABSTRACT

The procedures used to experimentally determine the quality parameters of a biodiesel are lengthy and expensive. Occasionally it may be impossible to obtain a sufficient amount of oil for the relevant analyses. This is often the case for algal biodiesel, for example. Here we report on a new software package, the BiodieselAnalyzer© Version 1.1, for predicting the properties of a prospective biodiesel. BiodieselAnalyzer© can estimate 16 different quality parameters of a biodiesel based on the fatty acid methyl ester profile of the oil feedstock used in making it. The current version of the BiodieselAnalyzer© is intended for the Windows platform and is publically available at http://www.brteam.ir/biodieselanalyzer.

* Corresponding author at:
Tel/fax: +982632703536, E-mail address: meisam_tabatabaei@abrii.ac.ir (M. Tabatabaei).

Please cite this article as: Talebi, A.F., Tabatabaei, M., Chisti, Y., 2014. BiodieselAnalyzer©: a user-friendly software for predicting the properties of prospective biodiesel. Biofuel Research Journal 2 (2014) 55-57.

1. Introduction

Supplying energy sustainably is a major challenge facing us. Consumption of fossil fuels continues to increase despite its severe and potentially irreversible consequences on the global climate. Biodiesel derived from renewable oils is a potential alternative to petroleum diesel.

Biodiesel typically consists of monoalkyl esters of fatty acids derived from vegetable oils and animal fats. Biodiesel is mostly produced through transesterification of the feedstock oil. Biodiesel derived from various oils is already in commercial use. Depending on the fatty acid composition of the feedstock oil used in making the biodiesel, its properties can vary greatly. Providing the end user with a sufficient assurance on fuel properties and quality is of great importance. Consequently, biodiesel standards have been developed in various regions. Examples are the European biodiesel standards EN 14214 and the American standard ASTM D6751. Experimental determination of the quality parameters of a biodiesel sample requires considerable amount of time and money. Examples of the attributes of interest are the kinematic viscosity, the oxidation stability (OS), the cold flow properties, and the cetane number (CN). In some cases, it may be impossible to obtain a sufficiently large sample of a biodiesel from an emerging feedstock oil for detailed analyses. Such is commonly the case for algal biodiesel, for example. Notwithstanding this, the properties of a biodiesel may be predicted using information on the fatty acid profile of the parent oil as all the relevant properties depend directly on the fatty acids (FAs) composition of the feedstock oil. A model relating the FA profile of the feedstock oil and the biodiesel produced from it may be used as a bioprospecting tool for rapidly estimating the potential usefulness of a new feedstock oil (Bigelow et al., 2001, Ramírez-Verduzco et al., 2012, Talebi et al., 2013).

Here we introduce a user-friendly public domain computer software, the BiodieselAnalyzer©, for estimating the properties of a biodiesel from the fatty acid profile of the parent oil. This software is based on the previously published highly-reliable modeling data including ours (Talebi et al., 2013).

2. Input data

The only input data required by the BiodieselAnalyzer© is the fatty acid profile of the feedstock oil as determined by gas-chromatography (GC). Once the weight percent of the individual fatty acids present in the oil has been entered (Figure 1), pressing 'continue' leads the user to a new page where the various calculated properties of the prospective biodiesel are given under different tabs (Figure 2).

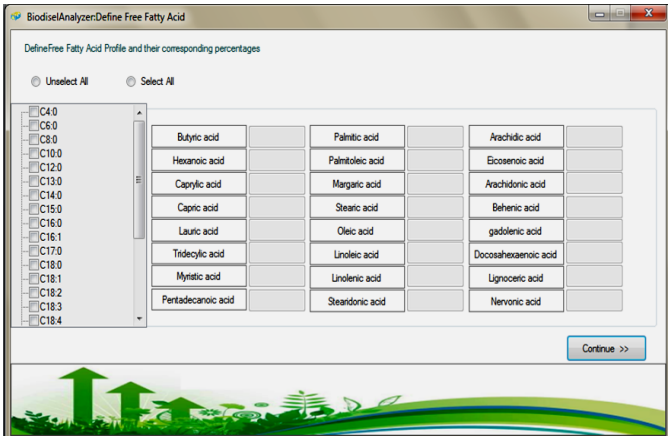

Fig. 1. Input data page for entry of the fatty acids profile as determined by gas chromatography.

Fig. 1. Results page where the prospective biodiesel properties are predicated.

3. Analysis

BiodieselAnalyzer© provides the estimated properties under the following tabs: Unsaturation Level, including the amount of the saturated and the unsaturated fatty acids and the degree of unsaturation (DU); the Cetane Number; the Cold Flow Properties including the cloud point (CP) and the cold filter plugging point (CFPP); the Oxidation Stability including the allylic (APE) and the bis-allylic position equivalents (BAPE); the Higher Heating Value (HHV); the kinematic viscosity; and the Density. The Equations 1–12 provided below are used in estimating the various properties from the fatty acid methyl ester profile (FAME) and the structure of the relevant fatty acids (Krisnangkura, 1986).

The cetane number (CN) is calculated as follows (Knothe, 2006):

$$CN = 46.3 + (5.458/SV) - (0.225 \times IV) \quad \text{(Eq. 1)}$$

The saponification value (SV) and iodine value (IV) for use in the above equation are calculated using the following equations:

$$SV = \sum(560 \times N)/M \quad \text{(Eq. 2)}$$
$$IV = \sum(254 \times D\ N)/M \quad \text{(Eq. 3)}$$

In the above equations D is the number of double bonds in the fatty ester, M is the molecular mass of the fatty ester, and N is the percentage of the particular fatty ester in the oil sample.

The degree of unsaturation (DU) is calculated using the amounts of the monounsaturated (MUFA) and polyunsaturated fatty acids (PUFA) present in the oil; thus:

$$DU = MUFA + (2 \times PUFA) \quad \text{(Eq. 4)}$$

The allylic position equivalents (APE) and bis-allylic position equivalents (BAPE) are calculated using the equations previously developed by Knothe (Knothe, 2002):

$$APE = \sum(ap_n \times A_{cn}) \quad \text{(Eq. 5)}$$
$$BAPE = \sum(bp_n \times A_{cn}) \quad \text{(Eq. 6)}$$

where ap_n and bp_n are the numbers of allylic and bis-allylic positions in a specific fatty acid, respectively, and A_{cn} is the amount (mass percent) of each fatty acid in the mixture.

The long-chain saturated factor (LCSF) and the cold filter plugging point (CFPP) are estimated:

$$LCSF = (0.1 \times C_{16}) + (0.5 \times C_{18}) + (1 \times C_{20}) + (1.5 \times C_{22}) + (2 \times C_{24}) \quad \text{(Eq. 7)}$$
$$CFPP = (3.1417 \times LCSF) - 16.477 \quad \text{(Eq. 8)}$$

The accuracy of the above empirical equations in estimating the quality of a biodiesel have been previously proven (Ramos et al., 2009).

Please cite this article as: Talebi, A.F., Tabatabaei, M., Chisti, Y., 2014. BiodieselAnalyzer©: a user-friendly software for predicting the properties of prospective biodiesel. Biofuel Research Journal 2 (2014) 55-57.

The cloud point (CP) (Sarin et al., 2009) is calculated using the following equation:

$$CP = (0.526 \times C_{16}) - 4.992 \quad \text{(Eq. 9)}$$

Eq. 9 is used to estimate the CP value based the C16:0 content (wt%) in the FA profile.

The kinematic viscosity (υ, mm^2/s) at 40 °C is estimated (Ramírez-Verduzco et al., 2012) as follows:

$$\ln(\upsilon) = \sum N_i(-12.503 + (2.496 \times \ln Mw_i) - 0.178 \times D_i) \quad \text{(Eq. 10)}$$

Here Mw_i is the molecular weight of a fatty acid, N_i is the percentage of the given fatty acid in the biodiesel and D_i is the number of double bonds in the given fatty acid (Ramírez-Verduzco et al., 2012).

The density (ρ, g/cm^3) of the biodiesel at 20 °C is estimated using the following equation (Ramírez-Verduzco et al., 2012):

$$\rho = \sum N_i(0.8463 + (4.9/Mw_i) + 0.0118 \times D_i) \quad \text{(Eq. 11)}$$

The higher heating value (HHV) of the biodiesel is estimated as follows (Ramírez-Verduzco, 2012):

$$HHV = \sum N_i(46.19 - (1794/Mw_i) - 0.21 \times D_i) \quad \text{(Eq. 12)}$$

4. Conclusions

BiodieselAnalyzer© Version 1.1 was released in the public domain on January 13, 2014, by the Biofuel Research Team (BRTeam). This software requires the Microsoft NET Framework 4 to operate. It is a especially useful tool for estimating the properties of a prospective biodiesel if the fatty acid profile of the parent oil is known, or a small sample of the oil is available for analysis.

References

Knothe, G., 2006. Analyzing biodiesel: Standards and other methods. J. Am. Oil. Chem. Soc. 83, 823–833.

Krisnangkura, K.A., 1986. A simple method for estimation of cetane index of vegetable oil methyl esters. J. Am. Oil. Chem. Soc. 63, 552–553.

Knothe, G., 2002. Structure indices in FA chemistry: How relevent is the iodine value? J. Am. Oil. Chem. Soc. 79, 847–854.

Ramos, M.J., Fernandez, C.M., Casas, A., Rodriguez, L., Perez, A., 2009. Influence of fatty acid composition of raw materials on biodiesel properties. Bioresour. Technol. 100, 261–268.

Sarin, A., Arora, R., Singh, N.P., Sarin, R., Malhotra, R.K., Kundu, K., 2009. Effect of blends of palm-jatropha-pongamia biodiesels on cloud point and pour point. Energy 34, 2016–2021.

Bigelow, N.W., Hardin, W.R., Barker, J.P., Ryken, S.A., Macrae, A.C., Cattolico, R.A., 2011. A comprehensive GC–MS sub-microscale assay for fatty acids and its applications. J. Am. Oil. Chem. Soc. 88, 1329–1338.

Ramírez-Verduzco, L.F., Rodríguez-Rodríguez, J.E., Jaramillo-Jacob, A.D.R., 2012. Predicting cetane number, kinematic viscosity, density and higher heating value of biodiesel from its fatty acid methyl ester composition. Fuel 91, 102–111.

Talebi, A.F., Mohtashami, S.K., Tabatabaei, M., Tohidfar, M., Bagheri, Zeinalabedini, M., Hadavand Mirzaei, H., Mirzajanzadeh, M., Shafaroudi, S.M., Bakhtiari, S., 2013. Fatty acids profiling; a selective criterion for screening microalgae strains for biodiesel production. Algal Res. 2, 258–267.

Please cite this article as: Talebi, A.F., Tabatabaei, M., Chisti, Y., 2014. BiodieselAnalyzer©: a user-friendly software for predicting the properties of prospective biodiesel. Biofuel Research Journal 2 (2014) 55-57.