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Full Length Article

Estimation of biodiesel cetane number, density, kinematic viscosity and heating values from its fatty acid weight composition

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A R T I C L E I N F O

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A B S T R A C T

A detailed statistical investigation was conducted in order to correlate some important biodiesel properties with the respective methyl ester weight composition in fatty acids. The examined properties were cetane number, density, kinematic viscosity and heating values (lower and higher). The chosen method for the correlation was the multiple linear regression analysis. A comprehensive data set was chosen for each interesting property as the basis for the formulation of the linear relations with respect to the eight, most important, fatty acids (lauric, myristic, palmitic, stearic, palmitoleic, oleic, linoleic, linolenic). The derived correlations were then verified against other experimental data, selected from various sources, with the aim to assess their predictive capability. It was found that for both the cetane number and density, the derived correlations were, on the one hand highly statistical, and, on the other, proved successful in predicting the corresponding properties from randomly selected samples reported in the literature. On the contrary, for both heating values and kinematic viscosity, the statistical correlations were weaker, although for the HHV the relative error between experimental and predicted values was adequately small.

1. Introduction

An extensive research has been carried out in the last decades regarding the use of biodiesel in engines. This is not surprising since methyl esters produced from agricultural or animal products succeed in reducing the dependence on oil imports, while at the same time they enhance the local economy and energy security, and manifest a positive CO_2 balance [1–6]. Furthermore, when burned in compression ignition engines, the combustion of biodiesel usually produces lower carbonaceous pollutant emissions [3,5].

One peculiar aspect of biodiesels (and their originating vegetable oils) is the fact that they are produced from a variety of feedstocks possessing different chemical composition. Since the structure of each oil/fat in fatty acids varies (sometimes by a lot) depending on its origin, the physical and chemical properties of biodiesel differ too; prominent examples here are the cetane number and the cold-flow properties [1–5]. Thus, the combustion characteristics and emissions from engines vary, sometimes by a lot, depending on the exact biodiesel used [3,5].

A logical question arises here, as to which feedstock possesses the 'best' composition, or, better still, what would be a superior fatty acid (FA) composition, with the ultimate goal to achieve 'better' engine performance and lower emissions. Many researchers have investigated such issues in the past [7–11], and it seems that a reasonable step is to try and correlate biodiesel properties with specific oil attributes such as fatty acid composition, chain length, molecular weight, degree of unsaturation or number of double bonds [e.g. [12–22]]. For example, Bamgboye and Hansen [12] reported one such correlation with respect to the FA composition for cetane number (CN) applying linear regression analysis. Piloto-Rodriguez et al. [13] focused on cetane number too applying both multiple linear regression (MLR) and artificial neural networks (ANN). The latter approach was the one followed by Ramadhas et al. [14], while the former (MLR) was chosen by Gopinath et al. [15]. Apart from CN, existing reports on other properties have correlated, for example, density with temperature [18]; density, viscosity, CN and higher heating value were inter-related with molecular weight and number of double bonds by Ramirez-Verduzco et al. [19]. Ramos et al. [20] correlated oxidation stability, cetane number, iodine value and cold filter plugging point with the methyl ester degree of unsaturation and long chain saturated factor. Lastly, a quadratic correlation with the number of carbon atoms in the original fatty acid and the number of double bonds was statistically selected as the most suitable by Lapuerta et al. [22], again for cetane number.

The research group involving the first author has studied broadly the use of biodiesels in engines, under both steady-state [23] and transient conditions [5,24]. Moreover, two extensive statistical analyses have been conducted, aiming to identify and analyze the effects of the

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Nomenclature

CN	cetane number
EU	European Union
FA	fatty acid
FAME	fatty acid methyl ester
HHV	higher heating value
LHV	lower heating value
ME	methyl ester
MLR	multiple linear regression
PME	palm methyl ester
RME	rapeseed methyl ester
SME	soybean methyl ester
TME	tallow methyl ester

biodiesel originating feedstocks on engine emissions [25], and on the properties of the fuel [26]. For the current work, which is, in a sense, continuation of [26], the focus is again on the biodiesel properties, but now aiming to formulate *predictive correlations with respect to the fatty acid weight composition applying multiple linear regression techniques.*

The target is to expand on previous analyses on the subject [12,13,15] as regards: a) the sample of oils/biodiesel feedstocks taken under consideration, b) the predictive capability of the obtained correlations and c) the number of investigated properties. With respect to the latter, the usually investigated property is cetane number. In this work, we also focus on density, kinematic viscosity and heating values (lower and higher).

2. Methodology

In order to proceed to the formulation of a reliable correlation between biodiesel properties and the respective fatty acid weight composition, the first step was the selection of an appropriately large and representative sample of reported (experimental) values from the literature. It was our intention to use a broad sample so as to include a great variety of published data from many sources and feedstocks, including also neat fatty acids. Particularly in regard to the fatty acids

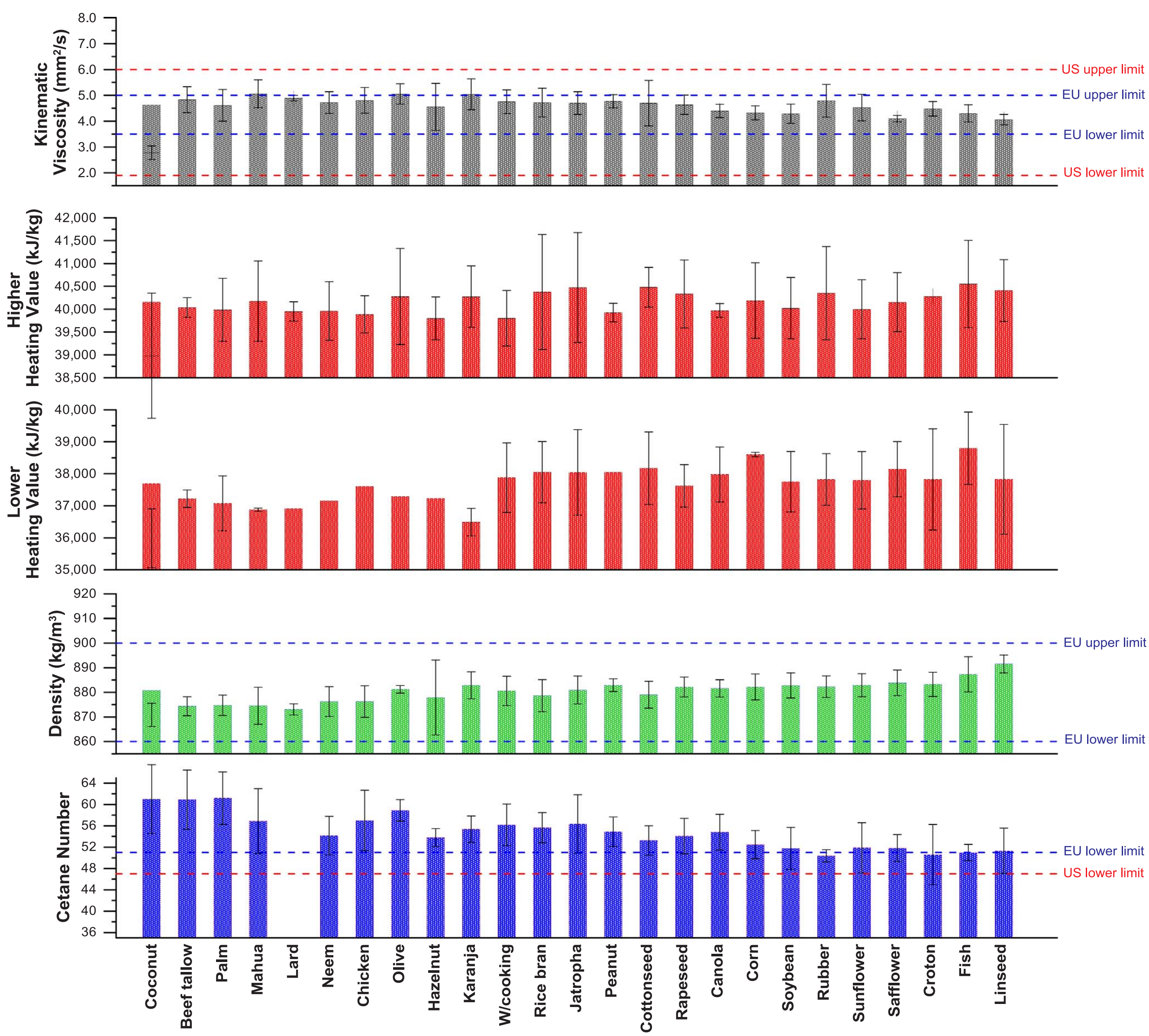

Fig. 1. Cetane number, density, heating values and kinematic viscosity for biodiesels from various feedstocks (data from [26]).