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Neural network prediction of biodiesel kinematic viscosity at 313 K

Xiangzan Meng [a], Ming Jia [b], Tianyou Wang [a,*]

[a] State Key Laboratory of Engines, Tianjin University, Tianjin 300072, China
[b] School of Energy and Power Engineering, Dalian University of Technology, Dalian 116024, China

HIGHLIGHTS

- An ANN method was developed to predict the kinematic viscosity of biodiesel at 313 K.
- The ANN method avoids the need of the kinematic viscosities of the individual FAMEs.
- The ANN method has a better performance than two previous prediction methods.
- The ANN method can be trained to account for the effect of double bond position on viscosity.

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ABSTRACT

Viscosity is an important fluid property because of its direct relation with the fuel injection process for engines. The kinematic viscosity of biodiesel at 313 K should satisfy the range specified by the international biodiesel standards. In this study, an artificial neural network (ANN) method was developed to predict the biodiesel kinematic viscosity at 313 K with the experimental data of 105 biodiesel samples collected from the literature. The ANN method only uses the mass fractions of 19 fatty acid methyl esters (FAMEs) as inputs, which avoids the need of the kinematic viscosities of the individual FAMEs required by the prediction methods using the mixing equations. Two previously reported methods based on empirical equations, the Knothe–Steidley method with the experimental or predicted (when experimental data are unavailable) viscosities of FAMEs as inputs and the Ramírez-Verduzco method with the predicted viscosities of FAMEs as inputs were also extensively evaluated to compare with the proposed ANN method. Results indicate that the proposed ANN method is able to predict overall more accurate biodiesel kinematic viscosities at 313 K with the mean squared error (MSE) of 0.0099 compared with the Knothe–Steidley method and the Ramírez-Verduzco method. In most cases, both the Knothe–Steidley method and the Ramírez-Verduzco method tend to under-predict the kinematic viscosities. The underestimation might be attributed to the viscosity contributions of minor mono-, di- and triacylglycerols resulting from incomplete transesterification and minor or trace amount of other FAMEs to the experimental viscosities, as well as the neglect of the interactions between the individual components in calculation of the mixture kinematic viscosities. However, the ANN method could learn to account for the viscosity contributions from the minor components and the interactions between the individual components to some extent during the training process. Overall, the ANN method realizes the best accuracy for the prediction of biodiesel kinematic viscosity with the highest correlation coefficient of 0.9774.

1. Introduction

With increasing energy demand and environment concern while continuing depletion of the petroleum-based energy, increasing attention is being paid for alternative renewable energy sources [1–3]. Biodiesel is one of the potential alternatives, which is renewable, biodegradable, nontoxic and environmentally friendly [4–6]. Biodiesel is a mixture of long chain fatty acid alkyl esters, which can be derived from various feedstocks including oil-bearing crops, animal fats and algal lipids through the transesterification reaction with alcohols [3]. Methanol is the most commonly used alcohol and the produced biodiesel is often referred to as fatty acid methyl esters (FAMEs). The properties of biodiesels derived from different feedstocks vary from one another due to the variation of fatty acid composition. To guarantee the fuel quality, biodiesel has to satisfy the international biodiesel standards [3], such as the European Standard (EN) 14214 in Europe [7] and the American Society for Testing and Materials (ASTM) D6751 in the United States of America [8].

Viscosity, a measure of resistance to flow of a liquid due to the internal fluid friction [9,10], is an important property because of its

* Corresponding author. Tel./fax: +86 22 27403434.
E-mail address: wangtianyou@tju.edu.cn (T. Wang).

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direct relation with the fuel injection process in engines [3,10]. Biodiesel viscosity is usually higher than that of diesel, which results in longer liquid penetration and worse atomization [11–13] compared with diesel fuel. The viscosity of biodiesel from different feedstocks varies with the FAME composition and the viscosity of FAME increases with the chain length and the degree of saturation [14]. Various feedstocks have been transesterificated to investigate their feasibility as the biodiesel sources recently [2,6,15–25]. The kinematic viscosity at 313 K of biodiesel from a newly investigated feedstock usually has to be determined experimentally to check if it is within the acceptable range specified by biodiesel standards, which is 3.5–5.0 mm^2/s in the EN 14214 [7] and 1.9–6.0 mm^2/s in the ASTM D6751 [8].

Accurate prediction methods are of great practical value in predicting the kinematic viscosity of biodiesel or FAMEs, and relevant studies can be found in the recent literature. Krisnangkura et al. [26] fitted empirical equations to predict the temperature-dependent kinematic viscosities of saturated FAMEs as a function of the carbon number in the corresponding fatty acid. Yuan et al. [27] developed a mixture topological index method to predict the kinematic viscosity of biodiesel. More recently, Ramírez-Verduzco et al. [28] correlated the kinematic viscosity at 313 K with the molecular weight and the double bond number of FAME. The simplified form of the Grunberg–Nissan equation [29] used by Allen et al. [30], which neglects the interactions between the individual components, was usually applied to determine the biodiesel kinematic viscosity from its FAME composition in the aforementioned work. Knothe and Steidley [31] further simplified the Grunberg–Nissan equation [29] by directly using the viscosity values rather than their logarithms and the biodiesel kinematic viscosity was computed based on the experimental kinematic viscosities of the individual FAMEs [14,31,32]. They also developed several methods to calculate the viscosity contributions from some long chain FAMEs, of which the kinematic viscosities at 313 K cannot be measured by experiment because their melting points are higher than 313 K [31].

It is worth noting that, in order to apply the above prediction methods to determine the biodiesel kinematic viscosity, the kinematic viscosities of the individual FAMEs must be experimentally measured or numerically computed. Moreover, some methods did not cover the kinematic viscosities for the long chain FAMEs with melting points higher than 313 K [26,27]. Knothe and Steidley [31] used the calculated viscosity contributions as the pseudo kinematic viscosities of the long chain FAMEs. The correlation developed by Ramírez-Verduzco et al. [28] can also be used to predict the pseudo kinematic viscosities of these FAMEs. However, both of these two methods have not been extensively validated yet. To avoid the need of the kinematic viscosities of the individual FAMEs, the artificial neural networks (ANNs), as an alternative, can be applied to predict the kinematic viscosity of biodiesel with only the FAME composition as the input.

ANNs are widely accepted as an information processing methodology inspired by the working process of the human brain [33]. ANNs are efficient in handling the nonlinear relationship in data [33,34] and have been used to predict biodiesel properties recently. Ramadhas et al. [35] evaluated four types of ANNs and found that the ANNs are effective and accurate methods in predicting the cetane number of biodiesel with the compositions of five FAMEs as inputs. Baroutian et al. [36] developed a feed forward back propagation neutral network to predict the temperature-dependent palm biodiesel densities and found the ANNs better reproduced the measured biodiesel density than the empirical and theoretical methods. Cheenkachorn [37] applied statistical models using best subset method and ANNs to predict the kinematic viscosity, high-heating value, and cetane number of biodiesel from fatty acid compositions. It was observed that the ANN models were more accurate and the need of detailed physical properties of the biodiesel mixture for the prediction of the kinematic viscosity was addressed as well. Balabin et al. [38] evaluated multiple methods in predicting biodiesel density, kinematic viscosity, methanol and water contents from near infrared (NIR) spectra and concluded that the ANN model was superior to the linear and the "quasi"-non-linear calibration methods. The possibility of using ANNs to predict the density and dynamic viscosity of biofuel compounds was also demonstrated by Saldana et al. [39]. More recently, Bhattacharyulu et al. [40] modeled the effect of operating conditions on the neem oil biodiesel viscosity using the ANN technique with acceptable accuracy. Piloto-Rodriguez et al. [41] successfully applied the ANNs to predict the cetane number of biodiesel with the compositions of ten FAMEs as inputs, and a better accuracy was achieved by the ANNs than the multiple linear regression model. The applications of ANNs in predicting biodiesel production, engine performance and emissions fueled with biodiesel were also reported [34,42–45].

It should be noted that the ANN model developed by Balabin et al. [38] were based on the NIR spectra data. In general, the FAME composition determined by the gas chromatography (GC) technology is the most commonly reported data for biodiesel samples rather than the NIR spectra data [10]. Therefore, this study aims at developing a biodiesel kinematic viscosity prediction method using the ANNs with only the FAME composition as the input to avoid the need of the kinematic viscosities of the individual FAMEs, which is required by the prediction methods using the mixing equations. Meanwhile, two previously reported prediction methods by Knothe and Steidley [31] and Ramírez-Verduzco et al. [28] for the prediction of biodiesel kinematic viscosity were extensively evaluated with more than one hundred biodiesel samples to compare their performance with the developed ANN method in this study.

2. Experimental data

In this study, the experimental data of 105 biodiesel samples were collected from the literature [2,5,6,12,15–26,28,46–78] to develop and validate the ANN method in comparison with two previously reported prediction methods. The components that compromise these biodiesel samples are 19 FAMEs and the detailed composition profiles can be found in the supplementary material. The number of the biodiesel samples containing specific FAMEs and the content distributions of different FAMEs are shown in Fig. 1(a and b), respectively. It can be seen that methyl esters C16:0, C18:0, C18:1, C18:2 and C18:3 are the most common components. Although several FAMEs are not the common components, they are the major components in some biodiesel samples. For example, methyl ester C10:0 with the mass fraction of 64.7% is the major component of cuphea oil biodiesel, which has a comparable kinematic viscosity with diesel [6]; methyl ester C12:0 with the mass fraction nearly 50% is the major component of babassu biodiesel [57], coconut biodiesel [26,49–51,57] and palm kernel biodiesel [12]. Other FAMEs are usually the minor components with the average mass fraction less than 10%.

3. Prediction methods

The Grunberg–Nissan equation [29] is a widely applied mixture equation for computing the viscosity of liquid mixtures [9] as

$$\ln \eta_m = \sum_{i=1}^{n} x_i \ln \eta_i + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1, j\neq i}^{n} x_i x_j G_{ij} \quad (1)$$