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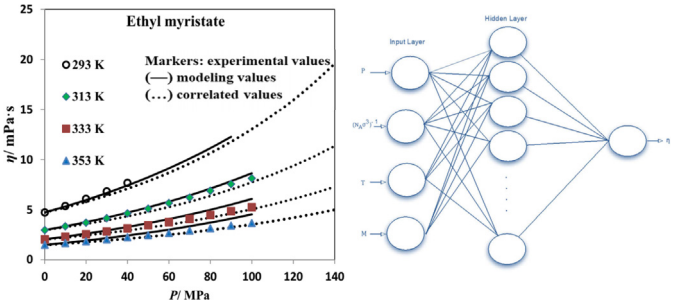
Full Length Article

Viscosities of some fatty acid esters and biodiesel fuels from a rough hard-sphere-chain model and artificial neural network

Sayed Mostafa Hosseini[a,*], Mariano Pierantozzi[b], Jalil Moghadasi[c]

[a] Department of Chemistry, Faculty of Sciences, University of Hormozgan, Bandar Abbas 71961, Iran
[b] SAAD, Università degli Studi di Camerino, 63100 Ascoli Piceno, Italy
[c] Department of Chemistry, Shiraz University, Shiraz 71454, Iran

GRAPHICAL ABSTRACT



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ABSTRACT

This work addresses the prediction of dynamic viscosities of several fatty acid esters and biodiesel fuels using a semi-theoretical model and artificial neural network as well. The semi-theoretical model used rough hard-sphere theory for the correlation and prediction of dynamic viscosities. In this respect, a smooth hard-sphere-chain expression and a coupling parameter of translational-rotational motions were employed to develop the rough hard-sphere-chain scheme. The three molecular parameters as well as the liquid densities required in this model were taken from previously developed perturbed Yukawa-chain equation of state (Fluid Phase Equilibria, 372 (2014) 105–112). Artificial neural network modeling employed a multilayer perceptron comprising one hidden layer and 21 neurons, managed according to the constructive approach. The performance of both semi-theoretical and ANN model have been checked by predicting dynamic viscosities over the temperature range within 283–393 K and pressures up to 140 MPa with the average absolute relative deviation of 3.10% (for 648 data points) and 0.91% (for 796 data points), respectively. The ANN model developed herein, has been trained, validated and tested for the set of data gathered, pointing that the efficiency of the neural network model was found excellent on the entire dataset.

1. Introduction

Biodiesels are promising alternative to the common diesel fuels because they are renewable and significantly reduce particulate matter, hydrocarbon, carbon monoxide and life cycle net carbon dioxide emissions [1,2] from combustion sources as well. Because of these

Abbreviations: FAE, fatty acid ester; S, soybean; R, rapeseed; S + R, soybean + rapeseed

* Corresponding author.
E-mail address: sm.hosseini@hormozgan.ac.ir (S.M. Hosseini).

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Nomenclature

b	van der Waals co-volume, m^3
x	mole fraction
C_η	coupling parameter
M_w	molar mass/g·mol^{-1}
P	pressure, Pa
R	gas constant, J/(mol·K)
T	absolute temperature, K
k_B	Boltzmann constant, J·K^{-1}
F_η	temperature-dependent function
c_1-c_3	coefficients that used in Eq. (12)
N	Avogadro's number, mol^{-1}

Greek letters

ε	dispersive energy parameter/J
σ	hard-core diameter/nm
ρ	molar density
η	dynamic viscosity/Pa·s
y	hard-sphere packing fraction
η^*	reduced viscosity

Subscripts

SHSC	smooth hard-sphere-chain
RHS	rough hard-sphere
SHS	smooth hard-sphere
SHS-MET	smooth hard-sphere expression taken from modified Enskog's theory

Superscripts

*	reduced
HSC	hard-sphere-chain

advantages, they gained considerably the scientific community attention over the past decade.

The knowledge of thermophysical property data of biodiesels is crucial to optimize the utilization of them in diesel engines. Among these properties, dynamic viscosity is one of the most significant properties affecting the utilization of biodiesel fuels due to its effect on the in-cylinder fuel atomization process in direct injection diesel engines [3]. The higher viscosity of biodiesels against the common diesel fuels could increase fuel penetration in the combustion chamber [4], consequently affecting combustion and emissions from the engine. Therefore the choice of qualified biodiesels for engine manufacturers is limited to the knowledge of their viscosity data over the vast pressure range, for which the available measured data are not still much in open literature. On the other hand, the knowledge of thermophysical properties of fatty acid esters such as their density and viscosity in the extended temperature and pressure ranging allows us to choose appropriate fatty acid profile that will give the desired biodiesel quality for the injection into the combustion chamber under high-pressures. In this case, some experimental data thermophysical properties of fatty acid esters have yet been reported in literature but those values are not enough available to determine the viscosity of biodiesel from the viscosity of pure fatty acid alkyl esters by using simple mixing rules [5].

Under these circumstances, the development of predictive models for thermophysical property data of biodiesels and fatty acid esters, in particular their viscosities over a wide pressure and temperature ranging is important task to supplement the available experimental data.

So far, numerous predictive methods for viscosities of biodiesels and fatty acid esters have been developed in literature based on the various approaches, from empirically-based equations [6] to those are coming from the group-contribution [7], Artificial neural network models [8,9] as well as fatty acid-composition-based approaches [10]. The semi-theoretical approaches have also been widely come into focus in literature for viscosity prediction of dense fluids, such as the friction theory (FT), free-volume theory (FVT) and Yarranton-Satyro (YS) correlation-based approaches [11,12].

Apart from this, several researchers tried to survey the predictive models for viscosities biodiesels and fatty acid esters by some review papers [13,14]. The first effort is the work of Freitas et al. [13] who evaluated the predictive capability of Ceriani's, Krisnangkura's, and Yuan's models, along with a revised version of Yuan's model for the description of the viscosities of biodiesels and their blend with other fuels. The latter, is the work of Verduzco [14] who not only reviewed the available empirical models for viscosities of biodiesels and fatty acid esters, also, suggested an alternative empirical model relating the molecular weight, fatty acid methyl ester type (saturated or unsaturated), and temperature to dynamic viscosity of fatty acid methyl esters. Then, some mixing rules in conjunction with empirical models of FAMEs were used to estimate the viscosity of biodiesels from 3 data sources. Verduzco 's model could estimate the dynamic viscosity of twenty two biodiesel samples, fourteen mixtures of FAMEs and one binary biodiesel mixture with the average absolute relative deviation (AARD, Eq. (1) of 6.39% which was more accurate than the models tested in the work of Feitosa et al. [13], where the AARD of 8.07% for Ceriani's model, 5.34% for Yuan's model, 4.65% for the revised Yuan's model and 7.25% for Krisnangkura's model were obtained. For each property, the average absolute relative deviation, AARD, is calculated as:

$$AARD\% = \frac{100}{NP}\sum_{i=1}^{NP}\frac{|x_i^{exp} - x_i^{calc}|}{x_i^{exp}} \quad (1)$$

where x is the property under consideration and NP is the number of points in the dataset.

Among the above-mentioned predictive and correlative methods, less emphasize has been placed on the assessment of the robustness of physical- and semi-theoretical-based approaches for transport property of biodiesels and fatty acid esters, in particular their viscosities based on the rough hard- sphere (RHS) theory [15–17] and the subsequent developments. Some aspects of the RHS-based approaches make them district when compared with other semi-theoretical approaches such as FT-, FVT- and YS correlation. It is necessary to define different sets of equations to be used in the above-mentioned approaches especially FT-based approaches which use different sets of equations for friction coefficients [11]. This aspect limits the generality of those approaches. Now, let's consider RHS-based approaches, they are user friendly to be adapted for various fluids of intermolecular forces regardless of the details of the molecular structures in contrary to FVT-based approaches [18]. Although RHS-based approaches use different sets of coefficients for the temperature-dependent parameter appearing in the characteristic molar volume of the liquid [16,19,20], the preceding works of Hosseini et al. [21,22] led to a general roughness factor being a universal function of reduced pressure which makes this approach distinct from other semi-theoretical-based viscosity prediction models.

This work is the continuation of our previous studies on the assessment of RHS-based models for transport properties of highly non-simple fluids [21–23]. It was found that, regardless of the fact that the RHS is based on the hard-sphere concept have to be extended by orders of magnitude, it is still an excellent scheme for the correlation and prediction of the properties of highly non-simple liquids; this fact is attributed to its theoretical basis.

Very recently, Hosseini et al. [21,22] developed some semi-