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APPLICATION OF ADAPTIVE NEURO-FUZZY INFERENCE SYSTEMS AND ARTIFICIAL NEURAL NETWORK AND FOR KINEMATIC VISCOSITY OF BIODIESEL PREDICTION

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ABSTRACT

This study investigates the applicability of adaptive neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) approaches for modeling the fatty acid methyl esters (FAMEs) property including kinematic viscosity at various temperatures and the volume fractions of biodiesel. An experimental database of kinematic viscosity of pure biodiesel was used for developing of models, where the input variables in the network were the temperature, the number of carbon atoms (NC) and the number of hydrogen atoms (NH) of the composition of methyl esters (C8:0, C10:0, C12:0, C14:0, C16:0, C16:1, C18:0, C18:1, C18:2, C18:3, C20:0, C20:1, C22:0, C22:1, C24:0 were considered as input variables on the ANFIS and ANN. Moreover, the models are divided into saturated species from C8:0 to C24:0 and unsaturated species, from C16:1 to C22:1. The model results were compared with experimental ones for determining the accuracy of the ANFIS and ANN predictions. The developed model produced idealized results and was found to be useful for predicting the kinematic viscosity of biodiesel blends with a limited number of available data. Moreover, the results suggest that the ANFIS approach can be used successfully for predicting the kinematic viscosity of biodiesel blends at various volume fractions and temperature compared to ANN approach.

KEYWORDS: Biodiesel blends; composition of methyl esters; kinematic viscosity; number of carbon atoms; number of hydrogen atoms

I. INTRODUCTION

Reducing sources of fossil fuels and their pollution has been the aim of extensive research performed on alternative energy sources, particularly renewable fuels. Biodiesel is an alternative renewable fuel for diesel fuel, which includes alkyl esters of fatty acids obtained from vegetable oils or animal fats by transesterification reaction. [1-3]

Biodiesel has many advantages, which have caused the consideration of this fuel in recent years. It is biodegradable, nontoxic, and renewable. In addition, biodiesel has a higher cetane number and a flash point than diesel oil and effectively reduces the release of hydrocarbons and carbon monoxide and suspends particles from combustion. Biodiesel dissolves in diesel oil completely so it can be combined in any percent. Differences between biodiesel and diesel fuels exist (higher density and viscosity, higher cloud point and pour point (in some cases), and lower heat of combustion), but biodiesel can be used pure or mixed with diesel, without modification in diesel equipment directly. [4-6]

Kinematic viscosity is considered the key of fuel properties according to diesel and biodiesel fuel standards. Biodiesel viscosity is usually higher than that of diesel, which results in longer liquid penetration and worse atomization [7-9] 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 [10]. Various feedstocks have been transesterificated to investigate their feasibility as the biodiesel sources recently [11-17].

Experimental methods are often used in the determination of fuel properties [11, 18-22] which provide good and high degree of accuracy results. This experimental determination of biodiesel fuel properties has to be conducted in accordance with standard test methods which have been provided for in the different standards world over. The cost of running these tests is high, and is technically challenging, energy and time consuming. In a case in which these three issues are considered to be a minor issue, the availability of a well equipped

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laboratory to perform these tests is scarce. Subject to the above, mathematical models [23, 24], statistical models [25-30], neuro fuzzy [31-33] and artificial neural network [34-39] have been used in predicting the properties of biodiesel including viscosity, density or cold flow properties.

This present study evaluated the efficiency of ANFIS and ANN in accurately predicting the kinematic viscosity of saturated and unsaturated biodiesel for wide ranges of temperature and hydrocarbon chain length. The details of the calculation method, numerical validation, and comparative statistical analysis are fully described in this work. The ANFIS and ANN to be developed in this paper address a more extensive database that published in other works.

II. METHODOLOGY

The adaptive neuro-fuzzy inference system (ANFIS) and Artificial neural networks (ANN) have been used extensively in biodiesel properties modeling, due to their ability to model nonlinear systems efficiently. The theoretical background of Artificial Neural Network (ANN) and Adaptive Neuro-Fuzzy Inference System (ANFIS) are given in [40-43]. The main steps that were followed in this work to develop predictive models of kinematic viscosity of biodiesel and fatty acid methyl esters (Biodiesel) are presented. Kinematic viscosity data of different biodiesel samples at different temperatures were gathered from the literature [44-49]. The experimental data was obtained from scientific publication (Table 1) to estimate the kinematic viscosity of biodiesel.

Table 1. Kinematic Viscosity in mm^2/s of FAMEs Data

T[K]	C6:0	C8:0	C10:0	C12:0	C14:0	C14.1	C16:0	C16.1	C18:0	C18.1	C18.2	C18.3	C20:0	C22:0
263.15			5.5			9.92		14.77		21.33	14.1	10.19		
			5.4			8.37		12.19		17.22	11.8	8.87		
			4.04			7.01		10.15		14.03	9.84	7.33		
268.15			4.68			6.13		12.19		11.66	8.47	6.59		
273.15	2.31		4.04		7						8.322	6.965		
278.15			3.378	5.45							8.46	6.9658		
			3.49								8.3219	6.966		
			3.378			5.35		7.33		9.869	7.3	5.53		
283.15	1.179	1.967	3.01	4.654							7.236	6		
		1.913	3.014	4.635							7.2365	6.176		
		1.931	3.014	4.79								6.1773		
				4.364								6.1774		
288.15	1.084	1.772	2.689	4.093		4.73		5.341		8.51	6.43	5.524		
		1.769	2.708	4.094				6.38		8.49	6.355	5.14		
			2.71	4.07							6.43	5.5241		
293.15	1.01	1.61	2.421	3.627	5.201	4.13		4.723		7.33	5.61	4.57		
	1.012	1.59	2.437	3.54				5.56		7.379	5.622	4.972		
	1.011	1.628	2.449	3.641						7.23	5.58	4.84		
		1.627	2.49	3.63						7.38	5.61	4.9722		
			2.45	3.64							5.6194			
			2.448			3.71		4.94		6.44	5.03	4.07		
298.15	0.9412	1.471	2.196	3.225	4.611			4.214		6.472	5.017	4.501		
		1.504	2.227	3.261	4.6105					6.47		4.5011		
			2.23	3.29		3.37		3.806		5.72				
				3.2614				4.42		5.724	4.53	3.88		
303.15	0.8822	1.368	2.004	3.892	4.12						4.508	4.099		
		1.396	2.037	2.942	4.1643						4.5079	4.0989		
		1.39	2.05	2.95								4.0973		
			2.036	2.942		3.04		3.96		5.08	4.08	3.32		
				2.942				3.432		5.099	4.075	3.75		
308.15	0.83	1.262	1.832	2.618	3.698		4.929					4.0504		
		1.3	1.871	2.668	3.697							3.7504		
		1.3001	1.87	2.69		2.73		3.064		4.51	3.65	3.09		
			1.871	2.668				3.67		4.573	3.703	3.298		
310.95	0.81	1.207	1.765	2.487	3.456		4.688		5.881	4.45	3.64	3.27		
313.15	0.785	1.17	1.686	2.384	3.338		4.32		5.61	4.721	3.702	3.14	7.4	6.955
	0.785	1.16	1.69	2.433	3.3		4.414		5.867			3.2898		
		1.215	1.726	2.431	2.73		4.38	2.85	5.58	4.125	3.383	3.028		
		1.19	1.71	2.41	3.3381		4.4136		5.867	4.123	3.103	3.0284		
313.15				2.43	3.0303						3.102			
				2.433	3.23						3.3826			
	0.7422	1.099	1.566	2.139	3.0303		2.977	2.57	5.241	3.742	3.103	2.811		
		1.138	1.589	2.229			2.9766	2.229	5.2451	3.121	2.644	2.434		
		1.138		2.228								2.263		
318.15	0.7014	1.028	1.452	2.014	2.764		3.602		4.706				5.736	
		1.069	1.485	2.05	2.763				4.705			2.4343	5.737	

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			1.06	1.184				1.918				2.1		

Table 1. Continued

T[K]	C6:0	C8:0	C10:0	C12:0	C14:0	C14.1	C16:0	C16:1	C18:0	C18.1	C18.2	C18.3	C20:0	C22:0
328.15	0.6668	0.966	1.353	1.859	2.533		3.28	2.06	4.254	2.871	2.453	2.09	5.154	
		1.006	1.384	1.893	2.5327			1.918	3.666	2.651	2.2832	2.1002	5.153	
			1.383						4.2537	2.6	2.25	2.0903		
	0.632		1.263	1.724	2.323		2.998		3.861	2.457	2.132	1.96	4.23	5.692
333.15	0.6332		1.276	1.732	2.33		3.001	1.792	3.666		2.1507	1.9621	4.657	5.691
			1.294	1.724	2.329				3.8611			1.9598		
			1.291	1.755				1.658			1.966	1.845		
										2.6		1.8455		
								1.573				1.742		

The development of the proposed approaches was performed as follows. In the first step, the experimental measurement data were separated into input data (independent variables, temperature, NC and NH of the composition of methyl esters (saturated, C8:0, C10:0, C12:0, C14:0, C16:0, C18:0, C20:0, C22:0, C24:0, and unsaturated, C16:1, C18:1, C18:2, C18:3, C20:1, C22:1,), and output data (dependent variable in term of kinematic viscosity)). Subsequently, different approaches (ANFIS and ANN) were proposed to describe the behavior of the kinematic viscosity, as a function of temperature and volume fraction of biodiesel. In this case, the database was randomly divided into three groups with 60% to training, 20% to testing and 20% to checking or validation. Since the input variables on the artificial neural network have different magnitude, a normalization of them is required. We use a range between 0.1 and 0.9 according with the proposal of Khataee and Kasiri [50,51], as follows:

$$\theta_n = 0.8\left(\frac{\theta - min(\theta)}{max(\theta) - min(\theta)}\right) + 0.1 \quad (1)$$

where θ_n is the normalized input variable, the minimum (min) and maximum (max) values are the shown in Table 2.

Table 2. Limit values for the input and output variables on ANFIS and ANN models

	Limit		Unit
Input	**Minimum**	**Maximum**	
Temperature	263.15	333.15	K
Number of Carbon	7.00	23.00	-
Number of Hydrogen	14.00	46.00	-
Output			
Viscosity	0.46	21.33	mm/s^2

In general, the calculation methodology used in this work had three stages:

1. Collect experimental data from the literature to make a robust database;
2. Develop ANFIS/ANN models able to predict the kinematic viscosity of biodiesel
3. Implement a comparative study between the simulated and experimental properties.

Furthermore, a sensitivity analysis was applied to find the variables of greater influence on the response variable (Figure 1). The Matlab2015 software was used for the application of the adaptive neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) approaches.

Appraisal of the Developed Models

The developed ANFIS and ANN models were evaluated comprehensively for predicting the biodiesel properties of biodiesel samples. The following statistical indicators were employed: correlation coefficients (R), coefficient of determination (R^2), mean squared error (MSE), root mean squared error (RMSE) and absolute average deviation (AAD).

$$R = \frac{\sum_i^n (a_{p,i} - a_{p,ave}).(a_{e,i} - a_{p,ave})}{\sqrt{\left[\sum_i^n (a_{p,i} - a_{p,ave})^2\right]\left[\sum_i^n (a_{e,i} - a_{p,ave})^2\right]}} \quad (2)$$

$$R^2 = 1 - \frac{\sum_{i=1}^n (a_{e,i} - a_{p,i})^2}{\sum_{i=1}^n (a_{p,i} - a_{e,ave})^2} \quad (3)$$

$$MSE = \frac{1}{n}\sum_{i=1}^n (a_{e,i} - a_{p,i})^2 \quad (4)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^n (a_{e,i} - a_{p,i})^2} \quad (5)$$

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$$AAD = \frac{100}{n}\sum_{i=1}^{n}\left|\frac{a_{cal,i} - a_{exp,i}}{a_{exp,i}}\right| \quad (6)$$

where n is the number of experimental data, $a_{p,i}$ is the predicted values, $a_{e,i}$ is the experimental values, $a_{e,ave}$ is the average experimental values, $a_{p,ave}$ is the average predicted values and *i* is the number of input variables.

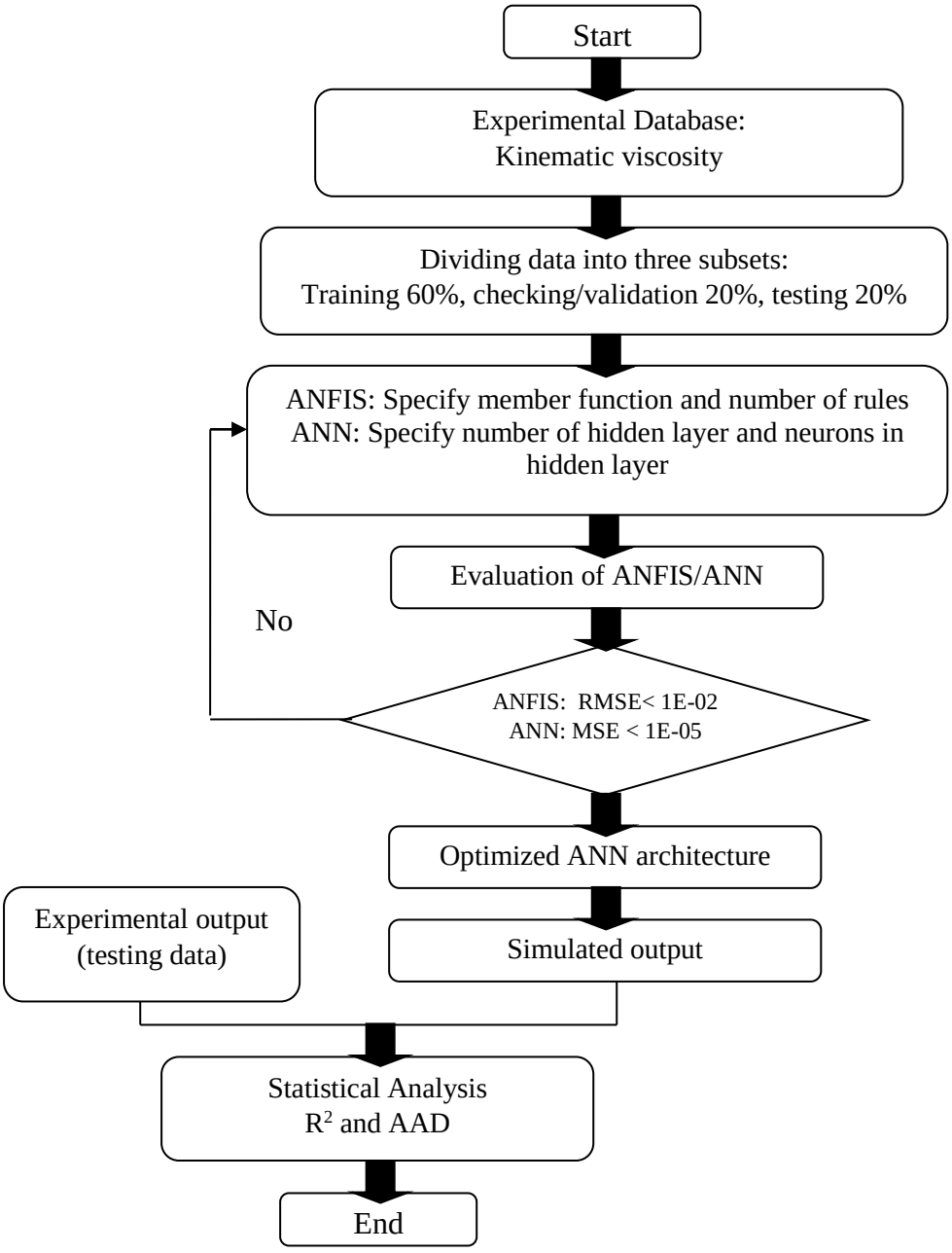

Figure 1. Algorithm used in this work for the development of the ANFIS and ANN models

III. RESULTS AND DISCUSSION

Adaptive Neuro–Fuzzy Inference System (ANFIS) Model for Saturated and Unsaturated FAMEs

The model was trained with part of the database derived from the experimental results of previous studies. The database was first split into training data and testing data. The training data set was also split into two parts, a training set (60%) and a checking set (20%). The use of checking sets in ANFIS learning beside the training set

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is a recommended technique to guarantee model generalization and to avoid over-fitting the model to the training data set.

In this study, by trial and error, the best number of membership functions for each input was determined as 5, the membership grades takes the Triangular-shaped membership functions and the output part of each rule uses a linear defuzzifier formula. In this research, two methods, hybrid and back propagation tested for generation ANFIS that the results is presented in Table 3. The results show the training error in the hybrid method is lower of back-propagation method. Therefore, the hybrid method has used for simulations. The developed ANFIS model for predicting the kinematic viscosity at different temperature, NC and NH is shown in Figure 2.

Table 3. The ANFIS information used in this study

	Saturated FAMEs		Unsaturated FAMEs	
	Hybrid	**Back-propagation**	**Hybrid**	**Back-propagation**
Epoch	1000	1000	1000	1000
Training error	0.0082	0.0088	0.0228	0.0237
Tasting error	0.0243	0.0345	0.0229	0.0264
Checking error	0.0218	0.0310	0.0540	0.0620
Number of nodes	286	286	286	286
Number of linear parameters	500	500	500	500
Number of nonlinear parameters	45	45	45	45
Number of fuzzy rules	125	125	125	125

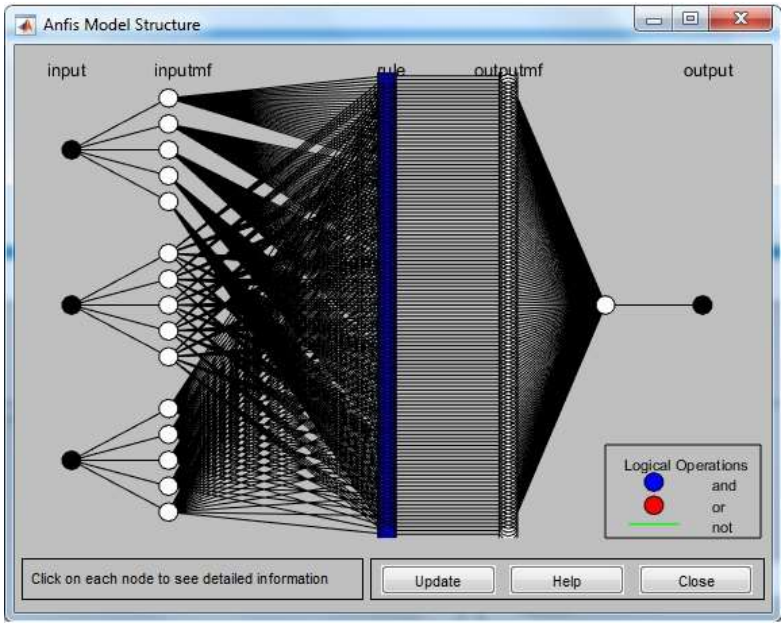

Figure 2. Structure of ANFIS models

The three-dimensional surface plots of kinematic viscosity of biodiesel against temperature and number of carbon atoms and number of hydrogen atom of biodiesel is depicted in Figure 3. The plot suggests strong interaction between the variables with significant influence on the viscosity of biodiesel. From the Figure, increasing in temperature leads to increase the viscosity of biodiesel.

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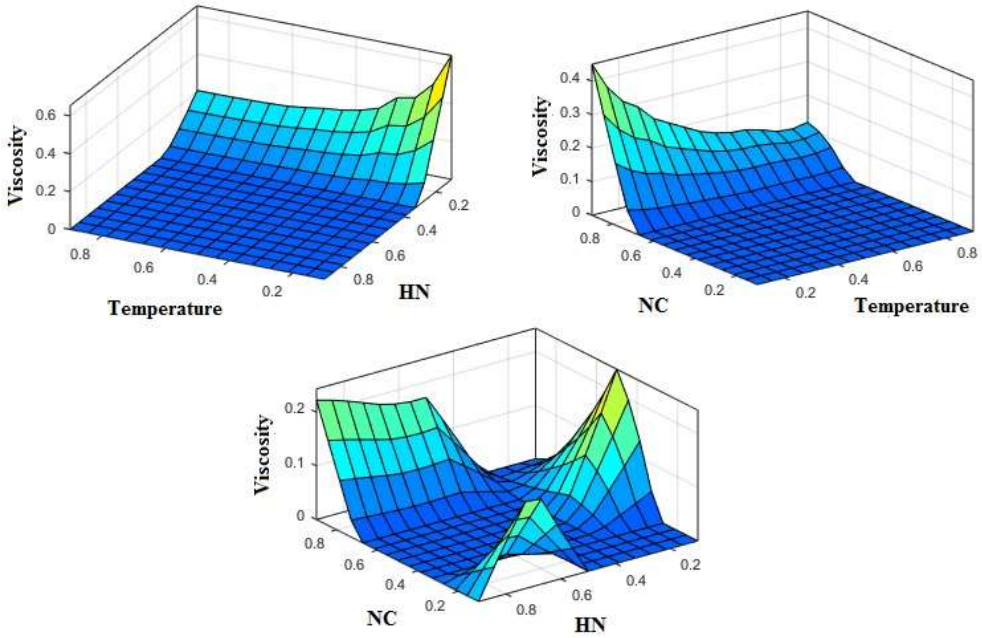

Figure 3. Surface viewer of ANFIS model for kinematic viscosity of saturated and unsaturated FAMEs

Artificial Neural Network (ANN) Model for Saturated and Unsaturated FAMEs

The development and the training of the network model in this study were carried out using the MATLAB 2015. In this study, the experimental data of biodiesel samples were randomly split into three data set, 60% in the training set, 20% in the validation set and 20% in the test set. Training of the network was performed by using the Levenberg–Marquardt, back-propagation algorithms. There is no general rule for the determination of the optimum number of hidden layers and usually it is determined through trial and error method [52]. Therefore, the number of neurons in the hidden layer was determined by trial and error test, where a mean squared error greater than 1×10^{-4} and a correlation coefficient higher than 0.95 was obtained. In addition, with the trial and error method, training results showed that the ANN with two hidden layers has the best performance. Consequently, the developed ANN model for predicting kinematic viscosity biodiesel blends is shown in Figure 4 and the training parameters can be found in Table 4. The developed network architecture has a 3-2-1 configuration with seven neurons in the input layer. Two hidden layers with varying neurons and seven neurons in the output layer representing viscosity are used.

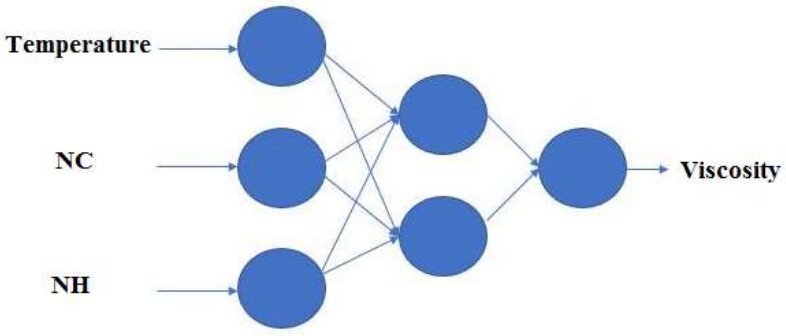

Figure 4. Neural network architecture for three inputs and one output

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Table 4. Neural network configuration for the training

Parameter	Specification
Training Function	Levenberg–Marquardt
Performance function	Mean square error (MSE)
Activation function	Tan-Sigmoid
Number of layers	2
Number of neurons	7
Normalized range	0.1 to 0.9

Figure 5 illustrates a linear relation for the training, validation, testing and performance of the network with high correlation coefficients (R) of kinematic viscosity. The straight lines in Figure 4.10 and 4.11 are the linear relationships obtained between the output (predicted) and the target (experimental) data of viscosity used in this study. The mean squared error (MSE) for saturated and Unsaturated Biodiesel network was 9.675×10^{-5} and 6.018×10^{-4}, respectively. The high coefficients of correlation (R) obtained during the training, validation and testing of the viscosity network display very good relationship between the output and the experimental values of viscosity.

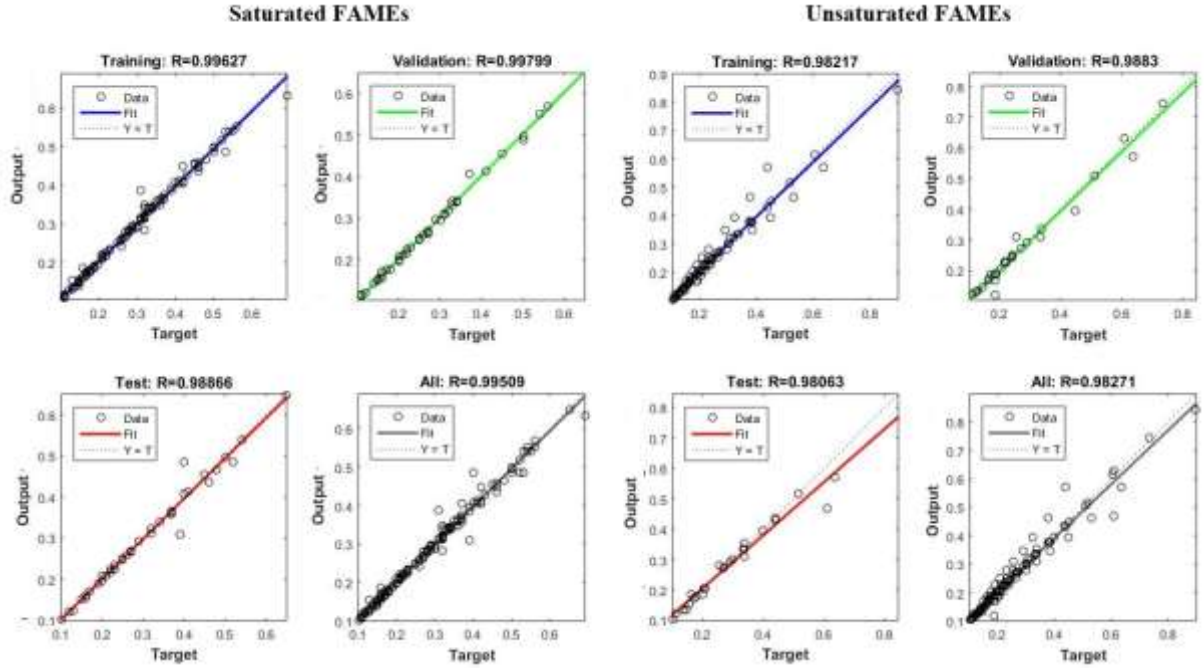

Figure 5. Regression plots for saturated and unsaturated FAMEs

Performance evaluation of ANFIS and ANN

The accuracy of the models obtained from ANFIS and ANN were examined by evaluating the values of both R^2 and AAD%. The results (Table 5) showed that the two optimization tools gave good predictions due to the values of R^2 and small values of AAD. However, ANFIS showed a clear lead over ANN because of higher value of R^2 and smaller value of AAD. ANFIS was better than ANN in the modeling and optimization studies for predicting the kinematic viscosity of saturated and unsaturated FAMEs.

Table 5. R^2 and ADD of ANFIS and ANN models

System	ANFIS models			ANN models		
	Temperature range [K]	R^2	ADD [%]	Temperature range [K]	R^2	ADD [%]
Saturated FAMEs	263.15-373.15	0.988	0.74	263.15-373.15	0.952	1.74
Unsaturated FAMEs	263.15-363.15	0.974	2.43	263.15-363.15	0.961	4.43

IV. CONCLUSION AND FUTURE WORKS

In this study, an ANFIS and ANN methods were developed to predict the kinematic viscosity of biodiesel at various temperatures with the experimental data collected from the literature. ANFIS and ANN methods

compared with the experimental data. The results showed that there is an excellent agreement between the experimental data and modeling data, with average errors very low. Comparison of the ANFIS and ANN predictions and the experimental results demonstrated that both models provide good quality predictions in terms of input variables. The results confirmed that the ANFIS model was more robust and accurate in predicting the values of kinematic viscosity of biodiesel blends compared to the ANN model. ANFIS model has performed more consistently than ANN and can be used as a very powerful and flexible tool for modeling the optimization process.

In future, ANFIS model can also be developed for predicting the kinematic viscosity, density and cold flow properties of biodiesel blends at various volume fractions of biodiesel and temperature.

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