

Biodiesel Production with Supercritical Ethanol Estimation using RBF-ANN Approach

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Abstract

Biodiesels as a renewable fuel can be an effective alternative for fossil fuels which can be obtained from transesterification of triglycerides method. In this study, a radial basis function neural network (RBFNN) was employed to predict the biodiesel yield in supercritical ethanol solvent. The result obtained by RBFNN model was analyzed with the statistical parameters (i.e., MSE, MAAE%, MEAE%, RMSE and R^2) and graphical method. The capability of RBFNN model was compared with the previous developed models. According to the result obtained the RBFNN has the best performance with $R^2=0.997$, $MSE=0.00075$ and $RMSE=0.0274$.

Keywords: Biodiesel; Radial basis function; Fossil fuels; Supercritical ethanol; Statistical parameters

Introduction

Today, search for suitable renewable energy is important due to global warming, environmental pollution, and depletion of world petroleum. Biodiesels as a renewable fuel can be an effective alternative for fossil fuels [1]. Biodiesels are derived from many sources such as vegetable oils, palm, soybean, rapeseeds, sunflower oils, animals' fats, and algae. Supercritical transesterification of triglycerides is an important method for producing the biodiesels [2,3]. The mathematical modeling of biodiesel production to estimate the effective parameters such as temperature, pressure, the molar ratio of reactant to oil and reaction time on biodiesel yield have complex analytical equations, costly and time-consuming [2].

There aren't many investigations about the prediction of biodiesels yield in supercritical fluids such as ethanol yet. Recently, intelligence tools have been mostly used in many applications for data analyzing in many fields of oil and gas industry [4-7].

The main objective of this paper was to predict the biodiesel yield using the radial basis function artificial neural network. To develop the model, four input values consisted of reaction temperature, pressure, time and oil-to-alcohol molar ratio, and one output, biodiesel yield, were considered. To evaluate the accuracy of the proposed model the statistical parameters (i.e., MSE, MAAE%, MEAE%, RMSE and R^2) and graphical method such as William plot and relative deviation plot were employed.

Radial Basis Function Neural Network (RBFNN)

The radial basis function neural network (RBFNN) as a feed forward structure is consist of three main layers, an input layer, a nonlinear hidden layer and a linear output layer. There are common transfer functions such as spline, multi quadratic and Gaussian function may be used for hidden neurons [8,9]. The output of the j^{th} hidden neuron to the input x_k can be expressed as:

$$\phi_j(x_k) = \exp\left(-\frac{1}{\sigma_j^2} \|x_k - u_j\|^2\right) \quad (1)$$

Where u_j is the centre vector for the j^{th} hidden neuron, σ_j is the spread of the Gaussian function and $\| \cdot \|$ refer to the Euclidian norm The response of output layer is obtained by:

$$y_i(x) = \sum_{j=1}^j \phi_j(x) w_j(x) \quad (2)$$

Where $w_j(x)$ is the output weight between the j^{th} hidden neuron and the output neuron, $j = 1, 2, \dots, j$; j is the number of hidden neurons; $\phi_j(x)$ is the output of the j^{th} hidden neuron (Table 1).

Statistical Parameters	Train	Test	All data
R2	0.996	0.999	0.997
MSE	9.2E-05	0.00023	0.00075
RMSE	0.0303	0.015	0.0274
MEAE%	1.82	0.49	1.5
MAAE%	6.34	4.91	6.34

Table 1: Statistical parameters of the developed model.

Data Processing

In this research, the data was collected using the supplied data in the work of Frapiccini and Marini [10]. The dataset were dividing into two parts for test and train data with 25 and 75 ratio percent respectively. The dataset was included reaction temperature, pressure, time and oil-to-alcohol molar ratio. The collected data were normalized between (0,1) to improve the performance of the model by employing the following formula [11]:

$$m_i = \frac{m - m_{\min}}{m_{\max} - m_{\min}} \quad (3)$$

Where m_i is normalized data, m is original data, n_{\min} and m_{\max} are minimum and maximum of m data respectively.

Result and Discussion

The purpose of this article was the development of a radial basis function artificial neural network (RBFNN) with high accuracy to estimate the biodiesel yield in supercritical ethanol. As mentioned, 4 parameters were considered as input variable included reaction temperature, pressure, time and oil-to-alcohol molar ratio. To investigation the capability of the established model, the statistical parameters were employed (MSE, MAAE%, MEAE%, RMSE and R²) which obtained as following formulations [12,13]:

$$MSE = \frac{\sum_{i=1}^k (a-e)^2}{k} \quad (4)$$

$$RMSE = \sqrt{\frac{1}{k} \sum_{i=1}^k (a-e)^2} \quad (5)$$

$$MEAE \% = \frac{1}{k} \sum_{i=1}^k \frac{|a-e|}{a} * 100 \quad (6)$$

$$MAAE \% = \frac{\max|e-a|}{a} * 100 \quad (7)$$

Where a is actual value and e is estimated value.

The statistical parameters were measured and expressed in Table 1 by obtained result the RBFNN has good performance to estimating biodiesel yield in supercritical ethanol. Evaluation of predicted values verses experimental data are shown in Figure 1. The accumulation of data points near the $Y = X$ line verifies the performance of the RBFNN model. The network shows an acceptable performance for Train and Test data with R² 0.996 and 0.999 respectively. The graphical method (relative deviation plot and William plot) was employed to evaluate the accuracy of the model. The relative deviation for both training and testing dataset has been computed and showed in Figure 2. The relative deviation values were obtained from equation (8) [14,15].

$$RD = \frac{e_i - a_i}{a_i} \quad (8)$$

Where RD is relative deviations, e_i is estimated values and a_i is the actual value. The accumulation of relative values near the $Y = 0$ line shows the appropriate performance of the RBFNN model.

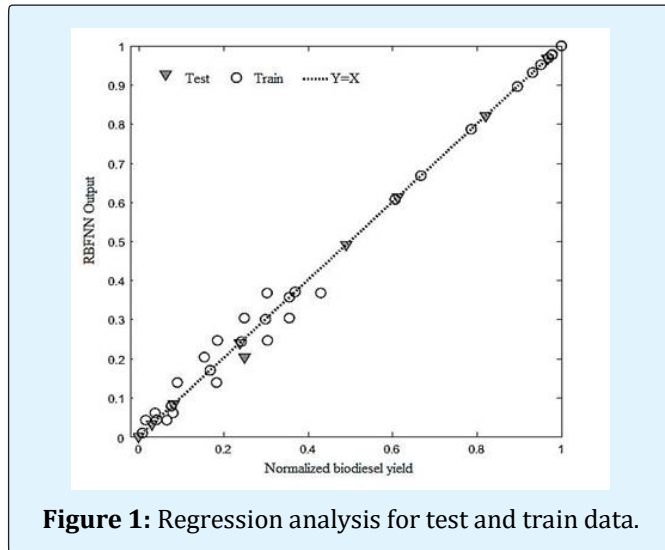


Figure 1: Regression analysis for test and train data.

Also applicability domain was used to evaluate the accuracy of the model. William plot was employed to this aim. This method generally used to distinguish between reliable and unreliable data point. The connection between estimated and observed values is obtained by the hat matrix [16,17].

$$H = X \left(X^T X \right)^{-1} X^T \quad (9)$$

Where H is symmetric matrix ($n \times n$), X is an ($m \times n$) matrix which m is data point and n is number of parameter.

William plot is consisting of the standardized residuals in horizontal axes and HAT values in vertical axes. Critical leverage value (H^*) obtained from $3 \cdot (p+1)/n$, where p is the number of parameters and n refer to the number of data point. The reliable values are located in $0 \leq H \leq H^*$ and between the standardized residual values ± 3 [18,19]. In Figure 3, as can be seen, the estimated values are in Applicability domain which shows the high accuracy of the model.

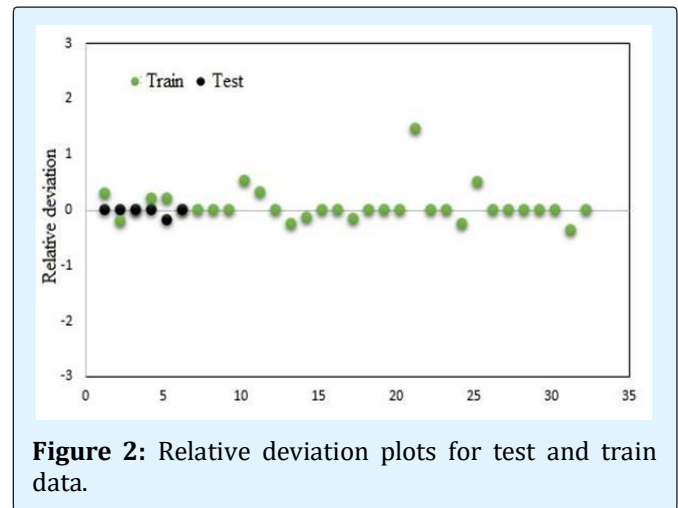


Figure 2: Relative deviation plots for test and train data.

In order to investigation the result of established model, the obtained results are compared to results of other published model in Table 2. As can be seen the RBFNN indicated the best performance for estimation of biodiesel yield against another intelligent algorithm. On the other hand, results from this comparison prove the better performance of RBFNN model for predicting the biodiesel yield.

Temperature	Pressure(M Pa)	Time	m/oil	Exp	Farobie et al., [2]	(Liu et al., [3])	Present Model
270	20	5	40	0.043	0.0299	0.42061	0.04298
270	20	15	40	0.132	0.1363	0.129361	0.1319
300	20	5	40	0.0916	0.096	0.093241	0.0916
300	20	25	40	0.5992	0.599	0.5934	0.5928
350	20	15	40	0.7893	0.839	0.7885	0.7892
350	20	25	40	0.9287	0.9282	0.92899	0.92865
400	20	5	40	0.9129	0.9024	0.9111	0.9129
400	20	20	40	0.9383	0.9287	0.9392	0.9382
325	10	3	20	0.0291	0.0225	0.0301	0.0526
325	10	15	20	0.161	0.157	0.1583	0.1623

Table 2: comparison of the proposed algorithms and published approaches.

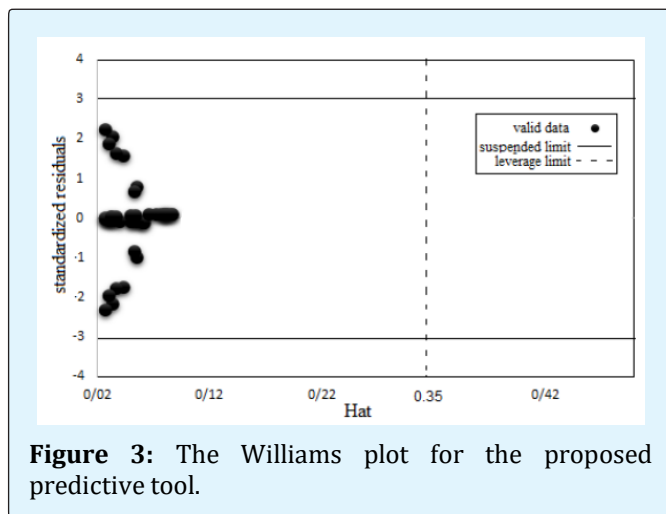


Figure 3: The Williams plot for the proposed predictive tool.

Conclusion

In this paper, the capability of RBFNN model was investigated to modeling to biodiesel yield in super critical ethanol solvent. The statistical parameters (i.e., MSE, RMSE, MAAE%, MEAE%, R^2) and graphical method (i.e., William Plot and relative deviation) are used to evaluate the performance of the model. The results show the radial basis function neural network (RBFNN) has good performance for estimating of biodiesel yield with statistical parameters. (MSE = 0.000753, RMSE = 0.0274, MAAE% = 6.34, MEAE% = 1.5, R^2 = 0.997). According to the results, the RBFNN can be considered as a suitable tool for modeling the biodiesel yield in super critical ethanol solvent.

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