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 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 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 predicting the biodiesel yield using the radial basis function artificial neural network. To developed 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 evaluated 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 jth hidden neuron to the input xk can be expressed as:

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

Where $$u_j$$ is the centre vector for the jth hidden neuron, $$\sigma_j$$ is the spread of the Gaussian function and $$|| \cdot ||$$ refer to the Euclidian norm. The response of output layer is obtained by:

$$y_j(x) = \sum_{j=1}^{k} \phi_j(x)w_j(x)$$ (2)

Where $$w_j(x)$$ is the output weight between the jth hidden neuron and the output neuron, $$j = 1, 2, \ldots, j$$; j is the number of hidden neurons; $$\phi_j(x)$$ is the output of the of the jth hidden neuron (Table 1).

<table>
<thead>
<tr>
<th>Statistical Parameters</th>
<th>Train</th>
<th>Test</th>
<th>All data</th>
</tr>
</thead>
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<tr>
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<tr>
<td>MAAE%</td>
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</table>

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]:

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

Where $$m_i$$ is normalized data, $$m$$ is original data, $$n_{\text{min}}$$ and $$m_{\text{max}}$$ 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 $$R^2$$) which obtained as following formulations [12,13]:

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

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

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

$$MAAE\% = \frac{\max|e - a|}{a} \times 100$$ (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 $$R^2$$ 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} (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.

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

Where H is symmetric matrix (n*n), X is an (m*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 $3*(p+1)/n$, 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 $\pm 3$ [18,19]. In Figure 3, as can be seen, the estimated values are in Applicability domain which shows the high accuracy of the model.

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Table 2: comparison of the proposed algorithms and published approaches.
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%, R²) 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% = 6.3 4, MEAE% =1.5, R² =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.

References


