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Neural-Network-Inspired Correlation (N2IC) Model for Estimating Biodiesel Conversion in Algal Biodiesel Units

Abdullah Bin Mahfouz [1], Abulhassan Ali [1,*], Mark Crocker [2], Anas Ahmed [3], Rizwan Nasir [1] and Pau Loke Show [4,*]

[1] Department of Chemical Engineering, University of Jeddah, Asfan Road, Jeddah 23890, Saudi Arabia
[2] Center for Applied Energy Research, University of Kentucky, Lexington, KY 40511, USA
[3] Department of Industrial and Systems Engineering, University of Jeddah, Asfan Road, Jeddah 23890, Saudi Arabia
[4] Department of Chemical and Environmental Engineering, Faculty of Science and Engineering, University of Nottingham Malaysia Campus, Jalan Broga, Semenyih 43500, Malaysia
* Correspondence: aquddusi@uj.edu.sa (A.A.); pauloke.show@nottingham.edu.my or showpauloke@gmail.com (P.L.S.)

Abstract: Algal biodiesel is of growing interest in reducing carbon emissions to the atmosphere. The production of biodiesel is affected by many process parameters. Although many research works have been conducted, the influence of each parameter on biodiesel production is not well understood when considering a complete system. Therefore, the experimental data from literature sources related to types of algae, methanol-to-algal-oil ratio, temperature, and time on the biodiesel production rate were reviewed and introduced into a neural-network-inspired correlation (N2IC) model to study the rate of transesterification. The developed N2IC model optimized for biodiesel production is based on the studied variables, specifically reaction time, temperature, methanol-to-algal-oil ratio, and type of algae. It was found from ANN analysis that the reaction time is the most significant parameter with 87% importance, followed by temperature (85%), alcohol-to-oil-molar ratio (75%), and type of algae (62%). Using error analysis, the results from the proposed N2IC model show excellent agreement with the experimentally obtained values with an overall 5% error. The results show that the N2IC model can be utilized effectively to solve the problem of industrial biodiesel production when various operating data are readily available.

Keywords: algal biodiesel; correlative modelling; ANN; N2IC model

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1. Introduction

Conventional energy sources, including crude oil, coal, and natural gas, are non-renewable. Moreover, their frequent usage results in global warming and damage to the environment due to the increasing carbon dioxide concentration in the atmosphere [1]. Despite this, the rapid population and social structure growth have instigated a rise in the use of fossil fuels. Consequently, researchers have recently begun to investigate alternative fuel sources. Considerable attention has been given to the conversion of various oils (e.g., vegetable, palm, sunflower, rapeseed, and waste cooking oil) for biodiesel production [1–3]. Biodiesel production is estimated to account for 69% of soybean oil, palm oil, and rapeseed oil [4]. This high proportion of edible oil use poses a challenge because of its effect on commodity prices and food security [5]. One viable yet renewable energy source is algae or microalgae, an emerging alternative for biodiesel production [6].

Among available renewable sources, microalgae-derived biofuel has attracted considerable attention in the last decade due to its many potential advantages. Microalgae contain many bioproducts, such as polysaccharides, pigments, vitamins, lipids, proteins, and bioactive compounds [7]. These compounds, and derivatives thereof, can be used to produce various products, including biofuels, medicinal products, cosmetics, and nutritional supplements [8]. From this, it follows that algae represent a promising feedstock for biorefineries, with the potential to produce high-value products along with lower-value, high-volume products such as biofuels. Given the wide variety of algae that occur in nature, many different types can be considered for such applications, including those belonging to the phyla Euglenophyta, Pyrrophyta, Chrysophyta, Chlorophyta, Rhodophyta, Xantheophyte, and Phaeophyta [9]. Problems associated with algal biodiesel production include high operational, maintenance, harvesting, and conversion costs [10,11]. However, improved cultivation methods and genetic engineering may, in the long term, help to increase algae productivity and, therefore, lower production costs [12]. In recent decades, many studies have been conducted to produce biodiesel from different microalgae. These studies typically investigate the effect of varying process parameters on biodiesel yield [13,14].

Several process parameters affect biodiesel production: these include pressure, temperature, reaction time, molar ratio, catalyst type, etc. Studying the effect of these parameters, individually or combined, is time-consuming and costly. Moreover, the combined effect of process parameters is also challenging due to their complex relationship [15,16]. To overcome these challenges and avoid costly and time-consuming experimentation, researchers employ several soft computing techniques intending to maximize biodiesel yield [17–19].

One effective prediction and modeling method is an artificial neural network (ANN). The ANN is a machine learning method that evolved from simulating the human brain. In engineering and research, ANNs represent a valuable tool for problem-solving, particularly when a problem is nonlinear or complex where traditional modeling methods fail [20]. The construction and application of the ANN model have been thoroughly examined in the literature. An artificial neural network (ANN) with trained, tested, and verified data could predict biodiesel-based fuel performance and emission characteristics [21]. ANNs have also been utilized to improve biodiesel production by enhancing microalgae growth and lipid production (i.e., the upstream process) [22,23]. In biodiesel production, ANN is also used to optimize the fatty acid esterification reaction (downstream process) [24,25].

Recently several researchers employed ANN to model and predict biodiesel synthesis using different algae feedstocks. For instance, a group of researchers used ANN to optimize the cultivation condition for Chlorella Vulgaris microalga, which was further used to produce biodiesel. They also compare the response surface methodology and ANN for the prediction and found that ANN is more accurate than RSM [26]. Kumar et al. used ANN to model the production of Chlorella-Vulgaris-based biodiesel [27]. They trained the ANN using the Levenberg–Marquardt (LM) algorithm, and the backpropagation learning algorithm was used to develop the model. The ANN was found to be highly accurate, with R^2 of 0.9976. The process input parameters were catalyst type, temperature, reaction time, and molar ratio. Garg and Jain used ANN and RSM to model the biodiesel synthesis from algal oil [28]. They chose the process parameters, including reaction time, alga-oil-to-methanol ratio, and catalyst concentration. They also found that ANN is more accurate (0.99 R^2) than RSM (0.97 R^2). Another study used ANN, RSM, and genetic algorithms to predict the optimum process conditions for biodiesel synthesis [29]. They used the supercritical temperature to avoid the catalyst used for synthesis process. They also concluded that the ANN is more accurate as compared to other prediction techniques. Several other researchers also used ANN to model and optimize the process conditions for biodiesel synthesis and growth of microalga [30,31].

Thus, it is evident from the literature that ANN is an excellent computational tool for predicting biodiesel yield. It can also help to optimize the process parameters for maximizing the biodiesel yield. The main objective of this study is to develop an ANN model to identify the process conditions at which the maximum biodiesel yield was obtained by identifying the significance of process parameters. Therefore, this research employs an artificial neural network modelling approach to develop a Neural-Network-Inspired Correlation (N2IC) model to estimate biodiesel conversion under the effect of various process parameters. The proposed model correlates the production of biodiesel via transesterification under the influence of types of algae, methanol-to-algae ratio, temperature, and reaction time. Experimental data for the neural network modelling approach is inserted randomly in the developed neural network model and correlated, as explained in the next section. The model is bound to optimize the correlation for the biodiesel conversion, seeking random inputs from feed and process parameters and assigning weight and biases to achieve the best correlation.

2. Methodology

In a MATLAB environment, the artificial neural network for correlating the biodiesel conversion was developed (R2021a). The code was written for a generic two-layer feed-forward neural network with backpropagation [32]. The designed neural network is shown in Figure 1. The data from four experimental sources [33–36] were used to train the neural network, which included temperature (in Kelvins), reaction time (in minutes), methanol-to-oil ratio (in the volume of weight ratio), and type of algae. Moreover, we searched the published literature and consciously selected experimental data from various studies using different catalysts. The step was taken to test and ensure the application of the N2IC model among various catalyst types and to demonstrate that the proposed model is flexible enough to accommodate different catalysts under the same algorithm. The results (presented later) show excellent correlation irrespective of the catalyst type but are sensitive to its concentration in the mixture. Therefore, the N2IC model is yet inconclusive about the comparative performance of different catalyst types and requires further studies. The hidden layer of the proposed ANN was developed in dual layers using a tangent sigmoid function, while the output layer was created using a non-linear transform function [37]. Three target layers were designed to incorporate different effects of the hidden layers into the target values, i.e., experimental biodiesel conversion. All the experimental data inserted into the ANN were normalized using Equation (1) to minimize the effect of data asymmetry. The input layers were distributed randomly into three sets. The training set contained 50% of the experimental data input, while the validation and testing set comprised 15% and 35% of the experimental data values, respectively [32].

$$Normalized(X) = \frac{X}{X_{\max}} \tag{1}$$

where $X_{\max}$ is the maximum value for a variable X.

The Bayesian coordinate optimization technique and the trial-and-error method were used to optimize the number of neurons in the hidden layer of the ANN [38]. Using a large number of hidden neurons usually helps improve the correlation; however, the complexity increases correspondingly, causing overfitting of the data values. This overshadows the experimental errors. Hence, the model becomes overfitted and may give erroneous values at non-tested conditions.

The designed ANN is tested against an incremental number of hidden neurons. The correlation test for a certain number of hidden neurons is started at a value of 1. It is then incremented by a value of 1 until a minimal mean square error is observed for all three data sets (train, validation, and test), using Equation (2). The system for the N2IC model was tested up to 19 hidden neurons as the mean square error value increased gradually after 15 hidden neurons, which yielded a minimal error value.

$$MSE = \arg\min \frac{1}{n} \sum_{i=1}^{n} (X_O - X_T)^2 \tag{2}$$

X_T and X_O represent the model's desired target (experimental data) values and output for each required output.

Figure 2 illustrates the change in mean squared error (MSE) values in relation to the number of hidden neurons in the created ANN. It can be observed that all MSE values for each data set drop with an increase in the number of hidden neurons. It is worth noting that all three training, validation, and testing datasets show similar peaks and troughs and show a gradual drop in the MSE values over the range. This shows an equal error distribution in the experimental data range and implies that the selected experimental data is reliable. Figure 2 demonstrates that when the created ANN has 15 hidden neurons, the mean square error values are at their lowest. Similarly, Figure 3 presents the R-square value, another statistical parameter for the correlation against increased neurons. The results in Figure 3 are somewhat like Figure 2, where the highest values of the R-square (nearing a unity) are seen at 15 hidden neurons. Hence, both figures indicate that the said N2IC model should be developed with 15 hidden neurons of the proposed ANN for optimal results and analysis.

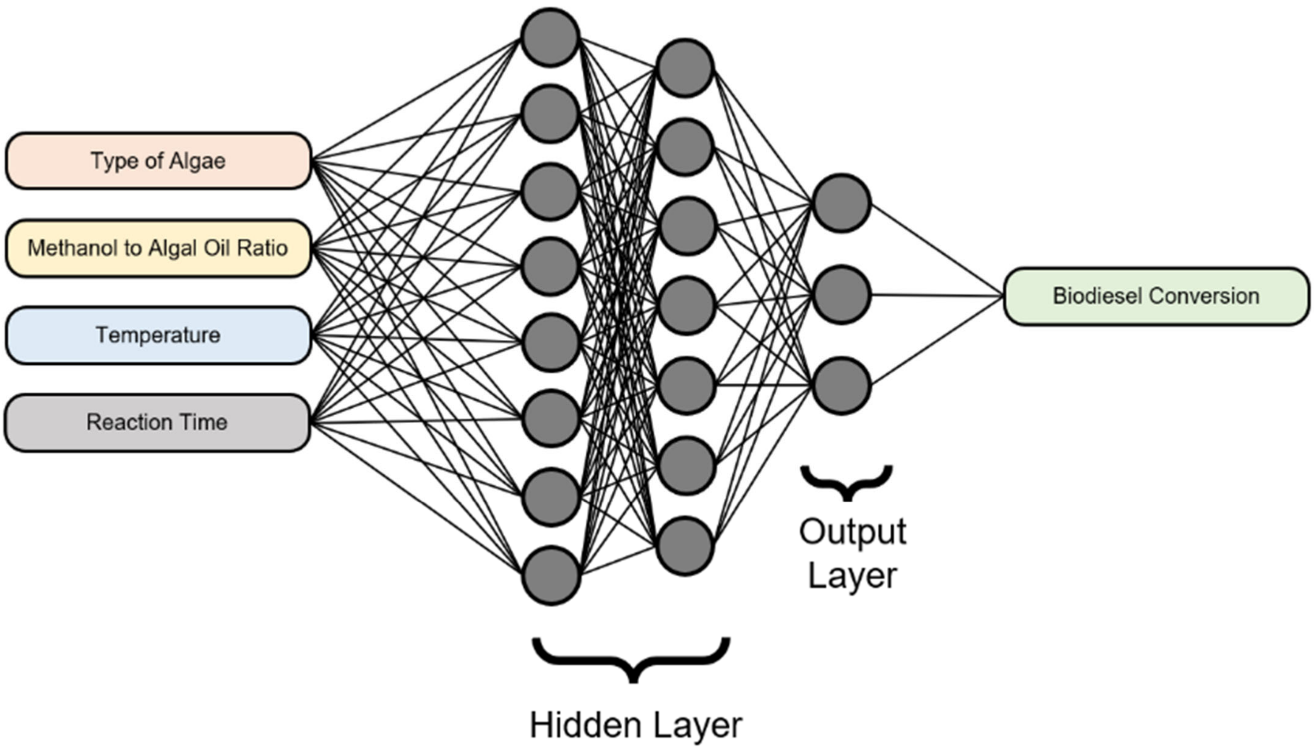

Figure 1. Illustrative representation of the artificial neural network design developed for the N2IC model.

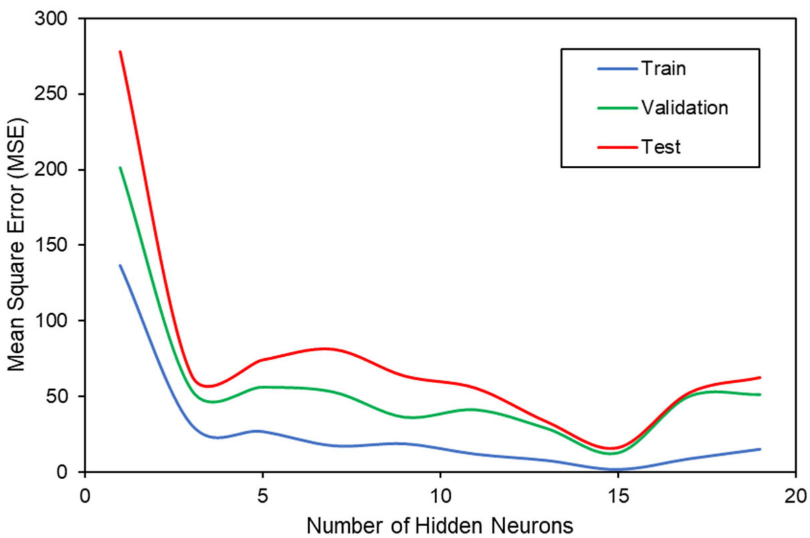

Figure 2. The change in the values of mean squared error against the number of neurons in the designed ANN.

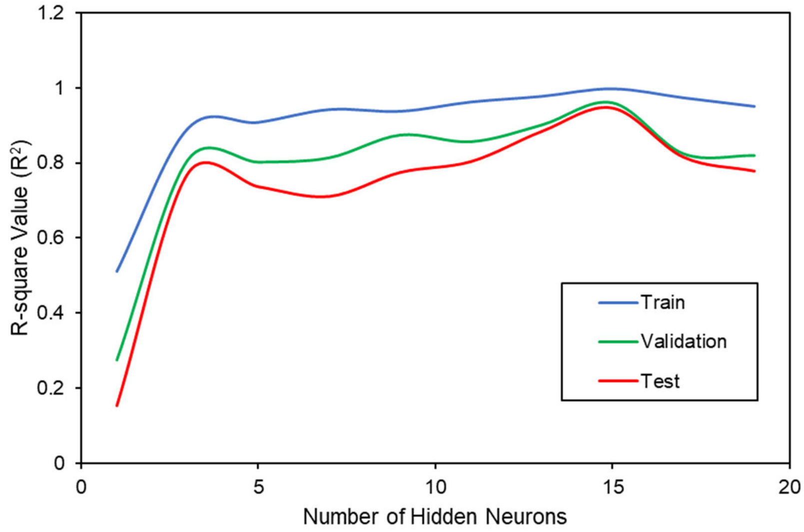

Figure 3. The variation in R-square values in relation to the number of neurons in the created ANN.

3. Results and Discussion

3.1. Effect of Temperature and Reaction Time on the Biodiesel Yield

Figures 4–6 illustrate how temperature and reaction time relate to biodiesel conversion for various algae and feed circumstances. Although the experimental data was taken from varied sources, which are not connected in any way, the results of the modelling study show that the N2IC model can correlate the experimental values with minimal error and high correlation. Despite variation in the temperature and reaction time, the absolute average relative error is below 5% among all experimental values described in the literature review above.

Figure 4 depicts the influence of reaction time on the biodiesel conversion for *Schizochytrium limacinum*-type algae at various temperatures with a constant methanol-to-oil ratio of 10. The modelling values excellently map the experimental values. Although the data values of biodiesel conversion lie in the near vicinity, the model shows a near-perfect duplication of the experimental values, which means that the model is both correlative and sensitive to the model parameters inserted as inputs.

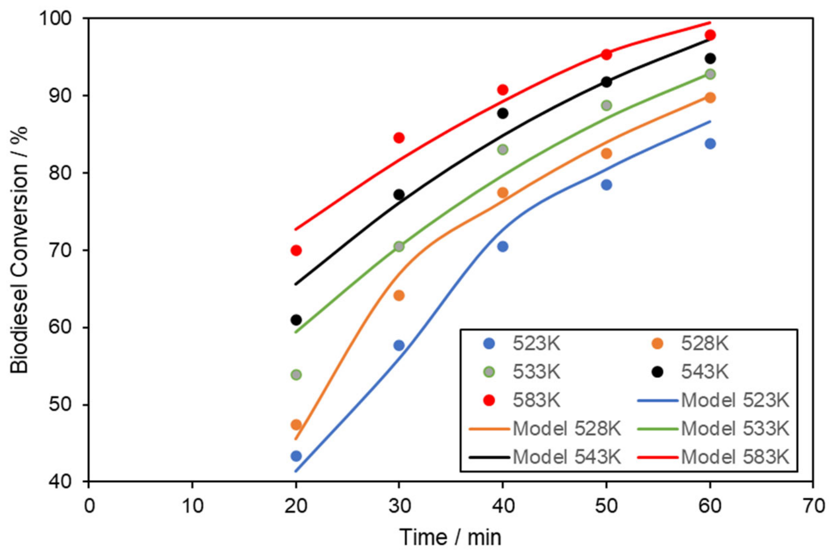

Figure 4. Effect of temperature and reaction time on oil conversion to biodiesel for constant methanol-to-oil ratio of 10, using oil derived from *Schizochytrium limacinum* algae. Experimental data were taken from [36].

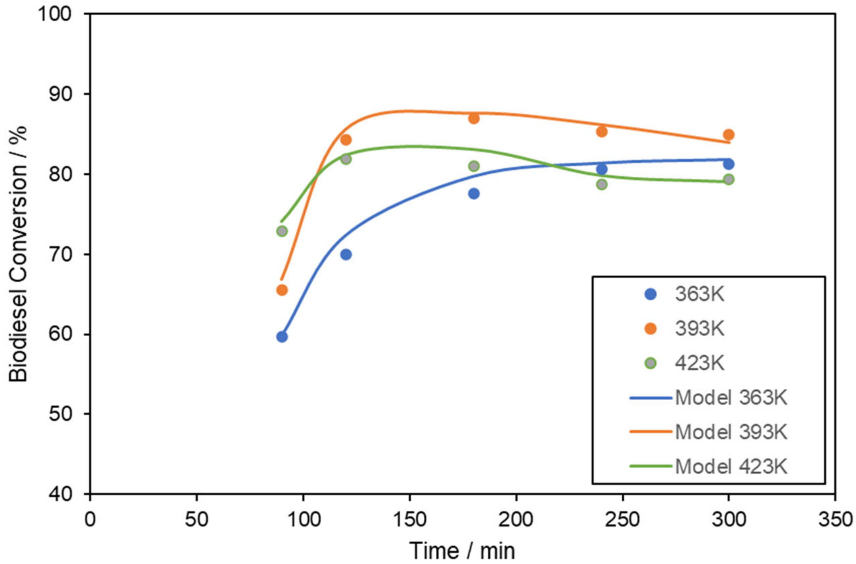

Figure 5. Temperature and reaction time effect on biodiesel conversion at constant methanol-to-oil ratio of 40, using oil derived from *Chlorella pyrenoidosa* algae. Experimental data were taken from [33].

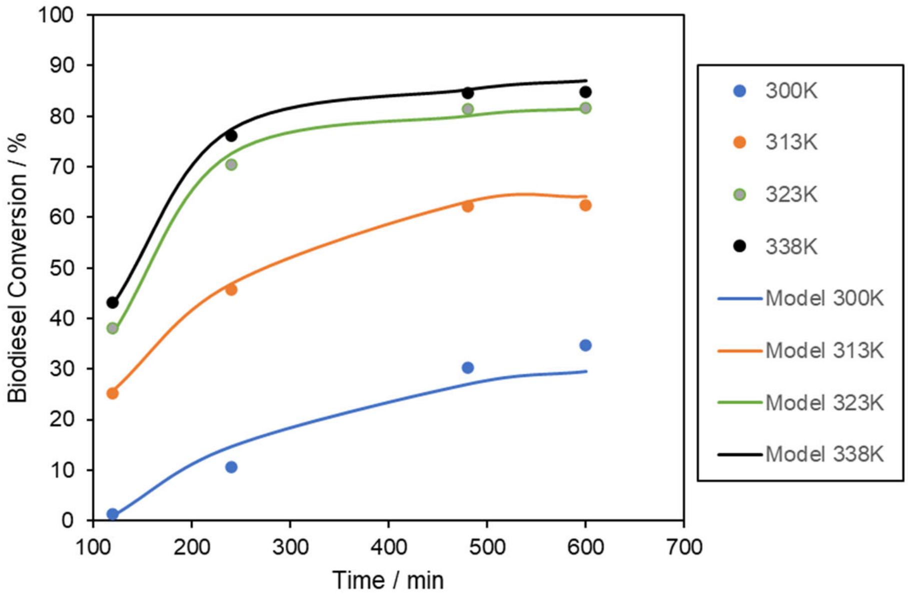

Figure 6. Temperature and reaction time effect on biodiesel conversion at a constant methanol-to-oil ratio of 5.33, using oil derived from *Spirulina platensis* microalgae. Experimental data were taken from [35].

Figure 5 shows a similar behavior as in Figure 4, where the experimental values criss-cross each other. The experimental data are taken from [33]. For example, the experimental values for biodiesel conversion deviate strongly from a linear relationship at temperatures of 393 K and 423 K. The overall experimental values for 423 K are lower than 393 K and match the trend shown by biodiesel conversions at 363 K. Interestingly, the N2IC model can replicate the experimental values with superb correlation and map the deviation shown at 423 K, which most linear relationships/models cannot easily do without using excessive regression and corrective factors. This must be taken as the strong point of the proposed ANN approach. Including three neurons, subsequent biases, and respective neuron weights in the output layers helps improve the off-trend observation at 423 K, proving that the

ANN is adequately sensitive to deviations from the general trend. Moreover, the Bayesian coordinate optimization algorithm maintains the correlation at all correlated values.

With a fixed methanol-to-oil ratio of 5.33 (vol/weight), Figure 6 shows the impact of temperature and reaction time on the biodiesel conversion for Spirulina platensis microalgae at various process temperatures. The experimental data shows a significant variation in the biodiesel conversion values from nearly 1% to 87%. The model provides an excellent prediction of the experimental values and caters to the large range of biodiesel values with average errors below 4% in the individual dataset. Interestingly, the increase in the temperature beyond 323 K does not improve the experimental biodiesel conversion much (i.e., at 338 K), which the proposed N2IC model can correlate satisfactorily. Surprisingly, the model results shown in Figure 6 are equally distributed along with the experimental values, different from Figures 4 and 5, where most of the values were either under-predicted (Figure 4) or over-predicted (Figure 5). This behavior is mainly attributed to the balanced distribution of model factors by the Bayesian coordinate optimization algorithm. A part of this correlation is also due to the smooth trend of the experimental values seen for the given data from [35].

3.2. Effect of Process Parameters on the Biodiesel Conversion

The methanol-to-oil ratio has a substantial effect on oil conversion to biodiesel. Theoretically, the higher the abundance of methanol, the greater the biodiesel conversion. However, the experimental data from two different sources [34,36] show that the methanol-to-oil ratio does not have a proportional/linear relationship with the other process parameters and biodiesel conversion. Due to limited experimental data, the N2IC model cannot create a holistic relationship between the studied parameters. However, the limited relationship it has developed shows an excellent correlation. Figures 7 and 8 show that the methanol-to-oil ratio has a non-linear relationship with biodiesel conversion. The experimental biodiesel conversion rises considerably and then drops after a certain value. The exact quantitative value for such a drop may be regarded as a function of the oil source/type of algae. Irrespective of that, the qualitative studies show that the observed biodiesel conversion drops in the third quadrant of the studied methanol-to-oil ratio range. This could be attributed exclusively to the range of the selected parameters when comparing experimental data values. Nevertheless, the model results can map the non-linear relationship shown by both datasets above. The peaks and troughs in Figure 8 are matched effectively, indicating that the model parameters are well-regressed, and the ANN model's parameters are optimized. Model values are slightly under-predicted in Figure 7. In contrast, they are well-distributed in Figure 8, where the model line draws a near-median through the experimental values yet follows the peaks and troughs within.

Overall, the ANN model accurately correlates biodiesel conversion for all the process parameters (i.e., reaction time, temperature type of algae, and methanol-to-oil ratio) with satisfactory R^2 values. Minor under- and over-prediction between the model results and experimental values are seen, yet they are within the range of experimental errors reported in their original studies. The results also indicate that the neural-network-based correlation models can reliably correlate the nonlinear experimental values for biodiesel production [39,40].

3.3. ANN Predictability

Figure 9 shows the prediction of the modelled biodiesel conversion against the experimental values of biodiesel conversion for the range of studied values taken from the open literature [33–36]. The coefficient of determination is 0.972 for the compared variables, exemplifying a good agreement and indicating between experimental and predicted values. The suggested N2IC model may provide a high correlation over the whole biodiesel conversion range (i.e., 0–100%) with the incorporation of a large range of process and feed parameters. The R^2-value is 0.986, calculated using the square root of the coefficient of determination (R^2) value [41]. A group of researchers optimized the process variable (time, temperature, oil-to-methanol ratio, and catalyst concentration) for biodiesel production from *Nannochloropsis salina* feedstock using ANN. They found the R^2 = 0.957, indicating a good agreement between mode and experimental data [22]. Muhammad et al. also studied the optimization of process parameters such as time, temperature, solvent-to-wet-biomass ratio, and hydrochloric acid concentration for enhanced biodiesel production from *Chlorella pyrenoidosa*. Their developed ANN model predicts accurately with an R^2 of 0.94 [42]. In contrast with previous studies, a good fit of our model was obtained with a small error (R^2 of 0.986).

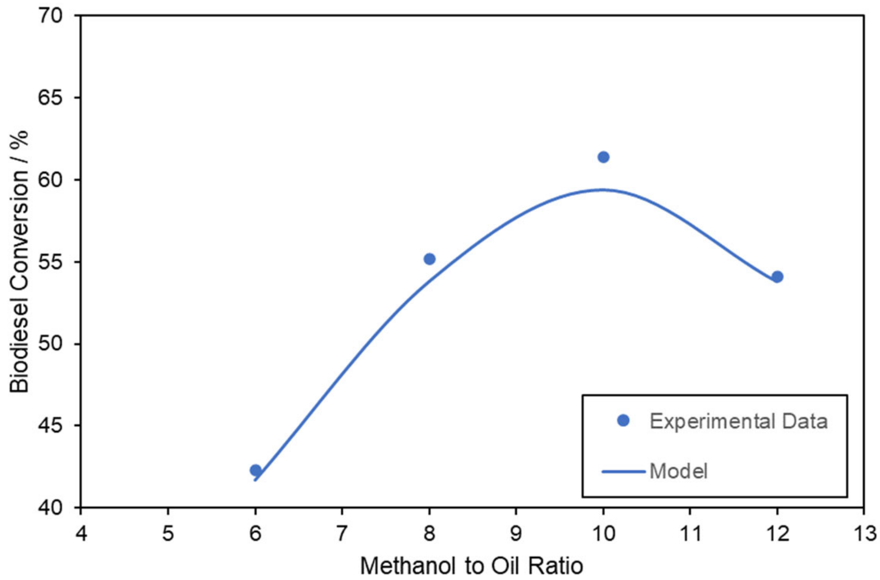

Figure 7. Methanol-to-oil ratio effect at a constant temperature of 533 K and reaction time of 20 min on the conversion to biodiesel, using oil derived from *Schizochytrium limacinum*. Experimental data were taken from [36].

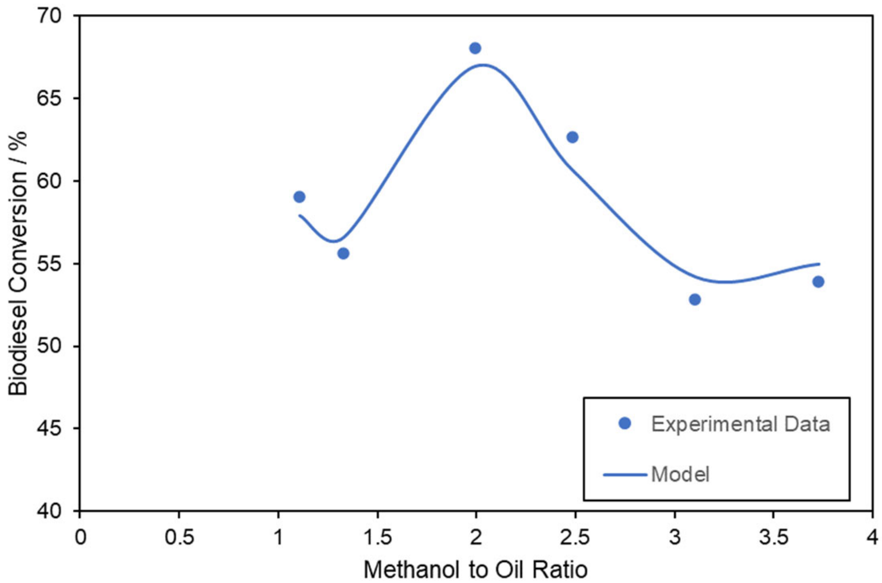

Figure 8. Methanol-to-oil ratio effect at a constant temperature of 303 K and reaction time of 420 min, using oil derived from *Chlorella protothecoides*. Experimental data were taken from [34].

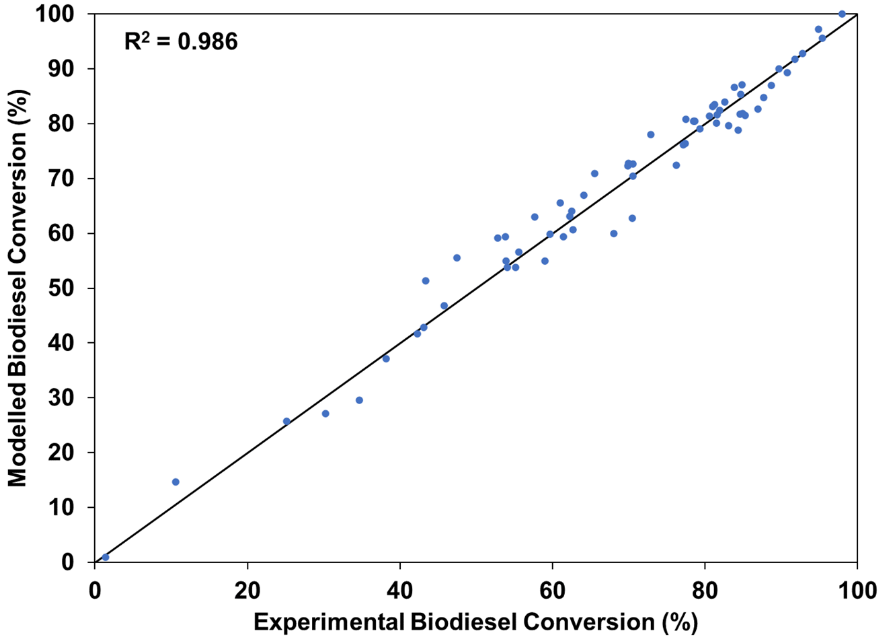

Figure 9. Parity plot for the modelled and the experimental data values for a range of biodiesel conversions studied to develop the N2IC model. Experimental data were taken from [33–36].

Another output layer that links the hidden layer to the target/output parameters might further help the N2IC model's correlation performance. The results can be optimized by tweaking the model parameters using conventional Levenberg–Marquardt and "fminsearch"-type optimization approaches. However, these approaches can impart uncontrolled overfitting to the model results and limit their application beyond the regressed range of parameters used to develop the N2IC model. We also recommend that future studies in this area use smoothened data points, which have been freed of data outliers and erroneous values. Moreover, experimental data for comparing types/sources of algae should be considered, which remains the most significant limitation of our work. For example, the N2IC model can provide an excellent correlation of the quantitative values for reaction time, temperature, and methanol-to-oil ratio. Still, it cannot exemplify the qualitative performance of the type of algae in the biodiesel conversion without common parametric data. Moreover, ANN-based models are not reproducible [43]. However, given the complexity of the experimental information, a reader would agree that advanced correlative techniques can only correlate such non-linear values. Furthermore, we suggest that the inclusion of linear variances can improve the model's sensitivity further and help reduce the consistent under-prediction and/or over-prediction seen in some modelling results.

3.4. Relative Importance of Variables

Analyzing the impact of process and feed factors on biodiesel conversion is crucial for the design, selection, and management of biodiesel production systems using microalgal sources. It is possible to examine the degree of the correlation between output and input parameters using the Cosine Amplitude Method (CAM). This approach states each data pair in a broad X-space [44]. The data pairs are used to make a data array X in the manner described below.

$$X = \{X_1, X_2, X_3, \ldots, X_m\} \tag{3}$$

Each element (Xi) in the data array X is a vector of length m.

$$X_i = \{X_{i1}, X_{i2}, X_{i3}, \ldots, X_{im}\} \tag{4}$$

Therefore, each of the data pairs may be shown at a specific location in m-dimensional space. Equation (4) provides the magnitude of the link between the data pairs, x_i and x_j. The calculated r_{ij}, is a pairwise comparison between two elements of the X-space [45,46].

$$r_{ij} = \frac{\sum_{k=1}^{m} x_{ik} x_{jk}}{\sqrt{\sum_{k=1}^{m} x_{ik}^2 \sum_{k=1}^{m} x_{jk}^2}} \tag{5}$$

The findings of the sensitivity analysis performed on the mentioned system are shown in Figure 10. The most sensitive variables that influence the conversion of algal oil to biodiesel in decreasing order are reaction time, temperature, methanol-to-oil ratio, and kind of algae.

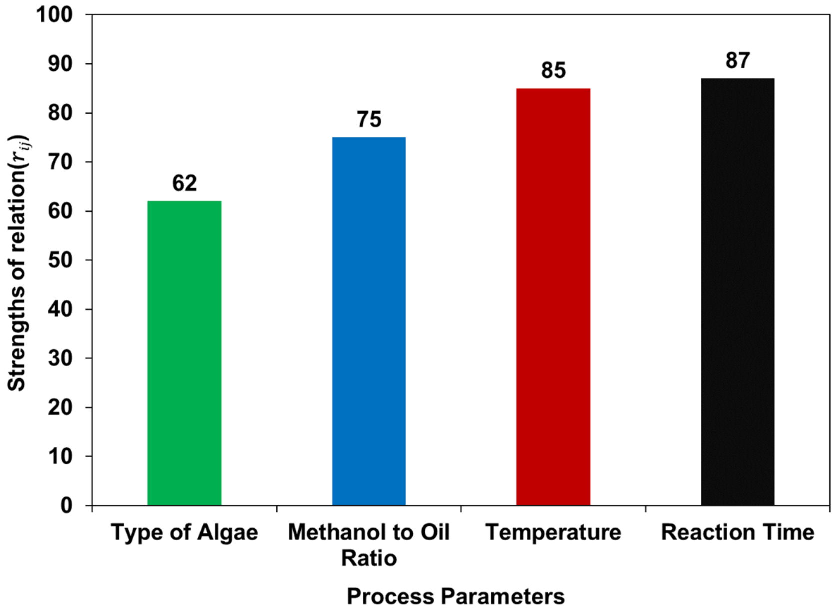

Figure 10. Sensitivity of process parameters in biodiesel production.

Moreover, the values given in Figure 10 are empirical and only valid within the limits of the studied datasets and their presented range of parameters in the literature. A hypothetical example can explain this behavior. The studied parameters and their weights in the developed model are distributed and balanced so that only significant variables are expressed in the model equation. However, their contribution does vary as is common with empirical relationships. According to the results presented in Figure 10, the reaction time is the most contributing variable compared to other variables. In theory, long reaction times are needed to achieve equilibrium conversion for both homogenous and heterogenous catalysis [15,47–50].

The model's results show an acceptable level of agreement with the experimental values. They show that it can confidently fully map the data under various conditions and algal sources.

4. Conclusions

The influence of process factors on biodiesel yield was predicted in this study. A Neural-Network-Inspired Correlation (N2IC) model was developed for estimating biodiesel conversion in algal units. The N2IC model shows an overall 5% error. The coefficient of determination for the compared variables is 0.972, indicating good agreement and implying that the proposed N2IC model is capable of excellent correlation for the full range of biodiesel conversion (i.e., 0 to 100%) with the incorporation of a wide range of process and feed parameters. The square root of the coefficient of determination value yields an R^2-value of 0.986. The model is sensitive to the rise and fall in biodiesel conversion with increasing methanol-to-oil ratio and is correlative enough to map the deviations in the experimental results. The N2IC model's results demonstrate excellent agreement with experimentally observed values when using error analysis. The ANN model presented here is a useful tool for understanding the qualitative and quantitative contribution of different process parameters on the conversion of biodiesel. The outcomes of this study are deemed essentially relevant for the non-linear correlation and modeling capability of ANN for biodiesel production.

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