Mathematical Models for Predicting the Biodiesel Properties

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Abstract: Density, viscosity and cetane number are important physical properties of biodiesel as they participate in one way or another in the fuel metering, calibration and nozzle process during combustion. High and good accuracy of the physical properties of biodiesel will therefore lead to improved combustion and therefore better efficiency. The aim of this study is therefore to seek good and high precision by combining properties and comparing the analysis between ANN and RSM. Studies have been made by researchers to collect data. In this study the combination of properties is exploited. A total of 1360 data from the various studies has been collected and exploited. From this data after elimination and treatment 39 possible combinations were analyzed and compared by ANN and RSM. The result of simulation is: The best combinations: \( p = f(Fa) \), \( v = f(Fa) \), \( cn = f(Fa) \) with \( R^2 \) respectively equal to (0.9998, 0.9998, 0.9987) and \( R \) equal to (0.9997, 0.99971, 0.9984) obtained with ANN simulation provide more accuracy than \( R^2 \) (0.9112, 0.799, 0.766) and \( R \) (0.837, 0.739, 0.920) obtained with RSM simulation in general \( R^2 \) obtained with ANN (0.9998, 0.9998, 0.9987) provide good accuracy than \( R^2 \) (0.9112, 0.799, 0.766) obtained with RSM. Also there is a good relationship between fatty acid and others properties since they provide good result. In general the overall regression coefficient \( R \) and the correlation coefficient \( R^2 \) values of the combinations obtained in the simulation with the ANN provide better and good accuracy since their values are close to each other and all close to 1, and their \( mse \) tend towards 0. While the one obtained with RSM are distant from each other and distant of 0 so they provide an acceptable accuracy. It is also important to note that high accuracy of properties using RSM must have at least combination of three parameters. Also after every combination, the conclusion says there is a good relationship between fatty acid and other properties. Then for the future work, it will be beneficial to combine fatty acid with others properties and evaluate result, also use another network to simulate.

Keywords: artificial neural network, cetane number density, fatty acid, regression coefficient, response surface methodology, overall coefficient, viscosity.

I. INTRODUCTION

A. BACKGROUNG

Inflate in rivalry and outbreak in energy resource costs lead researchers to pursue technologies that are in line with the international market. Despite the environmental quality of diesel problems, costs tend to rise due to the lack of coal reserves. In addition to all this, companies are increasingly turning to renewable sources of energy including biodiesel.

B. LITERATURE REVIEW

Researchers have developed various methods for predicting density, kinematic viscosity, cetane number, pour point, cloud point, biodiesel flash point, and FAME.
Nonetheless, due to their high involvement in the concept of fuel during the combustion process, their implications for engine design and parameter control during operation, biodiesel properties (density, viscosity and cetane number) are increasingly used (L. F. Ramirez – Verduzco, 2013). The viscosity and density allow for the size needed for proper operation during engine time (combustion), while the cetane number indicates the combustion efficiency. Thus, several steps and methods allow for the measurement of biodiesel properties to obtain high precision (Geacăi et al., 2015; Ebna Alam Fahd et al., 2014; Gülüm & Bilgın, 2016).

(Freitas et al. S.V.D. Freitas, M.J. Pratas, 2011) diversified models at various temperatures have made it possible to estimate the viscosity of biodiesel, thus the Kay method based on mixing and group contribution to estimate the density of ten samples were proposed (Pratas et al. M.J. Pratas, S.V.D. Freitas, 2011).

The hourly and monetary costs, the results and graphical interpretations, the models mentioned were used to estimate the properties of biodiesel (Betiku et al., 2014); (Wakil et al., 2015) dels Prieto et al., 2015); (Barabás & Todoruţ, 2011); (Barabás, 2013); (neuro fuzzy, Mostafaie et al., 2016); (Hosoz et al., 2013); and artificial neural neural network (Barabás, 2013).

(Piloto-Rodriguez et al. 2013) successfully implemented the ANNs to foresee the biodiesel cetane number with compositions of ten FAMEs as inputs, and multiple linear regression mode provided less accuracy than the ANNs process. (Yuan et al. 1949) elaborated a mixing topological index way to envisage the kinematic viscosity of biodiesel. In the aforementioned work, the biodiesel kinematic viscosity from its composition FAME was calculated by applying the simplified version of the Grunberg – Nissan equation (2009) used by (Allen et al. 1999), neglecting the interactions between the individual components.

Knothe and Steidley further simplified the Grunberg – Nissan equation (2009). By using the values, and neglecting their logarithms (viscosity) made it possible to calculate the kinematic viscosity based on the viscosities of the individual FAMES. Due to its chemical composition, the biodiesel properties (number, density, viscosity and higher heating value) have been established (Ramirez–Verduzco et al., 2012). The biodiesel properties (density and viscosity) of methyl esters of n-Alkanoic acids were expected (K.Y. Liew et al. 2000). Methyl esters were selected based on hexanoic acid, heptanoic acid, octanoic acid, decanoic acid, and dodecanoic acids.

At coeval time (Ramirez 2000), a four-parameter modifiable analytical model was anticipated to consider biodiesel properties (dynamic viscosity of FAMES). In connection with molecular burden, number of double bonds, and temperature, he measured biodiesel property (viscosity) with unsaturated FAMES.

Referring to the work done by Baroutian et al. and Veny et al., it has been observed that the application of the empirical method of Janarthanan, the Spencer, and the Danner model, to envisage the biodiesel densities of Jatropha and Pongamia at several temperatures, are in good agreement in order to obtain good accuracy.

Vogel equalization was used to make a correlation of the viscosity of some biodiesel samples with temperature by (Yuan et al., 2000). addition, combination and testing between the different components of biodiesel (density, viscosity and calorific value) have shown that there is a high regression between its properties. (Rao et al., 2010).

The calculation of the higher heating value of different vegetable oil and their biodiesel from their density, viscosity and flash point developed mathematical equations (A. Dermibas, 2008) research on the properties of the biodiesel soap nut oil mixture has been studied (Y.H. Chen, T.H. Chiang, J.H. Chen, 2013) and the correlation among diverse fuel properties was established and recommended. (Atabani et al. 2014) expanded and examined the physico-chemical properties of various mixed biodiesels such as Croton megalocarpus, Calophyllum inophyllum, Moringa olefera, Palm and Coconut biodiesel and, based on the results, found a strong affiliation between diesel and biodiesel mixture properties.

There is a good affiliation between biodiesel and blend after many experimentations, some study, Then (Raheman and Ghadge, 2007) and (Godigunur et al. 2009) proposed a very low mahuah biodiesel blend of up to 20 percent.

Research conducted by (Sarin et al. 2009, 2016, 2021) palm oil biodiesel was mixed with biodiesel Jatropha and Pongamia to improve low temperature flow properties such as cloud point and pour point temperature.

II. MATERIALS AND METHODS

A. Experimental Database

Many articles from different researcher have been exploited and data gathered. A total of 1360 data were obtained (228 data for density, 268 data for viscosity, 266 data flash point, 207 data for cloud point, 179 data for pour point and 220 data for cetane number) from references 3 to 35. Then a total of 39 combinations has been done and in each combination the calculation of the minimum value, maximum value and normalization value was made. Random data division was made in three groups: 20% to validation, 20% to testing and 60% to training before entering parameters for simulation (ANN). The same combinations was used to run data in Minitab (RSM). Table below shows different combinations used in this work.

B. Combinations

The goal of this study is to augur and find the best accuracy using biodiesel properties (density, viscosity, cetane number). Different combination have been made. Table below shows different combination used in this study for both simulations (ANN, RSM). Table II.1 shows network model with different input combinations.
Table II.1: Network Model with Different Input Combinations

| property       | Combination input | Model name |
|----------------|-------------------|------------|
| \( v = f(F_p)  \) | \( F_p \)          | Network1   |
| \( v = (\rho)  \) | \( \rho \)          | Network2   |
| \( v = f(cp)   \) | \( cp \)           | Network3   |
| \( v = f(pp)   \) | \( pp \)           | Network4   |
| \( v = f(cn)   \) | \( cn \)           | Network5   |
| \( v = f(F_a)  \) | \( F_a \)          | Network6   |
| \( v = f(F_p, cp) \) | \( F_p, cp \)      | Network7   |
| \( v = f(F_a, F_p) \) | \( F_a, F_p \)      | Network8   |
| \( p = f(F_p)  \) | \( F_p \)          | Network9   |
| \( p = f(cp)   \) | \( cp \)           | Network10  |
| \( p = f(pp)   \) | \( pp \)           | Network11  |
| \( p = f(cn)   \) | \( cn \)           | Network12  |
| \( \rho = f(F_p, cp) \) | \( F_p, cp \)      | Network13  |
| \( \rho = f(F_p, cp, pp) \) | \( F_p, cp, pp \) | Network14  |
| \( \rho = f(F_a) \) | \( F_a \)          | Network15  |
| \( F_p = f(cp) \) | \( cp \)           | Network16  |
| \( F_p = f(pp) \) | \( pp \)           | Network17  |
| \( F_p = f(cn) \) | \( cn \)           | Network18  |
| \( F_p = f(cp, pp) \) | \( cp, pp \)      | Network19  |
| \( F_p = f(cp, pp, cn) \) | \( cp, pp, cn \) | Network20  |
| \( cp = f(v) \) | \( v \)            | Network21  |
| \( cp = f(pp) \) | \( pp \)           | Network22  |
| \( cp = f(cn) \) | \( cn \)           | Network23  |
| \( cp = f(pp, cn) \) | \( pp, cn \)      | Network24  |
| \( pp = f(cn) \) | \( cn \)           | Network25  |
| \( cn = f(F_a) \) | \( F_a \)          | Network26  |
| \( Fa = f(F_p, cp) \) | \( F_p, cp \)      | Network27  |
| \( Fa = f(F_p, cp, pp) \) | \( F_p, cp, pp \) | Network28  |
| \( Fa = f(F_p, cp, pp, cn) \) | \( F_p, cp, pp, cn \) | Network29  |
| \( Fa = f(v) \) | \( v \)            | Network30  |
| \( Fa = f(\rho) \) | \( \rho \)          | Network31  |
| \( Fa = f(F_p) \) | \( F_p \)          | Network32  |
| \( Fa = f(cp) \) | \( cp \)           | Network33  |
| \( Fa = f(cn) \) | \( cn \)           | Network34  |
| \( Fa = f(v, F_p) \) | \( v, F_p \)      | Network35  |
| \( Fa = f(cp, pp) \) | \( cp, pp \)      | Network36  |
| \( Fa = f(F_a, cp, pp) \) | \( F_a, cp, pp \) | Network37  |
| \( Fa = f(F_a, cp, pp, cn) \) | \( F_a, cp, pp, cn \) | Network38  |

Table II.2: Network Model with Combinations, Output and Regression Values (RSM)

| Combination                               | Output                                    | \( R^2 \) | \( R^2(adj) \) | \( R^2(pre) \) |
|-------------------------------------------|-------------------------------------------|------------|---------------|---------------|
| \( v = f(F_p) \)                         | \( v = 3.78 + 0.00035F_p \)              | 2.19       | 1.66          | 0             |
| \( v = f(\rho) \)                        | \( v = 4.05 + 0.00032\rho \)            | 0.00       | 0.00          | 0.00          |
| \( v = f(cp) \)                          | \( v = 4.3375 + 0.023cp \)              | 4.00       | 3.10          | 0.32          |
| \( v = f(pp) \)                          | \( v = 4.4009 + 0.018pp \)              | 4.11       | 3             | 0.00          |
| \( v = f(cn) \)                          | \( v = 4.100 + 0.0042cn \)              | 1.12       | 0.21          | 0.00          |
| \( v = f(F_a, F_p, cp) \)                | \( v = 1.47 + 0.0031p + 0.0015F_p + 0.0058cp \) | 1.45       | 0.00          | 0.00          |
| \( v = f(F_a, F_p) \)                    | \( v = 2.69 + 0.0012p + 0.0037F_p \)     | 2.49       | 1.12          | 0.00          |
| \( v = f(F_a, F_p, cp) \)                | \( v = 4.23 - 0.070c14:0 + 0.000011c16:0 + 0.0037c16:1 + 0.0018c18:0 + 0.0049c18:1 + 0.0006c18:2 + 0.0060c18:3 + 0.042c20:20 + 0.0034c22:20 \) | 17.76      | 14.8          | 2.15          |
| \( \rho = f(F_p) \)                       | \( \rho = 8.78.43 - 0.0088F_p \)        | 0.04       | 0.00          | 0.00          |
| \( \rho = f(cp) \)                        | \( \rho = 878.88 - 0.14cp \)            | 0.32       | 0.00          | 0.00          |
| \( \rho = f(pp) \)                        | \( \rho = 876.30 - 0.25pp \)            | 1.98       | 0.65          | 0.00          |
| \( \rho = f(cn) \)                        | \( \rho = 898.4 - 0.35cn \)             | 2.78       | 0.00          | 0.00          |
| \( \rho = f(F_a, cp) \)                   | \( \rho = 861.9 + 0.10F_p - 0.029cp \)   | 3.79       | 0.97          | 0.00          |
| \( \rho = f(F_p, cp) \)                   | \( \rho = 865 + 0.08F_p - 0.089cp - 0.15pp \) | 7.36       | 1.57          | 0.00          |
| \( \rho = f(F_a) \)                       | \( \rho = 876.91 - 0.32c14:0 + 0.0018c16 + 0.045c18:0 + 0.071c18:1 - 0.057c18:2 + 0.47c18:3 - 0.51c20:0 - 0.37c22:0 \) | 6.56       | 0.00          | 0.00          |
| \( F_p = f(cp) \)                         | \( F_p = 150.96 - 0.247cp \)            | 0.14       | 0.00          | 0.00          |
| \( F_p = f(pp) \)                         | \( F_p = 145.59 - 1.24pp \)             | 5.57       | 4.77          | 1.95          |
| \( F_p = f(cn) \)                         | \( F_p = 95.6 + 1.057cn \)              | 2.54       | 0.00          | 0.00          |
| \( F_p = f(cp, pp) \)                     | \( F_p = 141.15 + 1.044cp - 2.05pp \)   | 8.17       | 6.23          | 0.53          |
| \( F_p = f(cp, pp, cn) \)                 | \( F_p = 123.2 + 1.79cp + 2.67pp + 0.37cn \) | 11.9       | 7.45          | 0.00          |

Table II.2 shows network model with combinations, output and regression values.
### Mathematical Models for Predicting the Biodiesel Properties

| Function | Equation | Model | Parameter | Coefficient |
|----------|----------|-------|-----------|-------------|
| $F_p = f(F_a)$ | $F_p = 144.26 + 0.007c14:0 + 0.111c16:0 + 0.15c16:1 + 0.28c18:0 + 0.16c18:1 + 0.18c18:2 + 0.37c18:3 + 4.36c20:0 - 4.12c22:0$ | 7.73 | 2.08 | 2.60 | 0.52 | 0.00 |
| $cp = f(v)$ | $cp = -4.88 + 1.71v$ | 4.00 | 3.10 | 1.25 | 0.00 | 0.00 |
| $cp = f(pp)$ | $cp = 4.09 + 0.59pp$ | 52.7 | 9 | 1.27 | 0.00 | 0.00 |
| $cp = f(cn)$ | $cp = 0.99 + 0.058cn$ | 0.57 | 0.00 | 0.00 | 0.00 | 0.00 |
| $cp = f(pp, cn)$ | $cp = 6.92 + 0.5138pp - 0.05cn$ | 46.3 | 9 | 16.1 | 1 | 0 |
| $pp = f(cn)$ | $pp = 0.58 - 0.022cn$ | 0.05 | 0.00 | 0.00 | 0.00 | 0.00 |
| $pp = f(Fa)$ | $pp = -1.25 - 0.036c14:0 + 2.98c16:1 + 0.21c18:0 - 0.035c18:1 - 0.055c18:2 - 0.017c18:3 + 0.49c20:0 + 2.82c22:0$ | 21.6 | 2 | 11.6 | 9 | 0 |
| $cn = f(Fa)$ | $cn = 50.32 + 0.046c14:0 - 0.0021c16:0 + 0.042c16:1 + 0.072c18:0 + 0.49c18:1 + 0.018c18:2 - 0.034c18:3 - 0.73c20:0 - 0.079c22:0$ | 8.95 | 0.05 | 0.00 | 0.00 | 0.00 |
| $Fa = f(Fp, cp, pp)$ | $Fa = 0.03 + 0.00031Fp - 0.0061cp + 0.0072pp$ | 1.27 | 0.00 | 0.00 | 0.00 |
| $Fa = f(Fa, Fp, pp, cp, cn)$ | $Fa = -0.256 + 0.00039Fp - 0.0093cp + 0.0108pp + 0.0059cn$ | 2.68 | 0.00 | 0.00 | 0.00 |
| $Fa = f(v)$ | $Fa = -0.077 + 0.077v$ | 0.08 | 0.00 | 0.00 | 0.00 |
| $Fa = f(\rho)$ | $Fa = -0.86 + 0.00107\rho$ | 0.18 | 0.00 | 0.00 | 0.00 |
| $Fa = f(FP)$ | $Fa = -0.102 + 0.00189Fp$ | 0.21 | 0.00 | 0.00 | 0.00 |
| $Fa = f(cp)$ | $Fa = 0.43 + 0.0015cp$ | 0.11 | 0.00 | 0.00 | 0.00 |
| $Fa = f(cn)$ | $Fa = 0.59 - 0.0074cn$ | 0.06 | 0.00 | 0.00 | 0.00 |

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**Figure II.1:** analysis description

### C FUNCTIONAL ANALYSIS

ANN is used to solve nonlinear, variables, multivariable and multivariable problem. ANN follows different and specific step to accomplish a specific model. Previous Figure II.1 shows the analysis description below shows synoptic used in this model for ANN development models.

### D TEST CONDITION

Input, unseen and output layer are three main layers which constituted ANN structure. Data from external source are arranged by ANN. In the input layer, Data are transferred from other source to unseen layer by handling elements (neurons). Burdens are the values of connection between cells. The information is obtained using data from neurons in the input and hidden layer, bias, and stimulation conditions.

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**Figure II.1:** analysis description
Constituted of outing layer, the outing of the network is obtained by handling data from unseen layer and send to external source. In this present work, the feedforward architecture with three layers (input, unseen and output) is used. Also TRAINLM is used as training function that updates the burden and bias values of neuron connections, according to Levenberg-Maquardt (LVM) optimization. Depending of the type of the neural network to be designed, tangent function and hyperbolic function, Threshold function, step stimulation function, sigmoid function are selected and regularly used. Figure below shows the functional diagram of neural network. Input Hidden layer Output

![Figure II.2: ANN model used in this work](image)

Referring to activation function, many studies used a sigmoid function. In the present study, this function is used as function which output is in between 0 and 1. It is defined by:

$$ f(x) = \frac{1}{1+e^{-x}} $$

(1)

Standardization of data in this study in the range of 0.01 to 0.09 is obtained by using the following equation:

$$ f(x) = \frac{x_{actual} - x_{min}}{x_{max} - x_{min}} $$

(2)

### E Empirical Models

Modelization of different combinations (kinematic viscosity, density, and cetane number) was made using:

- artificial neural network (ANN)
- response surface methodology (RSM)

Input data is obtained in function of target we want to obtain. (flash point, fatty acid, density, cloud point, pour point, cetane number) as input for viscosity, (flash point, cloud point, pour point, cetane number) as input for density, (fatty acid, f.a) as input for cetane number. Also to achieve this simulations, limit of input data and margin of determination of RRSME is listed. Figure II.3 and II.5 below show different limits and range.

### Table II.3: margin values for input and output variables

| Limits values | Units |
|---------------|-------|
| MIN           | MAX   |
| Viscosity     | 2.3   | 5.81 | mm²/s |
| Density       | 807   | 903  | kg/m³ |
| Flash point   | 11    | 264  | °C    |
| Cloud point   | -13.4 | 19   | °C    |
| Pour point    | -22.5 | 24   | °C    |
| Cetane number | 27.7  | 177  |       |
| Fatty acid    | 0     | 77   | mass fraction (w) |

The following table II.4 shows the condition followed in this work to run data in ANN network.

### Table II.4: ANN condition

| Network type | Multi – layer feedforward |
|--------------|---------------------------|
| Training function | TRAINLM |
| Adaptive learning function | LEARNINGDM |
| Performance function | MSE |
| Number of inputs | varied from 1 to 6 |
| Number of outputs | 1 |
| Number of hidden layer | varied from 2 to 8 |
| The optimum Number of neurons | 2 |
| Transfer function | Log sigmoid |

Also RSM design used number of continuous factors of 3, number of categorical factor of 1, number of block of 1 and number of replicate of 1. In order to have and to identify best ANN result, the relative root medium square erratum (RRSME) is used in this study and it is described as follow.

### Table II.5: RRSME margin

| Range of RRSME | Evaluation |
|----------------|------------|
| < 10%          | Excellent  |
| 10% < RRMSE < 20% | good  |
| 20% < RRMSE < 30% | fair  |
| > 30%          | poor       |
### III. RESULTS AND DISCUSSIONS

#### A. MODEL USED TO DEVELOP ANN

Response surface methodology (RSM) and artificial neural network (ANN) are used to identify the most variable, which affect the prediction of kinematic viscosity, density and cetane number. The input parameters identified are flash point, viscosity, density, cetane number, fatty acid, cloud point and pour point. In order to check the prediction accuracy using the identified parameters, 39 ANN and RSM models are developed. In order to evaluate and obtain good result, the parameters below were used: correlation coefficient ($R^2$), medium square error (mse), comparative root medium square (RRMSE). Depending on the value of mse, the number of neurons will be constantly increased and the action re-training. In this study hidden layer varies from 5 to 8. Following figure and table show different result obtained and explained.

**Table III.1: Network performance with regression values**

| S. no | Target | Network input | Network 1 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $f_p$  | Log sigmoid    | 5.80%                  | 0.9994 | 0.9995 | 0.000072 | 7     |
| 2     | $f_p$  | Log sigmoid    | 7%                     | 0.9992 | 0.9993 | 0.000106 | 0     |

| S. no | Target | Network input | Network 2 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $c_p$  | Log sigmoid    | 9.24%                  | 0.9983 | 0.9990 | 0.000124 | 0     |
| 2     | $c_p$  | Log sigmoid    | 10.5%                  | 0.9973 | 0.9984 | 0.000309 | 0     |

#### Network 3 performance

| S. no | Target | Network input | Network 3 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $p_p$  | Log sigmoid    | 6.95%                  | 0.9990 | 0.9994 | 0.000145 | 0     |
| 2     | $p_p$  | Log sigmoid    | 10%                    | 0.9959 | 0.9951 | 0.000472 | 0     |

#### Network 4 performance

| S. no | Target | Network input | Network 4 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $c_n$  | Log sigmoid    | 11.1%                  | 0.9983 | 0.9972 | 0.000262 | 0     |
| 2     | $c_n$  | Log sigmoid    | 10.25%                 | 0.9984 | 0.9987 | 0.000183 | 0     |
| 3     | $c_n$  | Log sigmoid    | 11.4850%               | 0.9983 | 0.9984 | 0.000130 | 0     |

#### Network 5 performance

| S. no | Target | Network input | Network 5 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $f_p,c_p$ | Log sigmoid    | 7.70%                  | 0.9994 | 0.9990 | 0.000296 | 0     |
| 2     | $f_p,c_p$ | Log sigmoid    | 6.80%                  | 0.9990 | 0.9954 | 0.000190 | 0     |

#### Network 6 performance

| S. no | Target | Network input | Network 6 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $f_p, c_p$ | Log sigmoid    | 7.50%                  | 0.9985 | 0.9989 | 0.000188 | 0     |
| 2     | $f_p, c_p$ | Log sigmoid    | 6.60%                  | 0.9992 | 0.9989 | 0.000655 | 0     |
| 3     | $f_p, c_p$ | Log sigmoid    | 6.65%                  | 0.9987 | 0.9979 | 0.000101 | 0     |

#### Network 7 performance

| S. no | Target | Network input | Network 7 performance | RRMS-E | $R$ | $R^2$ | mse   |
|-------|--------|---------------|------------------------|--------|-----|-------|-------|
| 1     | $F_a$  | Log sigmoid    | 9.50%                  | 0.9996 | 0.9993 | 0.000040 | 8     |
| 2     | $F_a$  | Log sigmoid    | 5.50%                  | 0.9997 | 0.9998 | 0.000034 | 7     |
| Network | Performance | ρ | fp | Log sigmoid | 6% | 0.9994 | 0.9997 | 0.000052 |
|---------|-------------|---|----|-------------|----|-------|--------|-----------|
| 1       |             | p | fp | Log sigmoid | 6.65% | 0.9994 | 0.9997 | 0.000073  |
| 2       |             | p | fp | Log sigmoid | 10.5% | 0.9989 | 0.9997 | 0.000087  |
| 1       |             | p | cp | Log sigmoid | 10.75% | 0.9980 | 0.9971 | 0.000237  |
| 2       |             | p | cp | Log sigmoid | 9.85%  | 0.9985 | 0.9972 | 0.000276  |
| 1       |             | p | pp | Log sigmoid | 10.22% | 0.9934 | 0.9971 | 0.000237  |
| 2       |             | p | pp | Log sigmoid | 11.5%  | 0.9922 | 0.9965 | 0.000522  |
| 1       |             | p | Fp,cp | Log sigmoid | 10.22% | 0.9986 | 0.9989 | 0.000291  |
| 2       |             | p | Fp,cp | Log sigmoid | 12.5%  | 0.874  | 0.642  | 0.000683  |
| 1       |             | p | Fp,cp,pp | Log sigmoid | 6.80%  | 0.9993 | 0.9973 | 0.000291  |
| 2       |             | p | Fp,cp,pp | Log sigmoid | 10.58% | 0.9962 | 0.9973 | 0.000230  |
| 1       |             | p | Fa  | Log sigmoid | 10.25% | 0.9981 | 0.9986 | 0.000236  |
| 2       |             | p | Fa  | Log sigmoid | 5.5%   | 0.9995 | 0.9996 | 0.000088  |
| 3       |             | p | Fa  | Log sigmoid | 4.35%  | 0.9997 | 0.9998 | 0.000032  |
| 1       |             | cn | Fa  | Log sigmoid | 4.88%  | 0.9997 | 0.9997 | 0.000051  |
| 2       |             | cn | Fa  | Log sigmoid | 12.2%  | 0.9962 | 0.9997 | 0.000054  |

Illustration of this statistical values are showed in the following figures. The best of each combination will be showed.
Figure III.1 shows the regression analysis for fatty acid comparison to viscosity. The validation and training of this combination give a good result between fatty acid and viscosity. The overall coefficient R and the correlation coefficient $R^2$ are closer each to other and they are near to 0. Then referring to this result we can assume that this combination give good accuracy. In order to predict biodiesel properties this combination is useful.

Figure III.2 shows viscosity versus fatty acid mse. Also the mse value of this combination is near to 0. This give more than more a good statements of good combination.

Figure III.3 shows the regression density versus flash point. In comparison with the previous result, this combination also give a good accuracy since theirs correlations coefficient and and overall coefficient are closer each other and near to 0. But error is 0.0003 and it is large than the combination viscosity and fatty acid which is 0.
Figure III.4 shows density versus flash point mse

The mse value of the combination density function flash point is fair since it is closer to 0. Figure III.5 shows the cetane number versus fatty acid.

Cetane number function fatty acid is very good combination since the training and validation values are almost the same and. Accuracy in this case is also fair since R and $R^2$ are closer.

Figure III.6 shows the mse regression value of cetane number function fatty acid.

Also in this combination the mse value of the combination density fatty acid and cetane number is fair since it tend to 0.

B Statistical observation of ann model

Many properties have been used to simulate combinations. The best performance is achieved by repeating the simulation until the minimum possible performance of mse is obtained. Likewise when the value of $R^2$ increases the value of mse must decrease, this indicates the correct functioning of the software. Otherwise the simulation is interrupted. Thus referring to what is said above and the assessment of RRSME the networks (7, 1, 14, and 4, 6) present combinations with good and high accuracy due to the fact that their margin of error is between 0 and 0.0003, R and $R^2$ are close to each other and close to 1. Also the RRSME values for this combination are less than 30%.

In other hand combinations (2, 3, 15, 5, 8, 9, 10, 11, 12, 13) have values with less and fair accuracy because of a large margin between their respective values of $R^2$ and R and also their percentage of RRSME between 10% and 20% for some and between 20% and 30% for others.

C Analysis of best performance

Table III.2 : Best performance analysis

| Network | Target | Combination | R   | $R^2$ | Mse  | Error % |
|---------|--------|-------------|-----|-------|------|---------|
| 1       | v      | $fp$        | 0.99| 0.99  | 727  | 0.00    |
|         | v      | $fp$        | 0.99| 0.99  | 0.0001| 0.00    |
|         | v      | $fp$        | 0.99| 0.99  | 0.0001| 0.00    |
|         | v      | $fp$        | 0.99| 0.99  | 0.0001| 0.00    |

Figure III.1: Cetane Number versus Fatty acid Regression
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| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| Model  | 1  | 1.433  | 1.4326 | 3.69    | 0.058   |

Linear

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| pour p | 1  | 1.433  | 1.4326 | 3.69    | 0.058   |

Error

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| Lack-of-Fit | 35 | 9.798  | 0.2799 | 0.60    | 0.941   |

Pure Error

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| Total  | 44 | 16.0322|        |         |         |

We can also observe that this configuration present almost the same configuration as the previous combination.

Figure III.7 shows response Surface Regression: viscosity versus density, flash p, cloud p, pour p.

Table III.3: Analysis of variance viscosity versus flash point

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| Model  | 1  | 1.433  | 1.4326 | 3.69    | 0.058   |

Figure III.8 shows Response Surface Regression: viscosity versus density, flash p, cloud point, pour p.

Table III.4: Analysis of variance viscosity versus density, flash p, cloud point, pour point

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| Model  | 4  | 0.5939 | 0.148472| 0.38    | 0.818   |
| Linear | 4  | 0.5939 | 0.148472| 0.38    | 0.818   |
| density | 1  | 0.0191 | 0.019062| 0.05    | 0.825   |
| flash p | 1  | 0.2565 | 0.256537| 0.66    | 0.420   |
| cloud p | 1  | 0.0552 | 0.055246| 0.14    | 0.707   |
| pour p | 1  | 0.0366 | 0.036598| 0.09    | 0.760   |
| Error  | 40 | 15.4383| 0.385957|         |         |
| Lack-of-Fit | 39 | 15.4383| 0.395853|         |         |
| Pure Error | 1  | 0.0000 | 0.000000|         |         |
| Total  | 44 | 16.0322|        |         |         |

D Analyze Using Response Surface Methodology

The same data cited in the literature review above are used for analysis with Minitab. Only the combinations used in the analysis with ANN will be used here and then compared each other.

Also like simulation with ANN, RSM simulation were also done and the following result are obtained.

Figure III.7 shows response Surface Regression: viscosity versus flash point

Table III.3: Analysis of variance viscosity versus flash point

| Source | DF | Adj SS | Adj MS | F-Value | P-Value |
|--------|----|--------|--------|---------|---------|
| Model  | 1  | 1.433  | 1.4326 | 3.69    | 0.058   |

Figure III.8 shows Response Surface Regression: viscosity versus density, flash p, cloud p, pour p.
Figure III.9: shows Response Surface Regression: viscosity versus density, flash p

Table III.5: Analysis of variance viscosity versus density, flash p

| Source          | DF | Adj SS  | Adj MS  | F-Value | P-Value |
|-----------------|----|---------|---------|---------|---------|
| Model           | 2  | 1.5196  | 0.75979 | 1.81    | 0.167   |
| Linear          | 2  | 1.5196  | 0.75979 | 1.81    | 0.167   |
| density         | 1  | 0.0368  | 0.03678 | 0.09    | 0.768   |
| flash p         | 1  | 1.4685  | 1.46852 | 3.50    | 0.063   |
| Error           | 14 | 59.5338 | 0.41925 |         |         |
| Lack-of-Fit     | 13 | 59.3538 | 0.44294 | 19.69   | 0.000   |
| Pure Error      | 8  | 0.1800  | 0.02250 |         |         |
| Total           | 14 | 61.0534 |         |         |         |

Figure III.10 shows Response Surface Regression: density versus flash p, cloud p

Table III.6: Analysis of variance density versus flash point, cloud point.

| Source          | DF | Adj SS  | Adj MS  | F-Value | P-Value |
|-----------------|----|---------|---------|---------|---------|
| Model           | 2  | 555.8   | 277.906 | 1.32    | 0.273   |
| Linear          | 2  | 555.8   | 277.906 | 1.32    | 0.273   |
| flash p         | 1  | 554.2   | 554.158 | 2.64    | 0.109   |
| cloud p         | 1  | 1.6     | 1.56    | 0.01    | 0.932   |
| Error           | 64 | 13427.2 | 209.8   |         |         |
| Lack-of-Fit     | 60 | 13418.2 | 223.637 | 99.62   | 0       |
| Pure Error      | 4  | 9       | 2.245   |         |         |
| Total           | 66 | 13983   |         |         |         |

Figure 4.11 shows Response Surface Regression: viscosity versus density, flash p, cloud p

Table III.7: Analysis of variance viscosity versus density, flash p, cloud p.

| Source          | DF | Adj SS  | Adj MS  | F-Value | P-Value |
|-----------------|----|---------|---------|---------|---------|
| Model           | 3  | 0.3238  | 0.10794 | 0.30    | 0.826   |
| Linear          | 3  | 0.3238  | 0.10794 | 0.30    | 0.826   |
| density         | 1  | 0.1257  | 0.12566 | 0.35    | 0.557   |
| flash p         | 1  | 0.0868  | 0.08680 | 0.24    | 0.626   |
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### Table III.8: Analysis of variance density versus flash p, cloud p, pour p

| Source     | DF | Adj SS | Adj MS | F-Value | P-Value |  
|------------|----|--------|--------|---------|---------|  
| Model      | 3  | 501.78 | 167.260| 1.27    | 0.295   |  
| Linear     | 3  | 501.78 | 167.260| 1.27    | 0.295   |  
| flash p    | 1  | 362.02 | 362.016| 2.75    | 0.104   |  
| cloud p    | 1  | 6.35   | 6.349  | 0.05    | 0.827   |  
| pour p     | 1  | 23.28  | 23.279 | 0.18    | 0.676   |  
| Error      | 48 | 6315.21| 131.567|         |         |  
| Lack-of-Fit| 45 | 6306.23| 140.138| 46.82   | 0.004   |  
| Pure Error | 3  | 8.98   | 2.993  |         |         |  
| Total      | 51 | 6816.99|        |         |         |  

### Table III.9: Analysis of variance viscosity versus fatty acid

| Source     | DF | Adj SS | Adj MS | F-Value | P-Value |  
|------------|----|--------|--------|---------|---------|  
| Model      | 9  | 21.017 | 2.3353 | 6.19    | 0.000   |  
| Linear     | 9  | 21.017 | 2.3353 | 6.19    | 0.000   |  
| c14:0      | 1  | 15.126 | 15.126 | 40.11   | 0.000   |  
| c16:0      | 1  | 0.000  | 0.0002 | 0.00    | 0.980   |  
| c16:1      | 1  | 0.103  | 0.1027 | 0.27    | 0.602   |  
| c18:0      | 1  | 0.019  | 0.0190 | 0.05    | 0.823   |  
| c18:1      | 1  | 2.913  | 2.9134 | 7.73    | 0.006   |  
| c18:2      | 1  | 0.054  | 0.0542 | 0.14    | 0.705   |  
| c18:3      | 1  | 0.410  | 0.4098 | 1.09    | 0.298   |  
| c20:0      | 1  | 0.005  | 0.0047 | 0.01    | 0.911   |  
| c22:0      | 1  | 0.007  | 0.0066 | 0.02    | 0.895   |  
| Error      | 25 | 97.674 | 3.777  |         |         |  
| Lack-of-Fit| 17 | 58.454 | 0.3359 | 0.73    | 0.959   |  
| Pure Error | 85 | 39.220 | 0.4614 |         |         |  
| Total      | 26 | 118.69 | 1       |         |         |  

Figure III.12 shows Response Surface Regression: density versus flash p, cloud p, pour p

Table III.10 shows Response Surface Regression: viscosity versus fatty acid

Figure III.13 shows Response Surface Regression: viscosity versus c14:0, c16:0, c16:1, c18:0, c18:1, c18:2, c18:3, c20:0, c22:0
Figure III.14 shows Response Surface Regression: density versus c14:0, c16:0, c16:1, c18:0, c18:1, c18:2, c18:3, c20:0, c22:0

Table III.10: Analysis of variance density versus fatty acid

| Source   | DF | Adj SS  | Adj MS  | F-Value | P-Value |
|----------|----|---------|---------|---------|---------|
| Model    | 9  | 1194.2  | 132.692 | 0.59    | 0.799   |
| Linear   | 9  | 1194.2  | 132.692 | 0.59    | 0.799   |
| c14:0    | 1  | 64.8    | 64.827  | 0.29    | 0.592   |
| c16:0    | 1  | 5.9     | 5.928   | 0.03    | 0.871   |
| c16:1    | 1  | 47.8    | 47.781  | 0.21    | 0.645   |
| c18:0    | 1  | 4.6     | 4.595   | 0.02    | 0.886   |
| c18:1    | 1  | 157.4   | 157.367 | 0.70    | 0.405   |
| c18:2    | 1  | 143.1   | 143.076 | 0.64    | 0.427   |
| c18:3    | 1  | 731.4   | 731.354 | 3.27    | 0.075   |
| c20:0    | 1  | 45.2    | 45.226  | 0.20    | 0.654   |
| c22:0    | 1  | 1.1     | 1.142   | 0.01    | 0.943   |
| Error    | 76 | 17021.0 | 223.960 |         |         |
| Lack-of-Fit | 53 | 12219.3 | 230.554 | 1.10    | 0.409   |
| Pure Error | 23 | 4801.6  | 208.767 |         |         |
| Total    | 85 | 18215.2 |         |         |         |

Figure III.15 shows Response Surface Regression: cetane n versus c14:0, c16:0, c16:1, c18:0, c18:1, c18:2, c18:3, c20:0, c22:0

Table III.11: Analysis of variance cetane number versus fatty acid

| Source   | DF | Adj SS  | Adj MS  | F-Value | P-Value |
|----------|----|---------|---------|---------|---------|
| Model    | 9  | 334.49  | 37.166  | 1.01    | 0.442   |
| Linear   | 9  | 334.49  | 37.166  | 1.01    | 0.442   |
| c14:0    | 1  | 2.20    | 2.201   | 0.06    | 0.808   |
| c16:0    | 1  | 9.54    | 9.542   | 0.26    | 0.613   |
| c16:1    | 1  | 10.99   | 10.988  | 0.30    | 0.587   |
| c18:0    | 1  | 6.74    | 6.744   | 0.18    | 0.670   |
| c18:1    | 1  | 110.77  | 110.772 | 3.00    | 0.087   |
| c18:2    | 1  | 18.01   | 18.012  | 0.49    | 0.487   |
| c18:3    | 1  | 5.43    | 5.434   | 0.15    | 0.702   |
| c20:0    | 1  | 107.03  | 107.031 | 2.89    | 0.092   |
| c22:0    | 1  | 3.30    | 3.298   | 0.09    | 0.766   |
| Error    | 92 | 3401.67 | 36.975  |         |         |
| Lack-of-Fit | 72 | 3179.75 | 44.163  | 3.98    | 0.001   |
| Pure Error | 20 | 221.92  | 11.096  |         |         |
| Total    | 101| 3736.16 |         |         |         |

E RSM result interpretation

The aim of the study is to find a good accuracy combination by using ANN and RSM combination result. The results obtained with the RSM method are less favorable since their p-value and f-value are very distant from each other. It is also important to note that obtaining an acceptable result using this method requires the combination of at least three other properties. Also the combination of viscosity,
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Density and cetane number properties with the fatty acid individually does not provide a better result.

\[ F \text{ Analysis of Comparison between } R^2(\text{ANN}) \text{ and } R^2(\text{RSM}) \]

| Combination | \( R^2(\text{ANN}) \) | \( R^2(\text{RSM}) \) |
|-------------|---------------------|---------------------|
| \( \nu = f(Fa) \) | 0.9998              | 0.9112              |
| \( \rho = f(Fa) \) | 0.9998              | 0.799               |
| \( \text{cn} = f(Fa) \) | 0.9987              | 0.766               |

IV. CONCLUSION AND FUTURE WORKS

Density, viscosity, and cetane number are important physical properties of biodiesel because of their direct implications in the combustion of fuel in the operation of machinery. Then poor accuracy prediction of these properties has a direct impact on engine performance. Throughout this thesis, different prediction methods were used to search for or obtain the best accuracy. Thus combinations obtained have been simulated and analyzed mathematically in two different software applications: ANN and RSM. As a result, it is clear that: The overall regression coefficient \( R \) and the correlation coefficient \( R^2 \) values of the combinations obtained in the simulation with the ANN provide better and good accuracy since their values are close to each other and all close to 1, and their mse tend towards 0. While the result obtained with RSM are distant from each other and distant of 0 so they provide an acceptable accuracy. It is also important to note that after analysis of the graphs obtained by the RSM method, the achievement of good and high accuracy requires the combination of at least 3 properties of biodiesel. It should be also added in this thesis that the combinations made with the FAME produce more and better yield meaning there is a good relationship between the FAME and the properties density, viscosity and cetane number. However some studies remain to discover since our goal in this study was focused only on viscosity, density and cetane number. Combining other properties will therefore be future objectives. The purpose of this study being to recover high accuracy, we have combined and simulated properties in two different software namely RSM and ANN, however our duty was based on three specific properties of biodiesel (density, viscosity, cetane number). Thus in forthcoming studies it will be discussed not only to focus on other properties of biodiesel (pour point, cloud point, flash point ), but also later use other software to find the best combination(s) needed to increase the power and efficiency of diesel engines.

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