MATHEMATICAL MODELS FOR PREDICTING THE BIODIESEL PROPERTIES
A THESIS SUBMITTED TO THE GRADUATE SCHOOL OF APPLIED SCIENCES OF NEAR EAST UNIVERSITY
By CONSTANT BANDE BAKANDE
In Partial Fulfillment of the Requirements for the Degree of Masters of Science In Mechanical Engineering
NICOSIA, 2019

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Constant BandeBakande: MATHEMATICAL MODELS FOR PREDICTING THE BIODIESEL PROPERTIES

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Department of Mechanical Engineering, NEU I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

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ABSTRACT

Density, viscosity and cetane number are important physical properties of biodiesel as they participate in the fuel metering, calibration and nozzle process during combustion. High accuracy of the properties of biodiesel will lead to improved better efficiency. The aim of this study is to seek good and high precision by combining properties and comparing the analysis between ANN and RSM. From previous study, A total of 1360 data have been collected and 39 possible combinations were analyzed and compared by ANN and RSM. The result of simulation is: The best combinations: $\rho = f(F)$, $\nu = f(F)$, c = f(F) with \mathbb{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 \mathbb{R}^2 (0.808, 0.799, 0.911) and R (0.837, 0.739, 0.920) obtained with RSM simulation. 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 \mathbb{R}^2 values of the combinations obtained in the simulation with the ANN provide 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 important to note that high accuracy of properties using RSM must have at least combination of three parameters. Also after many combination, fatty acid and others properties provide good result and it will be benefit for the future.

Keywords: viscosity; density;cetane number fatty acid; overall coefficient; regression coefficient; ANN; RSM

ÖZET

Yo unluk. viskozitevesetansayısı, yanmasırasındayakıtölçümü, kalibrasyonvenozuli leminekatıldıklarıiçinbiyodizelinönemlifizikselözellikleridir. Biyodizelinözelliklerininyüksekdo rulu u, dahaiyiverimliliksa lar. Bu çalı manınamacı, özellikleribirle tirerekve YSA ile RSM arasındakianalizikar ıla tırarakiyiveyüksekhassasiyeteldeetmektir. Öncekiçalı madantoplam1360veritoplanmı ve 39 olasıkombinasyonanalizedilmi ve YSA ve RSM ilekar ıla tırılmı tır. Simülasyonunsonucu: Eniyikombinasyonlar: = f (Fa), = f (Fa), cn = f (Fa)R ^ 2 sırasıyla (0.9998, 0.9998, 0.9987) ve R e ittir (0.9997) ANN simülasyonuileeldeedilen 0.99971,0.9984), RSM simülasyonuileeldeedilen R ^ (0.808, 0.799, 0.911) ve R (0.837, 0.739, 'den dahafazlado ruluksa lar. 0.920) Ayrıcaiyisonuçverdikleriiçinya asidivedi erözellikleriarasındaiyibirili kivardır. Genelolarak, simülasyondaeldeedilenkombinasyonların ANN ileeldeedilentoplamregresyonkatsayısı R R ۸ 2 vekorelasyonkatsayısı de erleri. de erleribirbirineyakınvetümü 1'e yakınoldu uvemse'nin0'ae ilimlioldu uiçiniyido ruluksa lar. RSM ileeldeedilen, 0 bunedenlekabuledilebilirbirdo ruluksa larlar. birbirindenuzakve uzaktır. RSM kullananözelliklerinyüksekdo rulu ununenazüçparametreninbirle iminesahipolmasıgerekti inibelir tmekönemlidir. Ayrıcabirçokkombinasyondansonra,

ya asidivedi erözellikleriyisonuçverirvegelecekiçinfaydasıolacaktır.

AnahtarKelimeler: viskozite; yo unluk; setansayısıya asidi; toplamkatsayı; regresyonkatsayısı; ANN; RSM

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LIST OF ABBREVIATIONS

ANN:	Artificial Neural Network
Cp:	Cloud point
Fp:	Flash point
Pp:	Pour point
RRMSE:	Relative root mean square error
RSM:	Response surface methodology
:	Kinematic viscosity
ρ:	density
с:	Cetane number

LIST OF ABBREVIATIONS (continued)

C14:0	Myristic

- C16:0 Palmitic acid
- C16:1 Palmitolcic acid
- C18:0 Stearic acid
- C18:1 Oleic acid
- C18:2 Linoleic acid
- C18:3 Alpha linoleic acid
- C20:0 Anahidic acid
- C22:0 Behenic acid

CHAPTER I

INTRODUCTION

I 1Background

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. Biodiesel is a sustainable and biodegradable fuel that can be made and processed domestically from vegetable oils, animal fat / tallow and restaurant grease recycled. Fuel consisting with monoalkyl ester of a long fatty acid chain is a Biodiesel in compliance with the American Society of Testing and Materials (ASTM) D6751 specifications and the European EN 14214 standard. Biodiesel is currently used extensively by automotive and thermal engines because of its accessibility, low cost and biodegradable. That energy source is long-lasting (Pratas et al, 2010). Diesel provides good safety in the domestic storage of liquids since it is less fuelefficient. Biodiesel has many physical properties but few are very significant as it helps to determine efficiency, fuel atomization, control process actuation, and possible engine design. Although viscosity and density are involved in fuel combustion during injection, cetane number, on the other hand, suggests fuel quality during the process of combustion. Several researchers are still developing new fashioned techniques to forecast physical properties present in diesel. Instead, a technique based on the Kay mixing rule and the contribution method for predicting the density of ten biodiesel samples as a function of temperature was applied by Freitas et al. to different models for contemplating the viscosity of biodiesel at multiple temperatures. More empirical correlations were established by Rodriguez-Rodriguez, Ramirez - Verduzco LF in (2011) and Geacais, Julian O, Nitra I in (2015) to predict the viscosity of biodiesel blends at different temperatures (T) and volume fraction (VF). Empirical

correlations were also extended by (Ramirez-Verduzco et al.) to predict the density, viscosity, cetane number and higher heating value (HHV) of biodiesel from its chemical composition. Ramirez – Verduzco recently developed analytical correlations to estimate the viscosity and density at different temperatures of the methyl esters of fatty acids and biodiesel. Average Relative Deviation (ADD) are expected values of 6.39 per cent for viscosity and 0.43 per cent for density.

Expansion of prediction methods provides more than greater value in estimating biodiesel properties. Relevant literature research studies have been found. Balabin et al tested other artificial neural networks that were developed and found that their artificial neural network had a slight mean square error referring to other models. Saldana et al., gave a description of different artificial neural network models with a coefficient of correlation between 0.985 and 0.995. Kumar and Bansal resulted in a mean square error of 0.02 and 5.510 (-6) for the viscosity of diesel and biodiesel blends.

I.2 Advantages of Biodiesel

Biodiesel is considered renewable energy and is biodegradable and can be mixed with other (diesel) fuels. It has lower Diesel flammability Comparing to diesel, materials used to manufacture biodiesel are cheap and available (Raimrez-Verduzco LF, 2013). Biodiesel may also be used as fuel engine for any other vehicle, such as diesel or other engines.

The material used for biodiesel processing, namely animal and vegetable fats, is accessible and cheaper.

Many plants are increasingly harvested and used also for the production of biodiesel. Which reduces production and manufacturing costs as compared to diesel which is much more costly to handle.

Referring to engine, Very good lubrication results in decreased engine wear when using biodiesel, it provides more oxygen, resulting in better combustion and therefore less fine particles, cleaner fuel.

I.3 Disadvantage of Biodiesel

Like any other side of the coin biodiesel also has disadvantages. It has higher viscosity and lower energy content disadvantage that can be solved by mixing both diesel and biodiesel (Ramirez – Verduzco LF.2013).

Referring to engine, with long operation, the engine oil must be changed more often. On a first use of biodiesel, the fuel filter must be changed no later than the second full, as biodiesel tends to clean the tank and lines.

Also during cold weather, there is a thickening of biodiesel, which increases its kinematic viscosity and therefore reduces engine performance. This problem is solved by blending the biodiesel with a diesel.

I.4 Aim of the Study

The purpose of this work is to predict biodiesel properties (density, viscosity, cetane number) using the artificial neural network (ANN) and surface response methodology (RSM) analysis curve for comparison and analysis results. To achieve this goal and obtain high accuracy prediction:

- 1. Data will be collected and properties combined.
- 2. Data will be analyzed with ANN and RSM approchs.

I.5 Thesis Outline

this section addresses design, description, advantages and disadvantages. Chapter 2 provides a study of the various methods used to predict biodiesel properties, descriptions of theories and explanations. Chapter 3 presents the collection of data grouped into two groups: first related to the collection of fatty acids, and second related to other properties (density, viscosity, flash point, cloud level, cetane number) also Result discussion and presentation of different curve are presented in chapter 4. Chapter 5concludes, and suggests future work.

CHAPTER 2

BIODIESEL

2.1Literature 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 (Geacai et al, 2015; EbnaAlam Fahd et al., 2014; Gülüm&Bilgin, 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&Todoru , 2011); (Barabás, 2013); (neuro fuzzy, Mostafaei et al., 2016);(Hosoz et al., 2013); and artificial neural neuralneural (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 Palm 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 amongdiverse fuel properties was

established and recommended. (Atabani et al. 2014) expanded and examined the physicochemical properties of various mixed biodiesels such as Croton megalocarpus, Calophylluminophyllum, Moringaolefera, 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 mahua 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.

2.2 Biodiesel

Biodiesel is a renewable fuel which can be made from vegetable oils, animal fat / tallow and restaurant grease recycled. Technically, biodiesel is a fuel composed of mono-alkyl ester from a long chain of fatty acids that obeys with the American Society of Testing and Materials (ASTM) D6751 (2003) and the European EN 14214 (2003) necessities. Biodiesel is used in many energy fields, due to its flexibility and various benefits. The raw material required for biodiesel (animal fat restaurant) production is accessible and less expensive. The high use as plant raw material for producing this same biodiesel also creates and develops more jobs in parallel. It is biodegradable and can be mixed with a variety of other sources of energy (diesel). Like every other side of coin, there are also drawbacks such as higher viscosity levels relating to diesel (Nogueira et al., 2010). Biodiesel at low temperatures poses a thickening problem that increases viscosity and decreases engine efficiency. Biodiesel also has a lower energy content and can be achieved by combining biodiesel with gasoline. There are many properties of biodiesel but density, viscosity and cetane number (cn) are very important due to their direct involvement in the determination of fuel quality during the combustion process, injection system operation and control (Ramirez-Verdasco, LF 2013).

2.3 Biodiesel Properties

2.3.1 Viscosity

Viscosity is a quantitative indicator of fluid flow resistance. On the other hand, it is known as internal fluid friction, there are normally two types of viscosity measurements: kinematicviscosity and dynamic viscosity

2.3.2 Dynamic viscosity

Defined as the measurement of fluid resistance to flow when applying external force, the constant proportionality between shear stress and velocity gradient is also defined in the other hand. The shear stress ratio with the fluid's velocity gradient is also known as absolute velocity. If two layers of fluid, the distance dy apart, travel at different speeds one over the other, the top layer causes shear stress on the adjacent lower layer while the lower layer causes shear stress on the adjacent top layer. The shear stress (ÿ) is proportional to the y-respect rate of change.



Figure 3.1: dynamic viscosity modelization

The external force:

$$\tau = \mu \frac{\partial}{\partial \tau} (3.1)$$
 with $\tau = \frac{F}{A}, \frac{\partial}{\partial \tau}$ the local shear velocity

 τ is Usually applied when the goal is to keep the top plate going at constant velocity. Centipoises is a traditional dynamic viscosity measurement device. It is of the poise of 1/1000. Poise is the name of the French scientist Jean Louis Poiseuille (1799-1869), (Tushar., 2007). Many other units are commonly used: Ns / m^2 , Pa. S or Kg/(m)s, N is the newton and Pa is the Pascal.

2.3.3 Kinematic viscosity

Is the measure of fluid resistance intrinsic to flow when there is no external force, except that gravity acts upon it. On the other hand, under the weight of gravity it is calculation of the resistive flow of air. It's expressed by the complex viscosity ratio to a substance's density at the same temperature.

 $v = \frac{\mu}{\rho}$ (3.2) Where is the kinematic viscosity in $\frac{m^2}{s}$, is the density of the fluid in k/m^2 and u is the dynamic viscosity. Fluid viscosity is generally affected by type of fluid, condition of utilization and inter molecules between fluid. Then it is useful to pay attention in order to check temperature of fluid.

2.3.4 Density

This means that the density of a substance should be the same regardless of how much of the material is present. The density of different materials is also different



In other hand, density is defined as the ratio of the mass over the volume and it is expressed by:

$$p = \frac{m}{V}(3.3)$$

Where ρ is the density in g/c^{3}

m, the mass in g

v , volume in c^{3}

Biodiesel density is a very important property since it is involved in atomizing fuels during combustion. High density promotes the combustion of the gas mixture needed for good combustion and performance.

2.3.5Cetane number

Cetane number is an indicator of diesel and biodiesel combustion efficiency. This is a significant expression of diesel fuel efficiency, a variety of other overall diesel fuel quality. These other diesel fuel quality metrics include pressure, lubricity, cold flow and sulfur content. Higher numbers of cetanes result in more efficient combustion. In comparison, cetane is the amount in volume of cetane in the mixture having the same value as the fuel being measured. It is also the measurement of the delay in the ignition of the fuel, the time period between the start of the injection and the first identifiable increase in the fuel pressure.Often essential biodiesel properties, it is useful to examine the fuel quality during the combustion process. It is dimensionless and a cetane number of 45 has been suggested by most automakers

2.4 Response Surface Methodology (RSM)

RSM is widely and extensively used based on statistical approach during problem solving. Defined as an assembly of mathematical and statistical modeling techniques applied to multiple regression and analysis, RSM (response surface methodology) is also used to calculate the relationship between one or more measured responses and the critical input measurement. On the other hand, it can also be described as a set of statistical techniques for experiment design, model construction, assessing the effects of factors and searching for optimum conditions (Kalil et al., 2000). Referring to (Montgomery and Douglas, 2005), RSM may be characterized as a modeling system used for complex process development, improvement, and optimisation. RSM is useful because it allows a reduction in the number of

experimental runs to obtain statistically acceptable result. Least squares were used to analyze the values of the parameters and it is define by:

$$y = \beta_0 \sum_{i=1}^n \beta_i x_i + \sum_{i=1}^{n=1} \sum_{j=i+1}^n \beta_i \ x_i x_j (3.3)$$

Where Y represents the predicted response (kinematic viscosity, density, CP or PP, FP); o is the offset term; i is the linear coefficient; ßij is the interaction coefficient; and xi and xj are the independent variables. Our studies will rely on curve analysis and statistical response.

2.5 Artificial Neural Network (ANN)

The persistent use of the ANN for the past two decades makes it an enticing inplement for modeling nonlinear and multivariable systems (K.M Desai, B.K. Vaidya, and R.S Singhal 2004). ANNs is a numerical approach which is based on processing units of artificial neurons that are connected together to form a direct graph (Haykin, 2009). More utilized, ANN method is frequently used as an option way to conventional technique and in a many energy application. ANN application can model various systems such as linear and nonlinear system. Input layer, hidden layer, connection weights and biases, activation function and summation node are the main components of ANN architecture.

There is two main stages of ANN: learning stage and generalization stage. The learning techniques includes reinforcement, evolutionary, supervised and unsupervised learning. This stage consist on simulation of a particular input that leads to a specific target output. According to the difference between the output and the target. The simulation in the network is adjusted. This action is repeated until the network output matches the target and the mean square error (mse) is determined. The mean square error permits to obtain the performance result. It evaluates the performance of network according to the mean of squared errors. Obtaining of the learning process result is done when the mse is minimized. This his result of try and error methodthat consist on simulation, analysis, resimulation by adding more layer if the discount result is not obtained.

CHAPTER 3

MATERIALS AND METHODS

During this study, several steps allowed us to obtain and collect data necessary for the estimation of biodiesel properties. In this thesis some essential and foremost steps will be listed.

3.1 Experimental Database

Many articles from different researcher has 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). Then a total of 39 combinations have been done and in each combination the calculation of the minimum value, maximum value and standardization 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.

3.2 Data Collection

Data have been grouped in two groups: first group related to fatty acid another to others properties. Table 4.1 and 4.2 give account of the data collected.

C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C22:0
	11.7		3.97	21.27	53.7	8.12	1.23	
	17.2		2.7	40.5	36.6	0.5	0.9	1.5
	11.4		1.3	27.1	60.2			
	4.9		2.3	32.6	59.4	5.6		0.5
	5.2		1.4	66	18.9		1.9	1
0.5	49.5		2.9	38.6	6.6			
4.8	11.5		1.4	15.9	1.8			
1.6	27.3		2.9	36.1	25.7	1.9		
	6.7		3.7	21.7	15.8	52.1		
	6.4		2.2	13.9	76	0.2		
	4.3		1.9	61.5	20.6	8.3		
	39.3		4.1	43.2	10.6	0.2		
0	14.2	1.4	6.9	43.1	34.4			
0	9.8		6.2	72.2	11.8			
0.2	11	0.8	5.7	20.6	66.2	0.8	0.4	
0.1	40.3	0.1	4	23.4	53.2	7.8	0.3	0.1
			3.1	43.4	13.2			
0.1	14.2		7.1	43.2	34.9	0.2	0.2	
0.9	44.5		4.9	39.6	9.3	0.2	0.4	
0.1	10.8		43	23.7	53.1	7.2	0.4	
0.07	5.41	0.25	1.89	62.14	21.79	6.14	0.57	0.3
0.14	10.54	0.65	4.02	54.71	28.07	0.29	0.37	0.65
0.28	9.91	4.52	4.19	41.13	35.65	0.35	0.3	0.56
0.08	10.35	0.12	4.53	21.39			0.42	0.38
0.31	14.22	0.93	4.09	36.37			0.44	0.21
0.06	5.58	0.25	1.94	55.11			0.64	0.32
0.96	25.32	0.59	2.79	15.91			0.18	0.1
1.01	44.39	0.22	4.28	38.48			0.39	0.68
0.08	13.74	0.91	6.84	44.26			0.21	
	3.92		1.13	13.62	15.15	13.39	0.65	
	2.98	0.16	1.19	16.04	15.11	13.29		
0.08	6.3	0.1	1.6	12.43	78.94	0.1	0.3	
	6.44	0.1	2.26	13.25	76.8	0.07	0.31	
0.1	14.6				21.0	0.2	0.2	
0.1	14.6		/.6		31.9	0.3	0.3	

Table 3.1: Fatty Acids Collection

Table 3.1: continued									
C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C22:0	
	11.5		4	24.5	53	7			
	12		4	25	53	6			
	17.2		4.4	15.7	55.6	7.1			
	16.4		4.8	16.5	55.3	2			
0.1	12.4	0.1	3.8	24.2	50.3	7.3	0.3		
1.5	21.9	3.2	12.3	41.9	17.9	1.1	0.2		
0.1	11.2	0.1	4.5	22.3	53.7	7.7	0.1		
1.2	17.4	3.2	9	33.2	26.3	1.5	0.2		
0	5.63		1.57	62.97	21.34	6.99	0.46		
0.1	37.29		4.04	40.42	17.84	0.18	0		
4.5	7		0.9	12.2	6.7				
0.6	47.2	0	3	40.8	8.2	0.2			
0.1	16.1	0	4	31.4	46.6	2.3			
0	11	0	4.2	22.6	55	7.2			
	11.76		5.23	26.43	46.62	6.96			
	12		5.3	26.79	49.26	6.65			
	12.28		5.18	28.25	48.32	6.17			
	12.69		5.22	29.16	47.23	5.7			
	11.95		4.94	27.91	49	6.2			
	12.08		4.69	29.03	48.69	5.51			
0.21	25.89		3.11	59.8	10.6				
	2.45	0.1	0.41	68.18	27.23	0.56		0.02	
0.8	21.53		18.9	39.1	19.35	0.16	0.62		
0.1	14.6		7.6	44.6	31.9	0.3	0.3		
18.3	9.2		2.9	6.9	1.7	0			
0.1	10.3		4.7	22.5	54.1	8.3			
1.3	43.9		4.9	39	9.5	0.3			
0	11		3.6	75.3	9.5	0.6			
0.1	3.9		3.1	60.2	21.1	11.1			
0	25.8		5.3	52.1	0	12			
0.5	23.4		5	29.4	34	3.2			
	4		6.23	47.61	13.69		3.66	2.6	
0.08	21.53		18.96	39.1	19.55	0.16	0.62		
	13.05		11.48	30.61	26.06	0.24			

	28.7	0	<u>^ </u>	10		0		
	3.5	0		• • • • •		8.2		
C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C22:0
	7.3	0	1.9	13.6	77.2	0		
	6.4	0.1	2.9	17.7	72.9	0		
	42.6	0.3	4.4	40.5	10.1	0.2		
	13.9	0.3	2.1	23.2	56.2	4.3		
	4.9	0.2	2.6	83.6	8.5	0.2		
	3.7		2.4	44.5				
0.09	12.01	2.5	12.95	34.05				
0.7	11.67		2.6	19.2				
2.2	8.7		8	17				
0.2	16	0.24	9	25				
0.045	5.85	0.3	5.47	20				
1.4	13.6		7.1	34.3				
0.6	6.9		3	75.2	12.4	1.2	0.4	
	3.8		1.9	63.9	19	9.7	0.6	
	4.9		1.6	33	20.4	7.9		
	4.2		2	57.4	21.3	11.2	1.2	
	9.4		4.1	22	55.3	8.9		
	10.8		3	26.5	47.3	9		
	4.2		3.3	63.6	27.6	0.2		
0.5	43.4		4.6	41.9	8.6	0.3	0.3	
	12.1		1.8	27.2	56.2	1.3	0.4	
	11.6		4.4	49.6	33.7	0.7		
	11.6		3.1	74.9	7.8	0.6		
2.9	24.3		22.8	40.2	3.3	0.7	0.2	
7.7	18.8		3.9	15	4.6	0.3	0.2	
	12.7		5.5	39.1	41.5	0.2	0.2	
	12.5		30.9	34.4	20.4			
	11.8		4.4	25.3	49.5	7.1	0.3	
	15.7		3.1	29.6	41.5	1		
	7.3		1.9	13.6	77.2			
	18.5		9.1	2.7	6.5	1.7		
	17.1		7.3	1.9	5.5	1.4		
			2.6	1.2	20.6	20.6	13.3	
	0.5		14.3	8	35.6	35	4	

C14:0	C16:0	C16:1	C18:0	C18:1	C18:2	C18:3	C20:0	C22:0
	18.22		5.14	28.46	48.18			
3.16	19.61	5.16	5.24	20.94	2.69	0.9	4.75	1.55
0.54	14.18	0.74	3.77	47.51	24.83	4.97	0.8	0.1
5.08	18.39	7.55	4	20.76	3.78	0.99	0.15	0.09
	6.8	0.5	1.98	81.46	3.72	2.78		
	5.45	3.71	2.13	1.78	30.71	38.87		
0.7	36.7	0.1	6.6	46.1	8.6	0.3	0.4	0.1
0	11.6	1	3.1	75	7.8	0.6	0.3	0.1
0.1	8	0	1.8	53.3	28.4	0.3	0.9	3
0	4.9	0	1.6	33	20.4	7.9	0	0
0	11.3	0.1	3.6	24.9	53	6.1	0.3	23
0	6.2	0.1	3.7	25.2	63.1	0.2	0.3	0.3
0.1	6.9	0.1	4	19	69.1	0.3	0.3	0.1
0	4.6	0.1	3.4	62.8	27.5	0.1	0.3	0
0	10.4	0.5	2.9	77.1	7.6	0.8	0.3	0
0	6.5	0.6	1.4	65.6	25.2	0.1	0.1	0.1
0.8	35.7	1.1	4.1	19.4	0	0	5.7	
21.4	23.6	33.2	0.8	1.5	0	0	0	
3.3	23.6	48.2	0.8	3.6	0	0	0	
0.5	16.8	1.2	3.4	15.5	35.8	14.9	2.1	
5.8	32.2	29.6	1	20.1	1.3	0	0	
6.6	25.6	60.6	0.9	3.2	0	0	0	
0.5	15.8	1.6	0.6	7.1	12.8	1	0	
0.6	12.9	1.4	0.5	4.4	8.5	1.2	0	
0.5	13.4	1.3	0.6	5.7	11.8	1	0	
2.7	6.1		2.8	16.8	17	35.6	1.4	

density	viscosity	flash p	cloud p	pour p	cetane n
885	4.1	175			51
886	5.3	193			54
886	4.4	167			55
886	4.4	183			52
886	4.6	177			55
885	4.7	189			62
878	3.2	131			62
877	4.9	167			55
900	3.8		-4	-5	
900	4.1		-5	-8	
900	4.3		-5	-13	
900	4				
	4.4	163	4		57
	4.2	141	4		55
	4.1	180	4		56
	4	160	4		58
	4.5	135	16		55
881	4.3				177
875	4.4				
885	4.3				
883	4.4				
887	5.2				
878	4.9				
886	4	177	0		
884	4.2	177	3		
885	4.4	183	-3		
882	4	173	9		
876	4.5	171	16		
880	4.4	176	2		
884	5.8	171	5.8	-3	
886	5.7	170	7.5	-3	
886	4.1	175	-5	-13	
860	4.9		-10	-12	

Table 3.2 : others properties

Density	viscosity	Flash p	Cloud p	Pour p	cetane
864	4.5				<u>.</u>
873	2.83	110	-3	-12	51
883	4.03				
885	4.3	169	6		
	4	116	0.5		47.1
	4.6	138	9.6		57.8
	4	176	-0.5		55.3
	4.4	171	6.4		61.8
			-3.5	-10	
			15	12	
	2.38		-10.1	-22.5	56.02
	4.52				
	4.55				
	4.06				
	4.03				
	4.16				
	4.1				
	4.24				
	4.35				
	4.09				
884	4.67	142			
887	4.69	169			49.2
882	4.2	170			
873.8	4.39				
870	4.1	180			
864.02	4.48				
874.2	2.726				
885.4	4.019				

Table 3.2: continued

Density	viscosity	Flash p	Cloud p	Pour p	Cetane I
880	4.6				49
884	4.1				46
880	5.7				62
876	4.9				54
	3.6				63
877	4.1				58
876	4.37	163	13	3	52
888.6	4.5	151	13.2	4.3	57.3
904	3.98	127	5	6	51
860	5.8		4	-8	37
874	4		1.7	-10	41.2
863		61	8	6	63.5
860	3.5			-12	49
912		34			51
865		108	1.7	4	28
879	4.9				52
864	3.7	162	10	5	46
879	4.52	170	-5		
	3.08		5	-3	
		115	0		
883	4.34	120	-1	-6	
884	4.18	110	-3	-9	
874	4.06	170	-3	-4	
887	3.98	170	6	-4	45.5
850	4.96		4		
870	4.8	178		-1	51
881.5	4	176	7	-5	48
	4.7	170	-2	-3	
			9	6	

2 2 .1 • . .

density	viscosity	Flash p	Cloud p	Pour p	Cetane n
864.4	3.7	178	13		56.2
876	4.84	176	1	5	
880.2	4.83	170	1	9	
	4.31	166		-6	56
880	4.03			-6	
833	4.4	149	3	5	49.8
872	4.03		3	3	45.5
	3.97	85		9	37
876	5.2	120	9	6	
888.5	4.1	100	-2	4	
920	5.81	124	6		
	5.7	141	1		
	5.66	125	4		54.9
		165			
	5.01	160	6	-9	
	5.2	162	0	-6	
		103			
	4.7	141			
876	4.63	181			
892	3.69	180			
880	4.31	147			
	4.5	176			61
	4.5	178			57
	4.6	176			53
	4.4	170			55
	4.2	171			49
	4.2	172			40
	4.1	175			48
	4.4	174			53
	4.2	172			57
	4.4	170			53

Table 3.2: continued

Density	viscosity	Flash p	Cloud p	Pour p	Cetane n
900	3.7				47.3
900	4				44
900	4.2				55
900	3.9				57.8
900	3.6				32.9
900	3.5				27.7
900	3.4				28.3
	3.8	136	3	-7	50.4
	4.38	153	-2	-6	53.7
	2.75	113	-3	-9	59.3
	4.19	171	-3	-2	55.7
	4.75	152	5	0	55.7
	4.61	163	14		61.9
	4.5	169	-3	-10	53.7
	4.14	174	-4	-7	51.1
	4.26	159	0	-4	51.3
	4.42	175	2	-2	51.1
	4.69	124	13	10	58.9
	4.8	161	8	3	56.9
875.78	3.96	174			
874.43	4.75	168			
866	2.64	162			
864.39	2.64	154			
862.94	4.55	172			
875.39	4.55	181.5			
877.58	3.97	152.5			
864	3.9	130.5			
864.69	3.62	127.5			
867.22	3.77	124			
870.43	3.14	126.5			
865.22	3.33	124.5			
866.22	3.14	146			
869.74	4.17	167.5			

Table 3.2: continued

Density	viscosity	Flash p	Cloud p	Pour p	Cetane n
867.88	3.89	150.5			
873.88	4.02	138.5			
870.14	3.92	136.5			
874.3	4.83	157.2		10	
881.6	4.4	159	-1.8	-8	54.8
917.6		160.5			42.1
876.3	4.81	162.2	7.5	4.4	57
870.8	2.78	127.7	-1.2	-3.8	
882.2	4.32	165.7	-3.2	-5.1	52.5
879	4.7	165.4	1.2	-0.2	53.3
883.2	4.48	174.5	-4	-6.3	50.6
887.3	4.3	162.6	-0.3	-4	51
877.9	4.55	163.5			53.8
878.7	4.72	158.5	5.7	-0.9	55.7
882.9	5.04	163.6	7.6		55.4
873	4.89	153.5			
891.5	4.06	170.3	1.7	-8	51.3
874.5	5.06	150.6	4	4	56.9
876.2	4.72	162.5		0.1	54.2
881.2	5.05	171	-2	-5	58.9
874.7	4.61	161.9			61.2
882.9	4.77	174.5	4.3	2.7	54.9
882.2	4.63	164.4	-3.3	-9.7	54.1
880.9	4.7	157.8	5	-0.9	56.3
882.3	4.79	158.3	3.6	-7	50.4
883.8	4.1	169.9	-4.9	-8.1	51.8
882.8	4.29	158.8	0.1	-3	51.9
882.9	4.53	172	0.9	-3.8	56.2
880	4.75	161.7	5.3	-0.3	
879	4.5				52
874	5.19	160	1		
892.5	3.75		-3.8		

Table 3.2: continued

Density	viscosity	Flash p	Cloud p	Pour p	Cetane n
884	4.9	178	1		
883	5.7	176	5		
876	4.95	164			
899	4.4				
885	4.8	170	-2.8		
879.5	3.98	135	2.7		
850	5.21				
884.5	4.2				
867.3	4.83	170	-6.8		
877.2	5.2				
882					
903	4.824		10		
874	4.55				
882			0		

885	2.3	117			
880	3.04	170			
874	3.59	183			
873	3.62	174			
871	3.75	170			
867	3.94	169			
866	4.03	167			
865	4.08	161			
885	4.08	124			
864	4.11				
Density	viscosity	Flash p	Cloud p	Pour p	Cetane n
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863	4.16	154			
860	4.18				
	4.41				
857	4.6	145			
876	4.8	131			
883	4.83	185			
	5.24				
872	5.78	160			
876		190			
832	3.6				53
840	3.63				52
848	3.97				51
875	4.71				50
879.4		181			52
862		135	6	2	
869		140	13.2	4.3	
880	4.37	163	13	3	
890	4	151	13.2	4.3	
904	3.98	130	4	1	
860	5.81	135	4.5	-8	
874	4		2	-10	
863		70	7	6	
860	3.5	152		12	
912		34			
865		108	1.7	-5	
879	4.9	181			
864	3.7	162	10	5	
870	4.7	85			50
860	5			4	51
870	4.5			-6	

Table 3.2: continued

density	viscosity	Flash p	Cloud p	Pour p	Cetane n
882	4.32				52.5
875	4.61				
861	3.23	114			
873	4.96	172			
869.9	4.83	153			
884.5	4.92	11			
883.7	4.41	125			
852	3.95	151			
878	4.88	172			58
874.5	5	174		12.5	
870		147		-3	52.8
876	.75	152		0	55.7
879	4.5	169		-10	53.7
882	4.26	159		4	51.3
862	4.6	113	-2.2	-12	
866	4.6	85		-1.9	
	3.8	151		10	
913	3.2	3			
930	3	98			
880	3.04	170			
865	4.08	161			
863	4.16	154			

Table 3.2: continued

3.3 Combinations

The goal of this study is to predict 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 thesis for both simulations (ANN, RSM)

Property	Combination of input	Model name
$\nu = f(F)$	F	Network1
$\nu = (\rho)$	ρ	Network2
$\nu = f(c)$	С	Network3
$\nu = f(p)$	p	Network4
$\nu = f(C)$	C	Network5
$\nu = f(\rho, F, c)$	ρ, F, c	Network6
$\nu = f(\rho, F)$	ρ, Γ ,	Network7
$\nu = f(F)$	c 14: 0, c 16: 0, c 16: 1, c 18: 0, c 18: 1, C18:2, c18:3, c20:0, c22:0	Network8
p = f(F)	F	Network9
$\rho = f(c)$	С	Network10
$\rho = f(p)$	p	Network11
$\rho = f(c)$	C	Network12
ho = f(F,c)	F,C	Network13
ho=f(F,c,p)	F , c , p	Network14
$\rho = f(F)$	c14: 0, c16: 0, c16: 1, c18: 0, c18: 1 c18:2, c18:3, c20:0, c22:0	Network15
F = f(C)	С	Network16
F = f(p)	p	Network17
F = f(c)	C	Network18
F = f(c, p)	с,р	Network19
F = f(c, p, c)	c, p, c	Network20
F = f(F)	c14: 0, c16: 0, c16: 1,c18:0,c18:1 c18:2, c18:3, c20:0, c22:0	Network21
c = f(v)	ν	Network22
c = f(p)	p	Network23
c = f(c)	C	Network24
c = f(p, c)	p , c	Network25
c = f(F)	c14:0, c16:0, c16:1, c18:0, c18:1, C18:2, c18:3, c20:0, c22:0	Network26
p = f(c)	C	Network27
p = f(F)	c14:0, c16:0, c16:1, c18:0, c18:1,C18:2, c18:3, c20:0, c22:0	Network28

Table 2.3: Network Model with Different Input Combinations

	Table 3.3 : continued	
c = f(F)	c14:0, c16:0, c16:1, c18:0, c18:1,	Network29
	C18:2, c18:3, c20:0, c22:0	
F = f(F, c, p)	F , c , p	Network30
F = f(F, c, p, c)	F , c , p , c	Network31
F = f(v)	ν	Network32
$F = f(\rho)$	ρ	Network33
F = f(F)	F	Network34
F = f(c)	c	Network35
F = f(c)	c	Network36
$F = f(\nu, \rho, F)$	ν, ρ, F	Network37
F = f(c, p)	с,р	Network38
F = f(F, c, p)	F , c , p	Network39

Combination	Output	B^2	R ² (adi)	R ² (pre)
f(E)	$n = 3.78 \pm 0.00035 F$	2 19	1 66	0
v = f(r)	$v = 4.05 \pm 0.00032$	0.00	0.00	0.00
v = f(p) v = f(c)	$v = 4.03 \pm 0.00032p$ $v = 4.3375 \pm 0.023c$	0.00 4 00	3.10	0.00
v = f(v)	$v = 44009 \pm 0.018$ n	4 11	3	0.00
v = f(p) v = f(c)	v = 4.100 + 0.0042	1.12	0.21	0.00
v = f(o E - c)	$v = 1.47 \pm 0.0031a \pm 0.0015E \pm 0.0058 c$	1.12	0.00	0.00
v = f(a E)	r = 1.17 + 0.00310 + 0.00131 + 0.003010	1.45 2 /0	1.12	0.00
$v = f(F_{1})$	$v = 4.23 \pm 0.070 \cdot 14 \cdot 0 \pm 0.00011 \cdot 16 \cdot 0$	2. 4) 17.71	1.12	2.15
$V = f(\Gamma)$	$= 4.23 = 0.070214.0 \pm 0.000011210.0$ $\pm 0.0037 - 16.1 \pm 0.0018 - 18.0 \pm 0.0049 - 18.1$	1/./1	14.05	2.13
	+0.003710.1 + 0.0010100.0 + 0.004910.1			
$a = f(E_{c})$	0.00008018.2 - 0.00000018.3 + 0.0042020.0 + 0.0034022.0	0.04	0.00	0.00
p = f(r)	p = 6.76.43 - 0.0086F	0.04	0.00	0.00
$\rho = f(c_1)$	$\rho = 8/8.88 - 0.14c$	0.52	0.00	0.00
$\rho = f(p)$	$\rho = 8/6.30 - 0.25p$	1.98	0.65	0.00
$\rho = f(c)$	$\rho = 898.4 - 0.35c$	2.78	0.00	0.00
$\rho = f(F, c)$	$\rho = 861.9 + 0.10F - 0.029C$	3.79	0.97	0.00
$\rho = f(F, c, p)$	$\rho = 865 + 0.08F - 0.089c - 0.15p$	7.36	1.57	0.00
$\rho = f(F)$	$\rho = 876.91 - 0.32c14:0 + 0.0018c16: +2.43c16:1$	6.56	0.00	0.00
	+ 0.045c18:0 + 0.071c18:1			
	-0.057c18:2+0.47c18:3			
	-0.51c20:0-0.37c22:0			
F = f(c)	F = 150.96 - 0.247c	0.14	0.00	0.00
F = f(p)	F = 145.59 - 1.24p	5.57	4.77	1.95
F = f(c)	F = 95.6 + 1.057c	2.54	0.00	0.00
F = f(c, p)	F = 141.15 + 1.044c - 2.05p	8.17	6.23	0.53
F = f(c, p, c)	F = 123.2 + 1.79c - 2.67p + 0.37c	11.92	7.45	0.00
F = f(F)	F = 144.26 + 0.007 c 14:0 +	7.73	2.08	0.00
	0.111@16:0+3.15c16:1+0.28c18:0+0.16c18:1+0.18c1			
	8:2+0.37c18:3+4.36c20:0-4.12c22:0			
c = f(v)	c = -4.88 + 1.71v	4.00	3.10	0.93
c = f(p')	c = 4.09 + 0.59p	52.79	52.43	51.14
c = f(c)	c = 0.99 + 0.058c	0.57	0.00	0.00
$c = f(\mathbf{p}, \mathbf{c})$	c = 6.92 + 0.5138 p - 0.05 c	46.39	44.92	40.95
c = f(F)	c = 4.97 - 0.22c14:0 - 0.0042c16:0 + 2.09c16:1	24.99	16.11	0.00
	+0.042e18:0 - 0.020e18:1 - 0.09e18:2	, ,		
	$-0.129 \cdot 18 \cdot 3 + 0.079 \cdot 20 \cdot 0$			
	+ 1.24c22.0			
n = f(c)	n = 0.58 = 0.022	0.05	0.00	0.00
	P = 0.30 = 0.022	0.05	0.00	0.00

Table 3.4: Network Model with Combinations, Output and Regression Values (RSM)

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	Table 3.4: continued			
p = f(F)	p = -1.25 - 0.53c14: 0 - 0.0036c16: 0 + 2.98c16: 1 + 0.21c18: 0 - 0.035c18: 1 - 0.055c18: 2 - 0.017c18: 3 + 0.49c20: 0 + 2.82c22: 0	21.62	11.69	0.00
c = f(F)	50.32 + 0.046c14: 0 - 0.0021c16: 0 + 0.042c16: 1 + +0.072c18: 0 + 0.049c18: 1 + 0.018c18: 2 - 0.034c18: 3 - 0.73c20: 0 - 0.079c22: 0	8.95	0.05	0.00
F = f(F, c, p)	F = 0.033 + 0.00031F - 0.00610c + 0.0072p	1.27	0.00	0.00
F = f(F , p , c , c)	F = -0.256 + 0.00039F - 0.0093c + 0.0108p + 0.0059c	2.68	0.00	0.00
F = f(v)	$F = -0.077 + 0.077 \nu$	0.08	0.00	0.00
$F = f(\rho)$	$F = -0.86 + 0.00107\rho$	0.18	0.00	0.00
F = f(F)	F = -0.102 + 0.00189F	0.21	0.00	0.00
F = f(c)	F = 0.43 + 0.0015c	0.11	0.00	0.00
F = f(c)	F = 0.59 - 0.0074c	0.06	0.00	0.00
$F = f(\nu, \rho, F)$	$F = -2.09 + 0.105\nu + 0.0020\rho - 0.0015F$	2.60	0.52	0.00
F = f(c, p)	F = 0.0586 - 0.0037c + 0.0056p	1.25	0.00	0.00
F = f(c, p, F)	F = 0.033 + 0.000317F - 0.0061c + 0.0072p	1.27	0.00	0.00

3.4 Functional Analysis

Used to solve nonlinear, variables, multivariable and multipart problem, ANN follows different and specific step to accomplish a specific model. Figure below shows synoptic used in this work for ANN development models.



Figure 3.3: analysis description

3.5 Test Conditions

input, unseen and output layer are three main layers which constitute ANN structure. Data from external source are called input. In the input layer, Data are transferred from outer source to unseenlayer byhandling elements (neurons). The burdens are the values of connection between cells. The outing information is obtained using data from neurons in the input and hidden layer, the bias, and stimulationfunctions. Constituted of outing layer, the outing of the network is obtained by handlingdata 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 regularlyused.Figure below shows the functional diagram of neural network.





HIDDEN LAYER

OUTPUT

Figure 3.4: ANN model used in this work

Referring to stimulation 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:

$$f(x) = \frac{1}{1 + e^{-x}} \tag{4.4}$$

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

$$f(x) = \frac{x_a - x_m}{x - x_m}$$
(5.5)

3.6 Empirical Models

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

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

Input data is obtained in function of target we want to obtain. (Density, flash point, cloud point, pour point, cetane number, fatty acid) as input for viscosity, (flash point, cloud point, pour point, cetane number) as input for fatty acid. (fatty acid) as input for cetane number. Also to achieve this simulations, limit of input data and range of determination of RRSME is listed. Figure 4.5 and 4.6 below show different limits and range.

	Limits values		Units
	MIN	MAX	
Viscosity	2.3	5.81	m^2/s
Density	807	903	k / m^{\exists}
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)

 Table 3.5: Margin values for input and output variables

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

Network type	Multi – layer feedforward
Training function	TRAINLM
Adaptive learning function	LEARNGDM
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

 Table 3.6: ANN condition

Also RSM design used number of unceasing 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 3.7: RRSME margin

Margin of RRSME	Evaluation
< 10%	Excellent
10 % < RRMSE< 20%	good
20 % < RRMSE< 30%	fair
> 30%	poor

CHAPTER 4

RESULTS AND DISCUSSIONS

4.1 Model Used to Develop ANN

Artificial neural network (ANN) and response surface methodology (RSM) are used to identify the most variable, which affect the estimation 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 .The following statistical indicators were employed correlation coefficient (\mathbb{R}^5), medium square erratum (mse), comparative root medium square(RRMSE) Depending on the value of mse, the number of neurons will be continuallyaugmented and the action re-training. in this study unseen layer varies from 5 to 8 . Following figure and table show different result obtained and explained.

Network 1 performance							
S. no	target	Network input	Transfer function	RRMSE	R	R^2	mse
1		f	Log sigmoid	5.80%	0.9994	0.9995	0.0000727
2		f	Log sigmoid	7%	0.9992	0.9993	0.0001060
			Network 2	2 performance	e		
1		С	Log sigmoid	9.24%	0.9983	0.9990	0.000124
2		C.	Log sigmoid	10.5%	0.9973	0.9984	0.000309
			Network 3	3 performance	2		
1		p	Log sigmoid	6.95%	0.99902	0.9985	0.000145
2		p	Log sigmoid	10%	0.9959	0.9951	0.000472
			Network 4	4 performance	e		
1		C:	Log sigmoid	11.1%	0.9983	0.9972	0.000262
2		C	Log sigmoid	10.25%	0.9984	0.9987	0.000183
3		C	Log sigmoid	11.48.50%	0.9983	0.9984	0.000130
			Network 5	5 performance	e		
1		ρ,f ,c	Log sigmoid	7.70%	0.9994	0.9990	0.000296
2		ho,f ,c	Log sigmoid	6.80%	0.9990	0.9954	0.000190
			Network 6	5 performance	9		
1		p,f,	Log sigmoid	7.50%	0.9985	0.9989	0.000188
2		ρ,f,	Log sigmoid	6.60%	0.9992	0.9989	0.000655

Table 4.1: Network performance with regression va	lues
---	------

		Table 4.	1 : continued			
3	p,f,	Log sigmoid	6.65%	0.9987	0.9979	0.000101
		Network '	7 performand	ce		
1	F	Log sigmoid	9.50%	0.9996	0.9993	0.0000408
2	F	Log sigmoid	5.50%	0.9997	0.9998	0.0000347
3	F	Log sigmoid	6%	0.9994	0.9997	0.0000524
		Network	8 performance	ce		
1	f	Log sigmoid	6.65%	0.9994	0.9991	0.0000738
2	f	Log sigmoid	10.5%	0.9989	0.9992	0.0000878
		Network	9 performance	ce		
1	с:	Log sigmoid	10.75%	0.9980	0.9971	0.000237
2	С:	Log sigmoid	9.85%	09985	0.9982	0.000276
		Network 1	0 performan	ce		
1	p	Log sigmoid	10.22%	0.9934	0.9971	0.000237
2	p	Log sigmoid	11.5%	0.9922	0.9965	0.000522
		Network 1	1 performan	ce		
1	с:	Log sigmoid	9.75%	0.9968	0.9973	0.000291
2	С:	Log sigmoid	11.78%	0.9946	0.9972	0.000683
		Network 1	2 performan	ice		
1	F,C	Log sigmoid	10.22%	0.9986	0.9989	0.000291

			Network 12	3 performanc	e		
1		F ,c.,p	Log sigmoid	6.80%	0.9993	0.9973	0.000291
2		F ,C ,p	Log sigmoid	10.58%	0.9962	0.9973	0.000230
			Network 14	4 performanc	e		
1		F	Log sigmoid	10.25%	0.9981	0.9986	0.000236
2		F	Log sigmoid	5.5%	0.9995	0.9996	0.0000884
3	ρ	F	Log sigmoid	4.35%	0.9997	0.9998	0.0000324
			Network 1	5 performanc	ce		
1	C.	F	Log sigmoid	4.88%	0.9997	0.9997	0.0000516
2	C.	F	Log sigmoid	12.2%	0.9962	0.9997	0.0000543

Illustration of this statistical values are showed in the following figures. The best of each combination will be showed.



Figure 4.1: Fatty Acid Regression with Viscosity

Figure 4.1 shows the regression analysis for fatty acid in 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 \mathbb{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 et good accuracy. In order to predict biodiesel properties this combination is useful.



Figure 4.2: Viscosity versus fatty acid MSE

Figure 4.2 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 4.3: Density versus Flash Point Regression Figure 4.3 density versus flash point regression

In comparison with the previous result, this combination also give a good accuracy since theirs correlations coefficient 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 4.4 shows density versus flash point mse

The mse value of the combination density function flash point is fair since the it is closer to 0.

Figure 4.5 : shows the regression analysis of cetane number function fatty acid



Figure 4.5: Cetane Number versus Fatty acid Regression

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 \mathbb{R}^2 are closer. Figure 4.6: shows the mse regression value of cetane number function fatty acid.



Figure 4.6: cetane n versus fatty acid mse

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

4.2 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 \mathbb{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 \mathbb{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 \mathbb{R}^2 and \mathbb{R} and also their percentage of RRSME between 10% and 20% for some and between 20% and 30% for others.

4.2.1 Analysis of best performance

Network	Target	Combination	R	R^2	Mse	Error%
1	ν	f	0.9994	0.9995	0.0000727	0.0001
	ν	f	0.9993	0.9994	0.000106	0.0001
7	ν	F	0.9996	0.9993	0.0000408	0.0003
	ν	F	0.9997	0.9998	0.0000347	0
	ν	F	0.9994	0.9997	0.0000524	0.0003
14	ρ	F	0.9981	0.9986	0.000236	0.0005
	ρ	F	0.9995	0.9996	0.0000884	0.0001
	ρ	F	0.9997	0.9998	0.0000324	0.0001
4	С	F	0.9984	0.9987	0.000183	0.0001
	С	F	0.9983	0.9984	0.000130	0.0001
6	ν	ρ, f	0.9985	0.9989	0.000188	0.0004
	ν	ρ, f	0.9992	0.9989	0.0000655	0.0003

 Table 2.3: Best performance analysis

4.22Analyze 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 the compared each other.

Combination	Output	R^2	R ² (adj)	R ² (pre)
v = f(F)	v = 3.78 + 0.00035F	2.19	1.66	0
$v = f(\rho)$	$v = 4.05 + 0.00032\rho$	0.00	0.00	0.00
v = f(c)	v = 4.3375 + 0.023c	4.00	3.10	0.32
$\nu = f(p)$	v = 4.4009 + 0.018 p	4.11	3	0.00
v = f(c)	v = 4.100 + 0.0042c	1.12	0.21	0.00
$\nu = f(\rho, F, c)$	$\nu = 1.47 + 0.0031\rho + 0.0015F + 0.0058c$	1.45	0.00	0.00
$v = f(\rho, F)$	$\nu = 2.69 + 0.0012\rho + 0.0037F$	2.49	1.12	0.00
v = f(F)	v = 4.23 - 0.070c14:0 + 0.000011c16:0 + 0.0037c16:1 + 0.0018c18:0 + 0.0049c18:1 0.00068c18:2 - 0.0060c18:3+0.0042c20:0+0.0034c22:0	17.71	14.85	2.15
$\rho = f(F)$	$\rho = 8.78.43 - 0.0088F$	0.04	0.00	0.00
$\rho = f(c)$	$\rho = 878.88 - 0.14c$	0.32	0.00	0.00
$\rho = f(p)$	$\rho = 876.30 - 0.25p$	1.98	0.65	0.00
$\rho = f(c)$	$\rho = 898.4 - 0.35c$	2.78	0.00	0.00
$\rho = f(F, c)$	$\rho = 861.9 + 0.10F - 0.029c$	3.79	0.97	0.00
$ \rho = f(F, c, p) $	$\rho = 865 + 0.08F - 0.089c - 0.15p$	7.36	1.57	0.00
$\rho = f(F)$	$\rho = 876.91 - 0.32c14:0$ + 0.0018c16: +2.43c16: 1 + 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 = f(C)	F = 150.96 - 0.247c	0.14	0.00	0.00
F = f(p)	F = 145.59 - 1.24p	5.57	4.77	1.95
F = f(c)	F = 95.6 + 1.057c	2.54	0.00	0.00
F = f(c, p)	F = 141.15 + 1.044c - 2.05p	8.17	6.23	0.53
F = f(c,p,c)	F = 123.2 + 1.79c - 2.67p + 0.37c	11.92	7.45	0.00
F = f(F)	$F = 144.26 + 0.007c14:0 + 0.111c16:0 + 3.15c16:1+0.28c18:0+0.16c18:1+0.1 \\ 8c18:2+0.37c18:3+4.36c20:0-4.12c22:0$	7.73	2.08	0.00
c = f(v)	$c = -4.88 + 1.71\nu$	4.00	3.10	0.93
c = f(p)	c = 4.09 + 0.59p	52.79	52.43	51.14

 Table 4.3: Network Model with Combinations, Output and Regression Values (RSM)

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Table 4.3 : continued

$\begin{array}{cccccccccccccccccccccccccccccccccccc$						
$\begin{array}{cccc} c = f(p,c) & c = 6.92 + 0.5138p - 0.05c & 46.39 & 44.92 & 40.95 \\ p = f(c) & p = 0.58 - 0.022c & 0.05 & 0.00 & 0.00 \\ p = -1.25 - 0.53c14: 0 - 0.0036c16: 0 & & & & & & & & & & & & & & & & & & $	c = f(c)	c = 0.99 + 0.058c	0.57	0.00	0.00	
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	c = f(p, c)	c = 6.92 + 0.5138p - 0.05c	46.39	44.92	40.95	
p = -1.25 - 0.53c14: 0 - 0.0036c16: 0 $+ 2.98c16: 1 + 0.21c18: 0$ $p = f(F)$ $- 0.035c18: 1 - 0.055c18: 2$ $21.62 11.69 0.00$ $- 0.017c18: 3 + 0.49c20: 0$ $+ 2.82c22: 0$ $50.32 + 0.046c14: 0 - 0.0021c16: 0$ $+ 0.042c16: 1 + +0.072c18: 0$ $- 0.034c18: 3 - 0.73c20: 0$ $- 0.079c22: 0$ $F = F = 0.033 + 0.00031F - 0.0093c$ $= f(F, p, c, c, p)$ $F = -0.256 + 0.00139F - 0.0093c$ $= f(F, p, c, c, c)$ $F = -0.077 + 0.077v$ $- 0.08 0.00 0.00$ $F = f(p)$ $F = -0.102 + 0.00189F$ $- 0.21 0.00 0.00$ $F = f(c)$ $F = 0.43 + 0.0015c$ $- 0.11 0.00 0.00$ $F = f(c)$ $F = -2.09 + 0.105v + 0.0020p - 0.0015F$ $2.60 0.52 0.00$ $F = f(c, p, F)$ $F = -0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = f(c, p, F)$ $F = -0.033 + 0.00037c + 0.0056p$ $- 1.25 0.00 0.00$ $F = f(c, p, F)$ $F = -0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = f(c, p, F)$ $F = -0.033 + 0.000317F - 0.0015F$ $- 1.27 0.00 0.00$ $F = f(c, p, F)$ $F = -0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = f(c, p, F)$ $F = -0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = 0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = f(c, p, F)$ $F = 0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = 0.033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = 0.0072p$ $F = 0.0033 + 0.000317F - 0.0061c$ $- 1.27 0.00 0.00$ $F = 0.0000 = 0.00000$ $F = 0.00000 = 0.00000$ $F = 0.000000000$ $F = 0.0000000000000000000000000000000000$	p = f(c)	p = 0.58 - 0.022c	0.05	0.00	0.00	
$50.32 + 0.046c14: 0 - 0.0021c16: 0$ $+ 0.042c16: 1 + +0.072c18: 0$ $+ 0.049c18: 1 + 0.018c18: 2$ $8.95 0.05 0.00$ $- 0.034c18: 3 - 0.73c20: 0$ $- 0.079c22: 0$ $F F = 0.033 + 0.00031F - 0.00610c$ $= f(F, p, c, p) F = -0.256 + 0.0039F - 0.0093c$ $= f(F, p, c, c) F = -0.256 + 0.0019F 0.08 0.00 0.00$ $F = f(v) F = -0.077 + 0.077v 0.08 0.00 0.00$ $F = f(p) F = -0.86 + 0.00107\rho 0.18 0.00 0.00$ $F = f(c) F = -0.102 + 0.00189F 0.21 0.00 0.00$ $F = f(c) F = 0.43 + 0.0015c 0.11 0.00 0.00$ $F = f(c) F = 0.59 - 0.0074c 0.06 0.00 0.00$ $F = f(c) F = -2.09 + 0.105v + 0.0020\rho - 0.0015F 2.60 0.52 0.00$ $F = f(c, p, F) F = -0.0586 - 0.00317F - 0.0061c$ $= f(c, p, F) F = 0.033 + 0.00317F - 0.0061c$ $= f(c, p, F) F = 0.033 + 0.00317F - 0.0061c$ $= f(c, p, F) F = 0.033 + 0.00317F - 0.0061c$ $= f(c, p, F) F = 0.033 + 0.00317F - 0.0061c$ $= f(c, p, F) F = 0.033 + 0.00317F - 0.0061c$ $= 1.27 0.00 0.00$	p = f(F)	p = -1.25 - 0.53c14:0 - 0.0036c16:0 + 2.98c16:1 + 0.21c18:0 - 0.035c18:1 - 0.055c18:2 - 0.017c18:3 + 0.49c20:0 + 2.82c22:0	21.62	11.69	0.00	
F $F = 0.033 + 0.00031F - 0.00610c$ $+ 0.0072p$ 1.27 0.00 0.00 F $F = -0.256 + 0.00039F - 0.0093c$ $+ 0.0108p + 0.0059c$ 2.68 0.00 0.00 F = $f(v)$ $F = -0.077 + 0.077v$ 0.08 0.00 0.00 F = $f(p)$ $F = -0.86 + 0.00107p$ 0.18 0.00 0.00 F = $f(F)$ $F = -0.102 + 0.00189F$ 0.21 0.00 0.00 F = $f(c)$ $F = 0.43 + 0.0015c$ 0.11 0.00 0.00 F = $f(c)$ $F = -2.09 + 0.105v + 0.0020p - 0.0015F$ 2.60 0.52 0.00 F = $f(c, p)$ $F = 0.033 + 0.000317F - 0.0061c$ 1.27 0.00 0.00 F = $f(c, p, F)$ $F = 0.033 + 0.000317F - 0.0061c$ 1.27 0.00 0.00	c = f(F)	50.32 + 0.046c14: 0 - 0.0021c16: 0 + 0.042c16: 1 + +0.072c18: 0 + 0.049c18: 1 + 0.018c18: 2 - 0.034c18: 3 - 0.73c20: 0 - 0.079c22: 0	8.95	0.05	0.00	
F $F = -0.256 + 0.00039F - 0.0093c$ $+ 0.0108p + 0.0059c$ 2.680.000.00F = f(v)F = -0.077 + 0.077v0.080.000.00F = f(p)F = -0.86 + 0.00107p0.180.000.00F = f(F)F = -0.102 + 0.00189F0.210.000.00F = f(c)F = 0.43 + 0.0015c0.110.000.00F = f(c)F = 0.59 - 0.0074c0.060.000.00F = f(c, p)F = -2.09 + 0.105v + 0.0020p - 0.0015F2.600.520.00F = f(c, p, F)F = 0.033 + 0.000317F - 0.0061c1.270.000.00F = f(c, p, F)F = 0.033 + 0.000317F - 0.0061c1.270.000.00	F = f(F, c, p)	F = 0.033 + 0.00031F - 0.00610c + 0.0072p	1.27	0.00	0.00	
$F = f(v)$ $F = -0.077 + 0.077v$ 0.08 0.00 0.00 $F = f(\rho)$ $F = -0.86 + 0.00107\rho$ 0.18 0.00 0.00 $F = f(F)$ $F = -0.102 + 0.00189F$ 0.21 0.00 0.00 $F = f(c)$ $F = 0.43 + 0.0015c$ 0.11 0.00 0.00 $F = f(c)$ $F = 0.59 - 0.0074c$ 0.06 0.00 0.00 $F = f(c, p)$ $F = -2.09 + 0.105v + 0.0020\rho - 0.0015F$ 2.60 0.52 0.00 $F = f(c, p)$ $F = 0.0586 - 0.0037c + 0.0056p$ 1.25 0.00 0.00 $F = f(c, p, F)$ $F = 0.033 + 0.000317F - 0.0061c$ 1.27 0.00 0.00	F = f(F, p, c, c)	F = -0.256 + 0.00039F - 0.0093c + 0.0108p + 0.0059c	2.68	0.00	0.00	
$F = f(\rho)$ $F = -0.86 + 0.00107\rho$ 0.180.000.00 $F = f(F)$ $F = -0.102 + 0.00189F$ 0.210.000.00 $F = f(c)$ $F = 0.43 + 0.0015c$ 0.110.000.00 $F = f(c)$ $F = 0.59 - 0.0074c$ 0.060.000.00 $F = f(c, p)$ $F = -2.09 + 0.105v + 0.0020\rho - 0.0015F$ 2.600.520.00 $F = f(c, p)$ $F = 0.0386 - 0.0037c + 0.0056p$ 1.250.000.00 $F = f(c, p, F)$ $F = 0.033 + 0.000317F - 0.0061c$ 1.270.000.00	F = f(v)	$F = -0.077 + 0.077\nu$	0.08	0.00	0.00	
F = f(F) $F = -0.102 + 0.00189F$ 0.21 0.00 0.00 $F = f(c)$ $F = 0.43 + 0.0015c$ 0.11 0.00 0.00 $F = f(c)$ $F = 0.59 - 0.0074c$ 0.06 0.00 0.00 $F = f(c, p)$ $F = -2.09 + 0.105v + 0.0020p - 0.0015F$ 2.60 0.52 0.00 $F = f(c, p)$ $F = 0.0586 - 0.0037c + 0.0056p$ 1.25 0.00 0.00 $F = f(c, p, F)$ $F = 0.033 + 0.000317F - 0.0061c$ 1.27 0.00 0.00	$F = f(\rho)$	$F = -0.86 + 0.00107\rho$	0.18	0.00	0.00	
$F = f(c)$ $F = 0.43 + 0.0015c$ 0.11 0.00 0.00 $F = f(c)$ $F = 0.59 - 0.0074c$ 0.06 0.00 0.00 $F = f(v, \rho, F)$ $F = -2.09 + 0.105v + 0.0020\rho - 0.0015F$ 2.60 0.52 0.00 $F = f(c, p)$ $F = 0.0586 - 0.0037c + 0.0056p$ 1.25 0.00 0.00 $F = f(c, p, F)$ $F = 0.033 + 0.000317F - 0.0061c$ 1.27 0.00 0.00	F = f(F)	F = -0.102 + 0.00189F	0.21	0.00	0.00	
$F = f(c)$ $F = 0.59 - 0.0074c$ 0.06 0.00 0.00 $F = f(v, \rho, F)$ $F = -2.09 + 0.105v + 0.0020\rho - 0.0015F$ 2.60 0.52 0.00 $F = f(c, p)$ $F = 0.0586 - 0.0037c + 0.0056p$ 1.25 0.00 0.00 F $F = 0.033 + 0.000317F - 0.0061c$ 1.27 0.00 0.00 $F = f(c, p, F)$ $+ 0.0072p$ 1.27 0.00 0.00	F = f(c)	F = 0.43 + 0.0015c	0.11	0.00	0.00	
$F = f(v, \rho, F)$ $F = -2.09 + 0.105v + 0.0020\rho - 0.0015F$ 2.600.520.00 $F = f(c, p)$ $F = 0.0586 - 0.0037c + 0.0056p$ 1.250.000.00 F $F = 0.033 + 0.000317F - 0.0061c$ 1.270.000.00 $F = f(c, p, F)$ $+ 0.0072p$ 1.270.000.00	F = f(c)	F = 0.59 - 0.0074c	0.06	0.00	0.00	
F = f(c, p) $F = 0.0586 - 0.0037c + 0.0056p$ 1.250.000.00 F $F = 0.033 + 0.000317F - 0.0061c$ 1.270.000.00 $= f(c, p, F)$ $+ 0.0072p$ 1.270.000.00	$F = f(\nu, \rho, F)$	$F = -2.09 + 0.105\nu + 0.0020\rho - 0.0015F$	2.60	0.52	0.00	
F $F = 0.033 + 0.000317F - 0.0061c$ 1.270.000.00 $= f(c, p, F)$ $+ 0.0072p$ 1.270.000.00	F = f(c, p)	F = 0.0586 - 0.0037c + 0.0056p	1.25	0.00	0.00	
	F = f(c, p, F)	F = 0.033 + 0.000317F - 0.0061c + 0.0072p	1.27	0.00	0.00	

However the biodiesel properties were used and at each combination the 3 parameter equation was obtained. Each combination equation is combined in table 4.3.



Figure 4.7 shows response Surface Regression: viscosity versus pour p

Figure 4.7:Response Surface Regression: viscosity versus flash point

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	1	1.433	1.4326	3.69	0.058
Linear	1	1.433	1.4326	3.69	0.058
pour p	1	1.433	1.4326	3.69	0.058
Error	86	33.413	0.3885		
Lack-of-Fit	35	9.798	0.2799	0.60	0.941
Pure Error	51	23.616	0.4631		
Total	87	34.846			

Table 4.4: Analysis of variance viscosity versus flash point

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



Figure 4.8 shows Response Surface Regression: viscosity versus density, flash p, cloud p,

Figure 4. 8:Response Surface Regression: viscosity versus density, flash p,cloud p, pour p

pour p

Table 4.5: 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		



Figure 4.9:Response Surface Regression: viscosity versus density, flash point Figure 4.9 shows Response Surface Regression: 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	142	59.5338	0.41925		
Lack-of-Fit	134	59.3538	0.44294	19.69	0.000
Pure Error	8	0.1800	0.02250		
Total	144	61.0534			

Table 4.6: Analysis of varianceviscosity versus density, flash point



Figure 4.10 shows Response Surface Regression: density versus flash p, cloud p

Figure 4.10: Response Surface Regression: density versus flash p, cloud p

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	1.560	0.01	0.932
Error	64	13427.2	209.800		
Lack-of-Fit	60	13418.2	223.637	99.62	0.000
Pure Error	4	9.0	2.245		
Total	66	13983.0			

Table 4.7: Analysis of variancedensity versus flash point, cloud point.



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

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

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Table 4.8: Analysis of varianceviscosity versus density, flash p, cloud p

Source	DF	Adj SS	Adj MS	F-Value	P-Value
Model	3	0.3238	0.107943	0.30	0.826
Linear	3	0.3238	0.107943	0.30	0.826
density	1	0.1257	0.125662	0.35	0.557
flash p	1	0.0868	0.086806	0.24	0.626
cloud p	1	0.0619	0.061917	0.17	0.680
Error	61	22.0281	0.361116		
Lack-of-Fit	60	22.0281	0.367134		

Pure Error	1	0.0000	0.000000
Total	64	22.3519	

Figure 4.12 shows Response Surface Regression: density versus flash p, cloud p, pourp



Figure 4.12: Response Surface Regression: 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		

 Table 4.9: Analysis of variancedensity versus flash p, cloud p, pour p

Total	51	6816.99
Total	31	0010.99

Figure 4.13 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 4.13: Response Surface Regression: viscosity versus c14:0, c16:0, c16:1, c18:0, c18:1, c18:2, c18:3, c20:0, c22:0

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	15.1260	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	

 Table 4.10: Analysis of variance viscosity versus fatty acid

c20:0	1	0.005	0.0047	0.01	0.911
c22:0	1 tinued	0.007	0.0066	0.02	0.895
Error	259	97.674	0.3771		
Lack-of-Fit	174	58.454	0.3359	0.73	0.959
Pure Error	85	39.220	0.4614		
Total	268	118.691			

Figure 4.14 shows Response Surface Regression: density versus c14:0, c16:0, c16:1, c18:0, c18:1, c18:2, c18:3, c20:0, c22:0



Figure 4.14: Response Surface Regression: density versus c14:0, c16:0, c16:1, c18:0, c18:1, c18:2, c18:3, c20:0, c22:0

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

Table 4.11: Analysis of variance density versus fatty acid

c14:0	1	64.8	64.827	0.29	0.592
c16:0	1	5. Table 4.1	L1 : continued	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 4.15 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



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			

 Table 4.12: Analysis of variancecetane number versus fatty acid
4.3 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, density and cetane number properties with the fatty acid individually does not provide a better result.

4.4 Analysis of Comparison between R^2 (ANN) and R^2 (RSM)

In this section there is a brief and comparison between R^2 obtained from ANN analysis and RSM obtained with RSM analysis. Table below shows a description.

Combination	$R^2(ANN)$	R ² (RSM)
$\nu = f(F)$	0.9998	0.9112
=f(F)	0.9998	0.799
c = f(F)	0.9987	0.766

Table 4.13: ANN and RSM Comparison

4.5 R² Evolution diagram (ANN)

In this section analysis done with ANN shows the ascending curve and it is almost near to 1



4.6 **R**² Evolution Diagram (RSM)



Figure 4.17: R² RSM Evolution

4.7 R²(ANN) and R² (RSM) Evolution Diagram

This figure shows in this combination and simulation done with ANN are more reliable due to the fact that it is constant while the combination and simulation done with RSM is not reliable since it change as far as possible and it decreases .

Figure 4.18 is a combination comparison between ANN and RSM



Figure 4.18: Combination and Comparison with ANN and RSM

CHAPTER 5

CONCLUSION AND FUTURE WORKS

5.1 Conclusion

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 \mathbb{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 were focused only on viscosity, density and cetane number. Combining other properties will therefore be future objectives.

5.2 Future Works

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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