NEAR EAST UNIVERSITY

INSTITUTE OF GRADUATE STUDIES

DEPARTMENT OF MECHANICAL ENGINEERING

QUADRATIC MODEL FOR PREDICTING KINEMATIC VISCOSITY AND DENSITY OF PURE BIODIESEL AND THEIR MIXTURES

M.Sc. THESIS

ADIVHAHO FRENE NETSHIMBUPFE

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NICOSIA, 2022

APPROVAL

We certify that we have read the thesis submitted by ADIVHAHO FRENE NETSHIMBUPFE titled **"QUADRATIC MODEL FOR PREDICTING KINEMATIC VISCOSITY AND DENSITY OF PURE BIODIESEL AND THEIR MIXTURES** " and that in our combined opinion it is fully adequate, in scope and in quality, as a thesis for the degree of Master of Educational Sciences.

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Declaration

I hereby declare that all information, documents, analysis and results in this thesis have been collected and presented according to the academic rules and ethical guidelines of Institute of Graduate Studies, Near East University. I also declare that as required by these rules and conduct, I have fully cited and referenced information and data that are not original to this study.

Adivhaho Frene Netshimbupfe

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ABSTRACT

QUADRATIC MODEL FOR PREDICTING KINEMATIC VISCOSITY AND DENSITY OF PURE BIODIESEL AND THEIR MIXTURES

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Machine learning in recent years has found applications in a number of fields. Its ability to make automate procedures and make well informed predictions based on a knowledge base developed with preexisting data is greatly advantageous to a lot of application processes.

The field of Biodiesel production and study has also seen its fair share of machine leaning applications. This is especially so because the biggest deterrent to mass adoption of biodiesel fuels is its cost of production, and uncertainty that still surrounds its behaviour under different situations. For this reason, Machine learning has been applied at different levels in study and production of biodiesels to reduce the cost of production, time spent and to help us better understand their properties and how they behave under different situations.

In this study, we use Response Surface Methodology (RSM) to predict the properties of Sunflower oil, Corn oil and Canola oil. We then analyse my results to see if these model is feasible for this application and to see what other Machine learning techniques might also work for this application. The results show that the RSM model is very effective for this problem and would generate accurate predictions with reasonable precision. We also suggest other models to be studied to see their level of effectiveness for this application.

Keywords: Biodiesel, Biofuel properties, Machine Learning, RSM, Neural Networks

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LIST OF ABBREVIATIONS

ANN:	Artificial Neural Networks
MLP:	Multi Layer Perceptron
ASTM:	American Society of Testing and Materials
CN:	Cetane Number
MLPNN:	Multi Layer Perceptron Neural Network
ELM:	Extreme Learning Machine
SOM:	Self Organizing Maps
FAME:	Fatty Acid Methyl Ester
ReLU:	Rectified Linear Unit
ANFIS:	Adaptive Neuro-Fuzzy Inference System
RBFNN:	Radial Basis Function Neural Network
RSM:	Response Surface Methodology

CHAPTER 1

INTRODUCTION

1.1 Historical Background of Biodiesel Technology

Today, more than 80% of the world's energy demand is met by fossil fuels such as oil, coal and natural gas, and human society is heavily dependent on these non-renewable energy resources. (Hosseini et al., 2015; Mandegari et al., 2016, 2017). Also, large scale use of these fossil fuels has created a lot of adverse effects for humans, such as the slow but irreversible deterioration of the environment as well as a lot of health problems (Farzad et al., 2020; Prakash Maran & Priya, 2015; Schalkwyk, 2020). It has in fact become the leading cause of pollution, environmental challenges and climate change globally (Tag & X, 2017). Among all the fossil fuels, diesel is undoubtedly the most used fossil fuel by-product, primarily because of the efficiency of diesel engines compared to petrol engines (Tabatabaei et al., 2019). This has led to it being the prefered engine type for heavy vehicles that are used in the transportation and industrial sectors (Hajjari et al., 2017). Consequently, diesel engines some of the biggest contributors to environmental problems as combustion of diesel produces gases that deplete the ozone layer and contribute to global warming (Hosseinzadeh-bandbafha et al., 2018). Issues like this have caused concern in the international community and have necessitated the improvement of engine technologies and the migration to the use of cleaner and safer alternative fuels for combustion engines (Khounani et al., 2019).

Nowadays, society is working to boost the use of renewable and alternative energy sources in order to minimize reliance on fossil fuels and reduce carbon dioxide emissions. Biomass is regarded as the sole carbon-based, long-term answer for replacing fossil fuels. Unfortunately, the variability of its properties (both physical and chemical), make it difficult to use for energy. Because energy biomass conversion systems are susceptible to significant variability in feedstock material properties and need continuous management, a new approach for measuring biomass parameters in real-time is necessary if biomass should be used as a replacement to fossil fuels. (Ahmed et al., 2019). As an example, some of the best alternatives to petrol and diesel that have been researched are vegetable oils and animal fats (Ali et al., 1995). Unfortunately, they are plagued with issues that have reduced their acceptance for use in ignition diesel engines (Kumar & Singh, 2019). Some of these issues include:

- High viscosity
- Low energy output
- High cloud and pour points
- Difficulty in pumping
- High copper strip corrosion levels, etc.

Nevertheless, various strategies have been looked into (like micro emulsion and transesterification) to solve this problem (Kumar & Singh, 2019).

A number of these strategies however have some bottlenecks. For example, dilution of these biomasses with pure diesel for use in diesel engines can sometimes lead to the formation of gum, partial combustion, high exhaust emissions, engine wear, among others (Aghbashlo, Tabatabaei, Hosseinpour, et al., 2018). Micro emulsion fuels for diesel engines have also been known to lead to a number of problems like heavy deposition of carbon residue, inferior combustion, and the thickening of lubricating oil (Sharma et al., 2008). The adoption of pyrolysis to alter the chemical composition of the vegetable oils and animal fats also requires very expensive machinery that can be quite difficult to operate and manage. It also leads to the production of deoxygenated short-chain molecules just like we have with gasoline (Aghbashlo, Tabatabaei, Hosseinpour, et al., 2018).

While most of these other strategies to help aid the use of biomass as a fossil fuel alternative are plagued with issues, the process of transesterification where biomass is converted into a diesel-like fuel called "biodiesel" appears to solve most, if not all of these problems effectively (Aghbashlo, Tabatabaei, Hosseinpour, et al., 2018). The efficient conversion rate coupled with the low cost of the process makes transesterification probably the best approach to aid the adoption of biomass for use in diesel engines (Lin et al., 2011).

With the advent of renewable diesel fuels developed to date, biodiesel is now the best known alternative to petrodiesel (Aghbashlo et al., 2016). It is more environmentally friendly and has a number of social security benefits (Aghbashlo, Tabatabaei, Hosseinpour, et al., 2018). Looking from the perspective of regulated emissions exhausted (like carbon monoxide (CO), smoke and particulate matter) , biodiesel performs way better than petrodiesel, with the single exception of nitrogen oxides emmision (NO_x) (Aghbashlo et al., 2017). Apart from the environmental and health benefits, Biofuels are also economically viable, because because they are easily reproducible, biodegradable, and less toxic. They also free of sulphur and benzene, have better lubricity, and are less flammable than petrodiesel (Aghbashlo, Tabatabaei, Rastegari, et al., 2018; Hosseinpour et al., 2016).

Tests and studies have shown that even with the issues that plague Biofuel use (Hoang et al., 2019; Saxena et al., 2013), already existing diesel engines can be reasonably powered with biofuels. This is possible even with little to no changes being made to the diesel engines (Aghbashlo, Tabatabaei, Khalife, et al., 2018; Amid et al., 2020). The issues that are faced in the use and production of biofuels are mostly related to the many physical and chemical similarities between biodiesel and petrodiesel (Aghbashlo, Tabatabaei, Jazini, et al., 2018).

Transesterifying triglycerides or esterifying free fatty acids (FFAs) with light alcohol in the presence of a catalyst produces long-chain fatty acid alkyl esters, which are used to make biodiesel fuel. (Reza et al., 2019). Under supercritical conditions the two methods of biodiesel production can be carried out without the presence of a catalyst.

1.2 Problem statement

Biodiesel has a higher combustion efficiency, a higher cetane number, is more biodegradable, and emits less carbon monoxide than diesel fuel. In addition to the inherent benefits of Biodiesel, the drawbacks of utilizing Biodiesel are worth considering. Biodiesel has a few drawbacks, including slightly higher NOx emissions, cold start issues, decreased energy content, increased copper strip corrosion, and fuel pumping trouble due to higher viscosity.

Biodiesel is now more expensive to generate than diesel, which appears to be the biggest barrier to its wider adoption. The current global production of vegetable oil and animal fat is insufficient to replace the consumption of liquid fossil fuels. Because of these factors, biodiesel blends with other fuels such as diesel, bioethanol, and other biofuels are becoming increasingly popular.

There is a lot of work done in the process design and manufacturing of Biodiesel from Biomass, but there is still a lack of data and studies for thermodynamic properties of Biomass and other important Biodiesel properties, according to the literature. The simulation tools requires thermodynamic data required for a thorough characterisation of Biomass.

These modeling tools, in reality, rely on correlations derived from a small number of data points. There is a scarcity of experimental data in the literature. There is a lot of potential in developing accurate models to anticipate the qualities of Biodiesel and, more crucially, their blends, as they are becoming more significant as the need for Diesel fuel grows.

1.3 Aim and objectives

My aim and objectives are as follows.

1.3.1 Aim

The aim of this thesis is to apply and analyse some machine learning techniques in order to predict certain biodiesel property (viscosity). The results would be analysed to see if the machine learning models are viable methods for the prediction of biodiesel properties. I would compare my results with other available results from machine learning application for biodiesel properties prediction.

1.3.2 Objectives

The objective of my research is to study the feasibility of the machine learning models for biodiesel properties prediction. Research into the field of machine learning has led to the development of many machine learning methodologies, and techniques. However, all this methods are not one-size-fits-all. Some methods work better for different problems.

In this study, I would develop a system to predict the state values for Viscosity and analyse the effectiveness of this method for this purpose. I would also compare it to other applications developed for the same purpose.

1.4 Significance

The negative environmental consequences of fossil fuel use, as well as the diminishing stocks of these fuels, necessitated and sparked a huge interest in alternative energy sources. Many governments have implemented policies such as stricter emission standards and tariffs to stimulate the use of renewable energy, with the goal of increasing the substitution of fossil fuels with biodegradable and environmentally friendly alternatives. Biodiesel is one of the alternatives for the transportation sector because it can be utilized in diesel engines without any modifications to the engine design.

1.5 Limitations of the study

The study was done with limited data in an idealistic scenario. Noise was not taken into consideration. This could create vague results or implications in the results. The hypothesis in this case is that the general trajectory of results would be maintained.

CHAPTER 2

EMPIRICAL MODELS

2.1 Machine Learning Models

Machine learning is one of the fastest growing fields of study in the world now, as it is the biggest topic now in the worls of technology. Machine learning provides the advantage of automating most of the tasks we do now as humans with even higher accuracy than can be achieved by humans in most cases. This increases convenience while also increasing efficiency and productivity, which is often not a small feat.

Machine learning is a subset of Artificial Intelligence based on the premise that computers can learn from data, detect and understand patterns and make predictions of conclusions based on what they've learned with little to no human help. There are numerous methods for Artificial Intelligence that have been developed. The methods are chosen based on the problem to be solved.

As an example Heuristic algorithms are used in problems where a quick approximate solution with a decent level of accuracy is needed. This can be considered as a simple "common sense" solution to a problem that saves time.

Fuzzy Logic is used in cases where a knowledge base for a specific field or topic is needed. Like an inference engine for medical diagnosis that has a knowledge base of diseases and can make a diagnosis based on detected symptoms.

Machine learning is used in cases where an outcome should be predicted on new data or input, based on patterns or trends that have been detected by previous analysis of large amounts of data. The machine learning model can be told what trends to look for (supervised machine learning) or It might be left to figure that out on its own (unsupervised learning).

Before any machine learning model is used for any application, its very important to investigate the problem, and understand the nature of the input, as well as the nature of the output to expected. This helps to determine the best machine learning model to be used. This is important because different machine learning models might handle the same problem differently. Some giving better results, solving the problem faster than others, or requesting more resources than others.

As an example, the table below shows preferred machine learning approaches for certain applications in biodiesel production, along with the input variables and expected output.

Table 2.1: Purposes, Recommended Machine learning models and the suggested input variables to solve those problems

Purpose	**Recommended ML Method/Model**	**Possible Input variables**
Quality Estimation	ANN, Least Squares Boosting (LSBoost), Regression models	Reaction temperature, reaction Time, Metal ratio, Calcination temperature, flow rate, pressure, reactor residence

		time, reflux rate, oil fraction, methanol-to-oil molar ratio, catalyst concentration
Yield Estimation	ANN, ANFIS, Linear Regression (LR)	Temperature, methanol-to-oil molar ratio, catalyst concentration, reaction time, organic loading rate, influent-effluent pH, pressure, reactor diameter, liquid height, ultrasound intensity
Quality and yield optimization	ANN-GA, SVM(Support vector machine) based on genetic algorithm,ANFIS-GA, multi-objective genetic algorithm	Methanol-tooil molar ratio, reaction temperature, reaction time, stirring speed,catalyst concentration, catalyst weight,humidity, impurities, mixing time, Free Fatty Acid (FFA) content

2.2 Biodiesel Properties

2.2.1 Viscosity

Viscosity is a measure of resistance to flow of a liquid due to internal friction of one part of a fluid moving over another. This is a critical property because it affects the behaviour of fuel injection. In general, higher viscosity leads to poorer fuel atomization. High viscosity can cause larger droplet sizes, poorer vaporization, narrower injection spray angle, and greater in-cylinder penetration of the fuel spray. This can lead to overall poorer combustion, higher emissions, and increased oil dilution. The viscosity of Biodiesel is typically higher than that of petroleum diesel often by a factor of two. 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:

kinematic viscosity and dynamic viscosity.

2.2.2 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 d_y 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 op layer. The shear stress (ÿ) is proportional to the y-respect rate of change.

2.2.3 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.

2.2.4 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 combustion and performance.

2.2.5 Cetane 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 sulphur 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

2.3 Applications Of Machine Learning In Modelling Biodiesel Properties

Despite biodiesel's positive attributes such as renewability, biodegradability and nontoxicity (Shamshirband et al., 2015), researchers and investors still often worry about some of its unfavorable physical and chemical features. (Hosseinzadeh-bandbafha et al., 2020). It is important to remember that biodiesel's production, storage, handling and combustion are all influenced by it's physical and chemical properties. Therefore, there are a number of international standards, such as ASTM D6751 and EN 14214 that it must adhere to that certifies its quality before it can be sold on the international market (Al-shanableh et al., 2016). However, determining the physical and chemical parameters of biodiesel using the experimental methodologies outlined in these standards is time-consuming, requires expert experience, is costly, and error-prone. Furthermore, using physical simulations to characterize biodiesel fuel is significantly more difficult than modeling the manufacturing process. This is due to the fact that the ester content of biodiesel fuel varies significantly depending on the origin feedstock. As a result, the scientific community will benefit greatly from establishing reliable models and simulations for determining biodiesel physical and chemical qualities from chemical and physical characteristics. The key structural aspects of a particular fatty ester molecule that determine its physical and chemical properties are chain length, unsaturation degree, chain branching, double bond number, and double bond configuration. (Aghbashlo et al., 2017; Jahirul et al., n.d.; Knothe, 2005).

2.3.1 Literature Review of Related Works

Various approaches for forecasting density, kinematic viscosity, cetane number etc, have been established by researchers. Nonetheless, biodiesel properties (density, viscosity, and cetane number) are increasingly used in engine design and parameter control during operation due to their vital role in the concept of fuel during the combustion process, their importance for engine design, and their implications for parameter control during operation. (L. F. Ramirez–Verduzco, 2013). The viscosity and density determine the size required for proper engine operation (combustion), whereas the cetane number determines the efficiency of combustion. As a result, numerous stages and methods are available for measuring biodiesel characteristics with great precision (Geacai et al, 2015; EbnaAlam Fahd et al., 2014; Gülüm&Bilgin, 2016). (Freitas et al. S.V.D. Freitas, M.J. Pratas, 2011) The viscosity of biodiesel may now be estimated using a variety of models at various temperatures. To estimate the density of 10 samples, the Kay approach based on mixing and group contribution was proposed. (Pratas et al. M.J. Pratas, S.V.D. Freitas, 201). The models described were used to estimate the attributes of biodiesel using the hourly and monetary costs, the results and graphical interpretations, and the models mentioned. (Betiku et al., 2014); (Wakil et al., 2015) delsPrieto et al., 2015); (Barabás&Todoruţ, 2011); (Barabás, 2013); (neuro fuzy, Mostafaei et al., 2016); (Hosoz et al., 2013); and artificial neural network (Barabás, 2013).

With 10 FAMEs as inputs, (Piloto-Rodriguez et al. 2013) successfully applied the ANNs to forecast the biodiesel Cetane number, and the multiple linear regression model gave less accuracy than the ANNs method. (Yuan et al. 1949) devised a method for calculating the kinematic viscosity of biodiesel using a mixing topological index. Cheenkachorn did a similar study that focused on assessing biodiesel fuel qualities only based on the fatty acid composition. However, other chemical compositions found in biodiesel, such as the amount of free glycerol, free fatty acid, methanol, and contaminants, were not considered through model input in these research, which could have an impact on the biodiesel's physical qualities.

In calculating the flash point, fire point, density, and viscosity of diesel and biodiesel blends, Kumar and Bansal examined the applicability of the standard technique of linear regression and ANN techniques. They used three training algorithms and ten different combinations of weights and biases to optimize the network. The findings of this study reveal that neural networks outperform the Linear Regression models in predicting the fuel qualities of various diesel and biodiesel blends. However, other training parameters such as objective, epochs, learning rate, gradient magnitude, and so on can boost the performance of a neural network even further.

The findings of previous studies, which also used explicit ML classifiers, differed from the test data, according to a review of relevant work. The Multilayer Perceptron (MLP) outperforms other classifiers, such as gullible Bayes and Forests, in assessing the number, with a score of 92.5 percent. More research using five different classifiers reveals that utilitarian trees (FT) have the highest dependability (95%) and genuine positive worth (TRP) (96.7 percent).

Using a similar Fisher test and the wellness test in the past, the potential risk of using the test was that the information used should be the recurrence or tally rather than the next kind. Meanwhile, regardless of whether the data is in recurrence or checks, the multilayer perceptron is capable of examining and testing it. The NVivo application, on the other hand, is straightforward and efficient to use. It also enhances the precision of subjective investigations.

Using the Multilayer Perceptron in the Adaboost algorithm, the cross-validation test is a reasonable strategy for recognizing the exhibition of understudy. Cross-validation is a technique for overlaying data numerous times and preparing it for precise accuracy. The accuracy of the Adaboost calculation is 92.23 percent based on the preparation dataset verification. It was formerly used to solve the issue of over-fitting and to broaden projections.

CHAPTER 3

METHODOLOGY

3.1 Data

As presented in table 3.1 below, a total of 5 properties were studied. Each property would be used as data points in the code. Temperature, w1 and w2 were the input variables used to predict the density(ρ) and viscosity(ν) of the biofuels. The data presented in the tables show the thermophysical properties of the biodiesel gotten from sunflower oil, corn oil, soy oil and canola oil.

Table 3.1 Table of Parameters for Sunflower Oil

Temperature	w1	w2	ρ	ν
10.15	0.25	0.75	829.772	3.248
20.15	0.25	0.75	828.535	2.563
30.15	0.25	0.75	825.134	2.074
40.15	0.25	0.75	820.126	1.701
50.15	0.25	0.75	816.655	1.484
10.15	0.5	0.5	847.247	4.711
20.15	0.5	0.5	845.777	3.566
30.15	0.5	0.5	842.213	2.875
40.15	0.5	0.5	837.374	2.333
50.15	0.5	0.5	833.995	1.926
10.15	0.75	0.25	868.402	6.471
20.15	0.75	0.25	864.902	4.857
30.15	0.75	0.25	860.647	3.815
40.15	0.75	0.25	858.004	3.161
50.15	0.75	0.25	853.172	2.586
10.15	1	0	887.599	9.926
20.15	1	0	883.41	7.441
30.15	1	0	879.324	5.546
40.15	1	0	874.962	4.571
50.15	1	0	871.035	3.827

Table 3.2 Table of Parameters for Corn Oil

Temperature	w1	w2	ρ	ν
10.15	0.25	0.75	829.391	3.264
20.15	0.25	0.75	827.96	2.598
30.15	0.25	0.75	826.171	2.077
40.15	0.25	0.75	821.161	1.715
50.15	0.25	0.75	817.566	1.437
10.15	0.5	0.5	850.079	4.751
20.15	0.5	0.5	846.229	3.575
30.15	0.5	0.5	842.385	2.911
40.15	0.5	0.5	837.412	2.379
50.15	0.5	0.5	834.579	1.936
10.15	0.75	0.25	866.85	6.406
20.15	0.75	0.25	864.811	4.806
30.15	0.75	0.25	860.124	3.793
40.15	0.75	0.25	856.715	3.163
50.15	0.75	0.25	853.437	2.595
10.15	1	0	885.86	9.542
20.15	1	0	880.947	7.162
30.15	1	0	877.259	5.58
40.15	1	0	873.728	4.329
50.15	1	0	869.248	3.674

Table 3.3 Table of Parameters for Soy Oil

Temperature	w1	w2	ρ	ν
10.15	0.25	0.75	832.996	3.422
20.15	0.25	0.75	831.477	2.678
30.15	0.25	0.75	829.256	2.115
40.15	0.25	0.75	824.848	1.763
50.15	0.25	0.75	823.573	1.499
10.15	0.5	0.5	847.067	4.507
20.15	0.5	0.5	844.68	3.43
30.15	0.5	0.5	840.803	2.732
40.15	0.5	0.5	836.604	2.209
50.15	0.5	0.5	833.107	1.83
10.15	0.75	0.25	866.688	6.163
20.15	0.75	0.25	863.352	4.658
30.15	0.75	0.25	860.324	3.66
40.15	0.75	0.25	856.162	2.998
50.15	0.75	0.25	853.202	2.477

10.15	1	0	886.327	9.315
20.15	1	0	882.993	6.997
30.15	1	0	877.678	5.651
40.15	1	0	873.945	4.44
50.15	1	0	868.716	3.655

Table 3.4 Table of Parameters for Canola Oil

Temperature	w1	w2	ρ	ν
10.15	0.25	0.75	833.458	3.462
20.15	0.25	0.75	832.249	2.678
30.15	0.25	0.75	828.011	2.136
40.15	0.25	0.75	823.277	1.747
50.15	0.25	0.75	819.552	1.49
10.15	0.5	0.5	847.431	4.768
20.15	0.5	0.5	845.047	3.608
30.15	0.5	0.5	841.294	2.945
40.15	0.5	0.5	836.685	2.358
50.15	0.5	0.5	833.835	1.968
10.15	0.75	0.25	868.717	6.564
20.15	0.75	0.25	866.209	4.983
30.15	0.75	0.25	863.269	3.927
40.15	0.75	0.25	859.241	3.188
50.15	0.75	0.25	855.067	2.634
10.15	1	0	886.431	10.317
20.15	1	0	882.418	7.699
30.15	1	0	878.945	5.835
40.15	1	0	874.511	4.679
50.15	1	0	871.732	3.89

For the development of the models, a data division of 15% for validation, 15% for testing, and 70% for training was selected. Input refers to data obtained from a third-party source entered into the model. Data is moved from the input layer to invisible layers made up of neurons. The weights are the values of cell connections. Data from neurons in the input and hidden layers, as well as the bias and activation functions, are used to generate the output information.

3.2 Response Surface Methodology (RSM)

Response Surface Methodology is a method that is used to investigate and explore the relationship between several causative variables and a response variable. The main aim of the model is to find the optimal resultant value of the response variable. RSM creates an emperical model to analyze or establish relationships between these variables using mathematical and statistical methods. It can also be used to analyze and understand the level of influence or effect of the causative variables on the response variables.

Another capability of RSM is that having established the relationship between the variables, it can now be used to predict values for its response variable outside of the domain experimented on. RSM has found a lot of application and use in the industrial sector due to its ability to make precise decisions in uncertain conditions (Sarabia & Ortiz, 2009).

Within this work, RSM is used because it is a statistical approach that can be used to maximize one factor by adjusting other factors. In history, RSM has been used to improve products and services. The model does this by making experimental changes to the causative or independent variables and analysing the response or dependent variables to choose the best response.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Results

The Results of my experiments with the dataset using RSM are discussed in this section. I used RSM to first predict the density of Sunflower oil, Corn oil and Canola oil, Then I did the same again, predicting the viscosity for each of them.

4.1.1 Density Results

The Regression equation used to establish the relationship between the emperature, w1, w2 and density is as follows:

ρ = 753,5 + 0,674 T(K) + 90,7 w1 - 0,00160 T(K)*T(K) + 9,02 w1*w1 - 0,1032 T(K)*w1

The results are as follows:

Table 4.1: Actual and predicted values for density of sunflower oil

T(K)	w1	w2	ρ (Actual)	ρ (Predict)
283.15	0.25	0.75	829.772	831.8375189
293.15	0.25	0.75	828.535	829.0925055
303.15	0.25	0.75	825.134	826.0273761
313.15	0.25	0.75	820.126	822.6421305
323.15	0.25	0.75	816.655	818.9367689
283.15	0.5	0.5	847.247	848.8916539
293.15	0.5	0.5	845.777	845.888728
303.15	0.5	0.5	842.213	842.5656861
313.15	0.5	0.5	837.374	838.922528
323.15	0.5	0.5	833.995	834.9592539
283.15	0.75	0.25	868.402	867.0732389
293.15	0.75	0.25	864.902	863.8124005
303.15	0.75	0.25	860.647	860.2314461
313.15	0.75	0.25	858.004	856.3303755
323.15	0.75	0.25	853.172	852.1091889
283.15	1	0	887.599	886.3822739

293.15	1	0	883.41	882.863523
303.15	1	0	879.324	879.0246561
313.15	1	0	874.962	874.865673
323.15	1	0	871.035	870.3865739

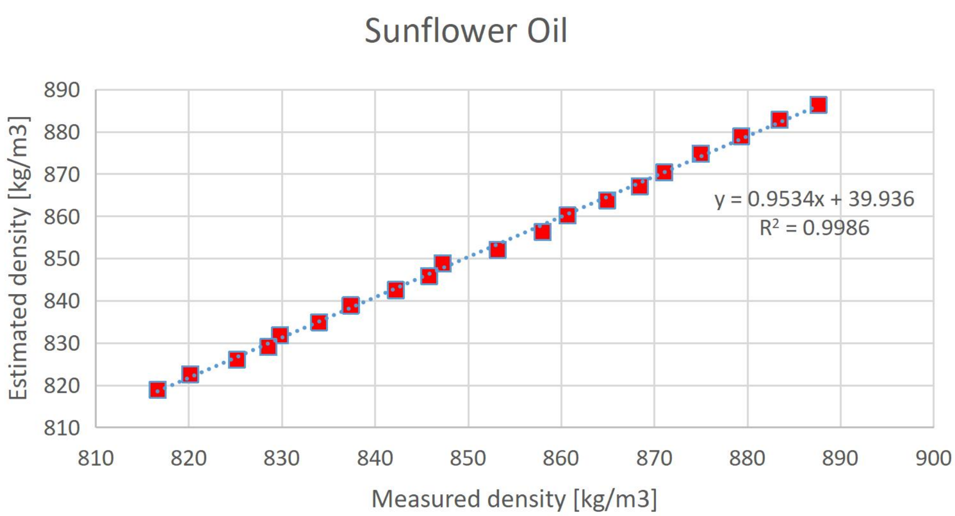

Figure 4.1: Graphical Representation of the Measured and Predicted values of the Density of Sunflower oil

Table 4.2: Actual and predicted values for density of corn oil

T(K)	**w1**	**w2**	**ρ (Actual)**	**ρ (Predict)**
283.15	0.25	0.75	829.391	831.8375189
293.15	0.25	0.75	827.96	829.0925055
303.15	0.25	0.75	826.171	826.0273761
313.15	0.25	0.75	821.161	822.6421305
323.15	0.25	0.75	817.566	818.9367689
283.15	0.5	0.5	850.079	848.8916539
293.15	0.5	0.5	846.229	845.888728
303.15	0.5	0.5	842.385	842.5656861
313.15	0.5	0.5	837.412	838.922528
323.15	0.5	0.5	834.579	834.9592539
283.15	0.75	0.25	866.85	867.0732389
293.15	0.75	0.25	864.811	863.8124005
303.15	0.75	0.25	860.124	860.2314461
313.15	0.75	0.25	856.715	856.3303755

323.15	0.75	0.25	853.437	852.1091889
283.15	1	0	885.86	886.3822739
293.15	1	0	880.947	882.863523
303.15	1	0	877.259	879.0246561
313.15	1	0	873.728	874.865673
323.15	1	0	869.248	870.3865739

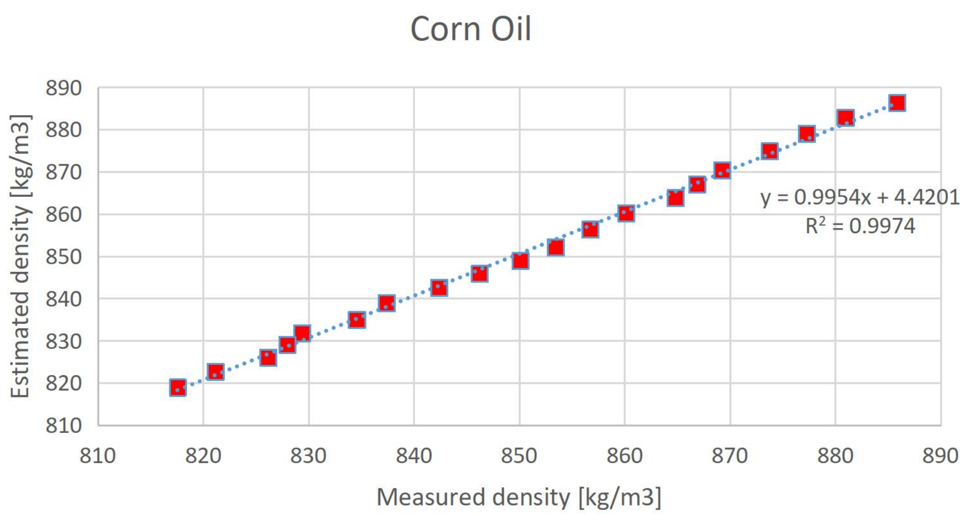

Figure 4.2: Graphical Representation of the Measured and Predicted values of the Density of Corn oil

Table 4.3: Actual and predicted values for density of canola oil

T(K)	w1	w2	ρ (Actual)	ρ (Predict)
283.15	0.25	0.75	832.996	831.8375189
293.15	0.25	0.75	831.477	829.0925055
303.15	0.25	0.75	829.256	826.0273761
313.15	0.25	0.75	824.848	822.6421305
323.15	0.25	0.75	823.573	818.9367689
283.15	0.5	0.5	847.067	848.8916539
293.15	0.5	0.5	844.68	845.888728
303.15	0.5	0.5	840.803	842.5656861
313.15	0.5	0.5	836.604	838.922528
323.15	0.5	0.5	833.107	834.9592539
283.15	0.75	0.25	866.688	867.0732389
293.15	0.75	0.25	863.352	863.8124005
303.15	0.75	0.25	860.324	860.2314461
313.15	0.75	0.25	856.162	856.3303755
323.15	0.75	0.25	853.202	852.1091889

283.15	1	0	886.327	886.3822739
293.15	1	0	882.993	882.863523
303.15	1	0	877.678	879.0246561
313.15	1	0	873.945	874.865673
323.15	1	0	868.716	870.3865739
283.15	0.25	0.75	833.458	831.8375189
293.15	0.25	0.75	832.249	829.0925055
303.15	0.25	0.75	828.011	826.0273761
313.15	0.25	0.75	823.277	822.6421305
323.15	0.25	0.75	819.552	818.9367689
283.15	0.5	0.5	847.431	848.8916539
293.15	0.5	0.5	845.047	845.888728
303.15	0.5	0.5	841.294	842.5656861
313.15	0.5	0.5	836.685	838.922528
323.15	0.5	0.5	833.835	834.9592539
283.15	0.75	0.25	868.717	867.0732389
293.15	0.75	0.25	866.209	863.8124005
303.15	0.75	0.25	863.269	860.2314461
313.15	0.75	0.25	859.241	856.3303755
323.15	0.75	0.25	855.067	852.1091889
283.15	1	0	886.431	886.3822739
293.15	1	0	882.418	882.863523
303.15	1	0	878.945	879.0246561
313.15	1	0	874.511	874.865673
323.15	1	0	871.732	870.3865739

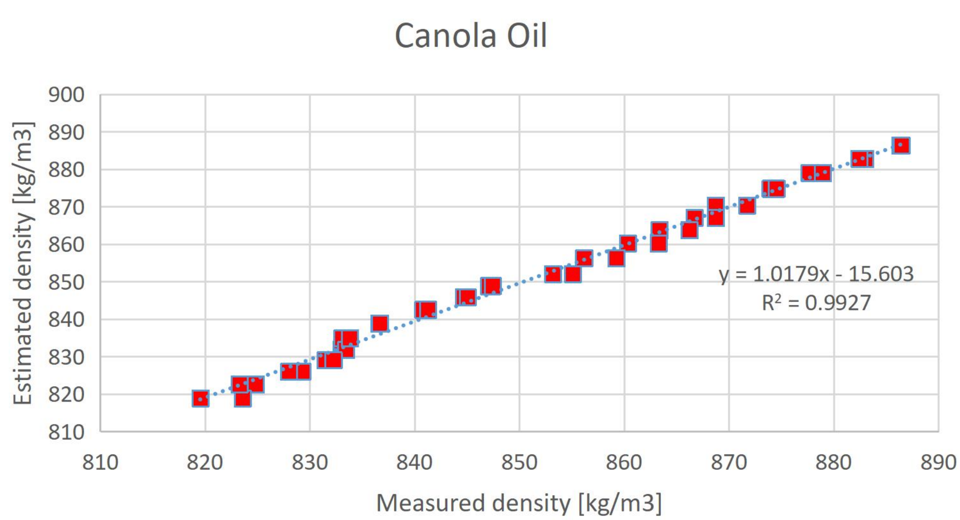

Figure 4.3: Graphical Representation of the Measured and Predicted values of the Density of Canola oil

The main effects plot, showing the effects of the causative variables Temperature, w1 and w2 at different levels on Density is shown below

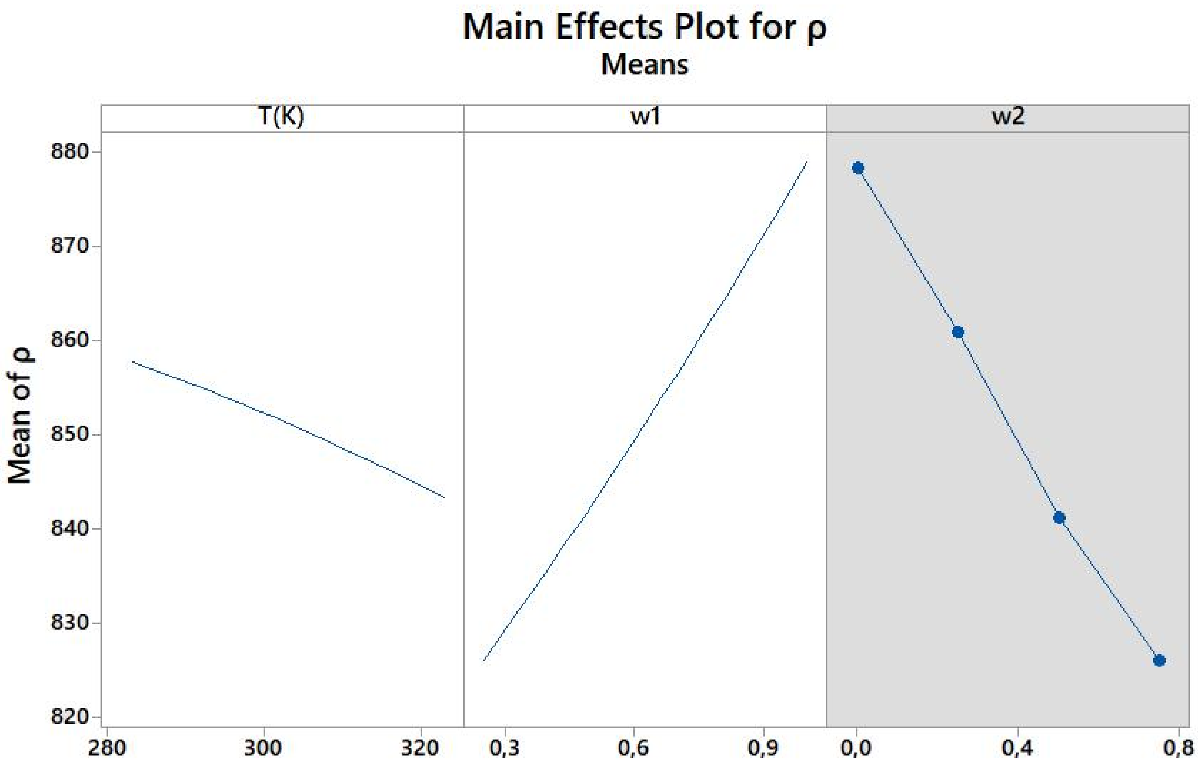

Figure 4.4: Main effect plots for Temperature, w1 and w2 on density

The steeper w1 and w2 plots in contrast to the Temperature plot shows that the w1 and w2 values had more effect on the density values.

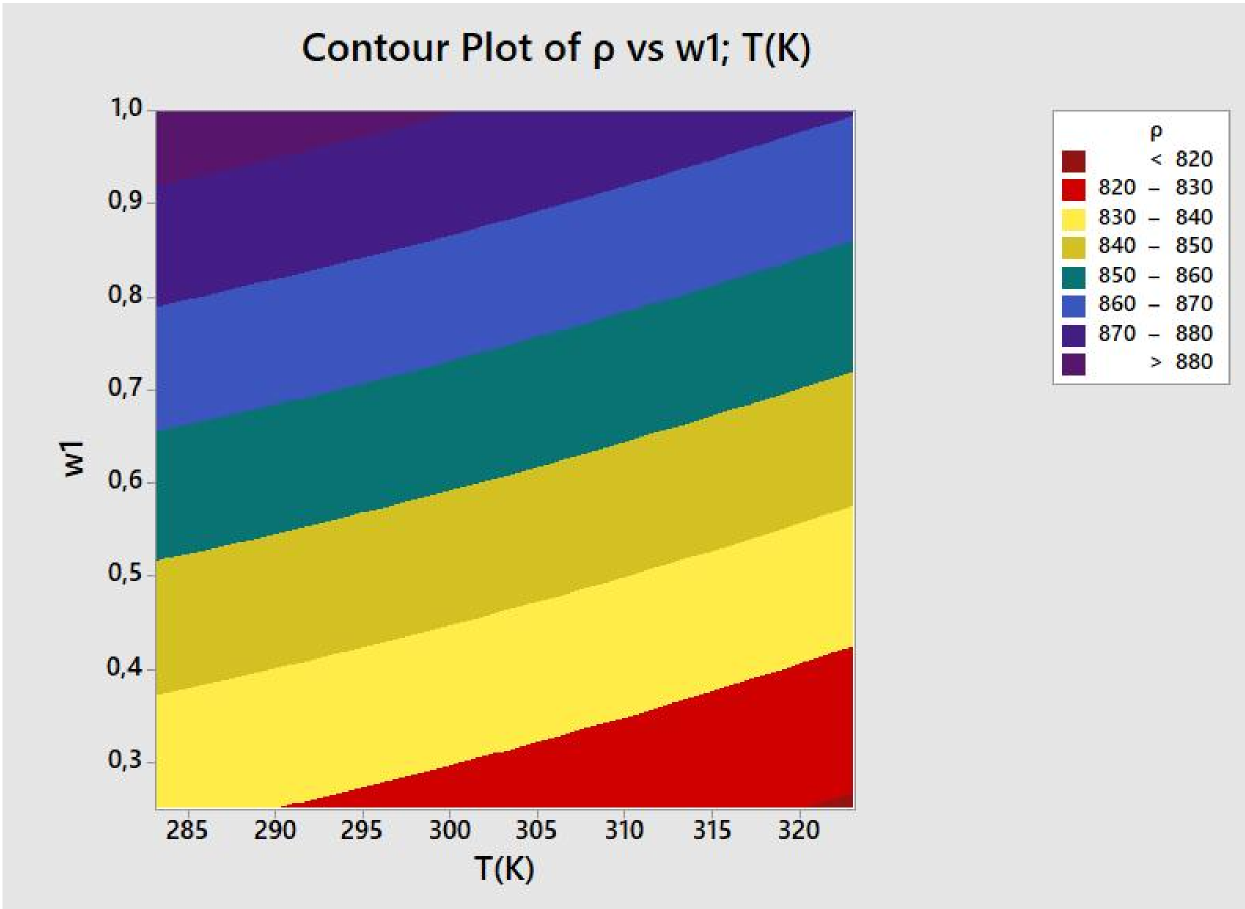

Figure 4.5: Contour plot of density and w1

4.1.2 Viscosity Predictions

The regression equation used tto establish the relationship between Temperature, w1, w2, and viscosity is as follows:

v = 151,9 - 0,983 T(K) + 39,19 w1 + 0,001612 T(K)*T(K) + 5,001 w1*w1

- 0,13284 T(K)*w1

The results for my viscosity experiments are as follows:

Table 4.4: Actual and predicted values for viscosity of sunflower oil

T(K)	w1	w2	v (actual)	v (predict)

283.15	0.25	0.75	3.248	3.3993925
293.15	0.25	0.75	2.563	2.52373875
303.15	0.25	0.75	2.074	1.9705225
313.15	0.25	0.75	1.701	1.73974375
323.15	0.25	0.75	1.484	1.8314025
283.15	0.5	0.5	4.711	4.7302975
293.15	0.5	0.5	3.566	3.52254625
303.15	0.5	0.5	2.875	2.6372325
313.15	0.5	0.5	2.333	2.07435625
323.15	0.5	0.5	1.926	1.8339175
283.15	0.75	0.25	6.471	6.6863025
293.15	0.75	0.25	4.857	5.14645375
303.15	0.75	0.25	3.815	3.9290425
313.15	0.75	0.25	3.161	3.03406875
323.15	0.75	0.25	2.586	2.4615325
283.15	1	0	9.926	9.2674075
293.15	1	0	7.441	7.39546125
303.15	1	0	5.546	5.8459525
313.15	1	0	4.571	4.61888125
323.15	1	0	3.827	3.7142475

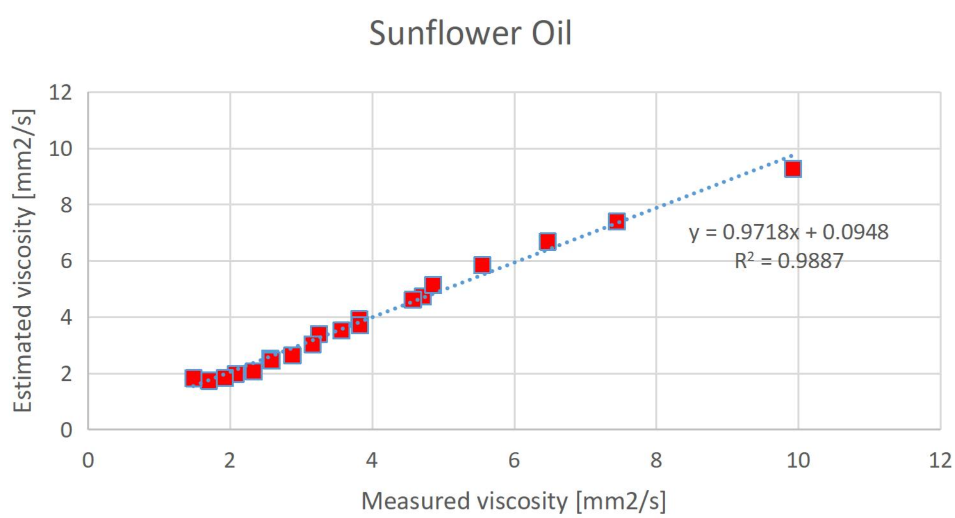

Figure 4.6: Graphical Representation of the Measured and Predicted values of the Viscosity of Sunflower oil

Table 4.5: Actual and predicted values for viscosity of corn oil

T(K)	w1	w2	v (actual)	v (predict)
283.15	0.25	0.75	3.264	3.3993925
293.15	0.25	0.75	2.598	2.52373875
303.15	0.25	0.75	2.077	1.9705225
313.15	0.25	0.75	1.715	1.73974375
323.15	0.25	0.75	1.437	1.8314025
283.15	0.5	0.5	4.751	4.7302975
293.15	0.5	0.5	3.575	3.52254625
303.15	0.5	0.5	2.911	2.6372325
313.15	0.5	0.5	2.379	2.07435625
323.15	0.5	0.5	1.936	1.8339175
283.15	0.75	0.25	6.406	6.6863025
293.15	0.75	0.25	4.806	5.14645375
303.15	0.75	0.25	3.793	3.9290425
313.15	0.75	0.25	3.163	3.03406875
323.15	0.75	0.25	2.595	2.4615325
283.15	1	0	9.542	9.2674075
293.15	1	0	7.162	7.39546125
303.15	1	0	5.58	5.8459525
313.15	1	0	4.329	4.61888125
323.15	1	0	3.674	3.7142475

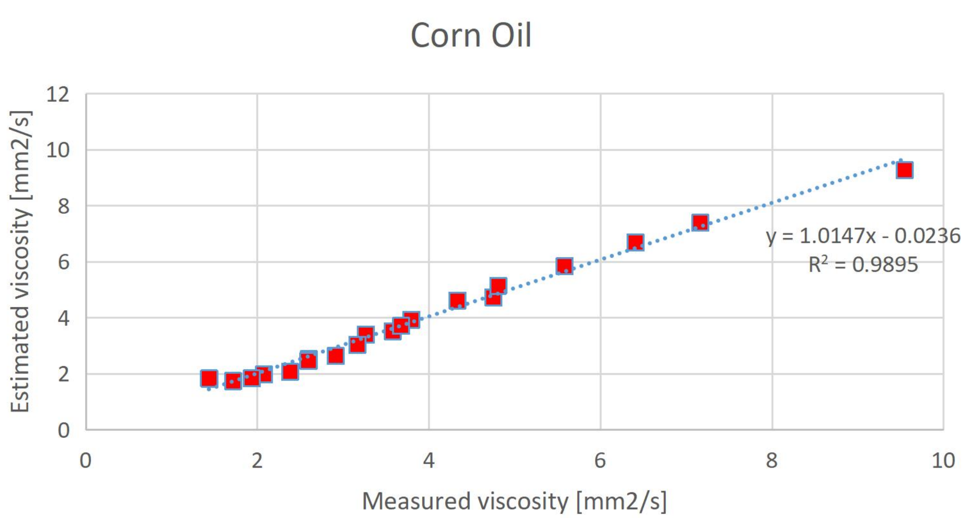

Figure 4.7: Graphical Representation of the Measured and Predicted values of the Viscosity of Corn oil

Table 4.6: Actual and predicted values for viscosity of canola oil

T(K)	w1	w2	v (actual)	v (predict)
283.15	0.25	0.75	3.422	3.3993925
293.15	0.25	0.75	2.678	2.52373875
303.15	0.25	0.75	2.115	1.9705225
313.15	0.25	0.75	1.763	1.73974375
323.15	0.25	0.75	1.499	1.8314025
283.15	0.5	0.5	4.507	4.7302975
293.15	0.5	0.5	3.43	3.52254625
303.15	0.5	0.5	2.732	2.6372325
313.15	0.5	0.5	2.209	2.07435625
323.15	0.5	0.5	1.83	1.8339175
283.15	0.75	0.25	6.163	6.6863025
293.15	0.75	0.25	4.658	5.14645375
303.15	0.75	0.25	3.66	3.9290425
313.15	0.75	0.25	2.998	3.03406875
323.15	0.75	0.25	2.477	2.4615325
283.15	1	0	9.315	9.2674075
293.15	1	0	6.997	7.39546125
303.15	1	0	5.651	5.8459525
313.15	1	0	4.44	4.61888125
323.15	1	0	3.655	3.7142475
283.15	0.25	0.75	3.462	3.3993925
293.15	0.25	0.75	2.678	2.52373875
303.15	0.25	0.75	2.136	1.9705225
313.15	0.25	0.75	1.747	1.73974375
323.15	0.25	0.75	1.49	1.8314025
283.15	0.5	0.5	4.768	4.7302975
293.15	0.5	0.5	3.608	3.52254625
303.15	0.5	0.5	2.945	2.6372325
313.15	0.5	0.5	2.358	2.07435625
323.15	0.5	0.5	1.968	1.8339175
283.15	0.75	0.25	6.564	6.6863025
293.15	0.75	0.25	4.983	5.14645375
303.15	0.75	0.25	3.927	3.9290425
313.15	0.75	0.25	3.188	3.03406875
323.15	0.75	0.25	2.634	2.4615325
283.15	1	0	10.317	9.2674075
293.15	1	0	7.699	7.39546125
303.15	1	0	5.835	5.8459525
313.15	1	0	4.679	4.61888125
323.15	1	0	3.89	3.7142475

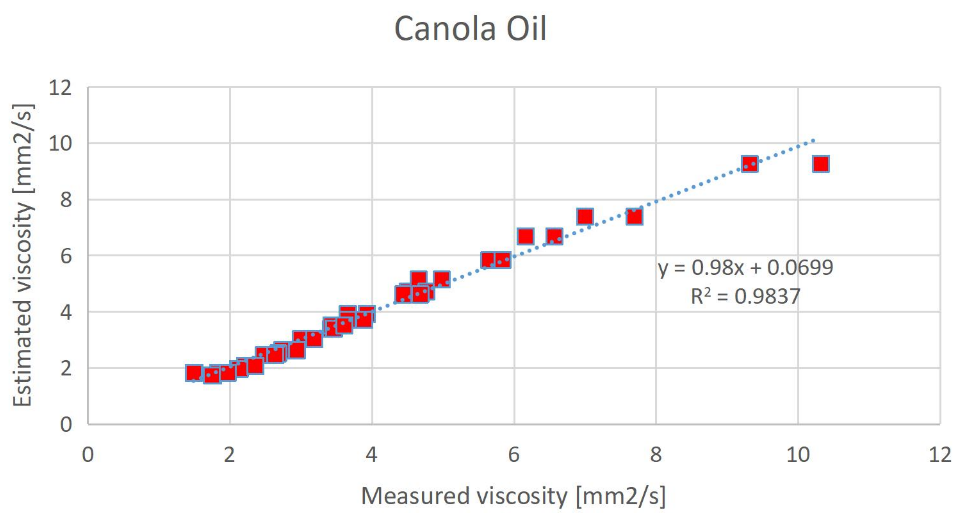

Figure 4.8: Graphical Representation of the Measured and Predicted values of the Viscosity of Canola oil

The main effects plot, showing the effects of the causative variables Temperature, w1 and w2 at different levels on Viscosity is shown below.

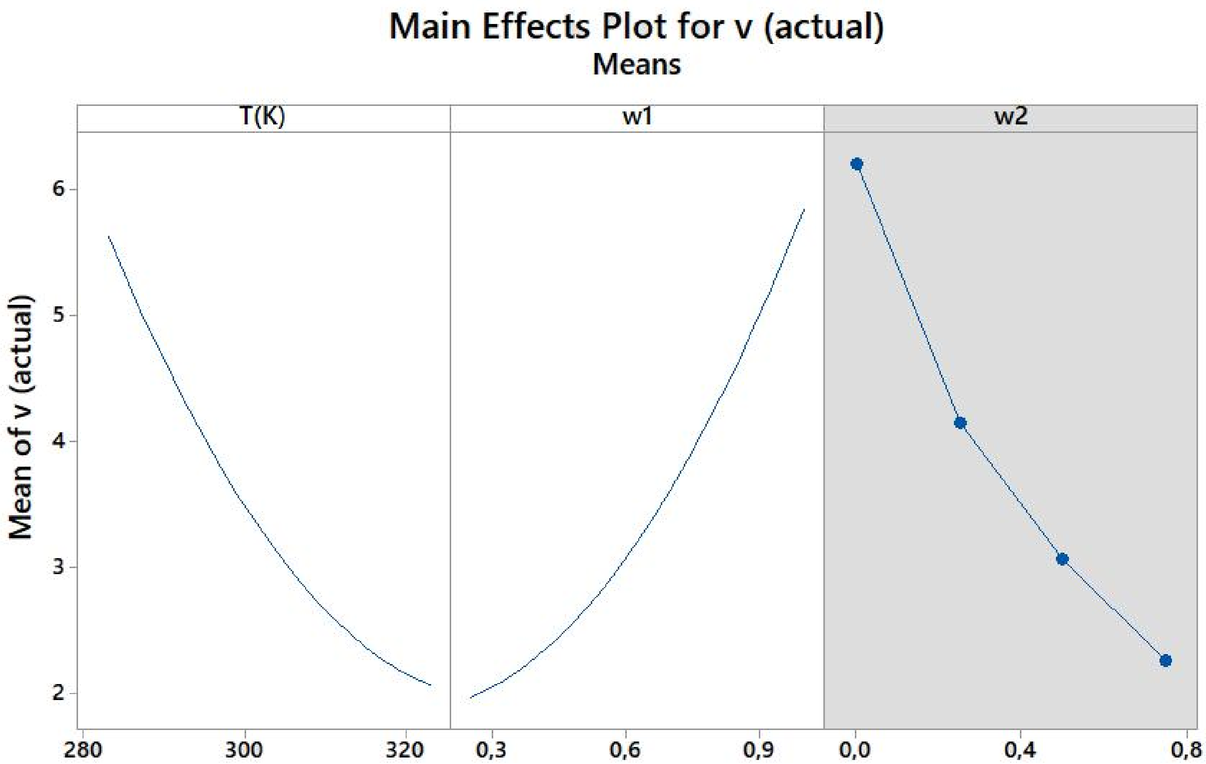

Figure 4.9: Main effect plots for Temperature, w1 and w2 on density

The steep Temperature, w1 and w2 plots show these causative or independent variables all have considerable effects on the response or dependent variable, viscosity.

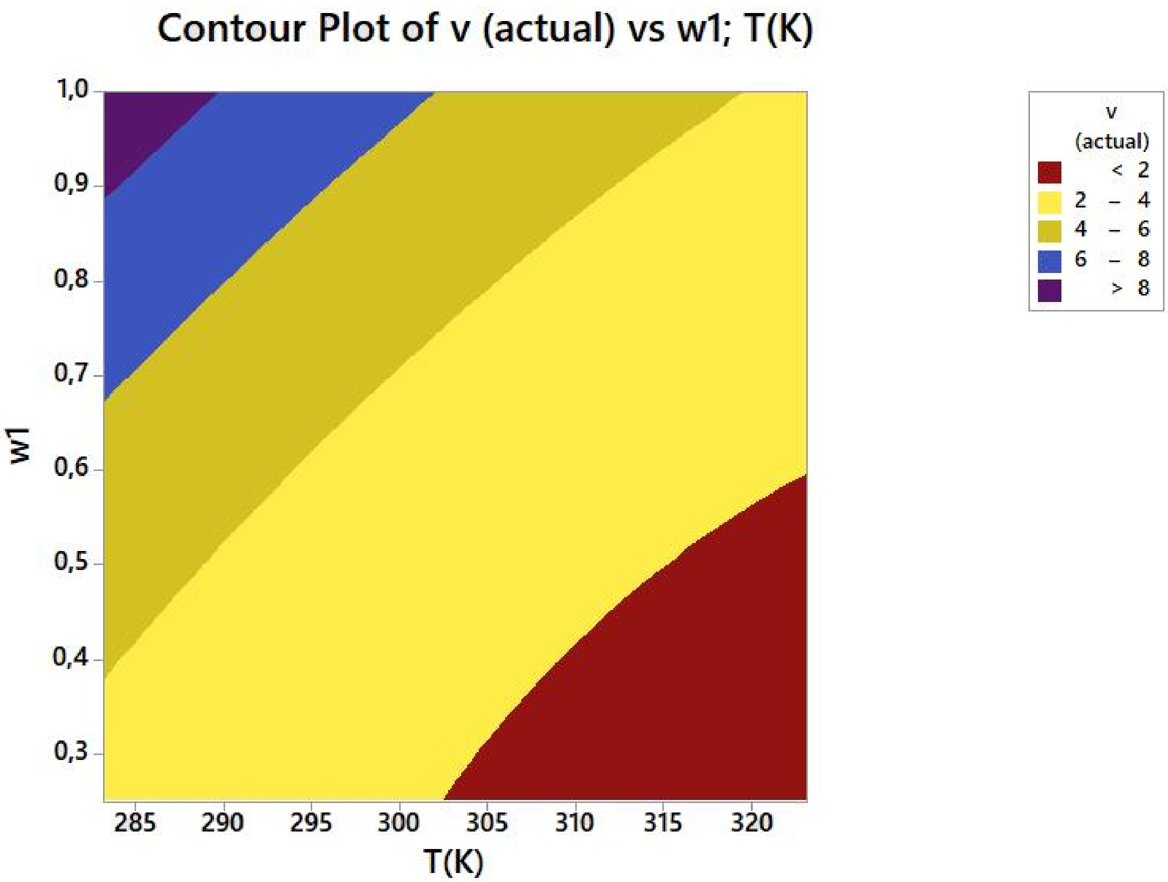

Figure 4.10: Contour plot of Viscosity and w1

4.2 Discussion

The results obtained are clearly satisfactory. R^2 Values of 0.9986, 0.9974, and 0.9927 were obtained for the density predictions for Sunflower oil, Corn oil and Canola oil respectively. Also, R^2 Values of 0.9887, 0.9895, and 0.9837 were obtained for the viscosity predictions for Sunflower oil, Corn oil and Canola oil.

Other properties can also be predicted using the same methodology. For example, Cetane number, as shown in Appendix A can also be predicted using a different set of input values. The results obtained shows that the model can adequately map the resultant attributes (Viscosity and Density) to the input attributes (Temperature, W1 and W2).

CHAPTER 5

CONCLUSIONS AND FUTURE WORK

In this thesis, the effectiveness of of Response Surface Methodology (RSM) was investigated. The model was developed and tested with the dataset to see how well it handled the data and was able to map the input to the target output.

The results obtained from this study are satisfactory and encouraging. They imply that with RSM, we can adequately predict the density and viscosity of Biodiesel. The accuracy of the model implies that the results are reliable enough and can be used to guide decision making in production of Biodiesel.

I also obtained results that were better than those shown for other models like Multilayer Perceptrons (MLP) as seen in other studies.

5.1 Future Work

Neural Network based Methodologies like adaptive neuro-fuzzy inference system (ANFIS), artificial neural network (ANN), radial basis function neural network (RBFNN) and response surface methodology (RSM) should also be studied to see how they measure up. Because these other models have different functioning principles, they could give better or worse results. Appendices B, C and D show the results obtained from predicting the Cetane number of other biofuels using one, two and three inputs attributes respectively on a number of machine learning models. This also goes to show that the number of independent variables used to predict the dependent variables also affects the obtained results.

ANFIS models for example are much more sophisticated Neural Networks and have an inference system that already does half of the work before the model even starts training. It is a hybrid between Neural networks and fuzzy systems (as the name implies) which means it would probably handle the data differently and might be faster.

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Appendices

Appendix A

Cetane Numbers of Some Biofuels

Biodiesel name	∑MUFAMs	∑PUFAMs	∑SFAMs	CN
Capric acid ester	0	0	100	47.2
Lauric acid ester	0	0	100	60.8
Myristic acid ester	0	0	100	66.2
Palmitic acid ester	0	0	100	74.3
Palmitoleic acid ester	100	0	0	51
Stearic acid ester	0	0	100	75.6
Oleic acid ester	100	0	0	56.5
Linoleic acid ester	0	100	0	38.2
Linolenic acid ester	0	100	0	22.7
Arachidic acid ester	0	0	100	100
Paullinic acid ester	100	0	0	64.8
Behenic acid ester	0	0	100	79.49
Erucic acid ester	100	0	0	76
Lignoceric acid ester	0	0	100	82.23
Anacardiaceae Rhus succedanea Linn	46.8	27.8	25.4	52.22
Annonaceae Annona reticulata Linn	52.6	21.7	25.7	53.47
Thevetia peruviana Merrill	60.9	12.6	26.5	57.48
Vallaris solanacea Kuntze	35.3	40.4	24.3	50.26
Balanitaceae Balanites roxburghii Planch	36.7	38.5	24.8	50.46
Burseraceae Canarium commune Linn	38.3	23	38.7	55.58
Terminalia chebula Retz	37.3	39.8	22.9	49.6
Compositaceae Vernonia cinerea Less	32	22	46	57.51
Croton tiglium Linn	56	29	15	49.9
Jatropa curcas Linn	40.8	32.1	27.1	52.31
Joannesia princeps Vell	45.8	46.4	7.8	45.2
Putranjiva roxburghii	33	3	118.99	
Sapium sebiferum Roxb Flacourtiaceae	27.4	0	72.6	30.72
Guttiferae Calophyllum apetalum Wild	48	30	22	51.57
Calophyllum inophyllum Linn	45.2	15.8	39	57.3
Garcinia combogia Desr	57.9	1.2	40.9	61.5

Garcinia indica Choisy	39.4	1.7	58.9	65.16
Garcinia echinocarpa Thw	52.6	0	47.4	63.1
Garcinia morella Desr	49.5	0.9	49.6	63.52
Mesua ferrea Linn	60	15	25	55.1
Icacinaceae Mappia foetida Milers	38.4	36.8	24.8	50.7
Illiciceae Illicium verum Hook	63.24	24.4	12.36	50.71
Labiatae Saturega hortensis Linn	12	80	8	25.46
Lauraceae Actinodaphne angustifolia	5.4	0	94.6	63.2
Neolitsea cassia Linn	4	3.3	92.7	64.05
Neolitsea umbrosa Gamble	21	6.7	72.3	60.77
Meliaceae Aphanamixis polystachya Park	21.5	42.6	35.9	48.52
Azadirachta indica	61.9	7.5	30.6	57.83
Melia azadirach Linn	22.3	67.7	9.4	41.37
Swietenia mahagoni Jacq	56	16.1	24.5	52.26
Menispermaceae Anamirta cocculus Wight & Hrn	46.4	0	53.6	64.26
Moraceae Broussonetia papyrifera Vent	14.8	72	13.1	41.25
Moringaceae Moringa concanensis Nimmo	83.8	0.8	15.4	56.32
Moringa oleifera Lam	81.5	0.9	17.6	56.66
Myristicaceae Myristica malabarica Lam	44.1	1	54.9	61.81
Papaveraceae Argemone mexicana	18.5	61.4	20.1	44.45
Papilionaceae Pongamia pinnata Pierre	51.8	19	29.2	55.84
Rhamnaceae Ziziphus mauritiana Lam	68.7	12.4	18.9	55.37
Rubiaceae Meyna laxiflora Robyns	32.5	39.7	27.8	50.42
Rutaceae Aegle marmelos correa Roxb	30.5	44.1	25.4	48.3
Salvadoraceae Salvadora oleoides Decne	8.3	0.1	91.6	66.13
Salvadora persica Linn	5.4	0	94.6	67.47
Sapindaceae Nephelium lappaceum Linn	49.5	0	50.5	64.86
Sapindus trifoliatus Linn	55.1	8.2	36.7	59.77
Sapotaceae Madhuca butyracea Mac	27.5	3	69.5	65.27
Madhuca indica JF Gmel	46.3	17.9	35.8	56.61
Mimusops hexendra Roxb	63	3	34	59.32
Urticaceae Urtica dioica Linn	14.6	76.4	9	38.73
Verbenaceae Tectona grandis Linn	29.5	46.8	23.7	48.31

Arachis hypoga Linn	40.07	40.69	19.39	48.86
Cocos nucifera	4.7	0.96	94.37	65.8
Oryza sativa	41.79	35.36	22.88	50.09
Elaeis guineensis	45.56	11.07	43.79	59.11
Glycine max (L.) merr	24.04	61.93	14.07	42.21
Helianthus annuus L.	22.52	67.12	10.39	41.41
Zea mays L.	35.3	48.58	16.15	46.3
Arachis hypogaea Linn.	63.57	16.46	20.21	54.03
Sesamum orientale L.	35.52	49.85	14.66	45.91
Sesamum indinum L.	41.21	44.61	14.2	46.92
Prunus dulcis	69.14	22.63	8.24	50.54
Brassica rapa (napus)	66.06	26.32	7.61	52.98
Carthamus tinctorius Linn.	14.19	76.72	9.12	39.32
Olea europoea Linn.	81.09	4.73	14.22	55
Irvingia malayana Oliv. ex A.W. Benn	3.07	0.44	96.21	66.13
Parinari anamensi Hance	43.52	19.59	36.89	56.35
Ceiba pentandra (L.) Gaertn.	26.51	43.76	29.64	49.52
Dipterocarpus alatus Roxb. ex G. Don	21.98	61.94	17	40.29
Ricinus communis L.	31.15	44.56	24.29	48.32
Jatropha currcas L.	41.79	38.88	19.34	48.91
Nicotiana tabacum L.	11.01	75.8	13.19	40.1
Citrus maxima (Burm.) Merr	24.7	45.32	30.02	49.29
Carica papaya Linn.	73.36	5.12	21.56	56.27
Nephelium lappaceum L.	56.21	3.98	39.6	61.17
Cucurbita moschata Duchesne	38.75	33.18	28.11	51.87
Citrus reticulate Blan co	21.38	52.45	26.03	46.48
Dasymaschalon lomentaceum Fiet & Gagnep	47	14.91	38.11	57.35
Rapeseed	64.1	30.5	5.4	46
Soybean	22.8	62.3	14.1	48
Rubber seed	27.8	51.1	21	51
Cottonseed	19.2	55.8	23.8	52.1
Jatropha	42.1	31.1	26.2	54
Karanja	53.2	19.1	17.8	52
Jatropha:palm 50:50	42.7	20.3	36.4	59
Neem	41.3	16.7	39.6	58.7
Sunflower	44	10.8	44.2	61.6

Palm	43.1	10.5	45.6	64
Mahua	36.4	16.1	46.2	61.4
SFCt 50:50	19.4	32.6	44.4	54.6
Beef Tallow	42.4	3.8	45.3	58.8
JCt 50:50	26.1	18.3	52.2	58
Coconut	8.2	2.7	81.5	60
Inedible tallow	41.9	6.7	45.6	61.7
Canola	60.3	28.5	7.8	55
Lard	41.9	13.7	40.9	63.6
Yellow grease	48.8	15.8	27.9	52.9
Linseed	20	73	7	52
Wild mustard	59.1	27.2	3.6	61.1
Waste palm oil	44.1	10.7	44.3	60.4
Palm	46.4	8.9	44.7	61
Olive	76	8.4	15.6	57
Peanut	55.7	28.7	15.6	53
Rape	65.3	28.3	6.5	55
Soybean	25.6	59.1	15.3	49
Sunflower	25.6	63.3	11.1	50
Grape	19.1	69.4	11.3	48
H.O. Sunflower	62.9	27.6	9.3	53
Corn	66.4	25.3	8.1	53
Almond	77.6	8.4	13.9	57
Apocynaceae Ervatamia coronaria Stapf	50.9	16.4	32.5	56.33
Cannabinaceae Cannabis sativa Linn	15	80	0	36.4
Combretaceae Terminalia bellirica Roxb	24	31	35	56.24
Corylaceae Corylus avellana	88	2.9	8.9	54.5
Aleurites moluccana Wild	10.5	77	12.2	34.18
Euphorbia helioscopia Linn	18.8	64.8	19.3	34.25
Perilla frutescens Britton	9.8	83.7	0	30.09
Litsea glutinosa Robins	2.3	0	96.3	64.79
Magnoliaceae Michelia champaca Linn	29.2	42.5	25.8	50.28
Rosaceae Princepia utilis Royle	32.6	43.6	22.4	48.94
Simaroubaceae Quassia indica Nooleboom	36	48	9	46.74
Sterculaceae Pterygota alata Rbr	44	32.4	23	51.09
Ulmaceae Holoptelia integrifolia	55.2	0	44.2	61.22

Appendix B

Some Model Performances With One Input To Predict Cetane Number

Model Name	Input	R^2	RMSE
MLP#1	∑MUFAMs	0.0153	10.4066
MLP#2	∑PUFAMs	0.6169	6.5181
MLP#3	∑SFAMs	0.4181	8.0070
RBFNN#1	∑MUFAMs	0.2987	8.8062
RBFNN#2	∑MUFAMs	0.6459	6.2417
RBFNN#3	∑MUFAMs	0.4579	7.7257
ME#1	∑MUFAMs	0.0078	10.4462
ME#2	∑MUFAMs	0.0565	10.1863
ME#3	∑PUFAMs	0.6270	6.4048
ME#4	∑PUFAMs	0.6277	6.3992
ME#5	∑SFAMs	0.4195	7.9899
ME#6	∑SFAMs	0.0048	7.9735

Appendix C

Some Model Performances With Two Input To Predict Cetane Number

Model Name	Input	R^2	RMSE
MLP#4	∑MUFAMs, ∑SFAMs	0.7079	5.7526
MLP#5	∑MUFAMs, ∑PUFAMs	0.6707	6.0516
MLP#6	∑PUFAMs, ∑SFAMs	0.6264	6.4513
RBFNN#4	∑MUFAMs, ∑SFAMs	0.6678	6.0784
RBFNN#5	∑MUFAMs, ∑PUFAMs	0.7528	5.3128
RBFNN#6	∑PUFAMs, ∑SFAMs	0.6711	6.0644
ME#7	∑MUFAMs, ∑SFAMs	0.7001	5.7841
ME#8	∑MUFAMs, ∑SFAMs	0.7086	5.7041
ME#9	∑MUFAMs, ∑SFAMs	0.7145	5.6471
ME#10	∑MUFAMs, ∑SFAMs	0.7170	5.6213
ME#11	∑MUFAMs, ∑PUFAMs	0.7039	5.7467
ME#12	∑MUFAMs, ∑PUFAMs	0.7198	5.5932
ME#13	∑MUFAMs, ∑PUFAMs	0.7058	5.7288
ME#14	∑MUFAMs, ∑PUFAMs	0.7205	5.5860
ME#15	∑PUFAMs, ∑SFAMs	0.7040	5.7460
ME#16	∑PUFAMs, ∑SFAMs	0.9880	5.5945
ME#17	∑PUFAMs, ∑SFAMs	0.7039	5.7472
ME#18	∑PUFAMs, ∑SFAMs	0.7221	5.5701

Appendix D

Some Model Performances With Three Inputs To Predict Cetane Number

Model Name	Input	R^2	RMSE
MLP#7	∑MUFAMs, ∑PUFAMs, ∑SFAMs	0.6491	6.2783
RBFNN#7	∑MUFAMs, ∑PUFAMs, ∑SFAMs	0.6986	5.8251
ME#19	∑MUFAMs, ∑PUFAMs, ∑SFAMs	0.7041	5.7451
ME#20	∑MUFAMs, ∑PUFAMs, ∑SFAMs	0.7215	5.5766
ME#21	∑MUFAMs, ∑PUFAMs, ∑SFAMs	0.7213	5.5784
ME#22	∑MUFAMs, ∑PUFAMs, ∑SFAMs	0.7294	5.4981

Appendix E

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