# Selection of Best Neural Network for Estimating Properties of Diesel-Biodiesel Blends

JATINDER KUMAR, AJAY BANSAL
Department of Chemical and Bio Engineering
Dr B R Ambedkar National Institute of Technology
Jalandhar-144011 Punjab
INDIA

*Abstract:* - Soybean oil was transesterified with methanol in the presence of alkaline catalyst to produce methyl esters commonly known as biodiesel. Biodiesel and diesel blends were prepared and tested in laboratory for flash point, fire point, viscosity and density. Seven neural network architectures, three training algorithms along with ten different sets of weight and biases were examined to predict the above-mentioned properties of diesel and biodiesel blends. The best suited neural network and training algorithm were selected and further generalized to improve its performance by using early stopping technique. The results showed that the neural network having an architecture 2-7-4 with Levernberg-Marquardt algorithm gave the best estimate for the properties of diesel-biodiesel blends.

*Key-Words:* - Biodiesel, Transesterification, Artificial Neural Network, Flash point, Fire point, Viscosity, Density.

## 1 Introduction

Increasing demand of diesel has forced the scientists and researchers to look for an alternative source, which should be having properties similar to that of usual diesel but with little or negligible contribution to the environment pollution and without necessitating a change in the specification of the engine. The biodiesel, having the advantage of being potential renewable source of energy, is known to be non toxic, eco-friendly (leading to lesser $CO_2$, CO, $NO_X$ emissions compared to commercial diesel), easy to store and to transport and has better lubricity properties [1]. However, it has the disadvantages of high cost compared to petroleum diesel, reduced cold flow properties, detergent characteristics in fuel tank may block fuel ways in the fuel injection system and high viscosity may affect the atomization process in the engine [2]. Biodiesel is completely miscible with diesel oil, thus allowing blends of diesel and biodiesel in any percentage, which may be used in any diesel engine without modifying engine specifications [3]. The various properties of blends like flash point, fire point, viscosity and density are of immense importance for the selection of any blend as an alternate to diesel as they affect the transportation, storage, handling, atomization and combustion. In present work, soybean oil was transesterified with methanol in the presence of alkaline catalyst to produce biodiesel [4-7].

The properties of biodiesel depend on many factors e.g. source of feedstock, method of esterification etc. and being significantly different from diesel, require a prior estimation before application to a particular combustion system [8-9]. As such a blend of diesel and biodiesel in a specified proportion will have different properties than either of pure diesel or biodiesel [10]. It may not always be convenient to make experimentation every time while switching over from one blend to another. Any tool helpful in estimation of these properties without experimentation can be of immense

utility and Artificial Neural Network (ANN) approach can be answer to the problem.

An artificial neural network has its origin in efforts to produce a computer model of the information processing that takes place in the nervous system [11-13]. In many applications, including the present work, the biological relevance of neural networks to nervous system function is unimportant. Rather, a neural network may simply be viewed as a highly parallel computational device. Neural network has shown to be useful in a variety of tasks including solving certain optimization problems and pattern recognition [14-16]. Selection of a neural network to a specific problem depends upon the network topology -that is, the number of layers, the size of each layer, and the pattern of connections and the assignment of connection strengths to each pair of connected units and of threshold to each unit [17-18]. In present work, seven neural network architectures, three training algorithms along with ten different sets of weight and biases were examined to predict the properties of diesel and biodiesel blends.

# 2 Problem Formulation

In the present study the biodiesel was prepared in the laboratory and the properties of its blends were experimentally measured. A set of seven ANNs with different training algorithms, weights and biases were used to select the ANN to give the best estimation of properties of diesel-bidiesel blends. The materials and methods used are as follows:

## 2.1 Materials

Refined soybean oil was procured from Amrit Banaspati Corporation Ltd, Rajpura, Punjab, India. Methanol (LR grade) with 99% purity was purchased from Loba Chemie Pvt. Ltd, Mumbai, India. Sodium Hydroxide pellets (LR grade) with 97% purity were purchased from S.D. Fine Chem Ltd, Mumbai, India. Commercial diesel was procured from the retail outlet of Indian Oil Corporation Limited, India. The Redwood viscometer was used for the measurement of viscosity. The flash point and fire point were measured with the help of Pensky –Marten Apparatus. The specific gravity bottle was used to measure density.

## 2.2 Preparation of Biodiesel

Biodiesel was prepared from soybean oil by the trans-esterification process, using methanol, in the presence of basic catalyst (NaOH). 900 gm of soybean oil was taken in the cleaned three-necked-round-bottom flask of capacity of 2.5 liters. A solution of sodium methoxide containing 5 g of NaOH and 250 ml of methanol was prepared separately in a beaker. The sodium methoxide mixture and oil were preheated to 65$^{o}$C separately. The reaction was started when both oil and sodium methoxide were mixed at 65$^{o}$C and it was continued for 1 hr. The reaction temperature was maintained at 65$^{o}$C throughout the process. Due to the presence of two distinct layers of methanol and oil and to have the proper contact between the phases, the mixture was continuously stirred with the help of a stirrer. To minimize the evaporation losses, the total reflux condenser was used. The resulting solution was allowed to stand for 18 hrs in a separating funnel. Two distinct layers were formed. Glycerol settled in the bottom layer and was separated as a by-product and then excess methanol was separated by distillation. The remaining solution was then washed twice with brine solution water and then kept in the separating funnel overnight. Biodiesel was then separated from water layer and collected in a bottle containing activated alumina gel to absorb the moisture present in biodiesel prepared. Different blends were made from the biodiesel and diesel with varying composition. The flash point and fire point were measured using Pensky-Marten Apparatus. The viscosity was measured using Redwood viscometer and

**Table 1 Experimental values of properties of various blends of diesel and biodiesel**.

| Blends | | Flash Point (°C) | Fire Point (°C) | Viscosity (cSt) | Density (g/ml) |
|---|---|---|---|---|---|
| Biodiesel (% v/v) | Diesel (%v/v) | | | | |
| 00 | 100 | 55.4 | 63.0 | 5.27 | 0.8424 |
| 10 | 90 | 55.6 | 66.0 | 6.21 | 0.8459 |
| 20 | 80 | 56.0 | 66.2 | 7.12 | 0.8504 |
| 30 | 70 | 57.2 | 67.0 | 7.40 | 0.8545 |
| 40 | 60 | 58.0 | 69.0 | 7.76 | 0.8583 |
| 50 | 50 | 59.0 | 70.0 | 8.25 | 0.8617 |
| 60 | 40 | 60.1 | 71.2 | 8.93 | 0.8666 |
| 65 | 45 | 61.7 | 73.3 | 9.52 | 0.8692 |
| 70 | 30 | 63.2 | 75.3 | 10.16 | 0.8720 |
| 75 | 25 | 66.4 | 78.2 | 10.41 | 0.8743 |
| 80 | 20 | 70.0 | 81.0 | 10.53 | 0.8746 |
| 85 | 15 | 71.2 | 82.3 | 10.81 | 0.8765 |
| 90 | 10 | 72.0 | 83.2 | 11.07 | 0.8790 |
| 95 | 05 | 76.2 | 85.2 | 11.38 | 0.8819 |
| 100 | 00 | 80.0 | 87.0 | 11.63 | 0.8847 |

calibrated specific gravity bottle was used to measure density. The values of different properties for various blends are shown in Table 1.

## 2.3 Neural Network Formulation

Seven numbers of neural networks having different architecture as shown in Table 2 were used. They were trained using three training algorithms i.e. Batch Gradient Descent with Momentum, Levenberg-Marquardt and Scaled Conjugate Gradient. The each algorithm with ten different sets of weights and biases was used to train each neural network for 1000 epochs using experimental values of properties as training data.

**Table 2 Different Neural Network used**

| Neural Network | Architecture |
|---|---|
| NN1 | 2-1-4 |
| NN2 | 2-2-4 |
| NN3 | 2-3-4 |
| NN4 | 2-4-4 |
| NN5 | 2-5-4 |
| NN6 | 2-6-4 |
| NN7 | 2-7-4 |

The goal (Overall Mean Square Error) was used to evaluate the performance of each neural network. The combination of neural network architectures, training algorithms, weights and biases with minimum goal was selected as the desired neural network. In order to check its validity the blend properties of fresh samples were predicted using selected neural network and compared with the experimentally measured. The selected neural network was further generalized using early stopping technique to enhance its performance and was further used to predict the properties of diesel and biodiesel blends.

## 3 Problem Solution

Table 3 summarizes the results of three different training algorithms for seven different neural network architectures. Each entry in the table represents ten trials with different initial weights and biases for 1000 epochs. The results show that the best combination of architecture and training algorithm for the present problem is NN7

**Table 3 Performance of different training algorithms**

| Algorithm | Overall Mean Square Error | | | | | | |
|---|---|---|---|---|---|---|---|
| | NN1 | NN2 | NN3 | NN4 | NN5 | NN6 | NN7 |
| Gradient Descent with Momentum | 13.672 | 30.224 | 23.3692 | 17.6159 | 8.70043 | 20.0793 | 16.6763 |
| Levenberg-Marquardt | 0.697215 | 0.364251 | 0.422187 | 0.512105 | 0.364263 | 0.364251 | 0.214461 |
| Scaled Conjugate Gradient | 3.53512 | 0.697979 | 0.797517 | 0.626841 | 0.70673 | 0.495826 | 0.456815 |

**Table 4 Comparison between predicted and actual properties**

| Blend | | Flash Point (°C) | | Fire Point (°C) | | Viscosity (cSt) | | Density (g/ml) | |
|---|---|---|---|---|---|---|---|---|---|
| Biodiesel (%v/v) | Diesel (%v/v) | Actual | Predicted | Actual | Predicted | Actual | Predicted | Actual | Predicted |
| 25 | 75 | 56.5 | 56.0 | 66.3 | 66.2 | 7.29 | 7.12 | 0.8523 | 0.8504 |
| 35 | 65 | 57.8 | 57.2 | 67.2 | 67.0 | 7.57 | 7.40 | 0.8563 | 0.8545 |
| 45 | 55 | 58.5 | 58.0 | 69.4 | 68.9 | 8.09 | 7.78 | 0.8594 | 0.8586 |
| 55 | 45 | 59.5 | 61.6 | 70.8 | 73.3 | 8.56 | 9.53 | 0.8640 | 0.8689 |

(2-7-4) and Levenberg-Marquardt respectively having minimum overall mean square error of 0.21. On the average, it is almost 1.7 times better than the next best combination of architecture and algorithm i.e. NN2 (2-2-4) and Levenberg-Marquardt respectively in terms of goal (overall mean square error). Figure 1 shows the comparison between Levenberg- Marquardt and Scaled Conjugate Gradient training algorithms.

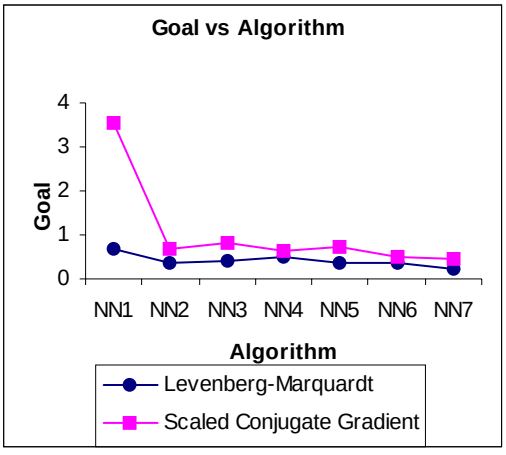


**Fig.1 Comparison of training algorithms**

It is very clear that the curve follows a zig-zag path indicating that error does not decrease linearly with the number of neurons in the hidden layer. Table 4 indicates the comparison between the values predicted by best neural network (i.e. NN7 having best combination of neural network architecture, training algorithm, weights and biases) and the actual values found by laboratory experiments for different blends. It was found that the selected combination gives an overall mean square error of 1.57. Table 5 shows the mean square error for individual properties.

**Table 5 Mean Square Error in prediction**

| Property | Mean Square Error |
|---|---|
| Flash point | 1.30 |
| Fire point | 1.65 |
| Viscosity | 0.27 |
| Density | 8.08E-06 |

After generalizing the selected network by early stopping technique, it was found that overall mean square error is reduced to 0.92.

**Table 6 Mean Square Error after Generalization.**

| Property | Mean Square Error |
|---|---|
| Flash point | 0.16 |
| Fire point | 0.74 |
| Viscosity | 0.02 |
| Density | 5.54E-06 |

Table 6 provides the information about mean square error for individual properties after generalization of the selected neural network. It is clear that the overall and individual mean square error is

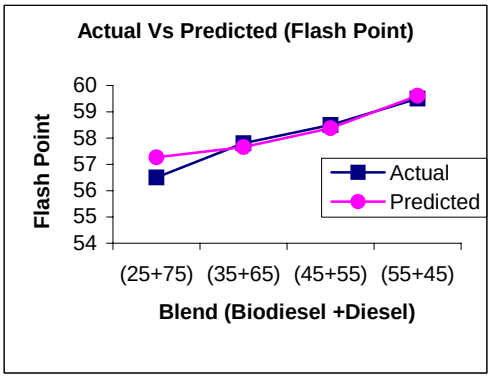


**Fig. 2 Parity plot for flash point**

comparatively much less in case of generalized neural network.
Figure 2, 3, 4 & 5 shows the comparison between the experimental and predicted flash point, fire point, viscosity and density respectively in case of generalized neural network.

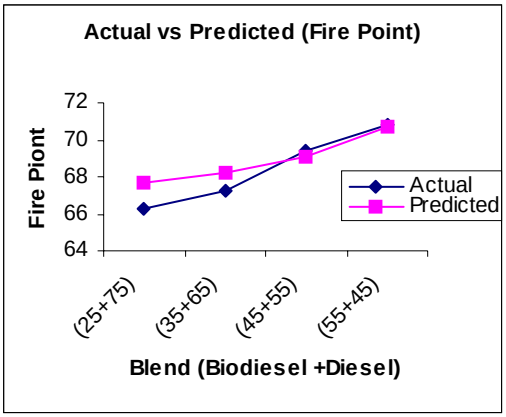


**Fig.3 Parity plot for fire point**

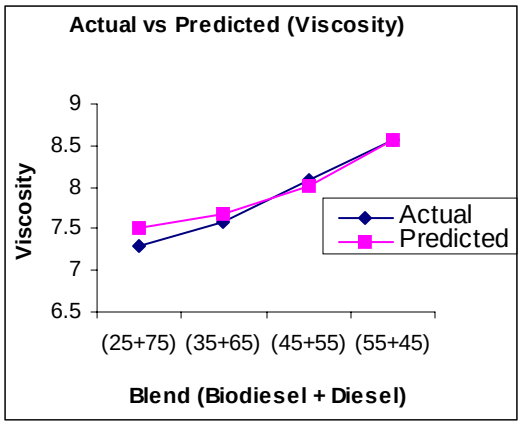


**Fig.4 Parity plot for viscosity**

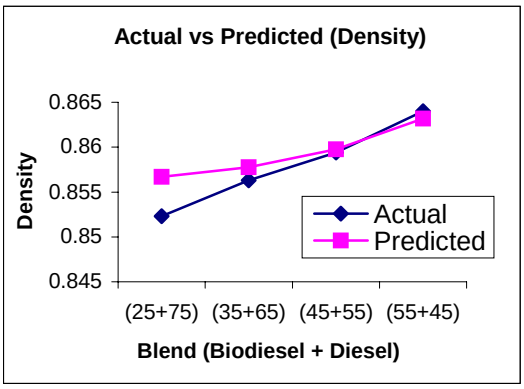


**Fig.5 Parity plot for density**

It is obvious from these graphs that there is a little difference between the experimental and predicted values of the properties

## 3 Conclusions

The generalized NN7 having an architecture 2-7-4 with Levernberg-Marquardt algorithm gives an overall mean square error of the 0.92 in the prediction of properties of diesel and biodiesel blends, which can be considered negligibly small and acceptable. Further, it is clear from figure 2, 3, 4 and 5 that the predicted and experimental values of the properties also have negligibly small error. Therefore, it can be inferred that the neural network NN7 (2-7-4) along with Levernberg-Marquardt algorithm can be relied upon to predict the above-said properties of blends of diesel and biodiesel. However,it is recommended that the Neural Network

should be extended to predict the other properties of the diesel and biodiesel blends like cetane number, pour point, cloud point etc. The performance of neural network may further be improved by adjusting the other training parameters like goal, epochs, learning rate, magnitude of the gradient etc.

*References:*


[1] Saka S. and Kusdiana D., Biodiesel Fuel from Rapeseed Oil as Prepared in Supercritical Methanol, *Fuel*, Vol. 80, 2001,pp.225-31.

[2] Graboski, M. S. and McCormick R.L., Combustion of Fat and Vegetable Oil Derived Fuels in Diesel Engines, *ProgEnergy Comust. Sci*., Vol. 24, 1998,pp125-164.

[3] Zhang, Y. ,Emissions and Combustion of Fatty Acid Esters of Soybean Oil in a Diesel Engine, *M. S. Thesis, Iowa State University*, 1994.

[4] Hideki F., Biodiesel Fuel by Transesterification of Oils, *Journal of bioscience and bioengineering*, 92,2001,pp. 405-416.

[5] Kinney A. J. and Clemente T.E.,Modifying Soyabean Oil Enhanced Performance in Biodiesel Blends, *Fuel Processing Technology*,Vol. xx , 2004, pp. 234-242.

[6] Hak-Joo Kim, 2004 Trans-esterification of Vegetable Oil Biodiesel Using Heterogeneous Catalyst, *Catalyst Today*, Vol. 93, 2004, pp. 315-320.

[7] Weiliang Cao , Preparation of Biodiesel from Soyabean Oil using Supercritical Methenol and Co-Solvent, *Fuel*, Vol 84, 2005, pp 347-351.

[8] Kalam M. A., and Masjuki H., Biodiesel from Palmoil – An Analysis of Its Properties and Potential, *and Bioenergy* , Vol. 23, 2002, pp.471- 479.

[9] Mohamad I., and Al- Shyoukh Ali O., Experimental Evaluation of The Transesterification of Waste Palm Oil into Biodiesel, *Biosource Technology* , Vol. 85, 2002, pp. 253-254.

[10] Violeta H., Solubility of Multi-Component Biodiesel Fuel Systems, *Biosource Technology*,Vol. 96, 2005, pp 611-616.

[11] Heeb D., *The organization of behavior* Wiley, New York 1949.

[12] Rosenblatt F., *Principles neurodynamics*, Spartan New York, 1962.

[13] Howard H. and Martin K,Protein Secondary Structure Prediction with Neural Network,*Proc. NatlAcad.Sci.USA*,Vol.86, 1989, pp.152-156.

[14] Mukherjee et. al., Cell Prediction of Bacillus through Artificial Neural Network at Simultaneous Multiple Variation in Concentration of Nutrients in Media *Proceedings of Indian Chemical Engineering Congress and 56$^{th}$ Annual Session of Indian Institute of Engineers*, 2003,pp. 16-17.

[15] Espinosa G. and Yaffe D. and Cohen Y. , Neural Network based Quantitative Structural Relations (QSPRs) for predicting Boiling Points of Aliphatic Hydrocarbons, *J.Chem.Inf .Comput Sci*.,Vol. 40, 2000, pp. 859-879.

[16] Rosa M. G. and Cesar H., Improving Artificial Neural Networks with a Pruning Methodology and Genetic Algorithms for their Applications in Microbial Prediction of Food, *Journal of Food Microbiology*, Vol. 72, 2002, pp.19-30.

[17] Jacek M.Zurada, 2003, Introduction to Artificial Neural Systems. *Publishing House*, 2003, pp.163-248.

[18] Venktasubramanian, V. and Vaidyanathan R., Fault Detection and Diagonosis using Neural Networks, *Computer Chem Engg*.,Vol 14, 1990, pp. 699-712.