Fatty Acid Composition of Some Seed Oils from Arid Zone of Rajasthan and their Iodine Values for Scope in Biodiesel Production using ANN Technique

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ABSTRACT
The Arid Zone of Rajasthan is a vast reservoir of desert plants. The seed oil is an important product obtained from the wild plants. The fatty acid composition of seed oil is a key point to determine the application of oil in a specific field. The properties of seed oils of eight plants from Arid zone of Rajasthan like fatty acid composition, saponification value, iodine value, viscosity, flash point, fire point, cloud point and pour point were determined by usual analytical methods. The Artificial Neural Network was applied to predict the relative significance of fatty acid composition of vegetable oil affecting the biodiesel properties. Iodine value predicted from ANN was found to be nearly the same as determined by analytical methods. It was concluded that the results predicted from ANNs were more precise as compared to the linear regression model. The effects of input variables show quantitative effect on seed oil properties.

Keywords
Seed oil, Bio diesel, Fatty acid composition, Iodine value, ANN.

1. INTRODUCTION
About 19.61 million hectares in Rajasthan, is arid zone, which is 61% of the total arid zone of India. The climate, soils, vegetation, animals, life styles and activities of people are diverse in these areas which is in contrast to other deserts of the world. About 628 species belonging to 87 botanical families are found in this region [1].

The seed oil is an important natural product obtained from almost all seed bearing plants, although the amount may vary from traces to 35-40 % by weight of the seed. The seed oils are being used by human population in domestic as well as industrial purposes since ancient times. One of the recent applications is the use of seed oil to produce biodiesel which is promising aspect. It is effective to reduce the demand supply gap of motor fuels especially from the wild growing unexploited plants.

Some adverse effects of fossil fuels and limited supply created a need for alternative fuel. This alternative fuel should have similar properties and area of applications to that of fossil fuel but should not pollute the environment and should be renewable. Biodiesel fulfills all the above requirements. It produces lower amounts of CO_2, CO, SO_2 as compared to petroleum biodiesel. It can be stored and transported easily. It has similar characteristics of diesel. So we can say that biodiesel is non toxic, environment friendly and convenient fuel [2-5].

In the vegetable oils, the alkyl esters of long chain fatty acids are present as triglycerides. These fatty acids are transesterified with short chain alcohols into biodiesel. Methanol and ethanol are frequently used alcohols. Since ethanol is obtained from waste biological material and being renewable and eco friendly, so it is more effective for transesterification.

The process of storage, transport and combustion is affected by the properties of fats and oils [2]. These are saponification value, iodine value, viscosity, flash point, fire point, cloud point; pour point etc. The chemical properties are predicted from its fatty acid profile i.e. the relative abundance of saturated, unsaturated polyunsaturated short or long chain fatty acid methyl esters in the seed oil. When seed oil is applied as a raw material for biodiesel, then the chemical composition of seed oil as well as the physical properties should be studied. By keeping these points in mind the scope of seed oil for biodiesel can be predicted [6, 7].

The important parameter for quality of diesel is cetane number. The cetane number of bio diesel derived from vegetable oil depends upon the fatty acid distribution of original oil. The biodiesel developed from long chain saturated fatty acid have high cetane number that of short chain or unsaturated ones [8].

There is a high regression between density and viscosity values of vegetable oil methyl esters. The viscosity is correlated with density of oil. The high heating value of a fuel is related with iodine value, saponification value and flash point [9]. The viscosity of biodiesel increases with increase in saturation. In this manner we can correlate the physicochemical characteristics of seed oil with the fuel properties of biodiesel generated from the oil.

2. PROPOSED TECHNIQUE
The above predictions have some limitations. It is quite difficult to compare such a large number of parameters and to develop a consolidated result. This type of short comes generate the requirement of some artificial intelligent system to produce results. Due to the above limitations in the prediction of results it is quite difficult to compare the properties.

The Artificial Neural Network is one of the AI methods, applied in a number of fields related to Chemistry; hence in this paper the attempt was made to train the ANN by analytical values to resolve the above mentioned problems.

ANN is the collection of small individually interconnected processing units. The information is passed between the processing units with interconnection weights. Some past data

are used to train the ANN with respect to that set data till network learning. It is very useful technique to predict and optimize the properties and impact of biodiesel.

ANN has been employed to predict biodiesel properties like heating value, cetane number from fatty acid compositions of various vegetable oils.

The present study is based on collection of seeds, extraction of oil and determination of various physico chemical characteristics and prediction of Iodine values for scope as biodiesel properties using ANN technique [10, 11].

ANNs are composed of simple parallel connected elements operating at the same time to compute the fast calculation. ANNs are trained by different algorithms to perform a particular function by adjusting the values of the connections, or weights, between elements until a particular input leads to a specific output. ANN operates like a 'black box' or nonlinear model. It does not require detailed information about the system being tested. Instead, it learns the relationship between the input parameters and the controlled and uncontrolled variables by studying previously recorded data, similar to the way a non-linear regression might perform. Another advantage of using an ANN is its ability to handle large and complex data with many inter-related parameters. Moreover, it predicts quite well even if the sample size is small [12].

The ANN consists of three types of layers: input layer, hidden layer, and output layer. These three layers are connected with each other. The input layer receives the input data outside the network and sends them to the hidden layer. The hidden layer contains interconnected neurons for recognition of patterns and the relevant information interpretation by adjusting the weights on the connections. Afterwards, the results from the hidden layer are sent to the output layer for the outputs.

All of the variables in the neuron can be continuous or discrete. The only defined value range in a neuron is the output which normally ranges from -1 to +1, but may have a different range if desired. Mathematically, for a layer of m neurons and neuron of index j and iteration n, the neuron can be defined as:

$$y_j(n) = \varphi_j(v_j(n)) \tag{1}$$

Where $y_j(n)$ the output of the current neuron is, φ_j is the activation function, and $v_j(n)$ is defined as:

$$v_j(n) = \sum_{i=1}^{m} w_i(n) y_i(n) + b \tag{2}$$

Where $y_i(n)$ is an output from a previous layer i, and $w_i(n)$ is the weight that connects the input to the neuron of index j.

The neurons contain several functions and variables including weights, non-linear transfer functions, methods to add up all inputs and bias values. The sum of all products of all the inputs multiplying the weights and the bias values passes through a non-linear transfer function as the output of each neuron. The basic concept of ANN is shown in Fig. 1.

The activation or transfer function determines the network output. Commonly used transfer functions are 'tansig', 'logsig' and 'purelin'. The log-sigmoid transfer function is given by

$$f(x) = \frac{1}{1+e^{-x}} \tag{3}$$

This form of the function keeps its output in the range of (0, 1) as the net input goes from $-\infty$ to $+\infty$. The general form of tangent sigmoid function is given by

$$f(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}} \tag{4}$$

And the 'purelin' function is given by

$$f(x) = x \tag{5}$$

In this study, the Back propagation ANN model was developed using MATLAB 2010 software for predicting the one of the important property of biodiesel i.e. Iodine Value as a function of fatty acid content. To evaluate the accuracy of the ANN predictions, the values predicted by ANN are plotted and compared with the straight line corresponding to the actual experimental data. The analysis has been restricted to a single hidden layer network since this is capable of mapping all data.

3. EXPERIMENTAL SETUP

A detailed literature and field survey was done in various regions of Rajasthan. The selected plants were identified and their seeds were collected. Seeds were dried and grounded. The oil was extracted by solvent extraction using petroleum ether.

The various physicochemical characteristics were determined according to AOCS methodology [13-18].

The fatty acid composition was determined by Gas Liquid Chromatography of methyl esters of seed oils. The data's obtained from analysis were used to train ANN.

The fatty acid composition and iodine values of eight seed oils were used to train the neuron.

Table 1. Introduction of plants

Sp.	Botanical Name	Common Name	Family
1	*Moringa oleifera*	Drum stick	Moringaceae
2	*Calotropis gigantean*	White aak	Asclepiadaceae
3	*Calotropis procera*	Aak	Asclepiadaceae
4	*Pergularia damea*	Gadaria re bel	Asclepiadaceae
5	*Jatropha curcus*	Ratanjot	euphorbiaceae
6	*Pongamia pinneta*	Karanj	leguminoceae
7	*Brassica nigra*	Black mustard	brassicaceae
8	*Glycine max*	soybean	leguminoceae

Table 2. Component fatty acids of seed oils

Sp. No.	14:0	16:0	18:0	18:1	18:2	18:3	20:0	20:1
1	-	-	4.56	56.16	19.53	17.03	2.65	-
2	0.90	36.35	11.95	12.10	29.57	2.9	5.6	-
3	-	16.43	-	2.60	77.27	3.7	-	-
4	11.6	1.68	0.60	51.6	31.63	2.52	0.34	0.11
5	-	14.9	9.5	40.5	34.7	0.3	-	-
6	-	11.6	7.5	51.6	16.6	-	-	-
7	-	2.0	2.0	18.0	13.0	8.0	-	-
8	-	13.9	2.1	23.2	56.2	4.3	-	-

Table 3. Physico chemical characteristics of seed oils

Sp. no.	Oil content (%)	Saponification Value (mg KOH/g oil)	Iodine Value (g Iodine /100 g oil)	Pour point (oC)	Cloud point (oC)	Flash point (oC)	Fire point (oC)	Viscosity (cSt)
1	38.9	252	140	11	10	268.5	288	3.2
2	23.3	270	99	0	2	170	188	4.8
3	30.0	275	189	-5	1	172	190	4.8
4	27.0	293	159	-4	0	165	182	4.5
5	36.0	195	96	-5	-3	170	191	4.6
6	32.0	186	87	-10	-5	160	178	3.9
7	30.0	192	82	0	2	173	195	4.2
8	25.0	195	122	-4	-0.5	131	152	4.3

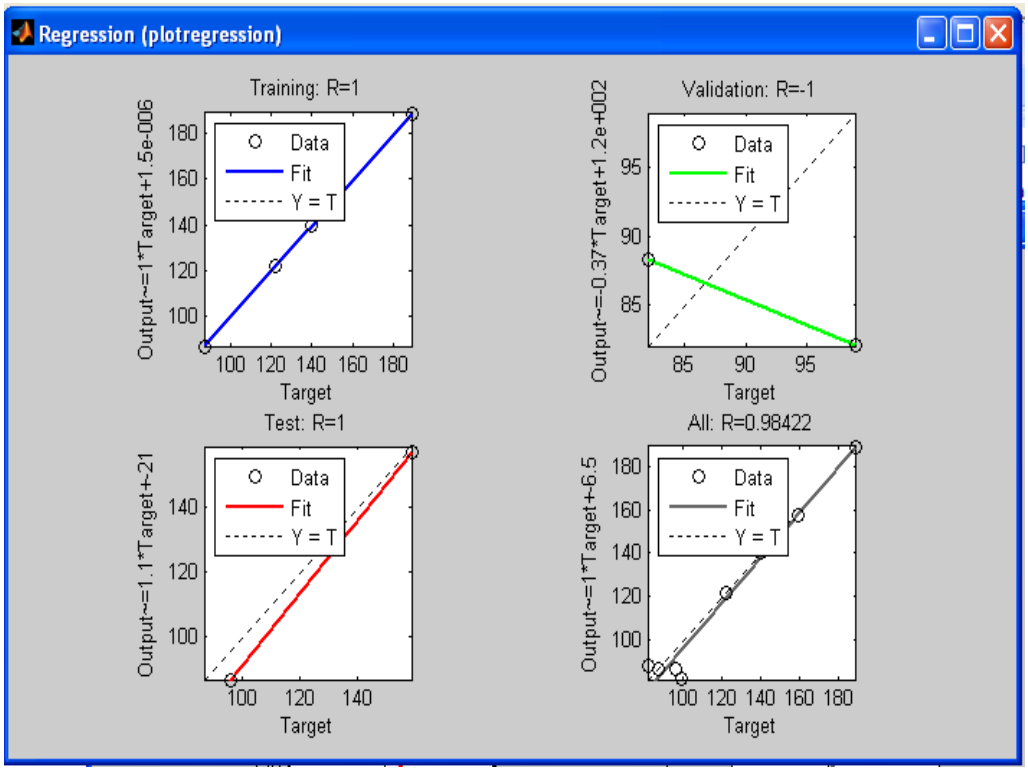

Fig. 1 Regression (Polyregression)

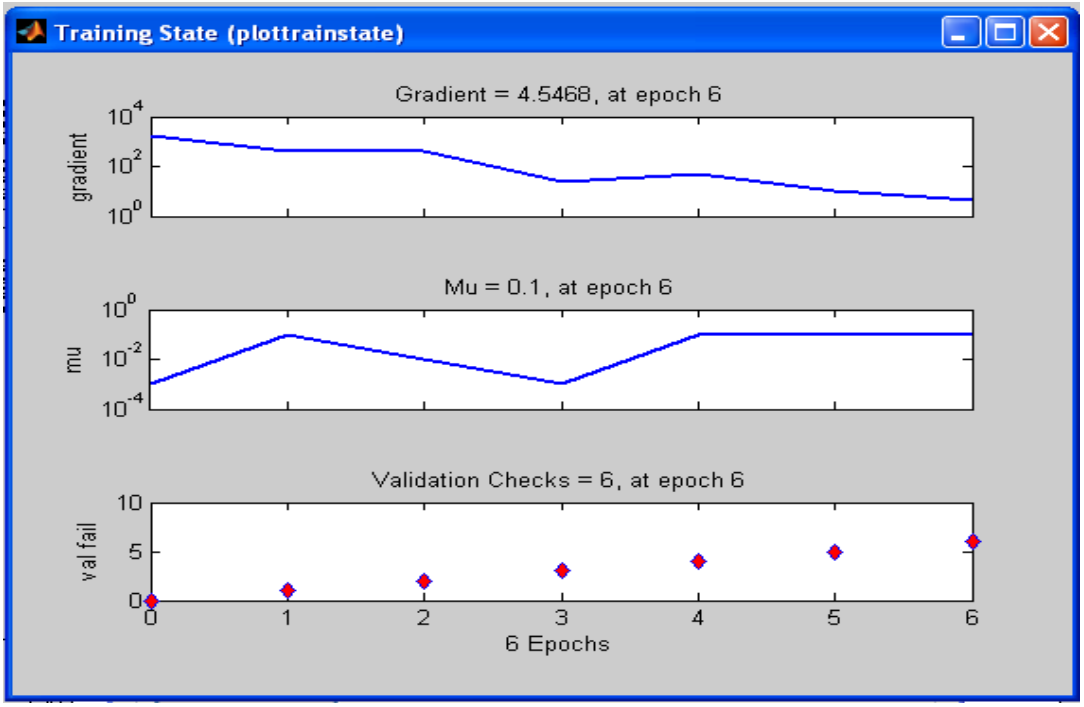

Fig. 2 Training state plot

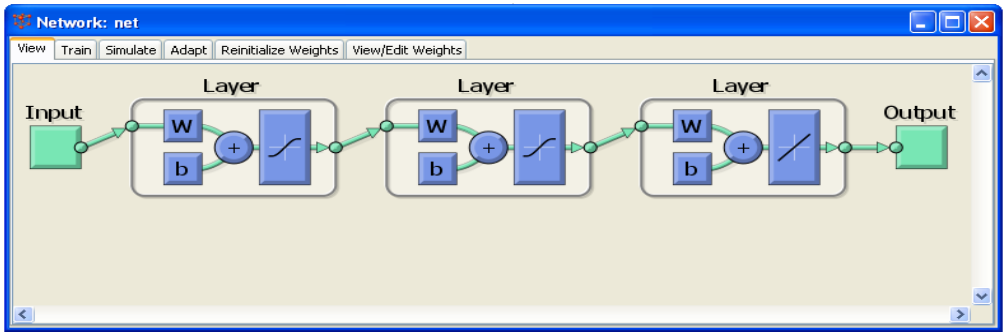

Fig. 3 Neural network for training (1 input layer, 2 hidden layers and 1 output layer)

Table 4. Values of inputs to train neuron

Sp. No.	X1	X2	X3	X4	X5	X6	X7	IV..
1	0	0	4.56	56.16	19.53	17.03	2.65	140
2	0.9	36.35	11.95	12.10	29.57	2.9	5.6	99
3	0	16.43	0	2.60	77.27	3.7	0	189
4	11.68	1.68	.6	51.6	31.63	2.52	0.34	159
5	0	14.9	9.5	40.5	34.7	0.3	0	96
6	0	11.6	7.5	51.6	16.6	0	0	87
7	0	2	2	18	13.0	8.0	0	82
8	0	13.9	2.1	23.2	56.2	4.3	0	122

4. RESULTS AND DISCUSSION

The physicochemical characteristics of seeds and oils are summarized in table 2 and 3. The seed oil of sp.1, 4, 5, 6 and 8 were found to contain rich amount of oleic acid. The seed oil of species 2,3,4,5 and 8 were found to contain linoleic acid in good amounts. Myristic acid was found only in species 4 as 11.68% and in species 2 in traces. The important saturated acid, palmitic acid was found in species 2,3,5,6 and 8. Linolenic acid was also found in almost all reported species. Arachadic acid was found in species 1, 2 and traces in species 4. The iodine values of seed oils obtained by analytical method are given in table 3.The properties related with fuel are also summarized in table 3. The regression obtained from ANN is given in figure 1.It is clear that there is a good regression between fatty acid composition and related Iodine value. Figure 2 represents the details of training state.

5. CONCLUSION AND SCOPE

It is clear from the above study that ANN is an effective tool to predict the property of seed oil by using related data. Obtained value by analytical method and predicted from ANN in effective manner can be correlated by the proposed technique. It has been concluded that the proposed model works very efficiently for the above experiment. By this method the Iodine Value can be predicted very accurately by the fatty acid composition of seed oil. This model would be helpful to predict the other values of biodiesel too.

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