Artificial Neural Networks for the Prediction of Thermo Physical Properties of Diacetone Alcohol Mixtures

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Abstract

A predictive method based on Artificial networks has been developed for the thermophysical properties of binary liquid mixtures of diacetone alcohol with benzene, chlorobenzene and bromobenzene at (303.15,313.15 and 323.15) K. In method 1, a committee ANN was trained using 5 physical properties combined with absolute temperature as its input to predict thermo physical properties of liquid mixtures. Using these data we found out the predicted data for intermediate mole fraction of different systems without conducting experiments. ANN with back-propagation algorithm is proposed, for Multi-pass Turning Operation and developed in MATLAB. Compared to other prediction techniques, the proposed ANN approach is highly accurate and error is <1%.

Keywords: Artificial neural network, Neurons (nodes), Perceptron, Network training, Diacetone alcohol

1. Introduction

In many real world applications, we want our computer to perform complex recognition problems. Since our conventional computers are obviously not suited to this type of field, we therefore borrow features from the physiology has come to be known as Artificial Neural Systems (ANS) Technology or Neural Networks. Artificial neural network is a branch of artificial intelligence (AI) that attempts to achieve human brain like capability. Traditional approaches of solving chemical engineering problems frequently have their limitations, as for example in the modeling of highly complex and nonlinear systems. Artificial neural networks (ANN) have proved to be able to solve complex tasks in a number of practical applications. The utility of artificial neural network models lies in the fact that they can be used to infer a function from observations. This is particularly useful in applications where the complexity of the data or task makes the design of such a function by hand impractical. Because ANN are nets of basis functions, they can provide good empirical models of complex nonlinear processes useful for a wide variety of purposes. The applications of ANN include detection of medical phenomena, stock market prediction, credit assignment, monitoring the condition of machinery and engine management. There are only few reports of using ANN in the prediction of physiochemical properties, these reports have generally been restricted to equilibrium rather than transport properties(John.et.al 1999). It is believed that so far there has been no attempt to truly predict the properties of liquid mixtures across their wide temperature range using ANNs. The present paper presents the findings of a programme of work devoted to the application of ANNs to thermo physical properties of binary mixtures. The thermo physical properties of binary mixtures are found by experimental work done by us. A predictive method based on Artificial Neural Networks (ANN) has been developed for ultrasonic velocity, density, kinematic viscosity, surface tension and refractive index for diacetone alcohol with benzene, chlorobenzene and bromobenzene at (303.15,313.15 and 323.15) K a wide range of mole fraction. The study of various properties like viscosity, refractive index, density, surface tension and ultrasonic velocity for different systems are very important to understand the molecular interaction, purity of compounds. Using these data we found out predicted data for intermediate mole fraction of different systems without conducting experiments.

2. Working procedure

A Neural Network is an interconnected assembly of simple processing elements, *units* or *nodes*, whose functionality is loosely based on the animal neuron. The processing ability of the network is stored in the inter-unit connection strengths, or *weights*, obtained by a process of adaptation to, or *learning* from, a set of training patterns. It has been shown that non linear feed forward neural networks are capable of universal functional approximation and that a single hidden layer is sufficient to uniformly approximate any continuous function Hornic.et.al.(1989). The neurons in a single hidden layer tends to interact globally but in complex functions this interaction makes it difficult to improve the approximation Heykin (1994), Maren .et.al (1990). The brain is principally composed of a very large number (circa 10,000,000,000) of *neurons*, massively interconnected (with an average of several thousand interconnects per neuron, although this varies enormously).

2.1 Artificial neurons

To capture the essence of biological neural systems, an artificial *neuron* is defined as follows:

• It receives a number of inputs (either from original data, or from the output of other neurons in the neural network). Each input comes via a connection that has a strength (or *weight*); these weights correspond to synaptic efficacy in a biological neuron. Each neuron also has a single threshold value. The weighted sum of the inputs is formed, and the threshold subtracted, to compose the *activation* of the neuron

• The activation signal is passed through an activation function (also known as a transfer function) to produce the output of the neuron.
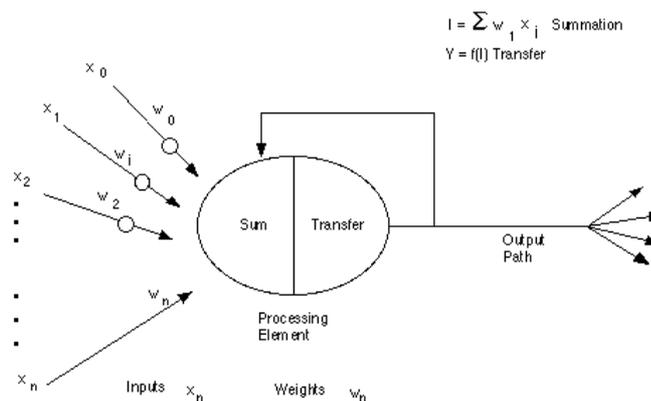

Figure 2.1 A Basic Artificial Neuron.

In Figure 2.1, various inputs to the network are represented by the mathematical symbol, x(n). Each of these inputs is multiplied by a connection weight. These weights are represented by w(n). In the simplest case, these products are simply summed, fed through a transfer function to generate a result, and then output. This process lends itself to physical implementation on a large scale in a small package. The commonest type of artificial neural network consists of three groups or layers of units: input, hidden, and output. The layer of input neurons receives the data either from input files or directly from electronic sensors in real-time applications. The output layer sends information directly to the outside world, to a secondary computer process, or to other devices such as a mechanical control system Necat(2006). Between these two layers can be many hidden layers. These internal layers contain many of the neurons in various interconnected structures. The inputs and outputs of each of these hidden neurons simply go to other neurons.

2.1.1Prediction Of Thermo physical Properties

Step 1: Collect data:

Things to be kept in mind while choosing the input data .

✓   The variables that are influential must be chosen

✓   Numeric and nominal variables can be handled. Convert other variables to one of these forms, or discard.

✓   Hundreds or thousands of cases are required; the more variables, the more cases.

Step 2: Define a network structure

An appropriate network topology is selected. Here for prediction problem, the neural network developed is fully connected feed forward multilayer perceptron. For this problem, the input variables are Temperature and mole fraction.

So, the number of Input nodes is 2. Here, we have to predict the density, kinematic viscosity, ultrasonic velocity, surface tension and refractive index of the systems. Hence, the number of output nodes is 5. After a number of experiments, the transfer function of the hidden layer and the number of epochs are set, the details of which are given below. For example consider a feed forward net with 30 hidden nodes in a single layer.
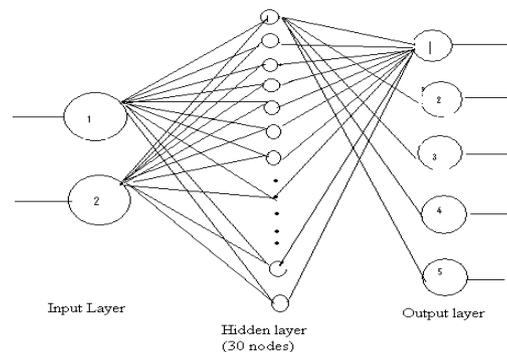

Figure 2.1.1 Feed forward net work

Step   3: Random initialization of weights and biases for the defined network

Step 4: Back propagation learning Mandic (2001), Reilly (1982) algorithm is selected for training the

       network

Step   5: Training parameters are set

       Number of iterations: 600

       Performance goal   : 0

Step   6: Start training

       During training, the input and output data are presented to the network.

Step   7: Termination

       The error for the network is calculated. The error calculation and weight updating process

       continues until the neural network reaches the performance goal or number of iteration.

3. Results and Discussion

Experimental thermo physical property values were extracted from the data base for all the mixtures studied. The list of binary liquid mixtures studied were displayed in Table 1. Input and output variables are listed in Table 2. Random experimental verification of ANN predicted thermo physical properties (not included in the training data) of mixtures with percent standard deviation are listed in Table 3. The thermo

physical properties were density, viscosity, refractive index, surface tension and ultrasonic velocity. The input to the ANN consisted of five thermo physical properties of three binary mixtures at   (303.15,313.15 and 323.15) K . The out put from the ANN consisted of five predicted thermo physical properties of three binary mixtures. A BPN simulator is designed and the input data were fed in. BPN simulator is trained several times using selected data from the collected data, which consists of normal as well as abnormal data. During training, the simulator is presented with both input and output pairs and the error is generated which is the difference between actual and desired output. The error is minimized using the steepest descent technique. When the error obtained is of acceptable value, then the simulator is said to be trained. Then, the data for prediction is presented to the neural network after training. The mean square error is calculated using BP algorithm and the learning curve is plotted between the mean square error and the number of generations (iterations) i.e. epochs. Performance and error graph of the trained committee ANN for the binary systems are presented in Figure 3.1- 3.3 While examining the results of these various neural networks, they were found to be in agreement with the desired results and within permissible error range. The algorithms traingdm or traingd are not producing satisfactory results for the 2 X 20 X 10 X 5 neural network for the maximum epochs of 800 and for a performance goal of 0. The trained algorithm with a single hidden layer with 30 nodes i.e 2 X 30 X 5 neural network.

(Figure2.1.1) is producing the desired result for the prediction of these properties. The predicted values of   other new mole fractions of the mixtures were taken and verified experimentally. The percentage of error is <1.

4. Conclusion

Due to high speed of processing, low consumption of memory, great robustness, possibility of self learning and simple incorporation into chips the approach ensures prediction condition in real time. It provides robust representation clue to the fault-tolerant nature of neural networks. Our future proposal is Extending the proposed idea of ANN prediction to systems at extremely high or low temperatures where conducting of experiments are difficult

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Table 1. Details of the systems studied

Sl.no	systems	Temperatures	Net work topology	Training algorithm
1	Diacetone alcohol + benzene	303.15, 313.15 and 323.15 K	Feed forward multilayer perceptron	Back propagation learning algorithm
2	Diacetone alcohol + chloro benzene			
3	Diacetone alcohol + bromobenzene			

Systems with temperatures, network topology and training algorithm used

Table 2. Input and output variables

Method	
Input	**Output**
Mole fraction	Predicted five thermo physical properties
Experimental five Thermo physical properties	

Input and output of this method

Table 3. Random experimental verification of ANN predicted thermo physical properties (not included in the training data) of mixtures with percent standard deviation.

x_1	T/ K	ρ (pre)	S %	η (pre)	S %	n_D (pre)	S %	σ (pre)	S %	U (pre)	S %
Diacetone alcohol + benzene											
0.1500	303.15	0.8885	0.15	1.1111	0.50	1.4876	0.62	30.10	0.11	622	0.87
0.5000	313.15	0.8821	0.21	1.6724	0.97	1.4517	0.84	24.74	0.45	785	0.99
0.9000	323.15	0.8944	0.71	2.4444	0.82	1.4266	0.41	26.82	0.13	1000	0.21
Diacetone alcohol + chloro benzene											
0.1500	303.15	1.0621	0.14	1.1225	0.29	1.5331	0.65	33.10	0.68	1228	0.99
0.5000	313.15	0.9887	0.24	1.8111	0.88	1.4872	0.98	30.80	0.14	1004	0.00
0.9000	323.15	0.9200	0.47	2.4889	0.68	1.4299	0.67	28.29	0.47	1078	0.14
Diacetone alcohol + bromobenzene											
0.1500	303.15	1.4001	0.54	1.3221	0.21	1.5321	0.18	33.31	0.64	1188	0.31
0.5000	313.15	1.1844	0.11	2.1254	0.31	1.4999	0.00	32.01	0.00	1149	0.22
0.9000	323.15	0.9520	0.44	2.6221	0.12	1.4384	0.00	29.11	0.98	1118	0.31

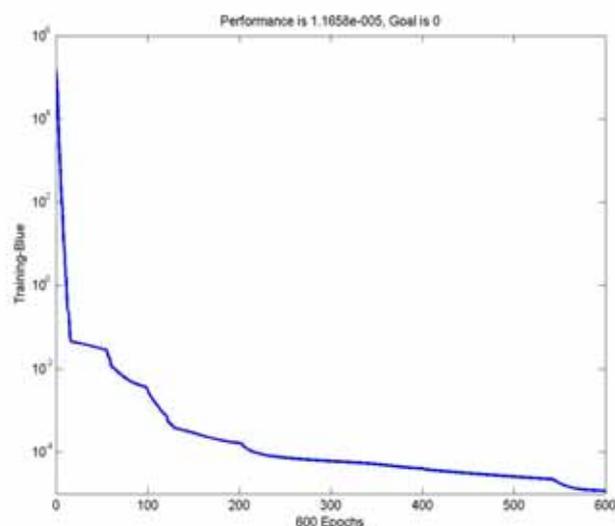Diacetone alcohol with benzene, chlorobenzene and bromobenzene mixtures

Figure 3.1 Plot of error and number of iterations

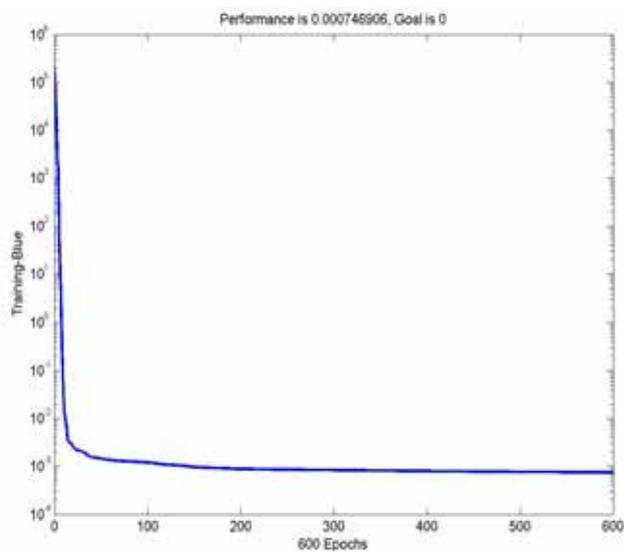Error performance for Diacetone alcohol   + benzene mixture

Figure 3.2 Plot of error and number of iterations

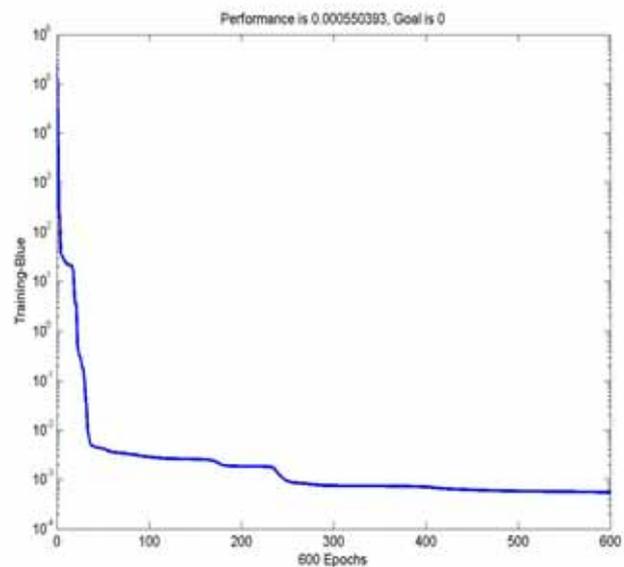Error performance for　Diacetone alcohol　+ chlorobenzene system

Figure 3.3 Plot of error and number of iterations

Error performance for Diacetone alcohol　+ bromobenzene system