THE PREDICTION OF THERMO PHYSICAL PROPERTIES OF DIFFERENT ACETOPHENONE LIQUID MIXTURES USING ARTIFICIAL NEURAL NETWORK

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Abstract: *In this present investigation, a predictive method based on Artificial Neural Networks (ANN) has been developed for the thermo physical properties of different acetophenone binary liquid mixtures at a temperature of 303.15 K and 323.15 K. For this analysis, the binary mixtures a) Acetophenone + n Butylamine, b) Acetophenone + Ethyl chloro acetone, c) Acetophenone + Nitrobenzene, d) Acetophenone + Ethyl cyano acetate has been used. The ANN was trained using 3 physical properties namely density, viscosity, ultrasonic velocity combined with absolute temperature as its input to predict thermo physical properties. 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, thermo physical properties, Acetophenone, MATLAB, viscosity, density, ultrasonic velocity.*

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1. INTRODUCTION

1.1. Artificial Neural Network (ANN)

An artificial neural network (ANN), often just called a "Neural Network" (NN), is a mathematical model or computational model based on biological neural networks. It consists of an interconnected group of artificial neurons and processes information using a connectionist approach to computation. In most cases an ANN is an adaptive system that changes its structure based on external or internal information that flows through the network during the learning phase. In more practical terms neural networks are non-linear statistical data modeling tools. They can be used to model complex relationships between inputs and outputs or to find patterns in data. A neural network is an interconnected group of nodes, akin to the vast network of neurons in the human brain.

1.2. Definition

An artificial neural network (ANN) is an information processing paradigm that is inspired by the way biological nervous systems, such as the brain, process information. ANN has some different names which are:

1) Connectionist model
2) Parallel distributed processing model
3) Natural intelligent systems
4) Neuron computing
5) Machine learning algorithm

1.3. Steps involved in the software simulation

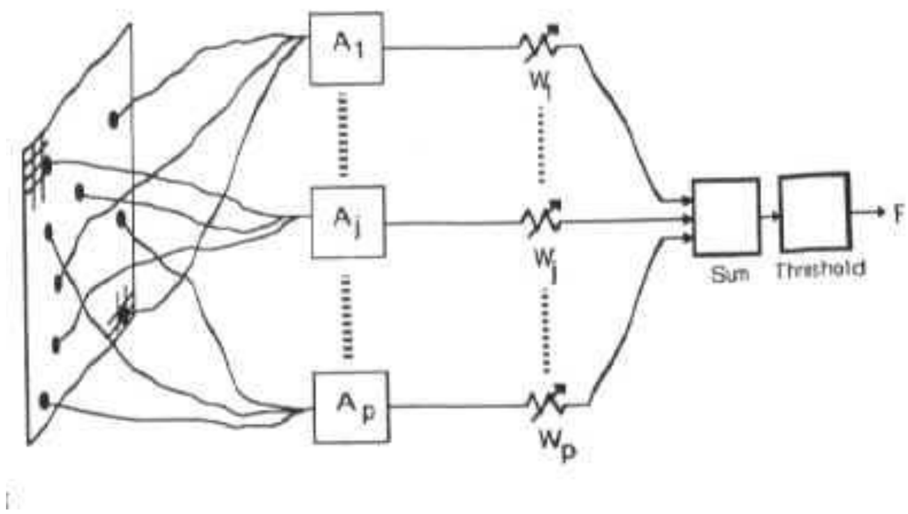

Figure 1: Neuron with weighted inputs

The sequences of steps are:

Step 1: Collect Data

Preparation of Known or Pre-determined inputs and outputs, which are used for Training and Testing of ANN.

Step 2: Define the Network Structure

After step 1, select the type and Architecture of the ANN. For that, the number of hidden layer and nodes for each layer and transfer function are defined.

Step 3: Select the Learning Algorithm

Network learning is a matter of adjusting the variable connection weights on the inputs of each processing element according to some neural based algorithm. This process of changing the weights of the input connections to achieve some desired result. Back propagation Learning Algorithm is most commonly used.

Step 4: Set Training Parameter Values

The rate at which ANN learn depend on several controllable factors one of that is Training parameters such as Learning rate, Momentum Factor, number of iteration or epochs, maximum allowed system error. There is no general rule for the selection of training parameters, only on the basis of experience.

Step 5: Start Training

Train the defined network, by using the Training set. Training is based on the simple idea of continuously modifying the strengths of the input connections to reduce the difference between the desired output value and the actual output It is done until it reach the maximum allowed error or number of Epochs.

Step 7: Start Test

The testing set is to be used to verify and validate the resultant neural network from supervised learning. If testing is successful and the error of prediction is within the permissible limits, the Neural Network Model is finished and ready for use. In case the testing is not successful, the training procedure must be repeated with another larger set of training data.

1.4. The biological neuron

The most basic components of neural networks are modeled after the structure of the brain. The most basic element of the human brain is a specific type of cell, which provides us with the ability to remember, think and apply previous experiences to our every action. These cells are known as neurons, each of these neurons can connect with up to 200000 other neurons. The power of the brain comes from the number of these basic components and multiple connections between them.

All natural neurons have four basic components, which are dendrites, soma, axon, and synapses. The figure shows a simplified biological neuron.

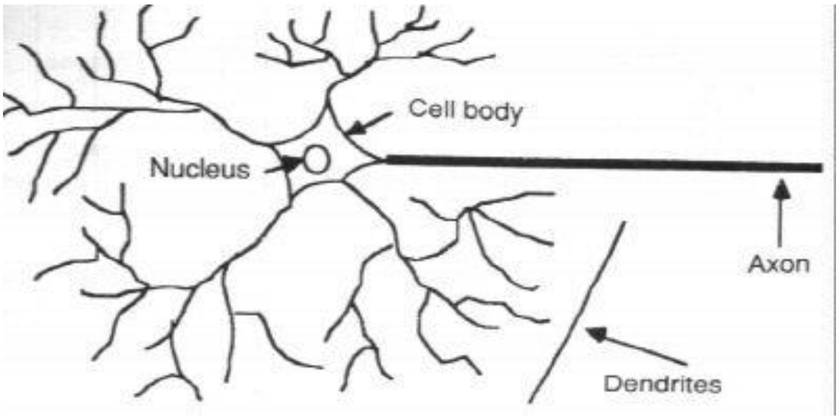

Figure 2: Components of a neuron

Dendrites are hair-like extensions of the soma which act like input channels. These input channels receive their input through the synapses of other neurons. The soma then processes these incoming signals over time. The soma then turns that processed value into an output which is sent spikes of electrical activity out to other neurons through a long, thin stand known as the axon and the synapses. Thus, each connection has an associated weight (synaptic strength) which determines the effect of the incoming input on the activation level of the unit.

1.5. Architecture of neural network

The commonest type of artificial neural network consists of three groups, or layers, of units: a layer of "input" units is connected to a layer of "hidden" units, which is connected to a layer of "output" units.

- The activity of the input units represents the raw information that is fed into the network.
- The activity of each hidden unit is determined by the activities of the input units and the weights on the connections between the input and the hidden units.

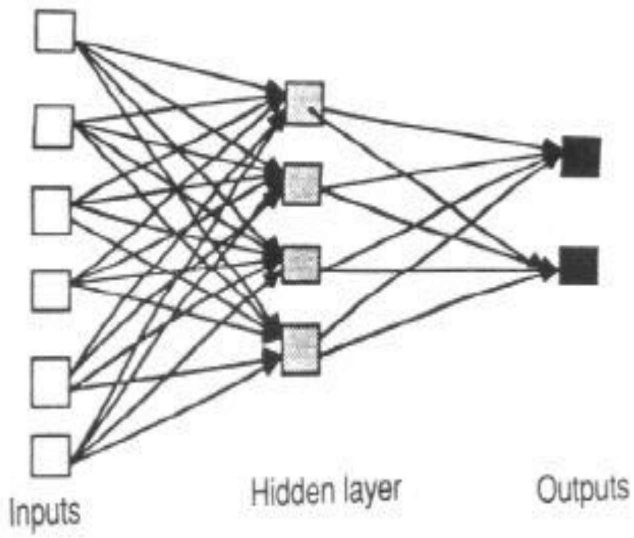

Figure 4: A Simple Neural Network Diagram

The behavior of the output units depends on the activity of the hidden units and the weights between the hidden and output units. This simple type of network is interesting because the hidden units are free to construct their own representations of the input. The weights between the input and hidden units determine when each hidden unit is active, and so by modifying these weights, a hidden unit can choose what it represents.

1.6. Advantages & Disadvantages of ANN

Advantages: There are many good points to neural networks and advances in this field will increase their popularity. 1. Neural networks, with their remarkable ability to derive meaning from complicated or imprecise data, can be used to extract patterns and detect trends that are too complex to be noticed by either humans or other computer techniques. 2. Adaptive learning: An ability to learn how to do tasks based on the data given for training or initial experience. 3. Self-Organization: An ANN can create its own organization or representation of the information it. 4. Real Time Operation: ANN computations may be carried out in parallel, and special hardware devices are being designed and manufactured which take advantage of this capability.

Disadvantages: There are quite a few down points to neural networks. They are: 1. our lack of hardware: The power of neural-networks lies in their ability to process information in a parallel fashion. Unfortunately, machines today are serial - they only execute one instruction at a time. Therefore, modeling parallel processing on serial machines can be a very time-consuming process. 2. The lack of defining rules to help construct a network for a given problem: There are many factors to be taken into consideration: the learning algorithm, architecture, number of neurons per layer, number of layers, data representation. 3. The internal mapping procedures are not well understood, and there is no guarantee that the system will converge to an acceptable solution. At the time of learning, network may get stuck in local minima.

1.7. Applications of ANN

Neural networks are applicable in virtually every situation in which a relationship between the predictor variables (independents, inputs) and predicted variables (dependents, outputs) exists, even when that relationship is very complex and not easy to articulate in the usual terms of "correlations" or "differences between groups." A few representative examples of problems to which neural network analysis has been applied successfully are: **1. Detection of medical phenomena.** A variety of health-related indices (e.g., a combination of heart rate, levels of various substances in the blood, respiration rate) can be monitored. The onset of a particular medical condition could be associated with a very complex (e.g., nonlinear and interactive) combination of changes on a subset of the variables being monitored. Neural networks have been used to recognize this predictive pattern so that the appropriate treatment can be prescribed. **2. Stock market prediction.** Fluctuations of stock prices and stock indices are another example of a complex, multidimensional, but in some circumstances at least partially-deterministic phenomenon. Neural networks are being used by many technical analysts to make predictions about stock prices based upon a large number of factors such as past performance of other stocks and various economic indicators. **3. Credit assignment.** A variety of pieces of information are usually known about an applicant for a loan. For instance, the applicant's age, education, occupation, and many other facts may be available. After training a neural network on historical data, neural network analysis can identify the most relevant characteristics and use those to classify applicants as good or bad credit risks. **4. Monitoring the condition of machinery.** Neural networks can be instrumental in cutting costs by bringing additional expertise to scheduling the preventive maintenance of machines. A neural network can be trained to distinguish between the sounds a machine makes when it is running normally ("false alarms") versus when it is on the verge of a problem. After this training period, the expertise of the network can be used to warn a technician of an upcoming breakdown, before it occurs and causes costly unforeseen "downtime." **5. Engine management.** Neural networks have been used to analyze the input of sensors from an engine. The neural network controls the various parameters within which the engine functions, in order to achieve a particular goal, such as minimizing fuel consumption. Some other areas where neural networks used are: Robotics, image processing, character recognition, voice recognition, optimization and scheduling.

2. LITERATURE REVIEW

The ability of artificial neural networks based on back propagation algorithm to predict densities of sulfur dioxide have been investigated [1]. To predict densities, several feed-forward neural networks with different architectures have been used. A feed-forward network with two hidden layers is used, in which temperature and pressure were input variables and density was the output variable. In addition, it has been proven that utilizing hyperbolic tangent sigmoid in the first layer and logarithmic sigmoid in the second layer will produce better results. The Levenberg-Marquardt algorithm has been applied as the training rule. Training a network for at least ten times indicates that using 15 and 10 neurons in the first and second layers, respectively has better results. Network predictions in comparison with several equations of state have proven that the ANN results are more accurate than predictions of EoSs. This has been shown with comparisons among several experimental set of PρT data, saturated liquid densities, and compressibility factors in contrast with the ANN predictions, too. These results show the capability of the presented network obviously.

N-propanol and toluene are frequently used as organic solvents in paints, varnishes, lacquers, glues, fuels, antifreeze, degreasing, cleaning agents, inks, pharmaceutical products, and laboratory processes. In spite of their wide usage, these solvents are considerably toxic and prolong exposure has an increase risk for cancer. Some alternatives for the use of solvents are available - for instance water based emulsions. Distillation, the most widespread technique for separating liquid mixtures, is in particular the chief separation method used in the petroleum and chemical industries. Experimental measurements of refractive indices and other property (density, surface tension, etc.) for binary mixtures have gained much importance in many chemical industries and engineering disciplines. From the values of the measured refractive indices, the excess refractive indices, of the mixed solvents were calculated. In this work [9] a simple neural network models and modular neural network for prediction excess refractive indices were developed. Good results are obtained both in training and validation phases, emphasizing the generalization capabilities of the neural models.

In this research [12], the ability of Multilayer Perception Artificial Neural Networks based on back-propagation estimate dimethyl ether (RE 170) densities and vapor pressures. The best network configuration for the layers network including 12, 15, 1 neurons in its layers, respectively, using Levenberg-Marquardt train between results show that there is a good agreement between experimental data and network prediction presented network for prediction of and saturated liquid, densities are less than 0.04% and 0.16%, ANN predictions, several equations of state, and experimental data sets show that the ANN results are experimental data better than EoSs. Another network for estimation of vapor pressure has been trained Results prove that artificial neural network can be a successful tool to represent thermo physical properties.

The determination of thermo physical properties of the refrigerants is very important for thermodynamic analysis of vapor compression refrigeration systems. In this paper [17], an artificial neural network (ANN) is proposed to determine properties as heat conduction coefficient, dynamic viscosity, kinematic viscosity, thermal diffusivity, density, specific heat capacity of refrigerants. Five alternative refrigerants are considered: R413A, R417A, R422A, R422D and R423A. The training and validation were performed with good accuracy. The thermo physical properties of the refrigerants are formulated using artificial neural network (ANN) methodology. Liquid and vapor thermo physical properties of refrigerants with new formulation obtained from ANN can be easily estimated. The method proposed offers more flexibility and therefore thermodynamic analysis of vapor compression refrigeration systems is fairly simplified.

The analysis of a ternary mixture can be done by using analytical instruments like TLC, GLC, HPLC, GC etc. which is time consuming & expensive. In the present work [14] artificial neural network modeling has been applied to estimate composition of a ternary liquid mixture with its physical properties such as refractive index, pH & conductivity. The work is extended in developing ANN model for estimation of composition of a known ternary mixture for the experimentally determined physical properties, refractive index, pH & conductivity. Samples having known compositions of a ternary liquid mixture, acetic acid-water ethanol have been prepared & analyzed for the physical properties, refractive index, pH & conductivity. ANN models 1 & 2 with different topologies have been developed based on the generated data. The predicted & the actual values using ANN models 1 & 2 have been compared based on the % relative error. The novel feature of this work has been the development of ANN model 1 with the accuracy of prediction between 0-3 % for output parameter, mole % water & 0-5% for output parameter, mole % acetic acid for training data set & ANN model 1 having accuracy level of 0-10% for output parameter, mole % water & 0-3% for output parameter, mole % acetic acid for test data set.

3. EXPERIMENTAL SETUP & PROCEDURE

3.1. Viscometers

A wide variety of instruments have been used for measurement of viscosity of liquids. For Newtonian liquids simple instruments are adequate. Capillary viscometers are the most commonly used instruments for Newtonian liquids. Most glass capillary viscometers are operated by force of gravity. Because of small driving force this class of devices is useful for low viscosity liquids ranging from 0.4 to 16000 centistokes. Glass capillary instruments are low stress instruments the shear stress ranges from 10 to 500 dynes/cm^2

Advantages:

1. Comparatively Cheap.
2. High Accuracy.
3. Require only small quantity of test liquid.
4. Flow in amenable to rigid mathematical treatment.

The principal of these instruments is derived from viscometer originally used by Ostwald. The original Ostwald viscometer has been modified in many ways to minimize certain undesirable effects in viscosity measurements to increase range of Viscosity or to meet specific requirements of certain test liquids.

The most important of these is the kinetic energy factor, which is necessary because a portion of original potential energy is used in imparting velocity to liquid rather than overcoming viscous resistance. This correction assumes considerable magnitude of liquids of low viscosity in instruments that permit rapid flow. The original Ostwald viscometer and its modification are still in wide use. One of its simple modifications is the U-tube viscometer as per British Standard Specification.

In the U-tube viscometer a sample of liquid was charged from tube 1 to bulb C, so that level in the arm stands at the mark. The viscometer with the sample is immersed in a water bath so that it attains the desired temperature. Suction is applied so that liquid is drawn up to mark a through bulb D. The efflux time of the liquid between marks A and B is noted after releasing the vacuum suction.

Thermostatic bath:

A thermostatic water bath was used for maintaining a constant temperature during the testing. It was capable of controlling temperature with an accuracy of $\pm 0.1^0$C.

Time recording device:

Stopwatch capable of reading up to 1/100th of second was used in all tests.

3.2. Pyknometers

Pyknometers are vessels with capillary necks in which volume of liquid is weighed. The volume is determined by weighing the vessel filled with water at definite temperature. The pyknometer used in the present investigation is bi capillary pyknometer or Ostwald-Sperngal pyknometer, the quantity of liquid is adjusted so that the liquid meniscus is at the mark on the horizontal capillary while the other arm is completely filled. Tilting the completely filled unit slightly makes this adjustment and drawing liquid slowly from other capillary by touching a piece of filter paper to it. The pyknometer is removed from the bath, wiped dry with lint less cloth and caps are placed on capillary arms. It is allowed to stand in the balance for few minutes before it is weighed.

3.3. Ultrasonic velocity

Speed of sound was measured by using a variable path, single crystal interferometer at a frequency of 2 MHz the interferometer was calibrated using toluene. The interferometer cell was filled with the test liquid and the temperature of the solution was maintained constant within ± 0.01K by circulation of water from thermostatically regulated water bath through the water jacketed cell. The uncertainty was estimated to be 0.1 ms^{-1}.

3.4. Procedure

The following liquid mixtures were considered. 1. Acetophenone + n-butykamine, 2. Acetophenone + ethyl chloro acetone, 3. Acetophenone + nitrobenzene, 4. Acetophenone + ethyl cyanoacetate. The charge for viscometer was prepared by taking 20 cc of the solution obtained by mixing the two liquids in different proportions. The thermostat was set to the desired temperature. After it had been cleaned and dried the viscometer was immersed in the bath so that the mark A is at least 2 cm below the surface of the bath liquid. The viscometer was adjusted so that the capillary did not deviate from the vertical in any plane more than 1^{o}. The solvent used for cleaning was acetone. The liquid mixture was charged into tube 1 of the viscometer so that the air bubbles were absent and the level in this arm stood at the mark at the bulb when the temperature was attained. After the sample had attained the bath temperature it was blown up to a point 2 cm above the mark A and the liquid was allowed to flow freely and time required for the liquid to flow from top to bottom mark was taken as the flow time. The above steps were continued and an average of 5 sets of flow time was reported. The stopwatch used had an accuracy of 0.01 sec.

4. RESULTS & DISCUSSIONS

4.1. Development of ANN model using MATLAB

MATLAB, which stands for matrix laboratory is an interactive system, originally written as software for matrix computation. MATLAB has evolved over the years as a tool for teaching courses in mathematics, engineering, and science and is used for research, development, and analysis. MATLAB toolboxes are collections of functions used to solve particular classes of problems. Areas in which toolboxes are available include signal processing, control systems, fuzzy logic, wavelets, simulation and neural networks. In the following section of this chapter, let us see a brief explanation of the different MATLAB toolbox functions Used in the developed of ANN model and the sample programs of ANN model.

4.2. Used MATLAB Functions; Syntax and Description

<u>Syntax</u>

P = a (: 1:2:3:4);

<u>Description</u>

Here ‘a’ is matrix with set of experimental data in which column 1,2,3,4 are read as input.

<u>Syntax</u>

T = a (: 5:9);

<u>Description</u>

Here ‘a’ is matrix with set of experimental datas in which column 5, 6,7,8,9 are read as output target. Using this, the architecture will be developed after simulating the whole datas.

Syntax

net = newff (PR, [t p],{'tansig' 'purelin'});

Where PR = MINMAX (P) takes one argument,

S - RxQ matrix.

and returns the Rx2 matrix PR of minimum and maximum values

for each row of S.

Description

The network net is created using the function newff.

The command newff is the feed forward function.

The tansig stands for the tan sigmoid transfer function.

The purelin function will stands for purelin neuron

The‘t’ stands for the no of hidden layers.

The ‘p’ stands to define the pureline function based on output we are targeting.

P = Network inputs.

Syntax

Y = sim (net, P);

Description

The output is obtained by simulating the network and the input datas.

sim simulates the neural network.

net = Network.

P = Network inputs.

Syntax

plot (P, T, P, Y,'o')

Description

The learning curve is plotted after simulating the datas.

P = Network inputs.

T = Network targets.

Y = Network outputs.

‘o’ = Network performance.

Syntax

net.trainParam.epochs = 1000;

Description

Train trains the network according to the number of epochs i.e. no of iterations. Train calls the function indicated by net.trainFcn, using the training parameter values indicated by net.trainParam.

Syntax

net = train(net,P,T);

Description

Network is finally developed after training the input and target values.

Syntax

Y = sim (net, P);

Description

The output with minimum error is obtained by simulating the network and the input datas.

Syntax

plot (P,T,P,Y,'o')

Description

Finally the learning curve with minimum error is plotted after simulating the datas.

Also the weights are calculated by following function

net.IW, net.LW, net.b

4.3. Algorithm

Feed-forward networks consist of Nl layers using the DOTPROD weight function, NETSUM net input function, and the specified transfer functions. The first layer has weights coming from the input. Each subsequent layer has a weight coming from the previous layer. All layers have biases. The last layer is the network output. Each layer's weights and biases are initialized with INITNW. Adaption is done with TRAINS which updates weights with the specified learning function. Training is done with the specified training function. Performance is measured according to the specified performance function. In order to choose the best architecture to the neural network it is necessary to conduct test to find the values for the following parameters:

1. Number of hidden layer and hidden nodes,
2. Number epochs,
3. Sum square error,

4. Learning rate,
5. Momentum, in order to obtain the minimum value of the network error,

4.4. The predicted output for intermediate mole fraction

1. Acetophenone + n-butyl amine mixture

P = [303.15; .0.1025]
1.0e+002 *
3.03150000000000
0.00102500000000

Y = sim (net, P)
1.0e+003 *

Density	=	0.0010165
Ultrasonic velocity	=	1.4
Viscosity	=	0.0001462

P = [303.15; .0.0784]
1.0e+002 *
3.13150000000000
0.00784000000000

Y = sim (net, P)
1.0e+002 *

Density	=	0.01086813981760
Ultrasonic velocity	=	8.20000005212407
Viscosity	=	0.00768634833452

P = [323.15; 0.1023]
1.0e+002 *
3.13150000000000
0.00998900000000

Y = sim (net, P)
1.0e+003 *

Density	=	0.00111867118888
Ultrasonic velocity	=	1.62997420847947
Viscosity	=	0.00296000963426

P = [323.15; .0.0784]
1.0e+002 *
3.23150000000000
0.0078400000000

Y = sim (net, P)
1.0e+002 *

Density	=	0.07213

Ultrasonic velocity = 1.5
Viscosity = 0.0501

2. Acetophenone + ethyl chloro acetone

P = [303.15; .0.1089]
1.0e+002 *
3.03150000000000
0.00108900000000

Y = sim (net, P)
1.0e+003 *
Density = 0.009475
Ultrasonic velocity = 1.4973
Viscosity = 0.00014784

P = [303.15;.0.9]
1.0e+002 *
3.23150000000000
0.00148500000000

Y = sim (net, P)
1.0e+003 *
Density = 0.00142896296683
Ultrasonic velocity = 1.12407819242328
Viscosity = 0.00079060383057

P = [323.15; 0.1089]
1.0e+002 *
3.23150000000000
0.00155000000000

Y = sim (net, P)
1.0e+003 *
Density = 0.00942691
Ultrasonic velocity = 1.12761447
Viscosity = 0.00079941

P = [303.15; .9]
1.0e+002 *
3.03150000000000
0.00555000000000

Y = sim (net, P)
1.0e+003 *
Density = 0.00127255287813
Ultrasonic velocity = 1.45887321690213
Viscosity = 0.00169495925561

3. Acetophenone + nitrobenzene

P = [303.15; .0]
1.0e+002 *
3.03150000000000
0.00133300000000

Y = sim (net, P)
1.0e+003 *

Density	=	0.00119593561484
Ultrasonic velocity	=	1.45011654885333
Viscosity	=	0.00195090764402

P = [303.15; .1333]
1.0e+002 *
3.23150000000000
0.00133300000000

Y = sim (net, P)
1.0e+003 *

Density	=	0.00118149593375
Ultrasonic velocity	=	1.26998059268027
Viscosity	=	0.00134545179711

P = [323.15; .0]
1.0e+002 *
3.23150000000000
0.00999900000000

Y = sim (net, P)
1.0e+003 *

Density	=	0.00111294145434
Ultrasonic velocity	=	1.57097943945014
Viscosity	=	0.00250365598007

P = [323.15; .5555]
1.0e+002 *
3.23150000000000
0.00555500000000

Y = sim (net, P)
1.0e+003 *

Density	=	0.00114320213841
Ultrasonic velocity	=	1.42125775850648
Viscosity	=	0.00196143370476

4. Acetophenone + ethyl cyanoacetate

P = [303.15; 0]
1.0e+002 *
3.03150000000000
0.00122000000000

Y =sim (net, P)
1.0e+003 *

Density	=	0.00089642270798
Ultrasonic velocity	=	1.37800090372941
Viscosity	=	0.00098213762939

P = [303.15; .1220]
1.0e+002 *
3.13150000000000
0.00122000000000

Y =sim (net, P)
1.0e+003 *

Density	=	0.00087662560760
Ultrasonic velocity	=	1.33200046482738
Viscosity	=	0.00089715505055

P = [323.15; 0]
1.0e+002 *
3.23150000000000
0.00122000000000

Y =sim (net, P)
1.0e+003 *

Density	=	0.00086948724463
Ultrasonic velocity	=	1.25100015439724
Viscosity	=	0.00071693298768

P = [323.15; .3030]
1.0e+002 *
3.23150000000000
0.00303000000000

Y =sim (net, P)
1.0e+003 *

Density	=	0.00091881219793
Ultrasonic velocity	=	1.31860293825671
Viscosity	=	0.00102259571392

P = [313.15; .8030]
1.0e+002 *
3.13150000000000
0.00803000000000

Y =sim (net, P)
1.0e+003 *

Density	=	0.00106496708813
Ultrasonic velocity	=	1.56443735081440
Viscosity	=	0.00265419527315

P = [303.15; .6030]
1.0e+002 *
3.03150000000000
0.00603000000000

Y =sim (net, P)
1.0e+003 *

Density	=	0.00102601990412
Ultrasonic velocity	=	1.54869745777667
Viscosity	=	0.00250675497005

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.

4.5. Error performance

A solution has been developed using the concepts of neural networks for the experimental problem to be free from the difficulties faced in the calculation by traditional techniques. A BPN simulator is designed and the data like viscosity, density, refractive index, ultrasonic velocity, surface tension are collected by experimental method. The 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.

1. Acetophenone + n-butyl amine system

Temp 'K'	Mole fraction	Density, g/cc	Viscosity, m.Pa.sec	Ultrasonic velocity, m/sec
303.15	0	1.0165	1.497	1462.4
303.15	0.102544	0.9665	1.213	1452.8
303.15	0.175962	0.9342	1.008	1428.8
303.15	0.223202	0.8999	0.992	1395.2
303.15	0.246472	0.8757	0.807	1304
303.15	0.248253	0.8478	0.746	1348.8
303.15	0.230512	0.8046	0.723	1446.4
303.15	0.195197	0.7733	0.676	1313.6
303.15	0.143985	0.7541	0.602	1284.8
303.15	0.078438	0.7257	0.544	1265.6
303.15	0	0.6807	0.501	1224
323.15	0	0.9982	1.383	695
323.15	0.102544	0.9655	1.105	738
323.15	0.175962	0.9326	0.857	758
323.15	0.223202	0.8976	0.777	850
323.15	0.246472	0.8638	0.71	955
323.15	0.248253	0.8442	0.646	1082
323.15	0.230512	0.7988	0.636	1170
323.15	0.195197	0.7593	0.63	1290
323.15	0.143985	0.7512	0.548	1365
323.15	0.078438	0.7213	0.501	1511
323.15	0	0.6796	0.47	1571

2. Acetophenone + ethyl chloro acetone

Temp 'K'	Mole fraction	Density, g/cc	Viscosity, m.Pa.sec	Ultrasonic velocity, m/sec
303.15	0	0.9475	1.4969	1478.4
303.15	0.1089	1.0005	1.1523	1430.4
303.15	0.2151	1.0024	1.1222	1472
303.15	0.3199	1.0069	1.0585	1396.8
303.15	0.4223	1.0473	1.015	1364.8
303.15	0.5231	1.0646	0.9312	1340.8
303.15	0.6224	1.07225	0.8809	1403.2
303.15	0.7191	1.0588	0.8474	1324.8
303.15	0.8144	1.0853	0.8273	1222.4
303.15	0.9086	1.0946	0.787	1390.4
303.15	1	1.13225	0.7164	1188.8
323.15	0	0.9277	1.3832	1044
323.15	0.1089	0.9828	0.9647	1124

323.15	0.2151	1.0004	0.9379	1156
323.15	0.3199	1.00575	0.8949	1208
323.15	0.4223	1.0422	0.8474	1265
323.15	0.5231	1.06225	0.7836	1323
323.15	0.6224	1.06985	0.7568	1383
323.15	0.7191	1.0554	0.7467	1440

3. Acetophenone + nitrobenzene

Temp 'K'	Mole fraction	Density, g/cc	Viscosity, m.Pa.sec	Ultrasonic velocity, m/sec
303.15	0	1.0199	0	1384
303.15	0.097908	1.0267	0.015957	1397.6
303.15	0.196275	1.048	0.040574	1400.7
303.15	0.295332	1.0635	0.01258	1406
303.15	0.394378	1.0829	-0.01142	1411.2
303.15	0.494139	1.0982	-0.00151	1425.6
303.15	0.594361	1.1043	0.018651	1428.8
303.15	0.695054	1.1196	0.055583	1436.8
303.15	0.796204	1.1434	0.061774	1439.2
303.15	0.886552	1.1531	0.063057	1442.4
303.15	1	1.163	0	1448
323.15	0	0.9832	1.517	1221
323.15	0.097908	0.9945	1.45	1270
323.15	0.196275	1.0145	1.35	1308
323.15	0.295332	1.0254	1.299	1336
323.15	0.394378	1.03845	1.256	1399
323.15	0.494139	1.04187	1.1823	1410
323.15	0.594361	1.053	1.149	1437
323.15	0.695054	1.068	1.065	1502
323.15	0.796204	1.0743	1.015	1533
323.15	0.886552	1.0991	0.971	1551
323.15	1	1.1245	0.917	1571

4. Acetophenone + ethyl cyanoacetate

Temp 'K'	Mole fraction	Density, g/cc	Viscosity, m.Pa.sec	Ultrasonic velocity, m/sec
303.15	1	1.0099	1.5704	1585.6
303.15	0.894243	9544	1.4468	1462.4
303.15	0.790192	0.9563	1.4902	1476.3
303.15	0.687192	0.9576	1.5137	1486.4

303.15	0.585575	0.95995	1.5538	1356.8
303.15	0.49082	0.9641	1.6039	1425.6
303.15	0.385578	0.9719	1.7744	1428.8
303.15	0.28546	0.9729	1.7911	1436.8
303.15	0.190476	0.9737	1.8312	1433.6
303.15	0.094406	0.9769	1.8946	1427.2
303.15	0	0.9817	2.0217	1448
323.15	1	1.0068	1.3521	1044
323.15	0.894243	0.9535	1.1657	1124
323.15	0.790192	0.9561	1.1925	1156
323.15	0.687192	0.9594	1.2661	1208
323.15	0.585575	0.9585	1.42	1265
323.15	0.49082	0.9637	1.3431	1323
323.15	0.385578	0.9683	1.3732	1383
323.15	0.28546	0.9681	1.4735	1440
323.15	0.190476	0.9679	1.5002	1476
323.15	0.094406	0.753	1.5203	1545
323.15	0	0.9774	1.5738	1571

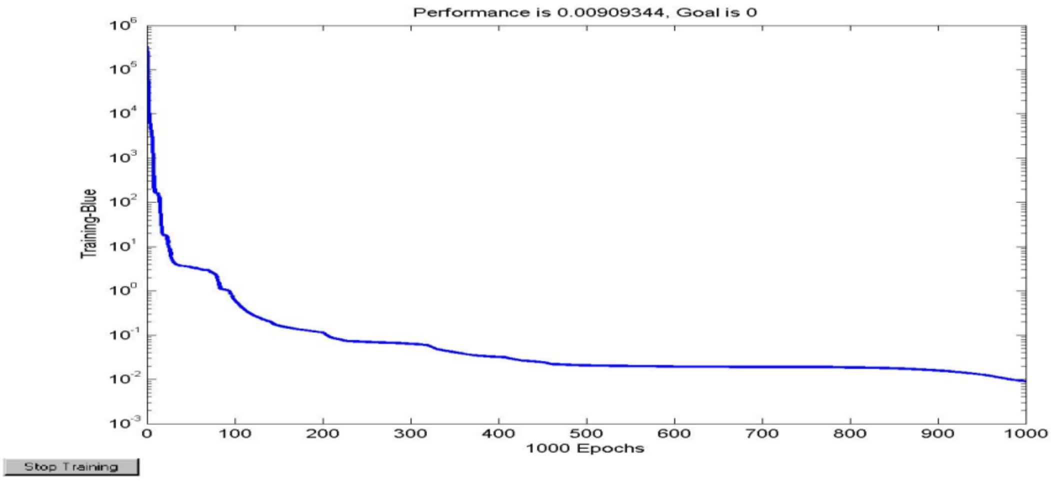

Figure 3: Error performance for Acetophenone + n-butyl amine system

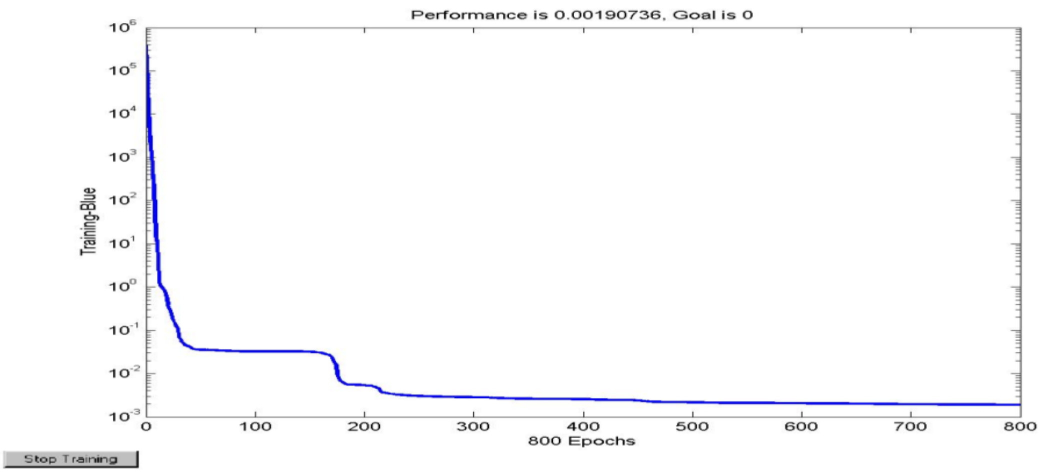

Figure 4: Error performance for Acetophenone + ethyl chloro acetone system

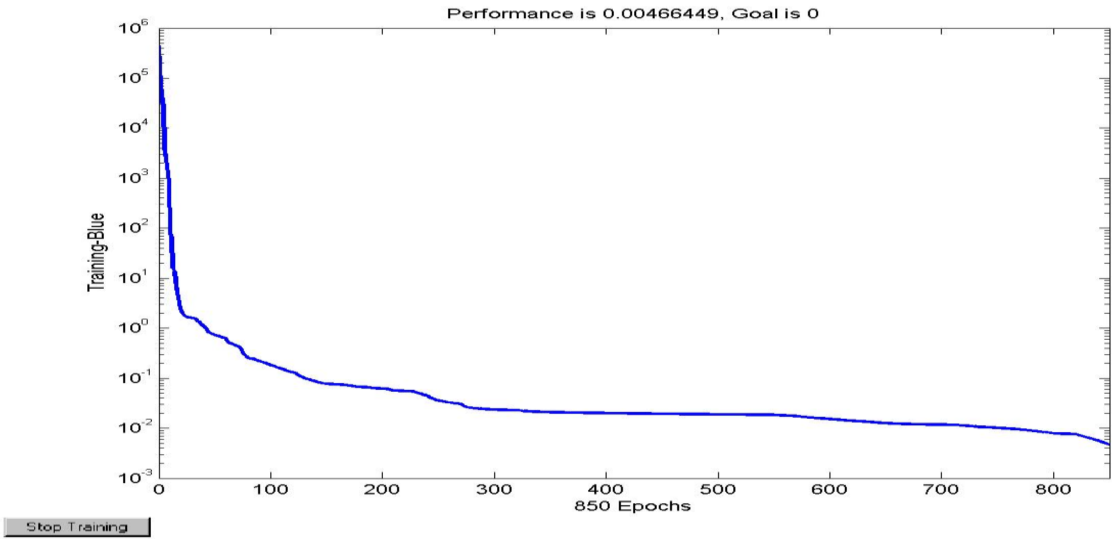

Figure 5: Error performance for Acetophenone + Nitrobenzene system

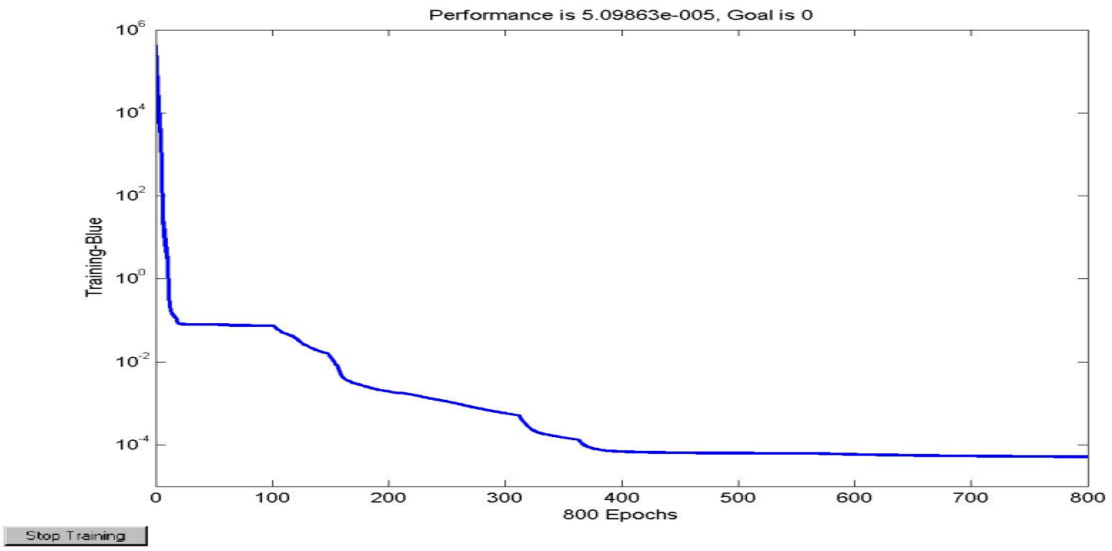

Figure 6: Error performance for Acetophenone + ethyl cyano acetate

CONCLUSION

The main advantage of this research is to measure the thermo physical properties of various Acetophenone liquid mixtures using Artificial Neural Network to get minimum error. From the output, we see that the error reduces as the number of iteration increases. Here, we have taken the number of input patterns is five and the number of output nodes is taken as the number of input patterns. The error has reduced to nearly zero which indicates that the network is trained. The network has to be run for several numbers of iterations for the error to be reduced. This network can be trained for more number of input patterns but has to be trained for more number of iterations. From the above graphs, we could find the mean square error and the number of iterations. From the output and the weight stored, the feed forward propagation was checked for the correctness of the result. Thus the structure of the proposed expert system model mainly consists of the following:

1. Designing PC-based Neural Network simulation software.
2. Collection and designing of data structures appropriately.
3. Presentation of data to the network.
4. Calculation of the mean square error of the output for each of the presentation.
5. Plotting of the learning curve for developing the architecture

Using this, an interactive system can be developed. This can happen only when the number of connectivity increases. Neural network studies can, without doubt, lead to important practical and scientific advances, but will require basic research in several areas and a thorough integration with many disciplines. Hope within a decade or two the neural network (expert system) in decision making of complicated problems in many fields including Medicine, Engineering, and Agriculture etc.

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