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An artificial neural network for prediction of thermodynamic properties; Case study: saturated and superheated water

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ABSTRACT

Water is an important natural fluid that plays significant roles in many processes. Consequently, knowledge of the thermodynamic properties of water is necessary for the interpretation of physical and chemical processes. In this work a new method based on artificial neural network (ANN) for prediction of water thermodynamic properties such as specific volume, entropy and enthalpy for both superheated and saturated regions has been proposed. The needed data is taken from steam tables[Perry's Chemical Engineering Handbook]. The accuracy and trend stability of the trained networks, were tested against unseen data their. Different training schemes for the back-propagation learning algorithm, such as; scaled conjugate gradient (SCG), Levenberg-Marquardt (LM), gradient descent with momentum (GDM), variable learning rate back propagation (GDA) and resilient back propagation (RP) methods were used. The SCG algorithm with seven neurons in the hidden layer shows to be the best suitable algorithm with the minimum mean square error (MSE) of 0.0001517. The ANN's capability to predict the water thermodynamic properties is one of the best estimating method with high performance.

KEYWORDS

Thermodynamic properties;
Steam table;
Artificial neural network.

INTRODUCTION

Water is an important natural fluid that plays significant roles in many processes, such as mineral deposits, hydrothermal venting, geothermal evolution, petroleum and natural gas formation, migration, and waste disposal, etc. The thermodynamic properties of water are important factor to study the mentioned processes[1]. Besides the high costs of the experimental work it is difficult if not impossible, to get a clear picture of the condition and possible problems of the work. Therefore a model based on some experimental results is proposed to predict the required data instead of doing more experiments. The major processes in the chemical engineering are unfortunately nonlinear. ANN is a model that attempts to mimic simple biological learning processes and simulate specific functions of human nervous system. This model creates a connection between input and output variables and keeps the underlying complexity of the process inside the system. The ability

to learn the behavior of the data generated by a system is the neural network's versatility and privilege[2]. Fast response, simplicity, and capacity to learn are the advantages of ANN compared to classical methods. This model has been widely applied to predict the physical and thermodynamic properties of chemical compounds. ANN has recently been used to predict some pure substances and petroleum fraction's properties[3], activity coefficients of isobaric binary systems[4], thermodynamic properties of refrigerants[5,6,7], and activity coefficient ratio of electrolytes in amino acid's solutions[8], etc. To the best of our knowledge no attempt has been made to model the thermodynamic properties of water by artificial neural network. Defining the ANN and selecting the best ANN predictor to predict the thermodynamic properties of saturated and superheated water instead of approximate and complex analytical equations are the main focus of this work. In the following sections after ANN introduction, the best ANN predictor is chosen. Finally results of the ANN model is evaluated against with the unseen data and then compared with the experimental work.

Artificial neural networks

In order to find relationship between the input and output data derived from experimental work, a more powerful method than the traditional ones are necessary. ANN is an especially efficient algorithm to approximate any function with finite number of discontinuities by learning the relationships between input and output vectors[3,9]. These algorithms can learn from the experiments, and also are fault tolerant in the sense that they are able to handle noisy and incomplete data. The ANNs are able to deal with non-linear problems, and once trained can perform prediction and generalization rapidly[10]. They have been used to solve complex problems that are difficult to be solved if not impossible by the conventional approaches, such as control, optimization, pattern recognition, classification, and so on. Specially if it is desired to have the minimum difference between the predicted and observed (actual) outputs[11]. Artificial neural networks are biological inspirations based on the various brain functionality characteristics. They are composed of many simple elements called neurons that are interconnected by links and act like axons to determine an empirical relationship between the inputs and outputs of a given system. Multiple layers arrangement of a typical interconnected neural network is shown in figure 1. It consists of an input layer, an output layer, and one hidden layer with different roles. Each connecting line has an associated weight. Artificial neural networks are trained by adjusting these input weights (connection weights), so that the calculated outputs may be approximated by the desired values. The output from a given neuron is calculated by applying a transfer function to a weighted summation of its input to give an output, which can serve as input to other neurons, as follows[12].

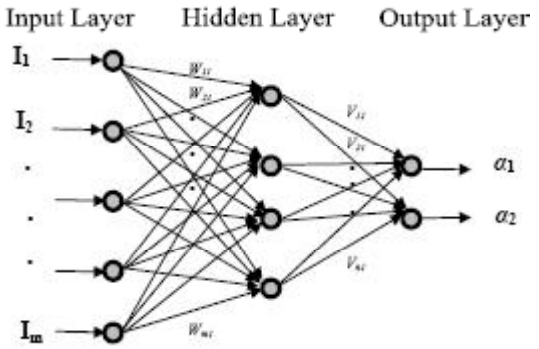

Figure 1 : Schematic of typical multi-layer neural network model

$$\alpha_{jk} = F_k\left(\sum_{i=1}^{N_{k-1}} w_{ijk}\alpha_{i(k-1)} + \beta_{jk}\right) \quad (1)$$

Where α_{jk} is neuron j's output from k's layer β_{jk} is the bias weight for neuron j in layer k. The model fitting parameters w_{ijk} are the connection weights. The nonlinear activation transfer functions f_k may have many different forms. The classical ones are threshold, sigmoid, Gaussian and linear function, etc…[13], for more details of various activation functions see Bulsari[14].

The training process requires a set of examples of proper network behavior; network input (I_i) and target output (t_i). During training the weights and biases of the network are iteratively adjusted to minimize the network performance function[15]. The typical performance function that is used for training feed forward neural networks is the Mean Squares of the network Errors (MSE) Eq. 2.

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(e_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(t_i - \alpha_i)^2 \quad (2)$$

There are many different types of neural networks, differing by their network topology and/or learning algorithm. In this paper the back propagation learning

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TABLE 1: Minimum and maximum of data used to train the neural network[14]

Saturated vapor-liquid region			Superheated vapor region		
Properties	**min**	**max**	**Properties**	**min**	**max**
Temperature (^{0}C)	5	370	Temperature (^{0}C)	50	1300
Vapor quality	0	1	Vapor quality	-	-
Pressure (kPa)	0.8721	21028	Pressure (kPa)	10	50000
Specific volume (m^3/kg)	0.001	147.118	Specific volume (m^3/kg)	0.001503	72.6025
Enthalpy (kJ/kg)	20.98	2804.14	Enthalpy (kJ/kg)	1699.51	5409.7
Entropy (kJ/kg K)	0.0761	9.0257	Entropy (kJ/kg K)	3.714	11.581

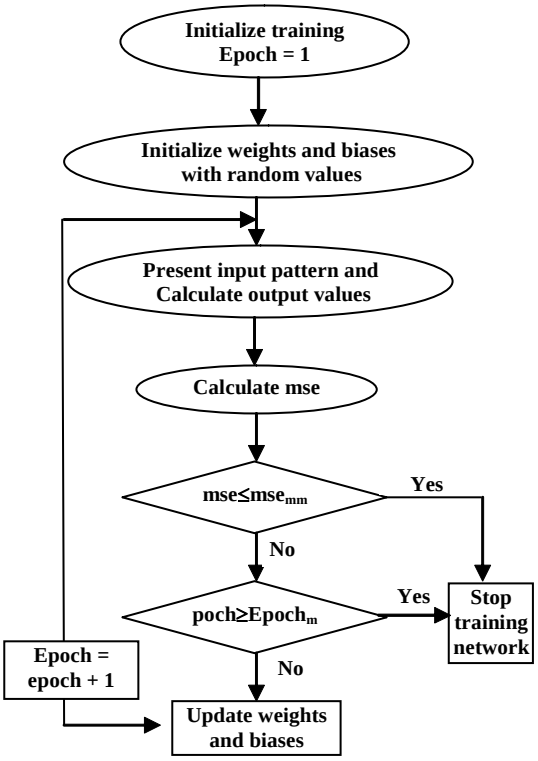

Figure 2 : A training process flowchart

algorithm, which is one of the most commonly used algorithms is designed to predict the thermodynamic properties of water. Back propagation is a multilayer feed-forward network with hidden layers between the input and output[16]. The simplest implementation of back propagation learning is the network weights and biases updates in the direction of the negative gradient that the performance function decreases most rapidly. An iteration of this algorithm can be written as follows[12].

$$x_{k+1} = x_k - l_k g_k \quad (3)$$

The details of this process are shown by a flow-chart as figure (2) for finding the optimal model. There are various back propagation algorithms. Scaled conjugate gradient (SCG), Levenberg-Marquardt (LM), gradient descent with momentum (GDM), variable learning rate back propagation (GDA) and resilient backpropagation (RP) are many types of them. LM is the fastest training algorithm for networks of moderate size and it has memory reduction feature for use when the training set is large. SCG is one of the most important back propagation training algorithms that is very good general purpose algorithm training[15,13].

The neural nets learn to recognize the patterns of the data sets during the training process. Neural nets teach themselves the patterns of the data set letting the analyst to perform more interesting flexible work in a changing environment. Although neural network may take some time to learn a sudden drastic change, but it is excellent to adapt constantly changing information. However the programmed systems are constrained by the designed situation and they are not valid otherwise. Neural networks build informative models whereas the more conventional models fail to do so. Because of handling very complex interactions, the neural networks can easily model data, which are too difficult to model traditionally (inferential statistics or programming logic). Performance of neural networks is at least as good as classical statistical modeling, and even better in most cases[16]. The neural networks built models are more reflective of the data structure and are significantly faster.

Neural networks now operate well with modest computer hardware. Although neural networks are computationally intensive, the routines have been optimized to the point that they can now run in reasonable time on personal computers. They do not require supercomputers as they did in the early days of neural network research.

EXPERIMENTAL

TABLE 1 lists the range of data that are used to model the water properties (taken from Perry's Chemical Engineering Handbook Steam tables[17]). The network inputs are temperature and quality in the case of vapor-liquid equilibrium (VLE) while the outputs are the pressure, specific volume, enthalpy and entropy. Similarly,

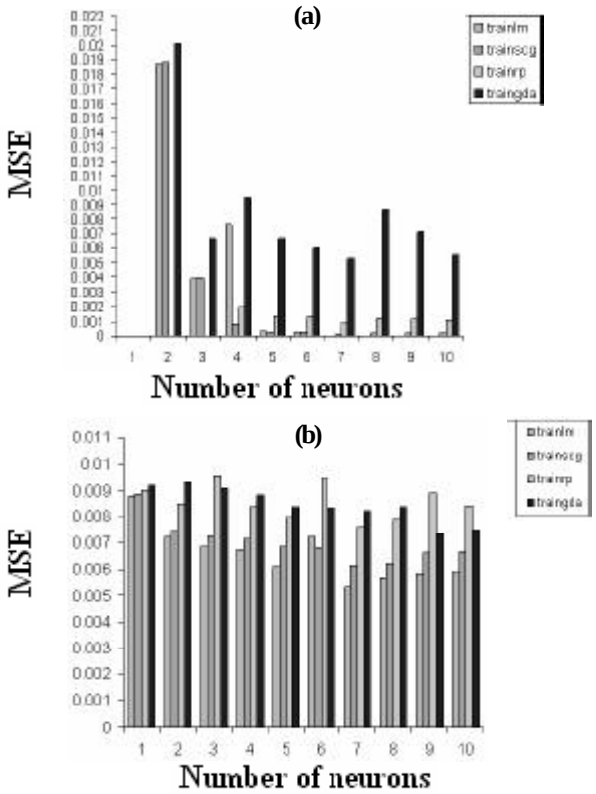

Figure 3: Determining the optimum number of neurons for some algorithms; Saturated region (a) superheated region (b) Networks

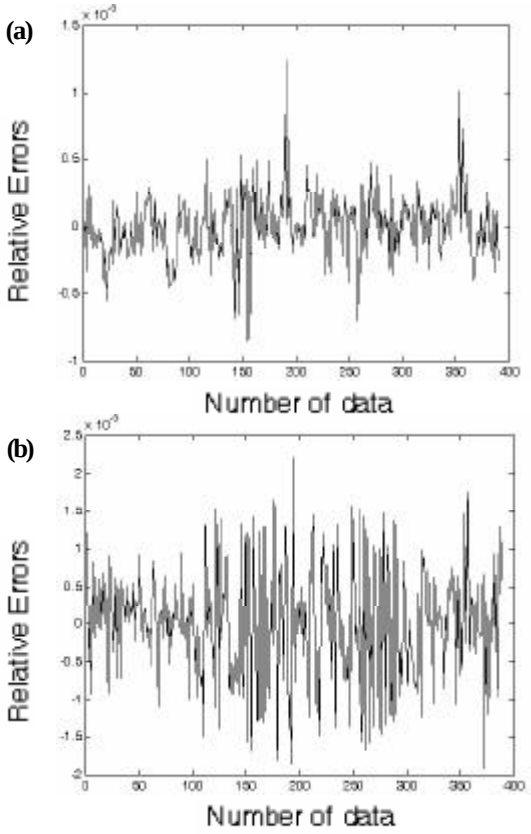

Figure 4: The relative errors between predicted data by ANN and Experimental data; Saturated water (a) Superheated water (b)

for the superheated vapor the inputs are the temperature and pressure while outputs are the specific volume, enthalpy and entropy.

Neural network model development

Developing the neural network model to accurately predict thermodynamic properties of water requires its exposure to a large data set during the training phase.

The back propagation method with SCG, LM, RP and GDA learning algorithm has been used in feed forward, single hidden layer network. Input layer neurons have no transfer functions. The neurons in the hidden layer perform two tasks: summing the weighted inputs connected to them and passing the result through a non linear activation function to the output or adjacent neurons of the corresponding hidden layer. The computer program has been developed under MATLAB. Two thirds of data set is used to train each ANN and the rest have been used to evaluate their accuracy and trend stability. The number of the hidden layer neurons is systematically varied to obtain a good estimate of the trained data. The selection criterion is the net output MSE. The

TABLE 2: MSE comparison between different algorithms for the training of ANN

Saturated vapor-liquid region		Superheated vapor region	
Algorithm	MSE of network training	Algorithm	MSE of network training
Trainlm	0.0000482	Trainlm	0.005835
Trainscg	0.0001571	Trainscg	0.005668
Trainrp	0.0009469	Trainrp	0.007897
Traingda	0.005305	Traingda	0.008218
Traingdm	0.02839	Traingdm	0.008806

MSE of various hidden layer neurons are shown in figure 3. As it can be seen the optimum number of hidden layer neurons is determined to be seven for minimum MSE.

Similarly the MSE of various training algorithms are calculated and listed in TABLE 2 for the obtained seven hidden layer neurons. As TABLE 2 shows the Levenberg-Marquardt (LM) and Scaled Conjugate Gradient (SCG) algorithms have the minimum MSE.

Now the trained ANN models are ready to be tested and evaluated against the new data. TABLE 3 lists the various MSE of the network testing. According

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TABLE 3: MSE comparison between different algorithms for the testing of ANN

Saturated vapor-liquid region		Superheated vapor region	
Algorithm	MSE of network testing	Algorithm	MSE of network testing
Trainlm	0.0932	Trainlm	0.02752
Trainscg	0.0005795	Trainscg	0.00006794
Trainrp	0.001208	Trainrp	0.011063
Traingda	0.01194	Traingda	0.00729
Traingdm	0.02451	Traingdm	0.001149

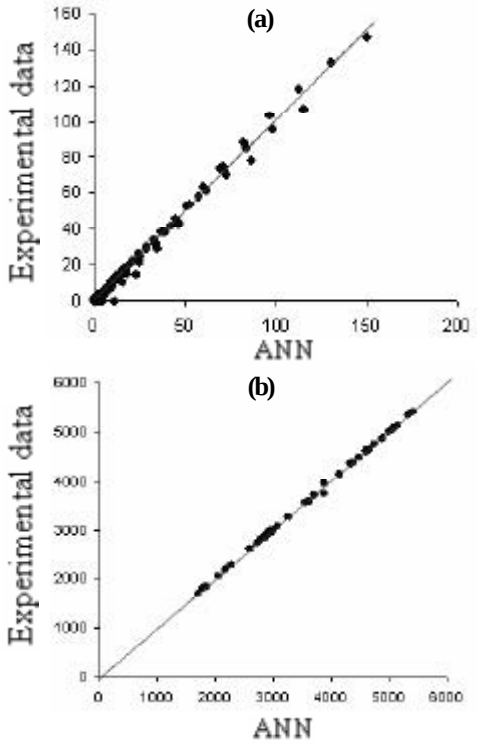

Figure 5 : Evaluation of ANN performance; A scatter plot of typically measured experimental data against the ANN model for unseen data; Saturated (a) and superheated water properties (b)

to this TABLE the scaled conjugate gradient (SCG) algorithm is the most suitable algorithm with the minimum MSE.

Consequently, SCG provides the best average minimum error for both training and testing of network. The fluctuations of relative error between experimental data and simulation by SCG algorithm are shown in figure 4 for both saturated and superheated.

A scatter plot of typically measured experimental data against the ANN model predictions was shown in figure 5. It is obvious from this figure that the ANN provides results very close to process measurements.

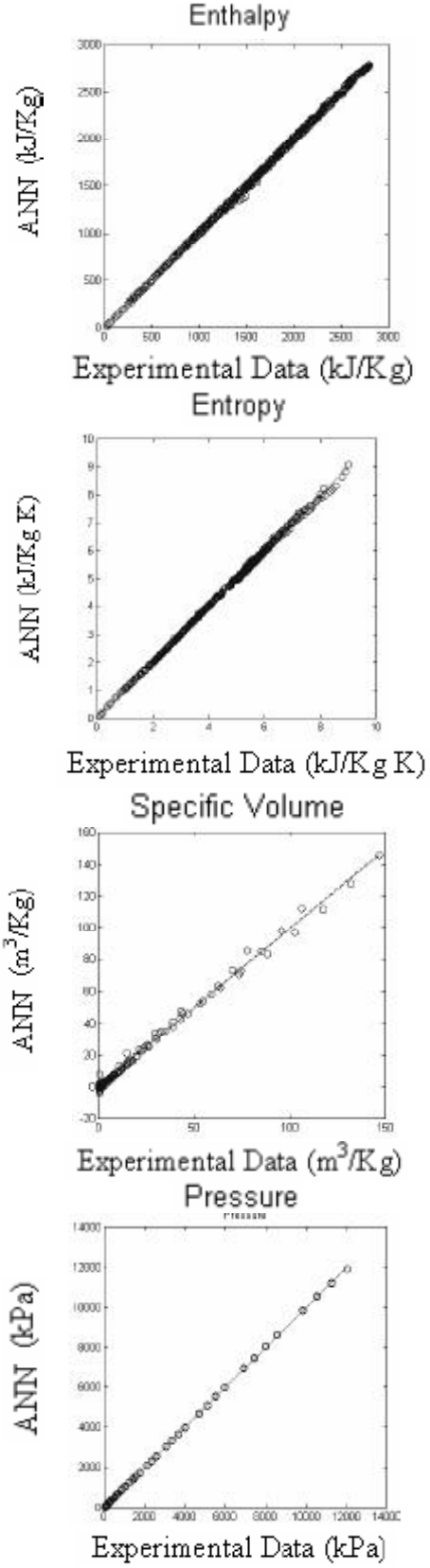

Figure 6: A Comparison between ANN and experimental data for saturated liquid-vapor region

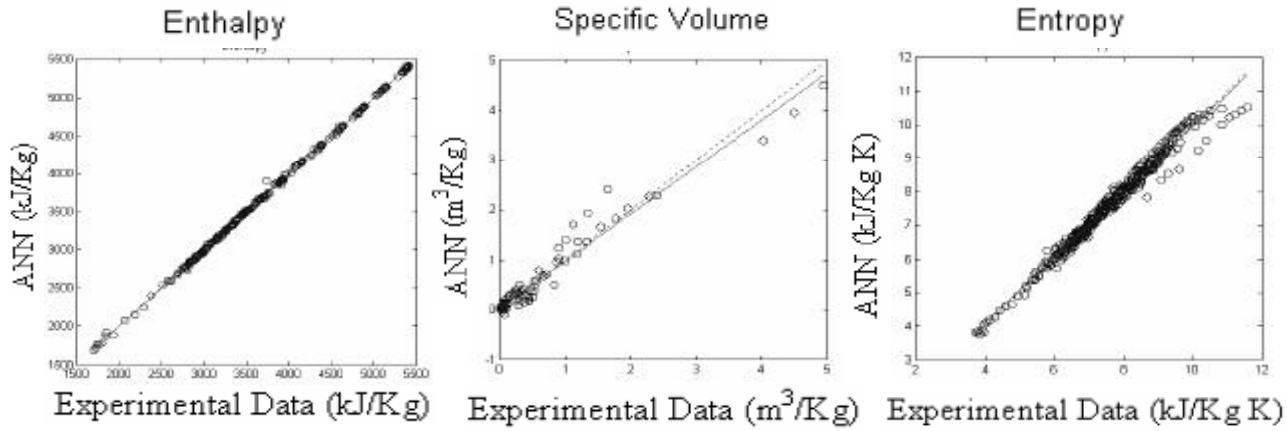

Figure 7: A Comparison between ANN and experimental data for superheated vapor region

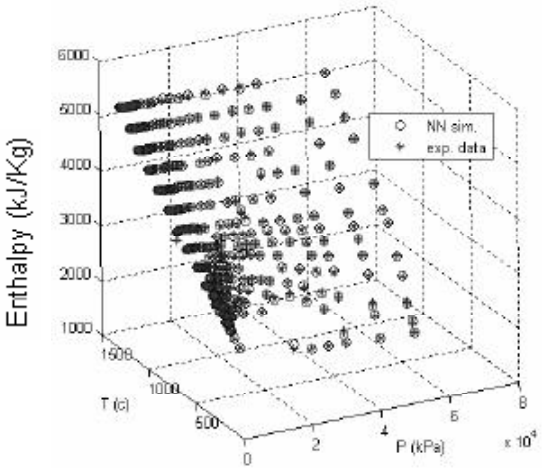

Figure 8: The comparison between predicted data by ANN and experimental data (The variation of enthalpy with pressure and temperature for superheated vapor phase)

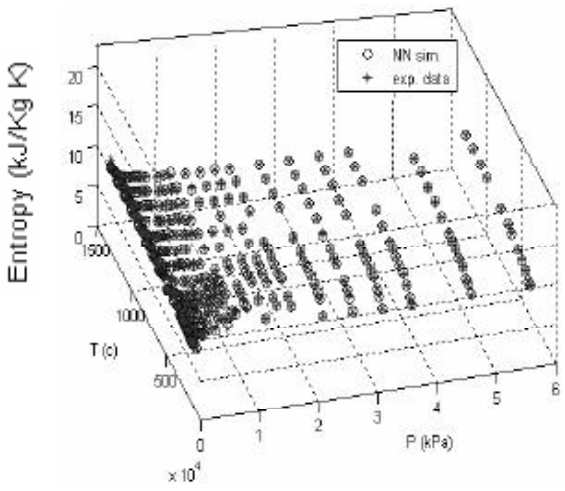

Figure 9 : The comparison between predicted data by ANN and experimental data (The variation of entropy with pressure and temperature for superheated vapor phase)

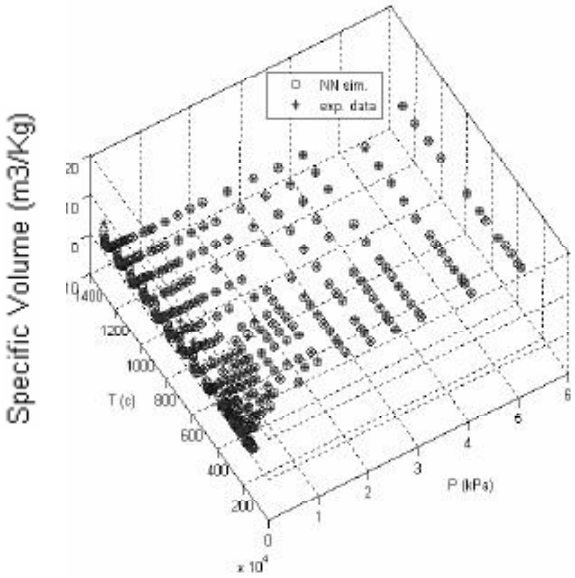

Figure 10: The comparison between predicted data by ANN and experimental data (The variation of specific volume with pressure and temperature for superheated vapor phase)

The predictions which match measured values should fall on the diagonal line. Almost all data lay on this line, which confirms the accuracy of the ANN model. ANN's results showed acceptable estimation performance for prediction of the water properties.

Results evaluation

The results show that the ANN predicts water properties very close to the experimentally measured ones. Figures 6 and 7 show the scatter diagrams that compare the experimental data versus the computed neural network data over the full range of operating conditions. As it may be seen, a tight cloud of points about the 45° line is obtained for the new data points. This

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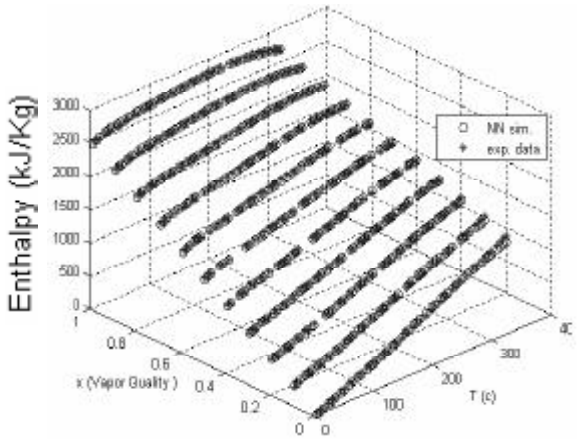

Figure 11: The comparison between predicted data by ANN and experimental data (The variation of enthalpy with temperature and vapor quality for saturated liquid-vapor phase)

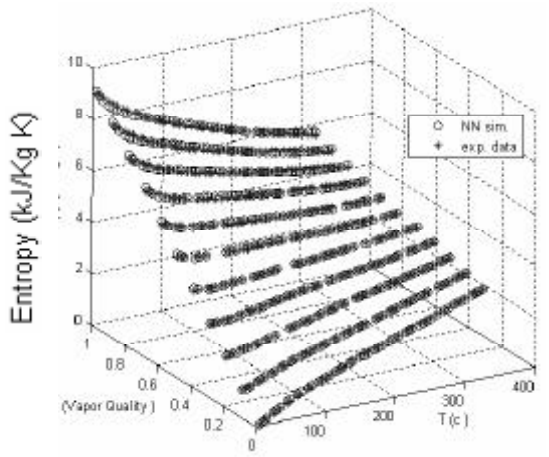

Figure 12: The comparison between predicted data by ANN and experimental data (The variation of entropy with temperature and vapor quality for saturated liquid-vapor phase)

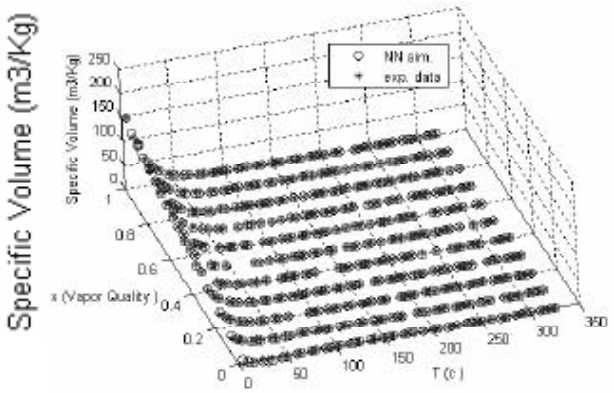

Figure13: The comparison between predicted data by ANN and experimental data (The variation of specific volume with temperature and vapor quality for saturated liquid-vapor phase)

indicates an excellent agreement between the experimental and the calculated data.

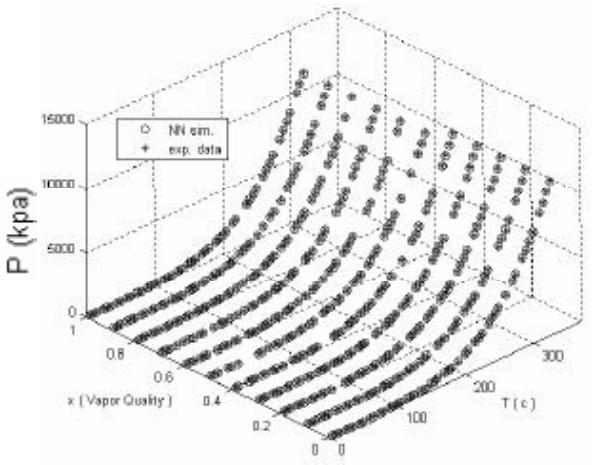

Figure 14: The comparison between predicted data by ANN and experimental data (The variation of pressure with temperature and vapor quality for saturated liquid-vapor phase)

Figures (8-10) illustrate comparison between ANN simulation and experimental data for change of enthalpy, entropy and specific volume against temperature and pressure in superheated vapor region. It is clear that the neural networks can give a very accurate representation of the experimental data over the full range of operating condition and indicates the good accuracy of the neural network to represent thermodynamic properties of water.

In figures (11-14), the variance of the enthalpy, entropy, specific volume and pressure versus temperature and vapor quality for saturated region have been shown.

List of symbols

e- Difference between target data and simulation ; F- Transfer function; g- Gradient; I- Input data; l- Learning rate; N- Number of data; t- Target data; x- Vector of weights; w- Connection weights ; α- Output of neuron; β– Bias weight

CONCLUSION

The ability of ANN with MLP neural network to model and predict saturated and superheated water properties have been investigated in this work. The MSE based analysis of the results, are used to verify the suggested approach. The results show a good agreement between experimental data and those predicted by ANN. An important feature of the model is that it doesn't require any theoretical knowledge or human

experience during the training process. It has been clearly shown that of the ANN calculates the water thermodynamic properties based on the experimental data only. Therefore it is not necessary to use approximate and complex analytical equations to calculate water thermodynamic properties. Also this new method can be applied in computational engineering software.

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