Chapter - 4

Applicability of ANN in Hydrodynamics Studies

This chapter deals with the applicability of ANN for the prediction of gas holdup and frictional pressure drop of the present system. The ANN with multilayer perceptron (MPL) with one hidden layer and four different transfer functions with backpropagation algorithm were used.

4.1 Introduction

An artificial neural network is a computational simulation of a biological neural network. The neural network is inspired by our brains. The human brain has about 10^{11} neurons and 10^{14} synapses. A neuron consists of a soma (cell body), axons (sends signals) and dendrites (receives signals). Fig. 4.1 shows two interconnected brain cells. A synapse connects an axon to a dendrite. Given a single, a synapse might increase (excite) or decrease (inhibit) electrical potential. A neuron fires when its electrical potential reaches a threshold. Learning might occur by changes to synapses. Similarly, an artificial neural network consists of units, connection and weights. Inputs and outputs are numeric. In a typical ANN, input units store the input, hidden unit transfer the input into an internal numeric vector, and an output unit transforms the hidden values into the prediction. The comparison of biological neural network and ANN is presented in Table 4.1.

In industrial practice the processes are often very complex and also poorly understood but it is essential to know how to control, optimization and prediction of the process behaviours. Thus, when the theoretical modelling is difficult, then empirical or data-driven modelling is the alternative solution. The artificial networks (ANNs) have been proposed to be a very promising tool for identifying empirical process models from process data (Bhat and McAvoy, 1990; Mah and Chakravarty, 1992; Sridhar et al., 1996). Himmelblau (2000) reviewed the applications of ANNs in chemical engineering field which include, fault diagnosis of chemical plants, dynamic modelling of chemical processes, system identification and control, sensor data analysis, prediction of product quality, chemical composition analysis and property prediction, inferential control, etc. Bar and Das (2011) critically reviewed the importance of the complex hydrodynamic parameter prediction through ANNs. The ANN based process modelling approach is to consider a number of possible candidate models (Transfer Function 1-4), and then predict the outputs from the given data (Clemen, 1989). The selected model is one that is expected to give the least prediction error in the future prediction. The prediction error of the candidate model is computed from the available input data for testing the model. Hence an optimal model assumes that ANN model which can predict accurately with minimum error using the data set than the other candidate models.

Artificial neural network has gained a widespread application in many engineering fields (Himmelblau, 2000). ANN model can learn from example incorporate a large number of variables and provide adequate quick response to the new information (Bar et al., 2010).

4.2 ANN Methodology

Figs. 4.2 and 4.3 show schematic diagram of artificial neural network for gas holdup and pressure drop respectively. It has three layers: an input layer, hidden layer and an output layer. Multilayer perception (MLP) is the most popular and widely used network for ANN studies (Bar and Das, 2011). Literature survey suggested that a network with single hidden layer using different popular transfer functions like sigmoid, hyperbolic tangent, etc. are extensively used for prediction and it performed successfully. Hence, this study is based on MLP using a single hidden layer. Presently there are many training algorithms in use, like Backpropagation (BP), Delta-Bar-Delta (DBD), Quickprop (QP), Conjugate gradient (CG), scaled conjugate gradient (SCG), Levenberg-

Marquart (LM), etc. Out of the entire training algorithm the most popular is the Backpropagation (BP). Hence, the prediction of gas holdup and frictional pressure drop are carried out using multilayer perceptron (MPL) with one hidden layer and four different transfer functions and is trained with backpropagation (BP) algorithm in MATLAB R2010b environment. The transfer functions used in the hidden layer are shown in Table 4.2, and the transfer function five represents the output function.

The backpropagation algorithm involves two steps. The first step is a forward pass, in which the effect of the input is passed forward through the network to reach the output layer. After the error is computed, a second step starts backwards through the network. The errors at the output layer are propagated back towards the input layer with the weights being modified according to equation (4.1),

$$\Delta w_{ij}(n) = -\varepsilon \times \frac{\partial E}{\partial w_{ij}} + \alpha \times \Delta w_{ij}(n-1) \tag{4.1}$$

where, $\Delta w_{ij}(n)$ and $\Delta w_{ij}(n-1)$ are the weight increments between node i and j respectively during the n^{th} and $(n\text{-}1)^{th}$ pass or epoch, E is Error, ε and α are known as learning coefficient and momentum factor and control the algorithm's rate of learning. To optimize the rate at which a network learns these factors must be set and/or adjusted properly during the training process. The valid range for both ε and α is between 0 and 1 (Qnet 2000 Manual, 1999). Once the network trained, the weights are frozen and then used to compute the output for new input data that is final prediction.

4.3 Performance of the ANN

The Range of variables investigated in the ANN study is shown in Table 2.3. Initially the total data was of 646 was randomized. The first 90% of the data are used for training, the next 10% for testing and prediction. The synapse that connects the hidden layer to the input layer adjusts the weights and learning rate. It is always desired that the number of processing elements in the hidden layer must be kept at a minimum to reduce the complexity of network. Hence one hidden layer is used. The numbers of nodes in the hidden layer are optimized by varying the nodes from 5 to 25 and each case the MSE was calculated.

Figs. 4.4 and 4.5 show the variation in MSE with the number of nodes for gas holdup and pressure drop. The optimum number of nodes is that node where the MSE is minimum. These optimum numbers of nodes are used for the analysis. The output is generated by using the transfer function 5 and compare with the desired output. The error passes to backpropagation for corrective adjustment of synaptic weight of network for training. The backpropagation process propagates the errors backward through the network and allows adaptation of hidden processing element and a closed-loop control system is thus established. The weights are automatically adjusted using a gradient-descent-based algorithm. The performance of the network is checked by calculating mean square error (*MSE*), Average absolute relative error (*AARE*), Standard deviation (σ), Cross-correlation coefficient [CCC (R)], Chi-square test (χ^2). As,

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(x_i - y_i)^2 \tag{4.2}$$

$$AARE = \frac{1}{N}\sum_{i=1}^{N}\left|\frac{(y_i - x_i)}{x_i}\right| \tag{4.3}$$

$$\sigma = \sqrt{\sum_{i=1}^{N}\frac{1}{N-1}\left[\left|\frac{(y_i - x_i)}{x_i}\right| - AARE\right]^2} \tag{4.4}$$

$$R = \frac{\sum_{i=1}^{N}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2 \sum_{i=1}^{N}(y_i - \bar{y})^2}} \tag{4.5}$$

$$\chi^2 = \sum_{i=1}^{N} \frac{(x_i - y_i)^2}{y_i} \tag{4.6}$$

The chi-square test was performed to find the best-fit network model when the values of cross-correlation coefficient are close to each other. The min value χ^2 give best model.

4.4 Prediction of Gas holdup

4.4.1 Input parameters are the physical and operating variables for prediction of gas holdup

Gas holdup is expressed as a function of liquid and gas physical properties, geometric variables of the system and dynamic variable. The operating variables include the gas flow rate (Q_g), Density of liquid (ρ_l), Surface tension of the liquid (σ_l), Consistency index (K), Flow behavior Index (n), Diameter of column (D_c), Gas-liquid mixture height in the column (H_m), Distributor hole diameter (D_n) and Taper angle (θ). The diameter of the column was calculated by first calculating the equivalent diameter of the base and at the gas-liquid interface then calculates the log mean diameter, D_c, of the column. Hence, for each gas flow rate the diameter, D_c, varies according to the height of the gas-liquid interface. For this system the optimum result was achieved using 2000 epochs for training. The gradual decrease of value of average MSE in this cases shows in Fig. 4.6 that the training in this cases are accurate. Also, Fig. 4.7 shows the training is good as CCC(R) in training is 0.99175.

Table 4.2 represents the performance of neural network for testing for different transfer functions used in the hidden layer after optimization. It is clear from this table that the cross-correlation coefficient [CCC (R)] value is greater than 0.97 for four different transfer functions used in the hidden layer. The low value of the average absolute relative error (AARE) also shows the accuracy of the result in this system. Because the cross-correlation coefficient value is greater than 0.97 for the entire best network, so the chi-square test was performed to find the best result. Table 4.3 contains the result for the chi-square test. The chi-square test confirms that the best network for prediction of gas holdup for tapered bubble column is the one that has the transfer function 1 with 14 processing elements in the hidden layer. This result indicates that the performance of the network output is excellent. Fig. 4.8 shows the comparison between the experimental to the predicted output. This comparison proves the effectiveness of the neural network analysis.

4.5 Prediction of frictional pressure drop

4.5.1 Input parameters are the physical and operating variables for prediction of frictional pressure drop

Frictional pressure drop is expressed as a function of liquid and gas physical properties, geometric variables of the system and dynamic variable. The operating variables include the gas flow rate (Q_g), Density of liquid (ρ_l), Surface tension of the liquid (σ_l), Consistency index (K), Flow behavior Index (n), Diameter of the column (D_c), Gas-liquid mixture height in the column (H_m), Distributor hole diameter (D_n), Gas hold up (ε_g) and Taper angle (θ) of the columns. The diameter of the column was calculated by first calculating the equivalent diameter of the base and at the gas-liquid interface then calculates the log mean diameter, D_c, of the column. Hence, for each gas flow rate the diameter, D_c, varies according to the height of the gas-liquid interface. The range of variables investigated and used as input variables in ANN is shown in Table 2.3.

For training the network 2000 epochs were used for each case. The gradual decrease of value of average MSE in this cases shows in Fig. 4.9 that the training in this cases are accurate. Also, Fig. 4.10 shows that the training is good as CCC(R) in training is 0.98512.

Table 4.4 represents the performance of neural network for testing for different transfer functions used in the hidden layer after optimization. This comparison proves the effectiveness of the neural network analysis. It is clear from this table that the cross-correlation coefficient [CCC(R)] value is greater than 0.97 for all four different transfer functions used in the hidden layer. The low value of the average absolute relative error (*AARE*) also shows the accuracy of the result in this system. Because the cross-correlation coefficient value is greater than 0.97 for the entire best network, so the chi-square test was performed to find the best result. Table 4.4 contains the result for the chi-square test. The minimum value of the chi-square in the chi-square test confirms the best network for prediction of frictional pressure drop for tapered bubble columns. The transfer function 4 with 25 processing elements in the hidden layer gives the best prediction. This result indicates that the performance of the network output is excellent. Fig. 4.11 shows the comparison between the experimental to the predicted output. This comparison proves the effectiveness of the neural network analysis.

4.6 Conclusions

A multilayer perceptron with backpropagation algorithm was used to predict the gas holdup and pressure drop in the present study. The ANN model accurately predicts the hydrodynamic parameters, gas holdup and pressure drop in the tapered bubble columns. All the transfer functions are predicted well but the chi-square test confirms that the transfer function 1 with 14 processing elements and the transfer function 4 with 25 processing elements in a hidden layer gives better predictability for gas holdup and pressure drop.

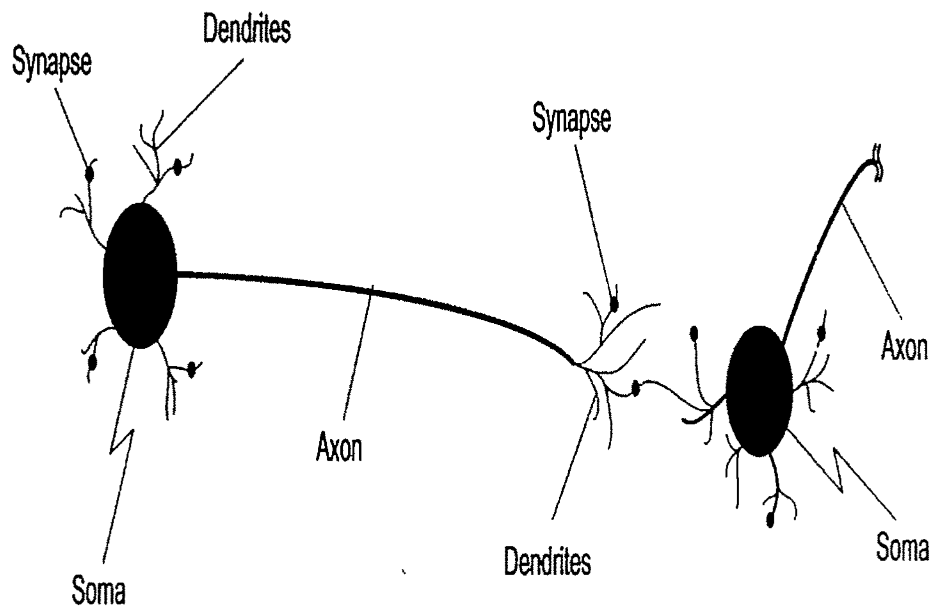

Fig. 4.1 Two interconnected brain cells (neurons)

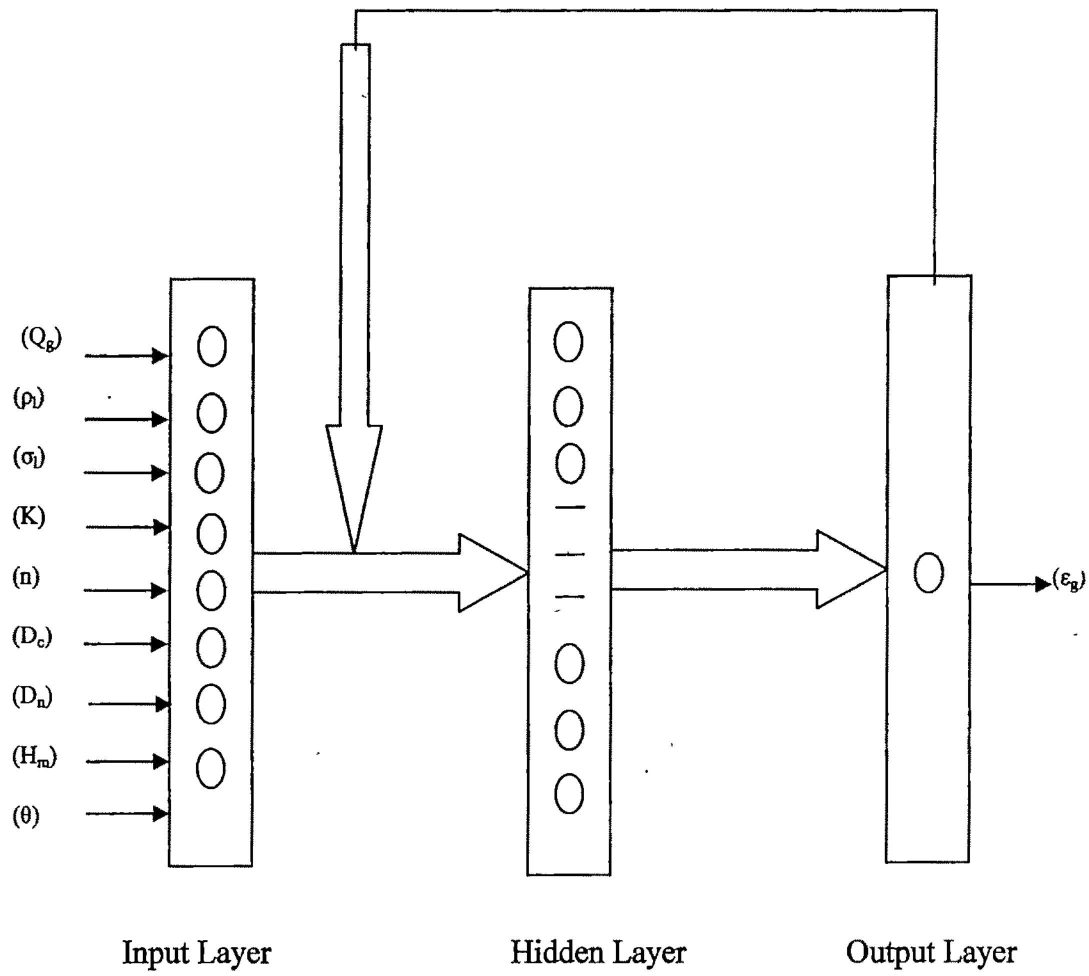

Fig. 4.2 Schematic diagram of neural network for gas holdup

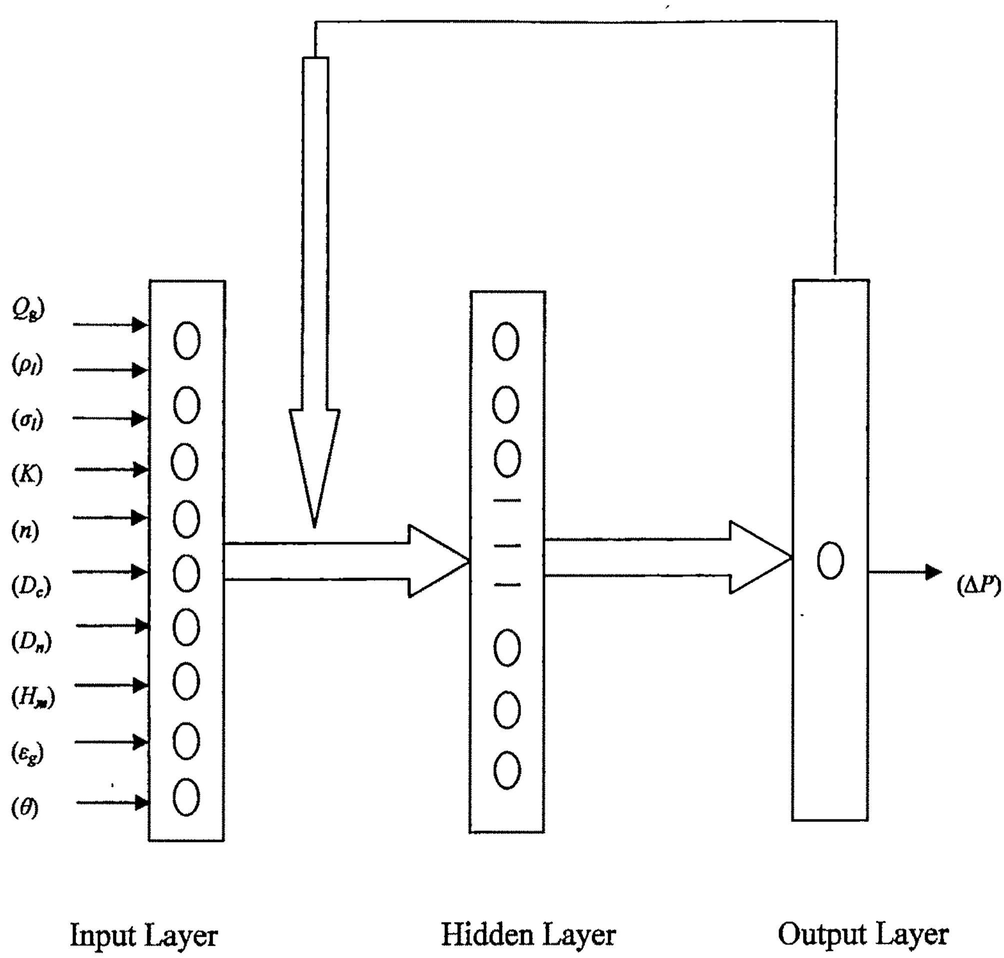

Fig. 4.3 Schematic diagram of neural network for pressure drop

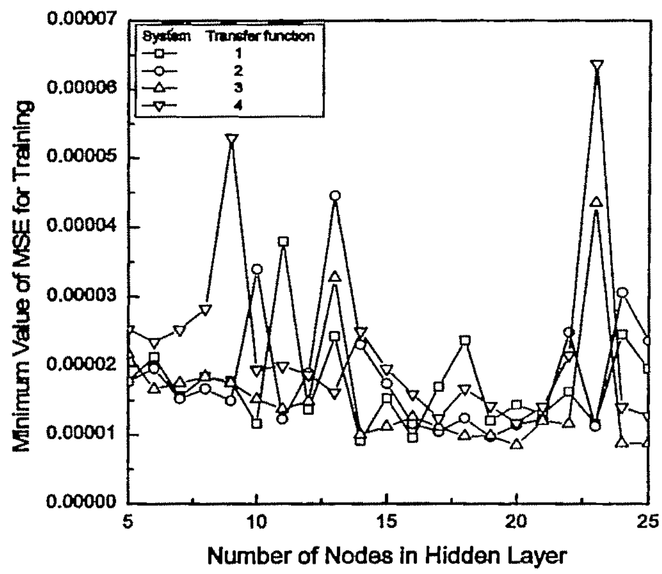

Fig. 4.4 Variation the minimum value of MSE with the number of nodes in a hidden layer for four different transfer functions for gas holdup

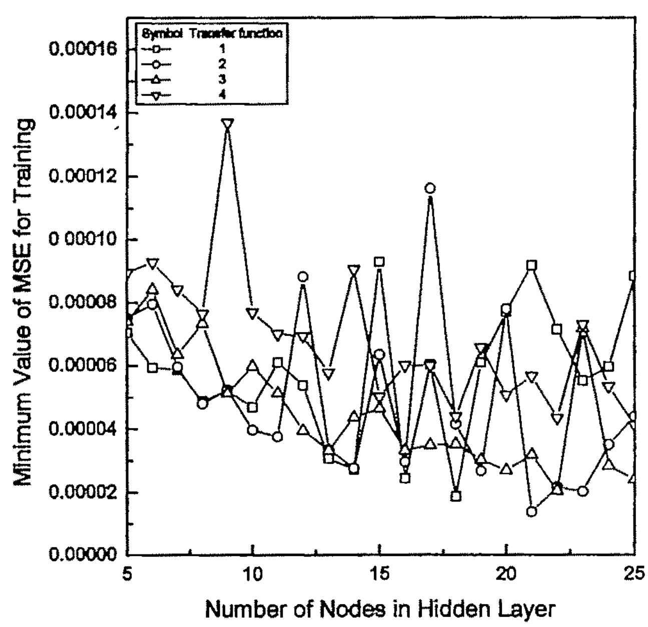

Fig. 4.5 Variation the minimum value of MSE with the number of nodes in a hidden layer for four different transfer functions for pressure drop

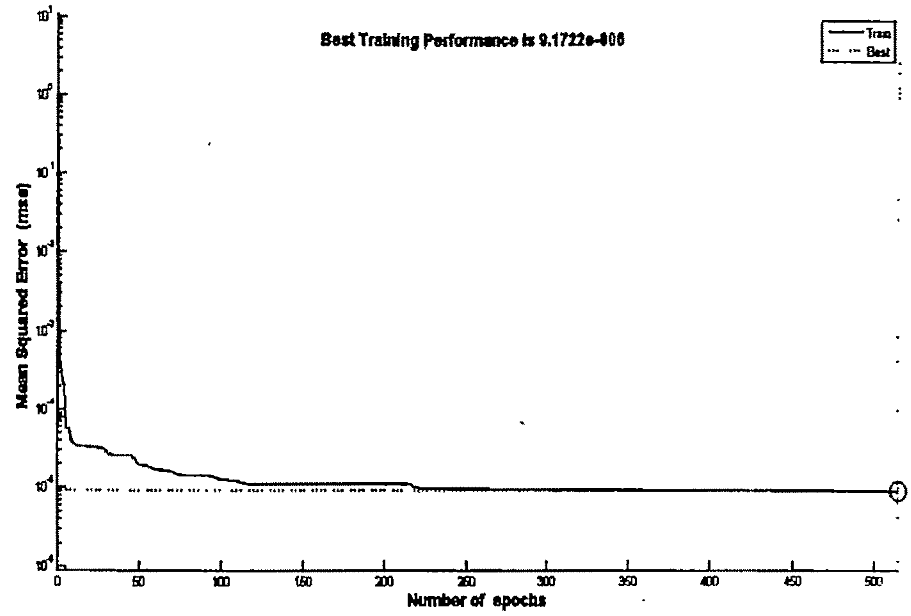

Fig. 4.6 Variation of the average MSE for training over 20 different runs vs the number of epochs for transfer functions 1 in the hidden layer for gas holdup

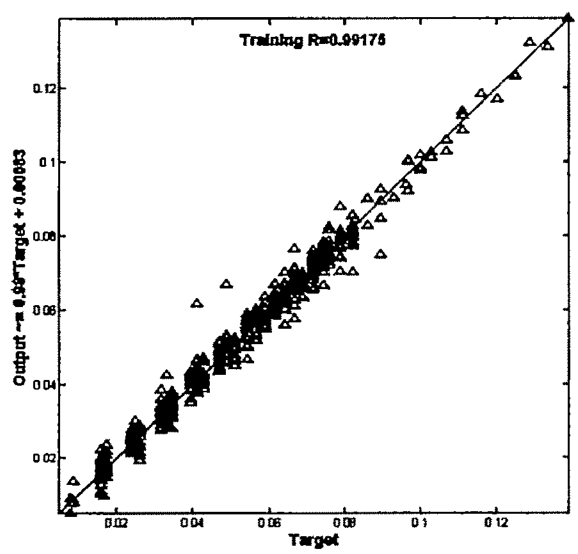

Fig. 4.7 Training curve for gas holdup

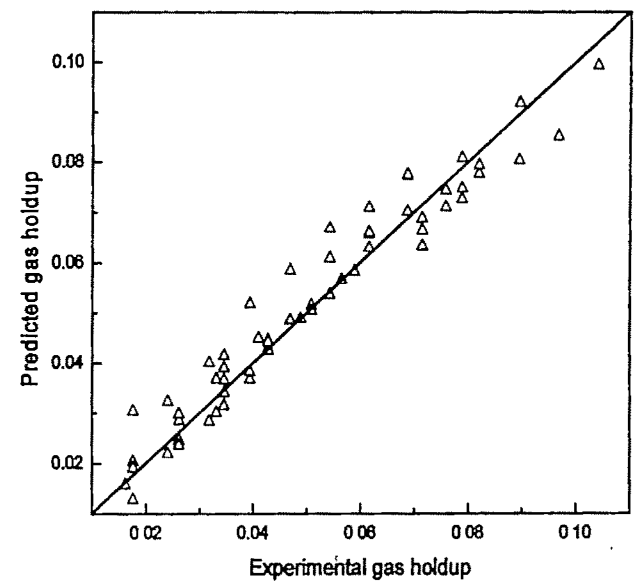

Fig. 4.8 Comparison of gas holdup for prediction by ANN

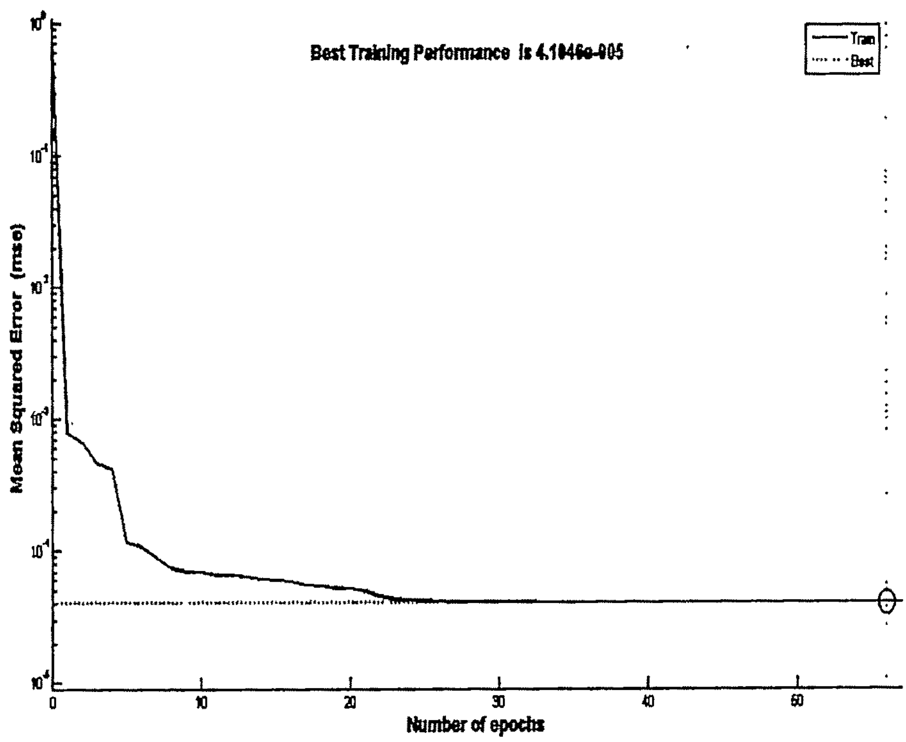

Fig. 4.9 Variation of the average MSE for training over 20 different runs vs the number of epochs for transfer functions 4 in the hidden layer for pressure drop

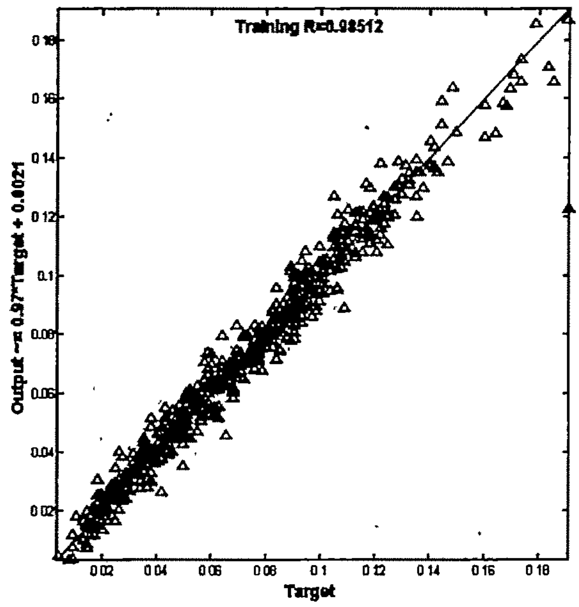

Fig. 4.10 Training curve for pressure drop

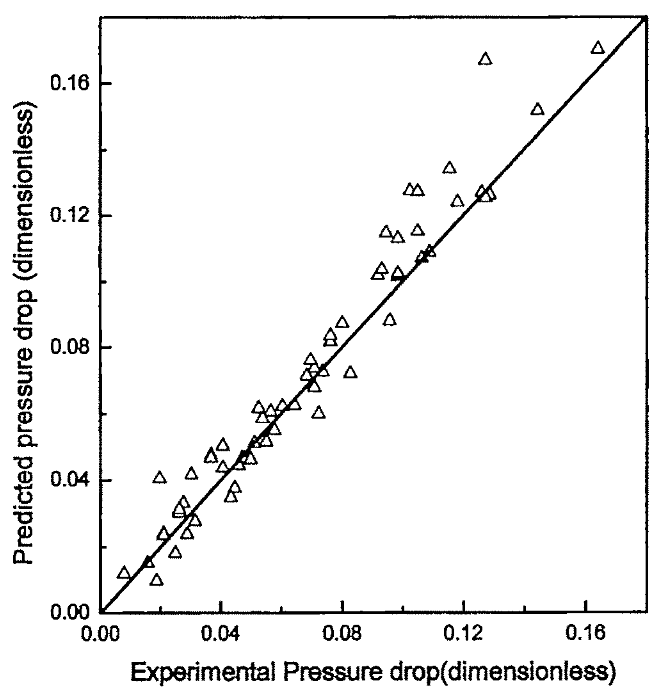

Fig. 4.11 Comparison of frictional pressure drop for prediction by ANN

Table 4.1 Comparison of biological neural networks and artificial neural networks

Biological Neural Networks	Artificial Neural Networks
Soma	Node
Dendrites	Input
Axon	Output
Synapse	Weight
Slow	Fast
Many neurons-10^9	Few neurons-100s

Table 4.2 Different activation function

Case	Name of activation function	Equation
Transfer function 1	tan hyperbolic function (tansig)	$y = \tanh(net)$
Transfer function 2	Logsigmoid function (logsig)	$y = \frac{1}{(1+\exp(-net))}$
Transfer function 3	Radial basis function (radbas)	$y = \exp(-net^2)$
Transfer function 4	Triangular basis function (tribas)	$y = 1 - abs(net)$ if -1≤(net)≤1 $y = 0$ otherwise
Transfer function 5	Linear function (purelin)	$y = (net)$

Where y is the output from node and net is the input to the node.

Table 4.3 Performance of best neural network for testing in gas holdup

Measurement type	Transfer function 1	Transfer function 2	Transfer function 3	Transfer function 4
AARE	**0.1001**	0.095332	0.100901	0.120589
SD(σ)	**0.11425**	0.114004	0.10781	0.10925
MSE	**0.0000288693**	0.0000276932	0.0000440029	0.10925
CCC(R)	**0.97284**	0.9713	0.97441	0.95798
χ^2	**0.035501**	0.03953	0.035601	0.049578
Optimum no. of processing elements in hidden layer	**14**	19	20	20

Table 4.4 Performance of best neural network for testing in pressure drop

Measurement type	Transfer function 1	Transfer function 2	Transfer function 3	Transfer function 4
AARE	0.12174	0.12295	0.13355	**0.14057**
SD(σ)	0.15715	0.13625	0.14514	**0.16194**
MSE	0.00007227	0.00019867	0.00009939	**0.000101006**
CCC(R)	0.96975	0.96244	0.97505	**0.97548**
χ^2	0.08607	0.09771	0.08870	**0.08258**
Optimum no. of processing elements in hidden layer	18	21	22	**25**