A
Project Report on

Application of ANN in predicting VLE data of CO_2-Aqueous-Alkanolamine System

In partial fulfillment of the requirements of

Bachelor of Technology
(Chemical Engineering)

Submitted By

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CERTIFICATE

This is to certify that that the work in this report entitled "Application of ANN in predicting VLE data of CO_2-Aqueous-Alkanolamine System" submitted by Deepak Ranjan Rout in partial fulfillment of the requirements for the degree of Bachelor of Technology in Chemical Engineering Session 2004-2008 in the department of Chemical Engineering, National Institute of Technology Rourkela, Rourkela is an authentic work carried out by him under my supervision and guidance. To the best of my knowledge the matter embodied in the thesis has not been submitted to any other University /Institute for the award of any degree.

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ABSTRACT

The removal of acid gases from gas streams by using suitable solvent like alkanolamine, commonly referred to as gas sweetening, is a technology that has been in use industrially for over half a century. For the rational design of gas treating processes the equilibrium solubility of acid gases like CO_2 and H_2S over alkanolamines (vapour-liquid equilibrium of the acid gases over alkanolamines) are essential besides the mass transfer and chemical kinetics. Representation of the experimental data with model is required, so that one can systematically correlate and predict the vapour-liquid equilibria (VLE) of these systems. In this work artificial neural network (ANN) has been used to predict the equilibrium solubility of CO_2 over the alkanolamine solvents like mono-ethanolamine(MEA), di-ethanolamine (DEA) and Piperazine (PZ) instead of using any rigorous thermodynamic model. A feed forward network with back propagation and a radial basis network have been used here in an effort to predict the VLE data of CO_2-MEA-water, CO_2-DEA-water and CO_2-Piperazine-water systems with a comparable accuracy to those predictions based on rigorous thermodynamic model. It has been found that the predictions are within accuracy of ±5%.

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Chapter 1

Introduction

1.1 Acid gas treating and Vapour-liquid equilibria

Removal of acid gas impurities such as carbon dioxide (CO_2), carbonyl sulfide (COS), and hydrogen sulfide (H_2S) from gas streams is a very important operation for natural gas processing, oil refineries, ammonia manufacture, coal gasification, and petrochemical plants. Many commercial gas-treating processes are still designed by experience and heuristics resulting in over design and excessive energy consumption. CO_2 and H_2S concentrations in the sour gas streams may vary widely, from several parts per million to 50% by volume of the gas streams. These impurities when present in the gas streams may lead to very serious problems in pipeline transportation and downstream processing of the gas. Some of the CO_2 is often removed from natural gas because at high concentrations it reduces the heating value of the gas and it is costly to compress this extra volume for pipeline transportation of natural gas. A wide variety of alkanolamines like mono ethanolamine (MEA), di ethanolamine (DEA), *N*-methyl diethanolamine (MDEA) and blended amine solvents are used for gas treating. The removal of acid gases by absorption into aqueous alkanolamines, falls under the category of regenerative chemical absorption into liquid, characterized as mass transfer enhanced by chemical reaction. Approximately 90% of the acid gas treating processes in operation today uses alkanolamine solvents because of their versatility and their ability to remove acid gases to very low levels.

For the rational design of gas treating processes knowledge of vapour liquid equilibrium of the acid gases in alkanolamines are essential, besides the knowledge of mass transfer and kinetics of absorption and regeneration. Moreover, equilibrium solubility of the acid gases in aqueous alkanolamine solutions determines the minimum recirculation rate of the solution to treat a specific sour gas stream and it determines the maximum concentration of acid gases which can be left in the regenerated solution in order to meet the product gas specification. One of the drawbacks of the conventional equilibrium stage approach to the design and simulation of absorption and stripping is that, in practice absorbers and strippers often do not approach equilibrium conditions. A better approach to design such non-equilibrium processes (mass transfer operation enhanced by chemical reaction) is by the use of mass and heat transfer rate based models. However, phase and chemical equilibria continue to play important roles in a rate-based model by providing boundary conditions to partial differential equations describing mass transfer coupled with chemical reaction. Accurate speciation of the solution is an integral part of

the equilibrium calculations required by the rate-based models. There is a need for the available data of acid gas-alkanolamine-water systems to be correlated so that the solubility predictions can be made confidently where data do not exist or where they are of poor precision. Therefore a robust model at all possible combination of temperature, amine concentration, and acid gas loading is needed. Besides thermodynamic modelling, the applicability of ANN based models can also be explored. The high cost of development and validation and large CPU time associated with complex numerical simulations have accelerated the endeavour to search for an alternative tool for VLE prediction instead of rigorous thermodynamic modelling.

Conventional thermodynamic approach to predicting VLE data of acid gas-alkanolamine systems is based on 'activity coefficient' based models, hence, encourages a certain amount of empiricism and assumptions regarding the various interaction parameters. ANN process models extract the desired information directly from data, thus becomes cost effective. They are time saving too, as instead of rigorous thermo-dynamic models, prediction can be done easily and accurately using computers. Hence this very futuristic topic with vast application in the chemical industry was undertaken as a project. In the present work, for a wide range of temperature, partial pressure of CO_2 and for a wide range of concentration of MEA, DEA and Piperazine solvents, the equilibrium liquid phase CO_2 loading have been predicted based on ANN model. Also based on loading, temperature and concentration values, partial pressure has also been predicted fairly accurately.

1.2 Artificial Neural Networks

Before using ANN to predict the VLE data, it is essential to know what a neural network is. A neural network is a powerful data modeling tool designed on the basis of the human brain. It resembles the human brain in that it acquires knowledge through learning. This knowledge is stored within inter-neuron connection strengths known as synaptic weights. The advantage of neural network is its ability to represent both linear and non-linear mathematical relationships and learn these relationships directly from given data. A neuron is the basic building block of a neural network.

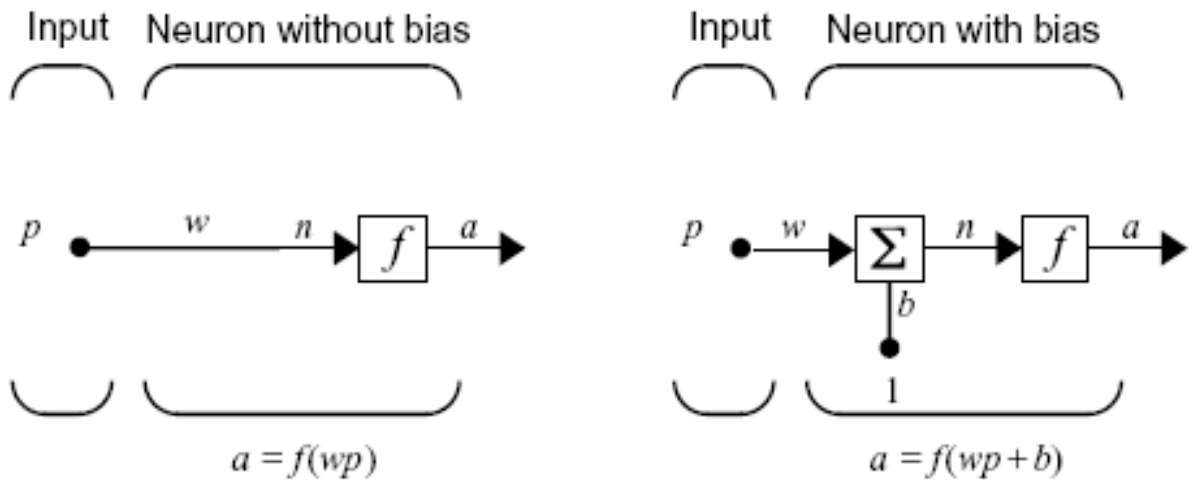

Figure 1.1 A neuron with and without bias

Figure 1.1 shows a simple neuron. It consists of an input signal *p*, which is connected to a transfer function *f* via a synaptic space signified by *w*. The output of the network is given by *a*. In a neuron with bias, the input *b* is connected directly to the transfer function *f*. Thus in this case, the whole input is presented by *wp+b*. This is the basic structure of a neuron. The input signals like *p* are connected to a neuron via adjustable weights *w*. *b* signifies the variable bias of a neuron. Thus when a network is trained, these weights and biases keep on getting automatically adjusted as the training goes on. On the completion of training, these networks can predict on the basis of these adjusted weights and biases. The best part is that these weights and biases are self-adjustable as per the training.

'f ' in above figure signifies the transfer functions. The result produced by a neural network on training is due to the transfer functions used. Following are the transfer functions generally used in a neural network.

1. Hard-limit transfer function.
2. Linear transfer function.
3. Tan-sigmoid transfer function.
4. Log-sigmoid transfer function

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In the current work, only tan-sigmoid transfer function has been used as the data is normalized and for normalized data, only tan-sig function can be used. A perceptron neuron has more than

one input. A perceptron neuron, which uses the hard-limit transfer function is shown below. It has R no. of input signals.

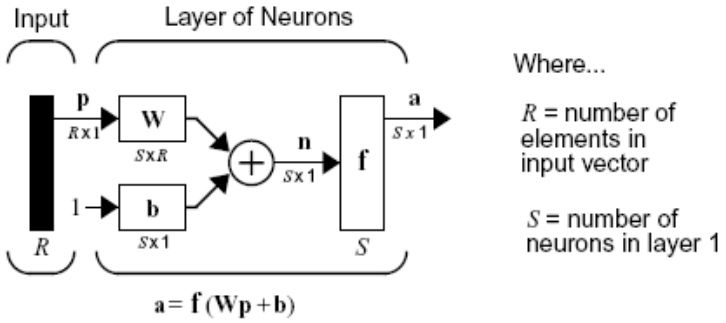

Figure 1.2 A Perceptron.

In this project we have used two types of networks. They are:

1. Feed-forward networks with back propagation
2. Radial basis networks

1.2.1. Feed-forward networks

A number of perceptrons connected together as in figure 1.3 form a single layer of feed-forward network.

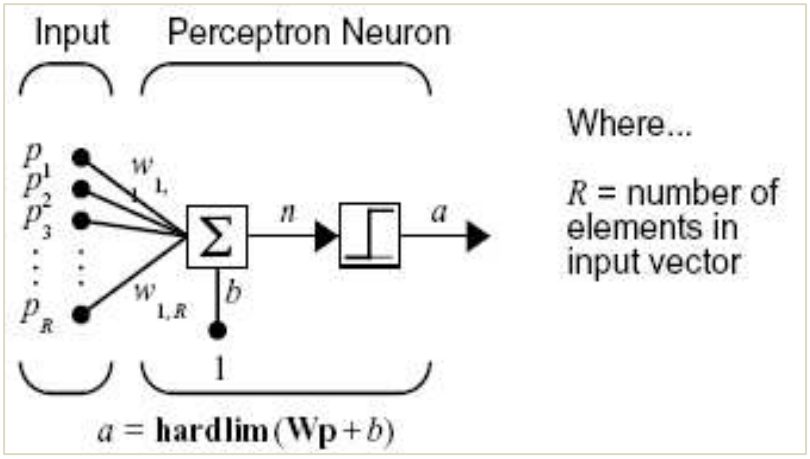

Figure 1.3 Feed forward network with perceptrons

Here R input signals are connected to S number of neurons, each via its own weight. This is the example of a single layer of feed-forward network. A feed-forward network can have more than one layer as shown in figure 1.4. In that case, the last layer consists of only linear transfer functions and is known as output layer. All other layers are known as hidden layers. The number of neurons in each hidden layer, as well as the number of hidden layers has a profound effect on the output of a feed-forward network.

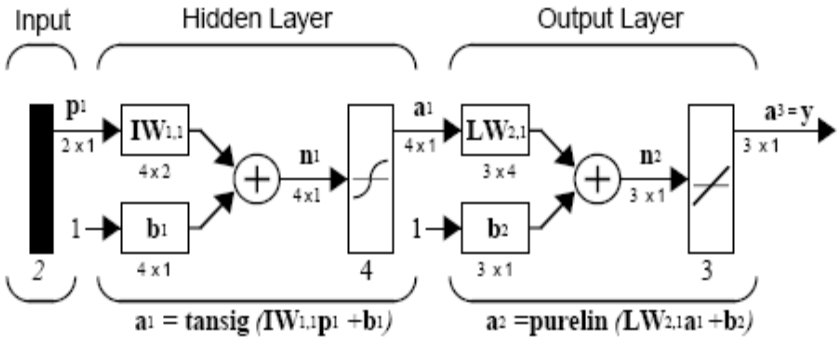

Figure 1.4 Multilayer feed forward network

There are 3 steps in designing a feed-forward network:

1. Creating a network.
2. Training a network.
3. Simulating a network.

For training a network using back-propagation algorithm the commonly used inbuilt MATLAB functions are train, traingd, traingda, trainrp. There is also different performance parameters used while training a network using MATLAB simulator like epochs, show, goal, time, min grad etc. Even though a number of techniques have been present for network topology selection, it still remains an iterative trial and error procedure (Sharma et al., 1999). Sharma et al., to reduce this trial and error selection process, used one heuristic approach. They determined the optimum architecture within 50-100 iterations without traversing the entire graph of absolute error as a function of the number of iterations for each topology. In this work the optimum architecture evolved out through an elaborate trial and error procedure. After a network has been created and trained with an optimal number of data, the network can be used to simulate unknown inputs to predict the result.

1.2.2 Radial basis networks

A Radial Basis Function (RBF) neural network has an input layer, one or more hidden layers and an output layer. The neurons in the hidden layer contain Gaussian transfer functions whose outputs are inversely proportional to the distance from the center of the neuron.

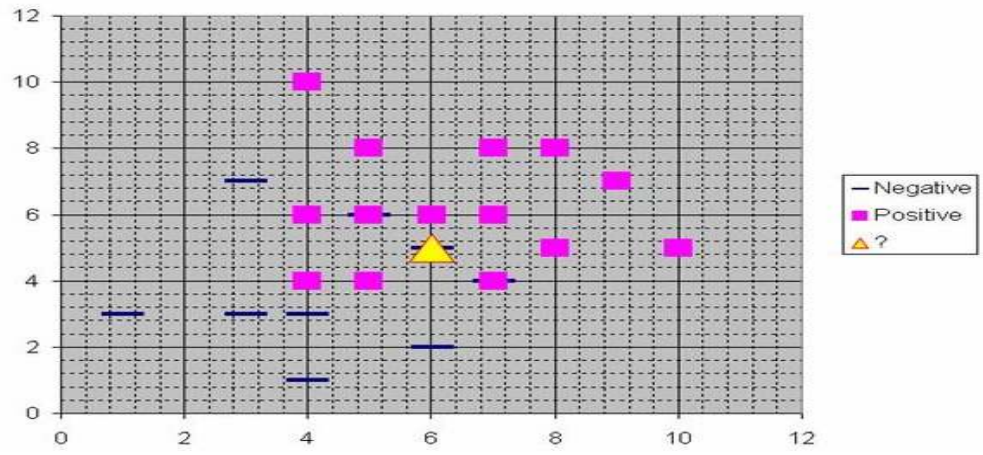

Figure 1.5 Prediction based on Clustering in radial basis network

A radial basis network works on the concept of clustering. The basic idea is that a predicted target value of an item is likely to be about the same as other items that have close values of the predictor variables. Assuming that each case in the training set has two predictor variables, *x* and *y*. The cases are plotted using their *x, y* coordinates as shown in the figure 1.5. Suppose we are trying to predict the value of a new case represented by the triangle with predictor values *x*=6, *y*=5.1. An RBF network positions one or more RBF neurons in the space described by the predictor variables (x,y in this example). This space has as many dimensions as there are predictor variables. The Euclidean distance is computed from the point to be evaluated (e.g., the triangle in this figure) to the center of each neuron, and a radial basis function (RBF) (also called a kernel function) is applied to the distance to compute the weight (influence) for each neuron. The radial basis function is so named because the radius distance is the argument to the function. The radial basis function for a neuron has a center and a radius (also called a spread). The radius may be different for each neuron. The further a neuron is from the point to be evaluated, the less influence it should have in prediction. The best predicted value for the new point is found by

summing the output values of the RBF functions multiplied by weights computed for each neuron. For a radial basis network, the parameters used for training are 'goal' and 'spread'.

In this project, both feed-forward with back propagation and radial basis networks have been used for theVLE prediction of the following three systems

1. MEA+water+CO_2 system
2. DEA+water+CO2 system
3. Piperazine+water+CO_2 system

1.3 Previous work

There are a few reported applications of ANN in VLE predictions (Naidu, 2004; Mehmet, 2004; Scalabrin *et al*., 2000; Sharma et al., 1999; Petersen et al., 1994). Chattopadhyay et. al. (2006) successfully predicted equilibrium solubility of CO_2 over aqueous MDEA and AMP solvent.

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Chapter 2

(MEA+Water+CO_2) System

Monoethanol amine (MEA) being a primary alkanolamine shows an equilibrium loading capacity of 0.5 moles of CO_2 per moles of amine at a fastest rate among all the alkanolamines. These days MEA being used as an accelerator in the blended alkanolamine solvents for its highest rate of absorbing CO_2. In view of this, correlation and prediction of VLE for (MEA+water+CO_2) system by ANN may be a useful and alternative tool.

For this system the training data set consists of total of 256 numbers of data and the simulation is done on 6 different data sets from different literature sources, which are shown in Table 2.1.

Data Type	No of Data	Literature Sources
Training Data	256	[1]
Simulation data	8,10,8,5,17,48	[2],[3],[4],[5],[6],[7]

Table 2.1 Data used in training and simulation for (MEA+water+CO_2) system

2.1 Prediction of Equilibrium Partial Pressure of CO_2

In predictionof equilibrium partial pressure of carbon dioxide, loading (moles of CO_2 per mole of amine solvent), temperature and alkanolamine concentration are used as the inputs and the partial pressure is predicted. Equilibrium partial prediction has been done using feed-forward networks and radial basis networks.

2.1.1 Feed-forward networks

For equilibrium partial pressure prediction of CO_2 in aqueous MEA system using FF networks, two types of networks have been designed. One uses TRAINGDA function for training the network while the other one uses TRAINRP function. This helps in comparison between them to find the better designed network for accurate equilibrium CO_2 partial pressure prediction. The network configurations along with the training performance of the networks using TRAINGDA and TRAINRP are shown in the Tables

2.2 and 2.3, respectively. The corresponding simulation results are shown in Tables 2.4 and 2.5 respectively.

Data Source	Temp (K)	No. of Data	No.of Neurons	Epochs	Mean square error (MSE)	Time (Sec)	No of hidden layer
[1]	313-393	256	5	5000	0.0057	17.5	1

Table 2.2 Network configuration using 'TRAINGDA' in equilibrium CO_2 partial pressure prediction

Data Source	Temp (K)	No. of Data	No.of Neurons	Epochs	Mean Square Error (Mse)	Time (Sec)	No of hidden layer
[1]	313-393	256	8	8000	0.0003770	27.313	1

Table 2.3 Network configuration using 'TRAINRP' in equilibrium CO_2 partial pressure prediction.

Data Source	Temp (K)	No. of Data Points	Aad%**
[2]	313	8	0.959
[3]	313	10	1.499
[4]	313	8	2.195
[5]	373	5	3.45
[6]	313-393	17	1.846
[7]	313-393	48	4.15

$$\text{AAD\%}=\left[\sum_{n}\left(p_{cal}-p_{exp}\right)/p_{exp}\right]/n\times 100 = \text{Average Absolute Deviation Percentage.}$$

Table 2.4 Simulation results using 'TRAINGDA' in in equilibrium CO_2 partial pressure prediction

Data Source	Temp (K)	No. of Data Points	Aad**
[2]	313	8	0.523
[3]	313	10	1.297
[4]	313	8	0.8031
[5]	373	5	4.8308
[6]	313-393	17	3.104
[7]	313-373	48	5.27

Table 2.5 Simulation results using 'TRAINRP' in in equilibrium CO_2 partial pressure prediction

From the simulation results of the two networks we find that the network using TRAINGDA is better for this particular case as it uses lesser number of epochs and takes lesser computation time to predict the VLE quite accurately (Less than 4 % AAD) in comparison to the network using TRAINRP. Figures 2.1 and 2.2 shows the training performance of the TRAINGDA and TRAINRP networks for partial pressure prediction.

2.1.2 Radial basis networks

To predict the VLE of (MEA+water+CO_2) system using radial basis networks, the designed network uses NEWRB function for training with a spread of 0.4373. The goal or target error is set as 10^{-3}. The result of simulation is shown in Table 2. 6. Figure 2.4 shows the training performance of radial basis network for (MEA+water+CO_2) system.

Data Source	Temp (K)	No. of Data	Mean Square Error	Time (Sec)	AAD%
[2]	313	8	0.00488	4.515	0.3065
[3]	313	10	0.00488	4.563	0.7009
[4]	313	8	0.00488	4.766	0.1412
[5]	373	5	0.00488	4.672	3.3764
[6]	313-393	17	0.00488	4.594	2.8744
[7]	313-373	48	0.00488	4.797	0.5630

Table 2.6 Simulation results using radial basis network in in equilibrium CO_2 partial pressure prediction

It is evident that the radial basis network is fairly accurate showing an average absolute deviation percentage of about 3%. It is better than the feed-forward network with respect to computation time as its execution time is 4-5 secs compared to 17-18 secs for feed-forward network with back propagation training algorithm.

2.2 Prediction of equilibrium CO_2 loading

In prediction of equilibrium loading of CO_2, partial pressure, temperature and concentration are used as inputs and the equilibrium loading of CO_2 is predicted. Equilibrium loading prediction has been done using only feed-forward network. For (MEA+water+CO_2) system using FF networks, two networks have been designed for this purpose. One uses TRAINGDA function for training the network while the other one uses TRAINRP function. This helps in comparison between them to find the better-designed network towards predicting the equilibrium loading of CO_2 in aqueous MEA system. The network configurations using TRAINGDA and TRAINRP along with the training performance of the networks are shown in the Tables 2.7 and 2.8, respectively. The corresponding simulation results are shown in Tables 2.9 and 2.10 respectively.

Data Source	Temp (K)	No. of Hidden Layers	No. Of Data	No.of Neurons	Epochs	Mse	Time (Sec)
[1]	313-393	2	256	6+4	5000	0.008	22.844

Table 2.7 Network configuration using 'TRAINGDA' in equilibrium CO_2 loading prediction

Data Source	Temp (K)	No. of Hidden Layers	No of Data	No.of Neurons	Epochs	MSE	Time (Sec)
[1]	313-	2	256	5+9	9000	0.00111	50.453

Table 2.8 Network configuration using 'TRAINRP' in equilibrium CO_2 loading prediction

Data Source	Temp (K)	No. of Data	AAD%
[2]	313	8	7.32
[3]	313	10	4.08
[4]	313	8	4.62
[5]	373	5	6.82
[6]	313-393	17	6.344
[7]	313-373	48	7.117

$$AAD\% = \left[\sum_{n} \left(p_{cal} - p_{exp} \right) / p_{exp} \right] / n \times 100$$

Table 2.9 Simulation results using 'TRAINGDA' in equilibrium CO_2 loading prediction

Data Source	Temp (K)	No. of Data Points	AAD%
[2]	313	8	2.158
[3]	313	10	1.782
[4]	313	8	2.289
[5]	373	5	1.387
[6]	313-393	17	2.503
[7]	313-373	48	4.435

Table 2.10 Simulation results using 'TRAINRP' in equilibrium CO_2 loading prediction

A comparison of hidden layer sensitivity using 'TRAINRP' is shown in Table 2.11. Using 2 hidden layers improved the predictions substantially. Figure 2.3 shows the training performance of TRAINRP network for equilibrium loading prediction.

Data Source	AAD%			
	2 LAYER(5,9)	1 LAYER (5 neurons)	1 LAYER (10 neurons)	1 LAYER (15 neurons)
[2]	2.158	8.092	7.748	9.466
[3]	1.782	6.368	7.973	6.096
[4]	2.289	6.394	4.118	4.844
[5]	1.387	6.318	20.136	2.87
[6]	2.503	11.756	14.641	15.544
[7]	4.435	8.992	8.702	8.526

Table 2.11 Hidden layer sensitivity of TRAINRP network in equilibrium CO_2 loading prediction using 9000 epochs

Conclusions

From the above comparison we find that the error percentage reduces appreciably for a 2 hidden layer network as compared to a 1 hidden layer network. Hence, for equilibrium CO_2 loading prediction using 'TRAINRP'as well as 'TRAINGDA', we have used a 2-layer network. It is evident from the above studies that the TRAINGDA network takes lesser time for computation but with higher error percentage in its prediction ability than the network using TRAINRP. Hence, It can well be concluded that between the two networks the TRAINRP network is preffered for prediction of equilibrium loading of CO_2.

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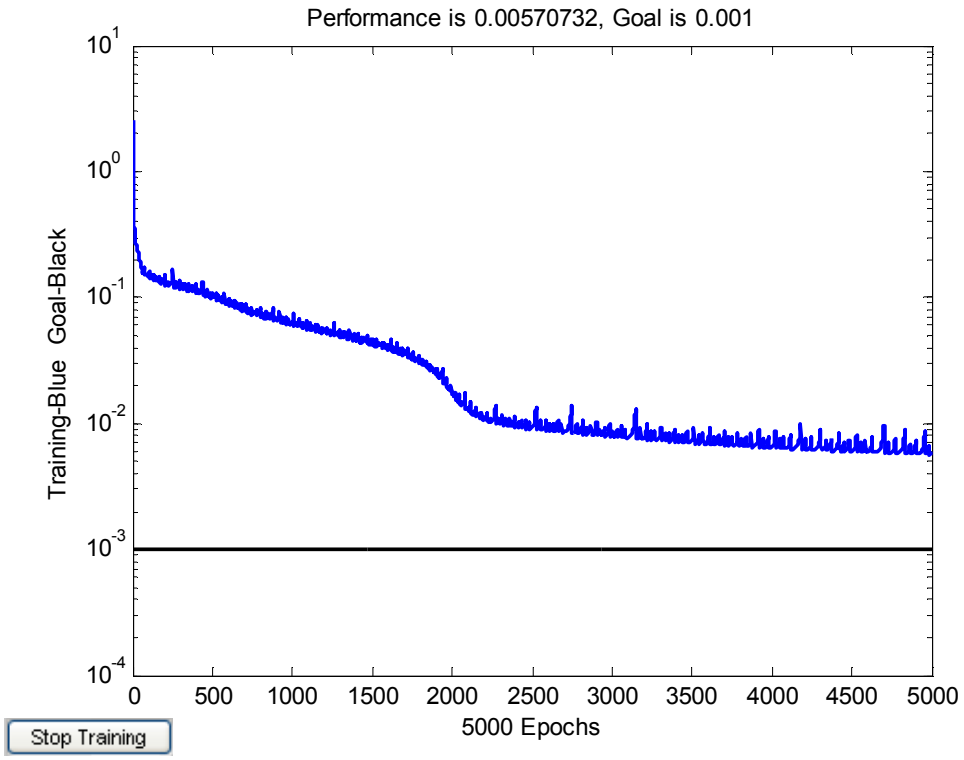

Figure 2.1 Training performance of feed forward TRAINGDA network in equilibrium CO_2 partial pressure prediction.

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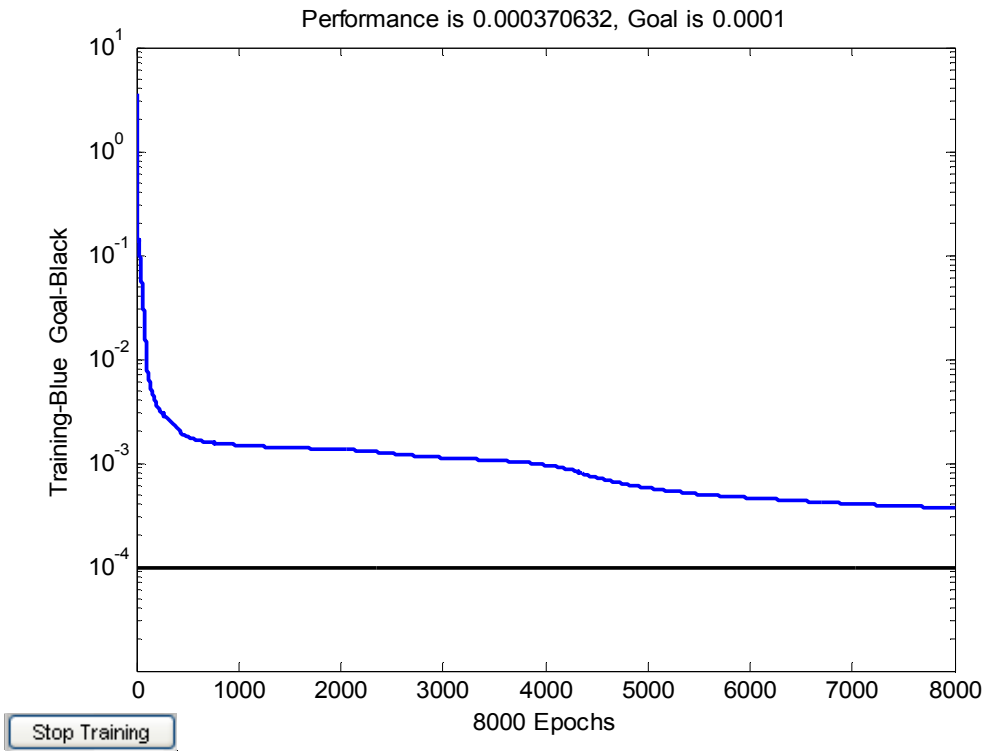

Figure 2.2 Training performance of feed forward TRAINRP network in equilibrium CO_2 partial pressure prediction.

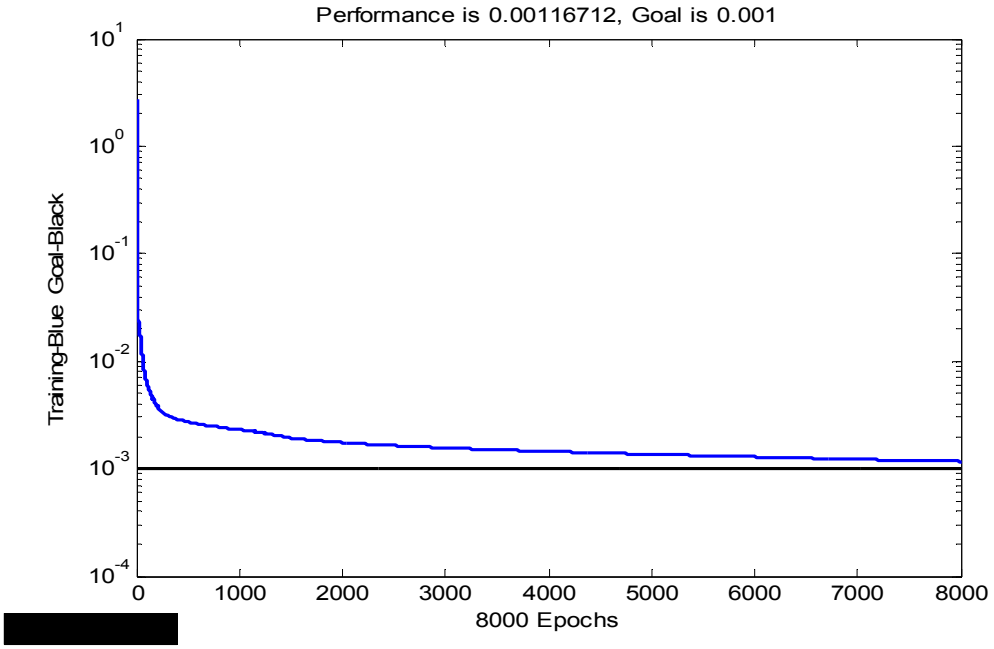

Figure 2.3 Training performance of feed forward TRAINRP network for prediction of equilibrium loading of CO_2.

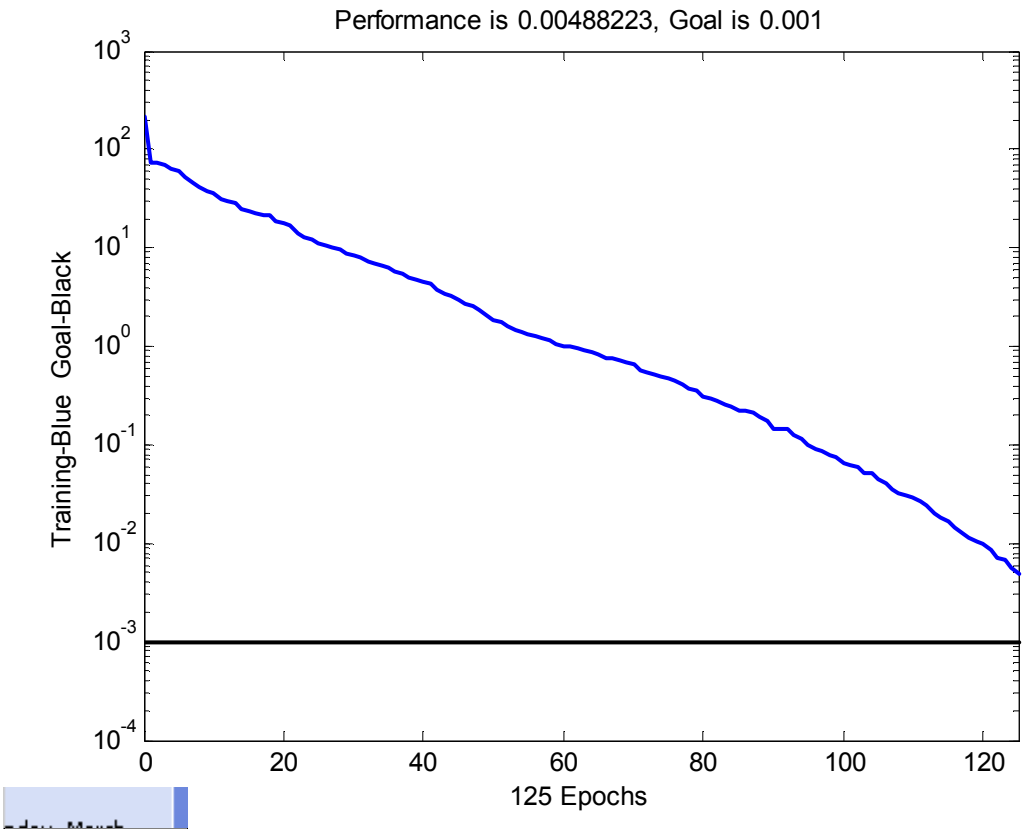

Figure 2.4 Training performance of radial basis network for prediction of equilibrium partial pressure of CO_2.

Chapter 3

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(DEA+water+CO_2) system

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Diethanolamine being the secondary amine is used extensively for acid gas treating processes for its lower vapor pressure, higher equilibrium loading and higher corrosion resistance than in comparison to MEA. These days it is being used in blended alkanolamine solvent preparation.

For this system the training data set consists of total of 292 numbers of data and the simulation is done on 4 different data sets from different literature sources, which are shown in Table 3.1.

Data Type	No of Data	Literature Sources
Training Data	292	[1]
Simulation data	8,10,8,5,17,48	[2],[3],[4],[5]

Table 3.1. Data used in training and simulation for (DEA+water+CO_2) system

3.1 Prediction of Equilibrium Partial Pressure of CO_2

In prediction of equilibrium partial pressure of carbon dioxide, loading (moles of CO_2 per mole of solvent), temperature and concentration are used as the inputs and the partial pressure is predicted. Equilibrium partial pressure prediction has been done using feed-forward networks and radial basis networks.

3.1.1 Feed-forward networks

For equilibrium partial pressure prediction of (DEA+water+CO_2) system using FF networks the network uses TRAINRP function. The network configuration along with the training performance of the network using TRAINRP is shown in the Tables 3.2. The corresponding simulation result is shown in Table 3.3.

Data Source	Temp (K)	No. of Data	No of hidden layers	No. of neurons	Epochs	Mean Square Error (MSE)
[1]	273-393	292	2	4+7	8000	0.00219

Table 3.2 Network configuration using 'TRAINRP' in equilibrium CO_2 partial pressure prediction

Data Source	Temp (K)	No. Of Data	AAD%**	Time(Sec)
[2]	313	25	0.291	42.891
[3]	313-353	13	1.239	42.063
[4]	310.928-	29	4.496	42.953
[5]	373	6	14.620	38.562

$$AAD\% = \left[\sum_{n} \left(p_{cal} - p_{exp} \right) / p_{exp} \right] / n \times 100 = \text{Average Absolute Deviation Percentage}$$

Table 3.3. Simulation results using 'TRAINRP' in equilibrium CO_2 partial pressure prediction

The results obtained are quite good with error within 4 %age except for the data set from Olukayode and Meisen data. Figure 3.1 shows the training performance of the network using TRAINRP function for equilibrium CO_2 partial pressure prediction.

3.1.2 Radial basis networks

To predict the equilibrium partial pressure of carbon dioxide in (DEA+water+CO_2) system using radial basis networks, the designed network uses NEWRB function for training with a spread of 0.32. The goal or target error is set as 10^{-3}. The result of simulation is shown in Table 3. 4.

Data Source	Temp (K)	No. of Data Points	Spread	MSE	AAD%	Time (Sec)
[2]	313	25	0.32	0.00087	0.9102	10.047
[3]	313-353	13	0.32	0.00087	2.9281	10.828
[4]	310.928-	29	0.32	0.00087	5.0181	11.172
[5]	373	6	0.32	0.00087	16.7131	10.797

Table 3.4 Simulation results using radial basis network in equilibrium CO_2 partial pressure prediction.

On comparison between the results for feed-forward network and radial basis network, we find that the error is almost identical for both. However, the time required by radial basis network is

only about 10-11 secs whereas feed-forward network takes about 40-42 sec. Thus the radial basis network may be a preferred one. Figure 3.2 shows the training performance of the radial basis network for equilibrium CO_2 partial pressure prediction.

3.2 Prediction of Equilibrium CO_2 Loading

In prediction of equilibrium CO_2 loading, partial pressure, temperature and concentration are used as inputs sets and the CO_2 loading is predicted. Equilibrium CO_2 loading prediction has been done using only feed-forward network. It uses TRAINGDA function for training the network. The network configuration using TRAINGDA along with the training performance of the network is shown in the Tables 3.5. The corresponding simulation result is shown in Table 3.6.

Data Source	Temp (K)	No. of Data	No of hidden layers	No. of neurons	Epochs	Mean Square Error (MSE)
[1]	273-393	292	2	3+3	3000	0.00829

Table 3.5. Network configuration using 'TRAINGDA' in prediction of equilibrium CO_2 loading.

Data Source	Temp (K)	No. of Data Points	AAD%**	Time (Sec)
[2]	313	25	18.016	42.891
[3]	313-353	13	7.959	42.063
[4]	373	6	6.920	38.562
[5]	310.928-380.372	29	4.514	42.953

Table 3.6. Simulation results using 'TRAINGDA' in prediction of equilibrium CO_2 loading.

The results show the error percentage, which is appreciably high with ANN irrespective of the type of the network being used. In prediction of equilibrium CO_2 loading, use of TRAINRP shows a higher AAD % than in comparison to TRAINGDA network. Figure 3.3 shows the training performance of the network using TRAINGDA function for equilibrium CO_2 loading prediction.

Conclusions

For equilibrium partial pressure prediction, we find that using feed-forward network shows la better performance than radial basis network. However radial basis network requires comparatively lesser computation time than the feed-forward network. Hence both the networks can be used for partial pressure prediction. For the equilibrium loading prediction the ANN, irrespective of the type of the network could not predict within 5% AAD, a desirable range.

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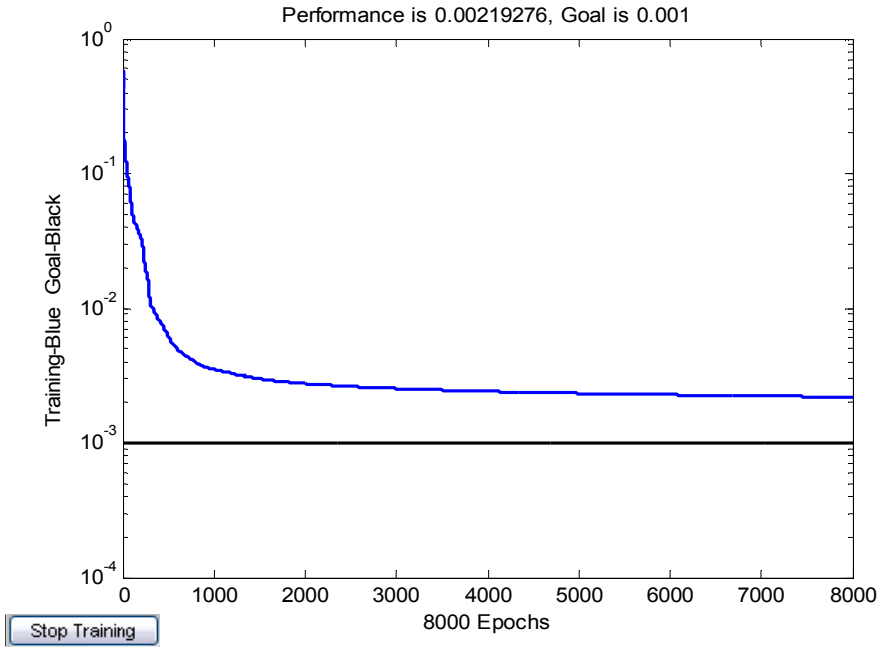

Figure 3.1 Training performance of feed forward TRAINRP network in equilibrium CO_2 partial pressure prediction (DEA+water+CO_2) system.

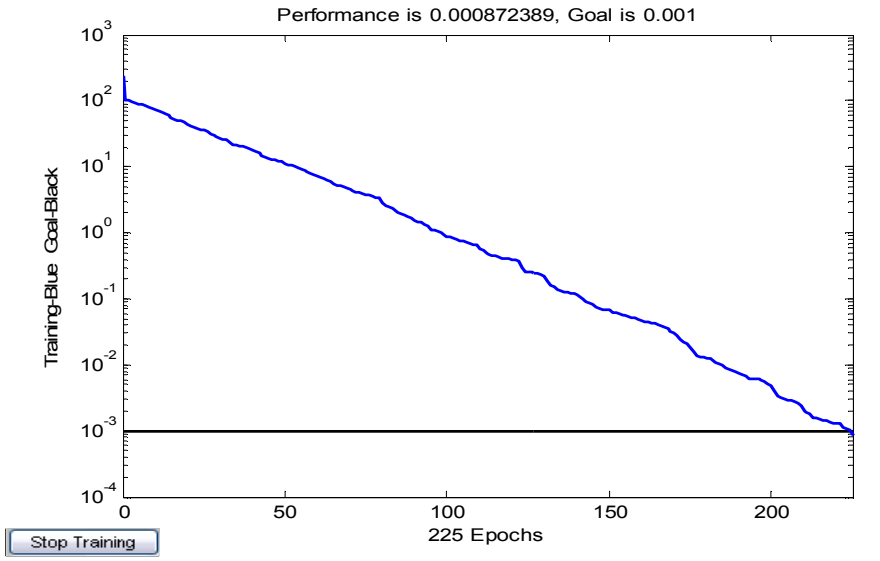

Figure 3.2 Training performance of radial basis network in equilibrium CO_2 partial pressure prediction (DEA+water+CO_2) system.

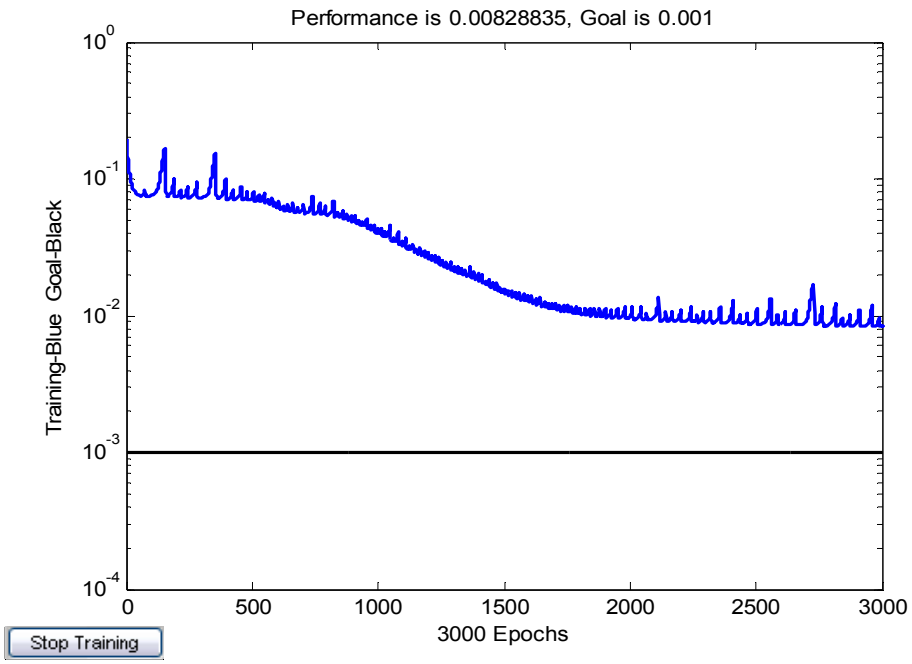

Figure 3.3 Training performance of feed-forward TRAINGDA network in equilibrium CO_2 partial pressure prediction (DEA+water+CO_2) system.

Chapter 4

(Piperazine+water+CO_2) system

In recent years, the importance of the chemical absorption process rises as a competitive process to reduce the discharge of CO_2 into atmosphere. The BASF activated MDEA technology used piperazine (PZ) as an activator in order to accelerate the absorption or desorption rate.
For this system the training data set consists of total of 82 numbers of data and the simulation is done on 84 numbers of data and the literature sources are shown in Table 4.1.

Data Type	No of Data	Literature Sources
Training Data	82	[1], [2]
Simulation data	84	[3]

Table 4.1 Data used in training and simulation for (Piperazine+water+CO_2) system.

4.1 Prediction of Equilibrium Partial Pressure of CO_2

In prediction of equilibrium partial pressure of carbon dioxide over aqueous PZ solvent, equilibrium loading (moles of CO_2 per mole of solvent), temperature and concentration are used as the inputs and the equilibrium CO_2 partial pressure is predicted. The prediction has been done using feed-forward network. The network uses TRAINRP function. The network configuration along with the training performance of the network using TRAINRP is shown in the Table 4.2. The corresponding simulation result is shown in Table 4.3. Figure 4.1 and 2.2 shows the training performance of the TRAINRP network for equilibrium CO_2 partial pressure prediction.

Data Source	Temp (K)	No. of Layers	No. of Neurons	Epochs	MSE	Time(Sec)
[1], [2]	298-353	1	3	2000	0.000162	12.328

Table 4.2 Network configuration using 'TRAINRP' in equilibrium CO_2 partial pressure prediction

Data Source	Temp (K)	No. Of Data Points	AAD%	Time(Sec)
[3]	298-353	84	0.7789	12.328

** [a] $AAD\% = \left[\sum_{n} \left(p_{cal} - p_{exp} \right) / p_{exp} \right] / n \times 100 =$ Average Absolute Deviation

Table 4.3 Simulation results using 'TRAINRP' in equilibrium CO_2 partial pressure prediction.

Conclusions

Since the Average Absolute Deviation Percentage %age is quite low (0.7789 %), and the time taken is only 12 sec, hence the TRAINRP network can be considered to be successful in prediction of equilibrium partial pressure of CO_2 over aqueous piperazine system.

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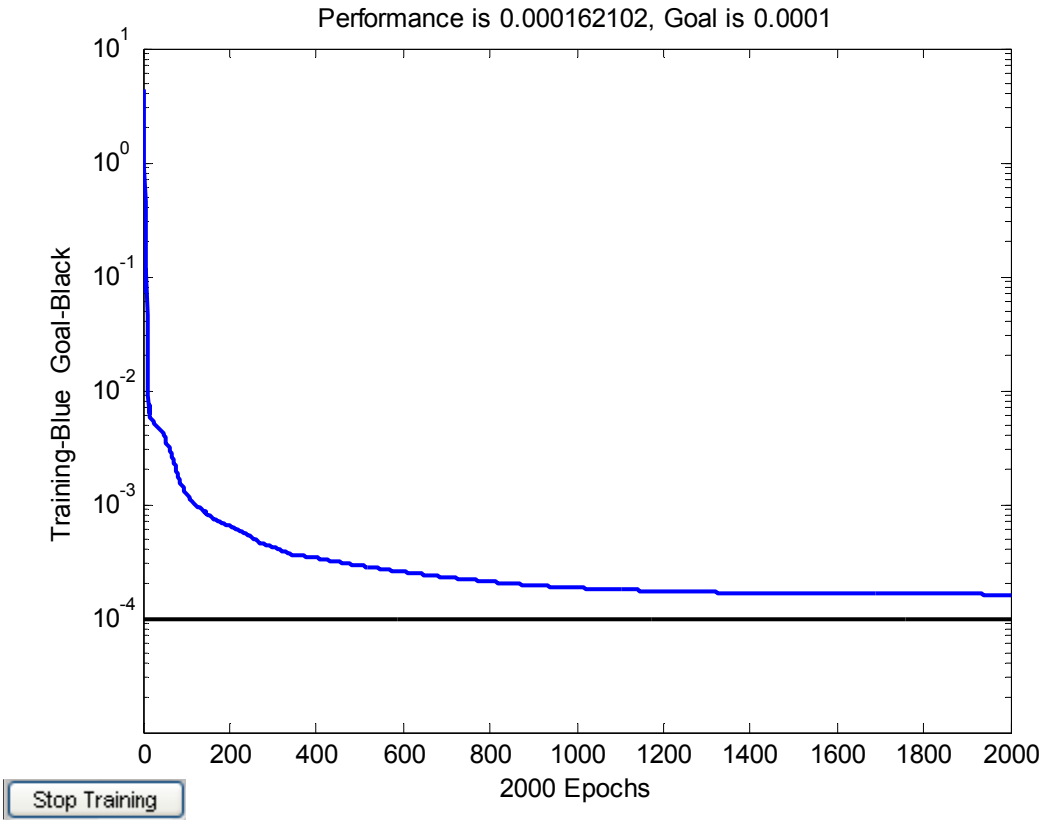

Figure 4.1 Training performance of feed forward TRAINRP network in equilibrium CO_2 partial pressure prediction.

Conclusion:

In this project both feed-forward networks as well as radial basis networks have been designed for prediction of VLE data of three aqueous-alkanolamine-CO_2 systems i.e. MEA+water+CO_2 system, DEA+water+CO_2 system, and piperazine+water+CO_2 system. From the results, it can be inferred that, for 95% cases, ANN has been able to predict VLE data within an error percentage of ± 5%. Thus the network designs can be considered to have been successful.

APPENDIX: The interested persons can ask for the programs from Dr. Madhushree Kundu, Dept. of Chemical Engineering, NIT Rourkela.