



# Journal of Applied Sciences

ISSN 1812-5654

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## Prediction of Vapor-Liquid Equilibrium for Aqueous Solutions of Electrolytes Using Artificial Neural Networks

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**Abstract:** In this study, an Artificial Neural Network (ANN) model has been developed for aqueous solutions of electrolyte systems. Multilayer Perceptron (MLP) and Radial Basis Function (RBF) networks were applied to estimate vapor-liquid equilibrium data for ternary system of  $\text{NH}_3\text{-CO}_2\text{-H}_2\text{O}$ . Experimental data, taken from the literature were divided into three sections of training, validating and testing. Mean Absolute Errors (MAE) of the networks for training set are used as network selection criterion and to find optimal design of the networks. The performance of ANN models to predict partial and total pressures of  $\text{NH}_3\text{-CO}_2\text{-H}_2\text{O}$  system were evaluated by comparing their results with the predictions of some thermodynamic models. The criterion for this comparison was the error between models predictions and the experimental data. The comparison indicated that both MLP and RBF models predict the system better than the thermodynamic models.

**Key words:** Artificial neural networks, vapor-liquid equilibria, electrolytes, ammonia, carbon dioxide

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### INTRODUCTION

Aqueous waste streams from petroleum or petrochemical plants and coal processing units often contain volatile weak electrolytes such as ammonia, carbon dioxide, sulfur dioxide, hydrogen sulfide and hydrogen cyanide. To prevent environmental pollution because of some ecological reason, these solutes must be removed by separation processes before they can be released into natural waters or sewage-disposal plants. Vapor-liquid equilibrium data for aqueous solutions of electrolytes play a vital role in designing equipment in the chemical industries. They are often nonlinear and complex in nature. VLE data are generally estimated using thermodynamic models based on the phase equilibrium criterion of equality of chemical potential in both phases (Arce *et al.*, 1996; Iliuta *et al.*, 1996). This process of calculating VLE is based on the Gamma/Phi approach. In this approach, activity coefficient models are used to describe the liquid phase (Smith *et al.*, 2001). Several activity coefficient models such as NRTL, UNIFAC, UNIQUAC and Wilson have been used to describe VLE (Iliuta *et al.*, 1998, 2000; Vercher *et al.*, 1996). Another method for phase calculation is based on Equations of State (EOS). Although EOS are derived based on strong physical principles, there is still certain amount of

empiricism involved in terms of several adjustable parameters that are required in mixing rules. However, while EOS can be applied well to hydrocarbon systems, it is difficult to apply EOS for systems containing polar compounds (Sharma *et al.*, 1999). In some cases empirical and semi-empirical equations are employed to predict VLE data. The constants in these equations are obtained from regression of the experimental measurements (Vega and Vera, 1976; Pitzer, 1973).

VLE data obtaining from the above mentioned methods, utilize an iterative algorithm that requires pure component properties, thermodynamic rules and experimental measurements. Iterative schemes require significant computational effort. These schemes are not suitable for rapid prediction of a dynamic behavior. Empirical equations do not account for detailed mechanism of VLE systems. Thermodynamic models and empirical equations have been traditionally serving the requirements of the industry. However these days, other faster alternative methods for the prediction of VLE data are more attractive to chemical engineers.

The development of numerical tools, such as Artificial Neural Network (ANN), has paved the way for alternative methods to predict the VLE (Petersen *et al.*, 1994; Guimaraes and McGreavy, 1995; Ganguly, 2003; Urata *et al.*, 2002). Recently many authors have reported

application of ANN for estimation of thermodynamic properties such as estimation of viscosity, density, vapour pressure and compressibility factor (Adnan *et al.*, 2004, 2007; Şencan, 2006, 2007; Jones *et al.*, 2006; Kürten, 1988). ANN offers nonlinear mapping capability that can be utilized for storage and recollection of VLE data. The associative property of artificial neural networks and their inherent ability to learn and recognize highly non-linear finds them ideally suited to a wide range of applications in chemical engineering. Many different types of ANNs have been developed (Hagan *et al.*, 1996; Haykin, 1994; Schalkoff, 1997). The Multilayer Perceptron (MLP) and Radial Basis Function (RBF) are the most popular networks in chemical engineering applications (Baughman and Liu, 1995; Dubdub, 2002; Jouyban *et al.*, 2004; Erol *et al.*, 2004). They have been widely used for estimation of VLE. They are both non-linear feed-forward networks and universal approximators. MLPs are usually trained with the back-propagation supervised algorithm, whereas RBF networks are usually trained one layer at a time with the first layer unsupervised (Hagan *et al.*, 1996; Schalkoff, 1997).

The application of ANNs to predict VLE was first conducted by Petersen *et al.* (1994). They introduced a new group-contribution model for prediction of liquid phase activity coefficients of binary systems. In their research, ANNs were defined as mathematical models of adaptive systems, originally inspired by studies on the human brain. The study by Petersen *et al.* (1994) used back-propagation algorithm for training a feedforward network. The calculated results were compared with UNIFAC model predictions and experimental data. A multi-layer perceptron with a single hidden layer has been used by Guimaraes and McGreavy (1995) to estimate VLE of benzene-hexane system. Sharma *et al.* (1999) have used multi-layer perceptron model to estimate VLE for methane-ethane and ammonia-water systems. Later on, Iliuta *et al.* (2000), Dubdub (2002), Chouai *et al.* (2002), Mohanty (2005), Urata *et al.* (2002) and Nguyen *et al.* (2007) applied MLP with the back-propagation algorithm to predict VLE of binary and ternary systems. On the other hand, Ganguly (2003) and Govindarajan and Sabarathinam (2006) have used RBF to estimate VLE for several binary and ternary systems. Table 1 presents a summary of the studies about VLE prediction using ANNs.

**Artificial neural networks model:** The aim of this study is applying RBF and MLP networks for numerical modeling very complex vapour liquid equilibria occurring in the aqueous solutions of electrolyte systems. Artificial neural networks are not good at evaluating inputs that are out of 0 to 1 interval. They require all training targets to be

Table 1: Summary of VLE prediction using ANNs

No.	Author	System	Network
1	Petersen <i>et al.</i> (1994)	Binary systems	MLP
2	Guimaraes and McGreavy (1995)	Binary systems	MLP
3	Sharma <i>et al.</i> (1999)	Binary systems	MLP
4	Iliuta <i>et al.</i> (2000)	Binary systems	MLP
5	Urata <i>et al.</i> (2002)	Binary systems	MLP
6	Dubdub (2002)	Binary systems	MLP
7	Ganguly (2003)	Binary and ternary systems	RBF
8	Mohanty (2005)	Binary systems	MLP
9	Govindarajan and Sabarathinam (2006)	Binary and ternary systems including two azeotropes	RBF
10	Nguyen <i>et al.</i> (2007)	Ternary systems saturated with salt	MLP

normalized between 0 and 1 for training. Without normalization, the variable with the largest scale will dominate the measure. To resolve this problem, all of the parameters were normalized between 0 to 1. The input parameters for networks are liquid solution variables that were normalized applying the following equations.

$$U_i = \frac{m_i - m_{i,min}}{m_{i,max} - m_{i,min}} \quad i = 1, 2, \dots, n-1 \quad (1)$$

In the aqueous solutions of electrolytes, water was assumed to be the nth component in both liquid and vapor phases that can be computed using Eq. 2.

$$U_n = \frac{1000/M_w}{1000/M_w + \sum_{i=1}^{n-1} m_i} \quad (2)$$

$$U_{n+1} = \frac{T - T_{min}}{T_{max} - T_{min}} \quad (3)$$

The normalized partial and total pressures in vapor phase are as output parameters of networks.

$$S_i = \frac{P_i - P_{i,min}}{P_{i,max} - P_{i,min}} \quad i = 1, 2, \dots, n \quad (4)$$

$$S_{n+1} = \frac{P_{total} - P_{total,min}}{P_{total,max} - P_{total,min}} \quad (5)$$

There are three criteria for stopping the networks training: maximum number of epochs, training time and target Mean Squared Error (MSE). However, in several cases, the Mean Absolute Error (MAE) and mean squared error as shown in Eq. 6 and 7 are used as network selection criterion. It has been applied in this study as well.

$$MAE = \sum_{k=1}^N (t(k) - a(k))^2 \quad (6)$$

$$MSE = \frac{1}{N} \sum_{k=1}^N \epsilon(k)^2 = \frac{1}{N} \sum_{k=1}^N (t(k) - a(k))^2 \quad (7)$$

The number of MLP hidden layers and neurons in the hidden layers are obtained during the training phase by trial and error method so as to minimize the error between the experimental partial pressures and estimated partial pressures in the vapour phase.

Average Relative Deviation (ARD), as shown in Eq. 8, has been used as a criterion to compare the results of ANN models with other models.

$$ARD = \frac{1}{Z} \sum_{k=1}^Z \frac{|t(k) - a(k)|}{a(k)} \quad (8)$$

**Vapor-liquid equilibria of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system:** The three-component system of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O occurs in many absorption processes of industrial waste gas purification. This system has been investigated both theoretically and experimentally by several researchers (Pexton and Badger, 1938; Badger and Wilson, 1947; Kervelen *et al.*, 1949; Otsuka *et al.*, 1960; Takahashi, 1962; Edwards *et al.*, 1975, 1978; Beutier and Renon, 1978; Chen *et al.*, 1979; Verbrugge, 1979; Pawlikowski *et al.*, 1982; Owens *et al.*, 1983; Muller *et al.*, 1988; Goppert and Maurer, 1988; Bieling *et al.*, 1989; Kurz *et al.*, 1995; Jadwiga, 1999; Thomsen and Rasmuesen, 1999; Pazuki *et al.*, 2006). In the literature there are plenty of VLE experimental data for NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system in wide range of temperature and component concentrations. A series of studies by Muller (1983), Müller *et al.* (1988), Göppert and Maurer (1988), Bieling *et al.* (1989) and Kurz *et al.* (1995) supplied a large amount of experimental data of the NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system. Table 2, shows an extensive database for VLE data of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system in different ranges temperature and ammonia and carbon dioxide liquid phase concentrations.

N is number of published experimental data. The ranges of the data that were used in networks are as follows:

$$T = 303 - 473\text{K}, m_{\text{NH}_3} = 0.5 - 25.8 \text{ mole kg}^{-1} \text{ H}_2\text{O},$$

$$m_{\text{CO}_2} = 0.17 - 12.7 \text{ mole kg}^{-1} \text{ H}_2\text{O}$$

$$P_{\text{NH}_3} = 0.1 - 2528\text{kPa}, P_{\text{CO}_2} = 0.1 - 6795\text{kPa},$$

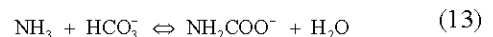
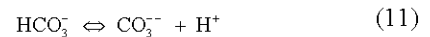
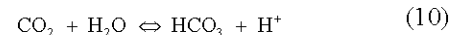
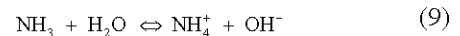
$$P_{\text{H}_2\text{O}} = 4 - 1885\text{kPa}, P_{\text{total}} = 11.5 - 8810\text{kPa}$$

The data that have been reported by the authors as mentioned in Table 2 were divided into training, validating and testing data sets. The training set was used to develop the ANN models, while the validating and testing sets were used to confirm the agreement between the ANN models with experimental data.

Table 2: VLE experimental data of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system used to develop the ANN models

Source	N	Temperature (K)	Concentration (mole/kg H <sub>2</sub> O)	
			m <sub>CO<sub>2</sub></sub>	m <sub>NH<sub>3</sub></sub>
Pexton and Badger (1938)	68	313, 293	0.03-2.3	0.1-2.3
Badger and Wilson (1947)	9	363	0.01- 0.8	0.4-1.9
Krevelen <i>et al.</i> (1949)	54	293-333	0.3-1.5	0.5-2.3
Otsuka <i>et al.</i> (1960)	50	293-373	0.5-5.6	2.0-15.3
Verbrugge (1979)	56	313-363	0-10	1-40
Pawlikowski <i>et al.</i> (1982)	19	373,423	0.9-5.4	3.1-9.6
Owens <i>et al.</i> (1983)	4	422,477.74	0.268-0.864	1.14-2.354
Muller (1983)	8	373-453	0-14	4-30
Goppert and Maurer (1988)	559	333-393	0.4-13	0.7-16
Muller <i>et al.</i> (1988)	294	373-473	2-13	0-26
Kurz <i>et al.</i> (1995)	55	313-353	0-10	6-12
Jadwiga (1999)	37	293-343	0.39-1.66	0.6-1.88

The gas phase of the vapor-liquid equilibrium in the ternary system of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O, contains NH<sub>3</sub>, CO<sub>2</sub> and H<sub>2</sub>O in molecular form and the liquid phase contains NH<sub>3</sub> and CO<sub>2</sub> not only in molecular, but also in ionic form. In the NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system, nine molecules and ion species exist in liquid phase; NH<sub>3</sub>, CO<sub>2</sub>, H<sub>2</sub>O, NH<sub>4</sub><sup>+</sup>, HCO<sub>3</sub><sup>-</sup>, CO<sub>3</sub><sup>2-</sup>, H<sup>+</sup>, OH<sup>-</sup> and NH<sub>2</sub>COO<sup>-</sup>. It is assumed that NH<sub>3</sub> and H<sub>2</sub>O dissociations, the first and the second dissociation of CO<sub>2</sub> and the formation of carbonate are the most important chemical reactions. The following equilibrium reactions take place in the solution:



Total components concentrations are expressed as follows:

$$m_{\text{NH}_3} = \text{NH}_3 + \text{NH}_4^+ + \text{NH}_2\text{COO}^- \quad (14)$$

$$m_{\text{CO}_2} = \text{CO}_2 + \text{NH}_2\text{COO}^- + \text{HCO}_3^- + \text{CO}_3^{2-} \quad (15)$$

In the present study, both input and output layers of the networks consist of four neurons. Table 3 and 4 show networks inputs and outputs with their ranges, respectively.

**RESULTS AND DISCUSSION**

Normalized concentrations of CO<sub>2</sub>, NH<sub>3</sub> and H<sub>2</sub>O in the liquid phase and normalized temperatures (Table 3) were fed as inputs to MLP and RBF for training the networks whereas normalized partial and total pressures (Table 4) were kept as outputs. Table 5 contains mean squared error and mean absolute error for both MLP and RBF networks in training, validating and testing phases.

It is a useful diagnostic tool to plot the training, validation and test mean squared errors to check the progress of training. The result is shown in the Fig. 1. Since the test set error and the validation set error have similar characteristics, the result is reasonable and it does not appear that any significant over fitting has occurred. A multi-layer perceptron with two hidden layers consisting of twenty three neurons in the first layer and twenty one neurons in the second layer was found to be the best network design, since it satisfactorily estimated partial and total pressures of NH<sub>3</sub>, CO<sub>2</sub> and H<sub>2</sub>O in the vapor phase. In the MLP network tang functions were applied for all layers except the output layer.

The prediction of total pressure of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system is demonstrated in Fig. 2. It indicates that a satisfactory training has been achieved for both MLP and RBF, since there is a good agreement between predicted total pressure and experimental data.

Experimental data and MLP model predictions for total and partial pressures of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system are

Table 3: Set of the input variables

No.	Input scaled variable	Range
1	$U_1 = \frac{m_{NH_3} - m_{NH_3,min}}{m_{NH_3,max} - m_{NH_3,min}}$	0-1
2	$U_2 = \frac{m_{CO_2} - m_{CO_2,min}}{m_{CO_2,max} - m_{CO_2,min}}$	0-1
3	$U_3 = \frac{55.49}{m_{NH_3} + m_{CO_2} + 55.49}$	0.6-1
4	$U_4 = \frac{T - T_{min}}{T_{max} - T_{min}}$	0-1

Table 4: Set of the output variables

No.	Output scaled variable	Range
1	$S_1 = \frac{P_{NH_3} - P_{NH_3,min}}{P_{NH_3,max} - P_{NH_3,min}}$	0-1
2	$S_2 = \frac{P_{CO_2} - P_{CO_2,min}}{P_{CO_2,max} - P_{CO_2,min}}$	0-1
3	$S_3 = \frac{P_{H_2O} - P_{H_2O,min}}{P_{H_2O,max} - P_{H_2O,min}}$	0-1
4	$S_4 = \frac{P_{Total} - P_{Total,min}}{P_{Total,max} - P_{Total,min}}$	0-1

shown in Table 6 (Similar results were obtained for RBF model). Comparisons between these values indicate that

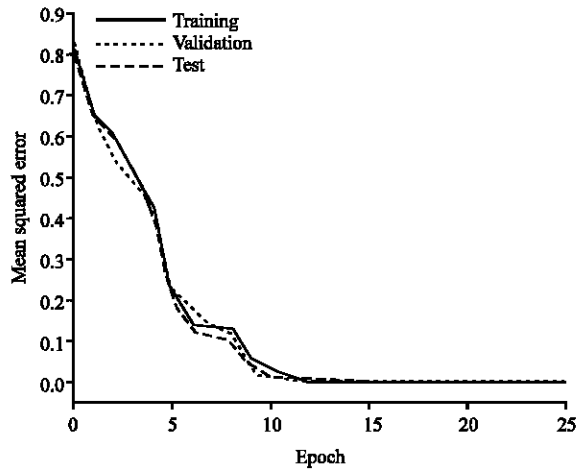


Fig. 1: Mean squared error of training, validation and test sets in each epoch

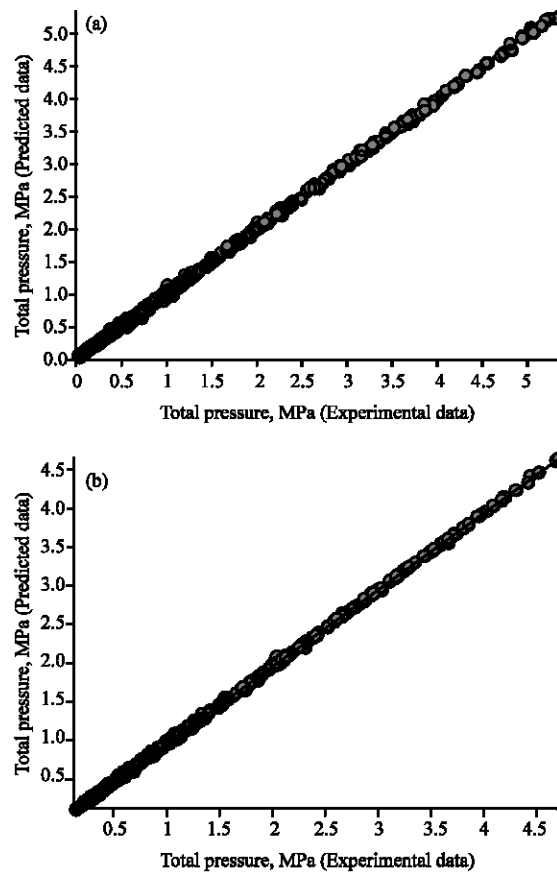


Fig. 2: ANN predictions versus experimental data of total pressure, (a) by MLP network for training set and (b) by RBF network for training set

Table 5: Performances and statistical tests of neural networks for NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system

Parameter	Data set	MLP				RBF			
		P <sub>NH<sub>3</sub></sub>	P <sub>CO<sub>2</sub></sub>	P <sub>H<sub>2</sub>O</sub>	P <sub>Total</sub>	P <sub>NH<sub>3</sub></sub>	P <sub>CO<sub>2</sub></sub>	P <sub>H<sub>2</sub>O</sub>	P <sub>Total</sub>
MAE	Training data	0.0017	0.0020	0.0018	0.0012	0.0043	0.0033	0.0018	0.0017
	Validating data	4.4e-4	2.6e-4	9.4e-5	1.8e-4	1.8e-5	5.9e-5	5.9e-5	3.3e-5
	Testing data	9.8e-4	1.6e-4	1.4e-4	5.8e-5	3e-5	1.1e-4	1.8e-4	6e-5
	Whole data	0.0037	0.0021	0.0035	0.0013	0.0047	0.0036	0.0020	0.0018
MSE	Training data	4.6e-6	5.6e-6	5.2e-6	3.2e-6	7.3e-6	5.6e-6	3.1e-6	2.9e-6
	Validating data	1.0e-4	1.4e-4	3.9e-5	1.2e-4	2.2e-6	7.4e-6	7.4e-6	4.1e-6
	Testing data	4.2e-5	7.2e-6	6.0e-6	2.5e-6	1.3e-6	4.7e-6	7.8e-6	2.6e-6
	Whole data	9.5e-6	5.5e-6	9.2e-6	3.2e-6	7.8e-6	5.7e-6	3.4e-6	3.0e-6

Table 6: Comparison between the published experimental data and ANN testing set predictions of NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system

No.	T,K	Published data (Goppert and Maurer, 1988; Muller <i>et al.</i> , 1998)						MLP predicted data			
		m <sub>NH<sub>3</sub></sub> , mole/kg H <sub>2</sub> O	m <sub>CO<sub>2</sub></sub>	P <sub>NH<sub>3</sub></sub>	P <sub>CO<sub>2</sub></sub>	P <sub>H<sub>2</sub>O</sub>	P <sub>T</sub>	P <sub>NH<sub>3</sub></sub>	P <sub>CO<sub>2</sub></sub>	P <sub>H<sub>2</sub>O</sub>	P <sub>T</sub>
		Kpa						Kpa			
1	353.15	5.930	3.326	17.3	171	39.1	227.4	17.70	173	38.5	233.5
2	353.15	9.030	5.009	26.1	204	37.4	267.5	25.50	211	37.4	279.5
3	353.15	9.030	5.639	17.9	436	37.6	491.5	17.40	450	36.7	506.8
4	353.15	12.170	7.736	20.3	649	34.0	703.3	21.13	655	35.9	709.8
5	360.15	4.780	2.898	11.6	342	55.6	409.2	11.32	336	54.2	404.3
6	360.15	6.520	3.296	25.9	170	57.1	253.0	26.20	168	54.1	253.6
7	360.15	7.754	3.888	31.1	176	53.2	260.3	30.50	175	53.2	264.8
8	360.15	9.824	5.015	36.4	213	50.5	299.9	34.71	209	51.3	302.5
9	360.15	12.490	7.306	23.3	556	46.3	625.6	22.60	550	45.6	624.3
10	360.15	14.080	8.667	17.7	896	43.6	957.3	18.90	901	43.8	965.7
11	360.15	16.520	9.465	29.2	596	41.3	666.5	29.70	598	43.1	665.4
12	373.15	3.963	2.038	24.5	321	93.3	438.8	23.80	313	93.5	429.3
13	373.15	7.872	3.689	54.8	311	73.3	439.1	54.70	321	81.2	465.1
14	373.15	8.144	3.921	54.7	343	88.8	486.5	51.50	366	80.0	506.6
15	373.15	11.240	6.163	44.1	789	77.6	910.7	44.30	786	74.9	912.8
16	373.15	14.150	6.600	94.4	368	65.9	528.3	93.50	382	65.7	547.9
17	393.15	3.855	1.672	45.3	634	171.7	851.0	43.30	637	165.8	840.9
18	393.15	5.822	2.284	92.3	531	159.0	782.3	86.20	562	164.0	813.9
19	393.15	9.923	4.362	134.0	858	154.9	1146.9	127.80	897	152.2	1152.0
20	393.15	11.770	4.251	267.0	418	134.8	819.8	271.20	413	135.2	801.4

Table 7: Results of thermodynamic models and ANN models for the NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system

Source of data	T, K	P	Average relative deviation (%)								
			N	Kurz <i>et al.</i> model (1995)		Thomsen K. model (1999)		Krop model (1999)		MLP	RBF
Kurz <i>et al.</i> (1995)	313-353	P <sub>NH<sub>3</sub></sub>	18	2.1	13	2.2	37	12.7	7	3.2	3.6
		P <sub>CO<sub>2</sub></sub>	24	10.3	16	6.2		10.4		2.4	4.1
		P <sub>H<sub>2</sub>O</sub>	-	-	-	-		4.1		5.2	6.3
		P <sub>total</sub>	47	5.6	47	3.3		7.5		2.3	2.6
Muller <i>et al.</i> (1998)	373-433	P <sub>NH<sub>3</sub></sub>	212	11.4	48	9.9	104	7.8	20	3.1	3.6
		P <sub>CO<sub>2</sub></sub>	214	7.6	32	29.0		9.8		6.3	7.9
		P <sub>H<sub>2</sub>O</sub>	254	9.2	-	-		6.4		2.9	4.8
		P <sub>total</sub>	254	4.9	61	6.8		3.3		2.1	2.2
Goppert and Maurer (1988)	333-393	P <sub>NH<sub>3</sub></sub>	117	13.5	83	10.0	489	17.9	23	5.6	5.8
		P <sub>CO<sub>2</sub></sub>	494	7.3	401	4.7		10.3		4.9	3.0
		P <sub>H<sub>2</sub>O</sub>	341	14.9	-	-		15.7		5.3	5.9
		P <sub>total</sub>	562	5.2	459	3.9		7.5		2.5	2.2
Total number of data and average relative deviation		P <sub>NH<sub>3</sub></sub>	347	11.6	144	9.3	630	15.9	50	4.3	4.6
		P <sub>CO<sub>2</sub></sub>	732	7.5	449	6.5		10.2		5.1	5.1
		P <sub>H<sub>2</sub>O</sub>	595	12.5	-	-		13.5		4.4	5.5
		P <sub>total</sub>	863	5.1	567	4.2		6.8		2.3	2.3

MLP model adequately predicts partial pressure of the system. Table 7 shows the results of neural network and thermodynamic models for ternary NH<sub>3</sub>-CO<sub>2</sub>-H<sub>2</sub>O system. Comparisons between these results and experimental data indicate both types of ANN models can predict the system better than thermodynamic models.

### CONCLUSION

The applicability of artificial neural networks for numerical description of vapour-liquid phase equilibria of electrolyte aqueous solutions have been investigated in this work. MLP and RBF networks correlations for vapor

liquid equilibrium of  $\text{NH}_3\text{-CO}_2\text{-H}_2\text{O}$  system were successfully developed employing an extensive database in a wide range of vapor and liquid phase conditions. Therefore, the model profile could be fitted in any range of liquid concentrations in the test data set. MLP and RBF networks were designed using mean absolute error. Optimal design of MLP network was found to have four inputs, twenty three neurons in the first hidden layer, twenty one neurons in the second hidden layer and four outputs. The ANN models were compared with thermodynamic models based on their ability to predict total and partial pressures of  $\text{NH}_3$ ,  $\text{CO}_2$  and  $\text{H}_2\text{O}$ . Average relative deviation between the predictions and published experimental data were used as a criterion in this comparison. The results indicated that both MLP and RBF models have higher accuracy than thermodynamic models.

In this study, the ANN model was developed for certain ranges of pressure and temperature. However, if experimental data for any other ranges of data are available similar model can also be developed.

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