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 NH3-CO2-H2O. 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 NH3-CO2-H2O 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

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 non-linear 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 obtained form 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
The 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 Sabarantham (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 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.

\[ U_i = \frac{m_i - m_{\text{min}}}{m_{\text{max}} - m_{\text{min}}} \quad i = 1, 2, ..., n \quad (1) \]

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.

\[ U_n = \frac{1000/M_w}{1000/M_w + \sum_i m_i} \quad (2) \]

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

\[ S_i = \frac{P_i - P_{i,\text{min}}}{P_{i,\text{max}} - P_{i,\text{min}}} \quad i = 1, 2, ..., n \quad (4) \]

\[ S_{nt} = \frac{P_{nt} - P_{nt,\text{min}}}{P_{nt,\text{max}} - P_{nt,\text{min}}} \quad (5) \]

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.

\[ \text{MAE} = \sum_{k=1}^{n} (t(k) - u(k))^2 \quad (6) \]
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.

\[
\text{ARD} = \frac{1}{N} \sum_{k=1}^{N} \frac{|t(k) - a(k)|}{a(k)}
\]

### Vapor-liquid equilibria of NH₃-CO₂-H₂O system:

The three-component system of NH₃-CO₂-H₂O occurs in many absorption processes of industrial waste gas purification. This system has been investigated both theoretically and experimentally by several researchers (Peixton 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; Göppert and Maurer, 1988; Bieling et al., 1989; Kurz et al., 1995; Iadwiga, 1999; Thomsen and Rasmussen, 1999; Pazuki et al., 2006). In the literature there are plenty of VLE experimental data for NH₃-CO₂-H₂O 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 NH₃-CO₂-H₂O system. Table 2, shows an extensive database for VLE data of NH₃-CO₂-H₂O 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:

\[ T = 303 - 473K, m_{NH₃} = 0.5 - 25.8 \text{ mole kg}^{-1} \text{ H₂O}, \]
\[ m_{CO₂} = 0.17 - 12.7 \text{ mole kg}^{-1} \text{ H₂O} \]
\[ P_{sat} = 0.1 - 2528kPa, P_{CO₂} = 0.1 - 6795kPa, \]
\[ P_{NH₃} = 4 - 1885kPa, P_{NH₃} = 11.5 - 8810kPa \]

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 NH₃-CO₂-H₂O system used to develop the ANN models

<table>
<thead>
<tr>
<th>Source</th>
<th>N</th>
<th>Temperature (K)</th>
<th>( m_{CO₂} )</th>
<th>( m_{NH₃} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peixton and Badger (1938)</td>
<td>68</td>
<td>313, 293</td>
<td>0.03-2.3</td>
<td>0.1-2.3</td>
</tr>
<tr>
<td>Badger and Wilson (1947)</td>
<td>9</td>
<td>363</td>
<td>0.01-0.8</td>
<td>0.1-2.3</td>
</tr>
<tr>
<td>Kervelen et al. (1949)</td>
<td>54</td>
<td>290-333</td>
<td>0.3-1.5</td>
<td>0.5-2.3</td>
</tr>
<tr>
<td>Otsuka et al. (1960)</td>
<td>50</td>
<td>293-373</td>
<td>0.5-5.6</td>
<td>2.0-15.3</td>
</tr>
<tr>
<td>Verbrugge (1979)</td>
<td>56</td>
<td>313-363</td>
<td>0-10</td>
<td>1-10</td>
</tr>
<tr>
<td>Pawlikowski et al. (1982)</td>
<td>19</td>
<td>373, 423</td>
<td>0.9-5.4</td>
<td>3.1-9.6</td>
</tr>
<tr>
<td>Owens et al. (1983)</td>
<td>4</td>
<td>422-477, 74</td>
<td>0.268-0.864</td>
<td>1.14-2.354</td>
</tr>
<tr>
<td>Muller (1983)</td>
<td>8</td>
<td>373-453</td>
<td>0.4-14</td>
<td>0.4-40</td>
</tr>
<tr>
<td>Göppert and Maurer (1988)</td>
<td>224</td>
<td>373-473</td>
<td>2.13</td>
<td>0.26</td>
</tr>
<tr>
<td>Muller et al. (1988)</td>
<td>294</td>
<td>373-473</td>
<td>2.13</td>
<td>0.26</td>
</tr>
<tr>
<td>Kurz et al. (1995)</td>
<td>55</td>
<td>313-353</td>
<td>0-10</td>
<td>6-12</td>
</tr>
<tr>
<td>Iadwiga (1999)</td>
<td>37</td>
<td>293-343</td>
<td>0.39-1.66</td>
<td>0.6-1.88</td>
</tr>
</tbody>
</table>

The gas phase of the vapor-liquid equilibrium in the ternary system of NH₃-CO₂-H₂O contains NH₃, CO₂ and H₂O in molecular form and the liquid phase contains NH₃ and CO₂ not only in molecular, but also in ionic form. In the NH₃-CO₂-H₂O system, nine molecules and ion species exist in liquid phase: NH₃, CO₂, H₂O, NH₄⁺, HCO₃⁻, CO₃²⁻, H⁺, OH⁻ and NH₄COO⁻. It is assumed that NH₃ and H₂O dissociations, the first and the second dissociation of CO₂ and the formation of carbonate are the most important chemical reactions. The following equilibrium reactions takes place in the solution:

\[
\text{NH}_3 + \text{H}_2\text{O} \leftrightarrow \text{NH}_4^+ + \text{OH}^- \quad (9)
\]
\[
\text{CO}_2 + \text{H}_2\text{O} \leftrightarrow \text{HCO}_3^- + \text{H}^+ \quad (10)
\]
\[
\text{HCO}_3^- \leftrightarrow \text{CO}_3^{2-} + \text{H}^+ \quad (11)
\]
\[
\text{H}_2\text{O} \leftrightarrow \text{OH}^- + \text{H}^+ \quad (12)
\]
\[
\text{NH}_3 + \text{HCO}_3^- \leftrightarrow \text{NH}_4\text{COO}^- + \text{H}_2\text{O} \quad (13)
\]

Total components concentrations are expressed as follows:

\[ m_{NH₃} = \text{NH}_3 + \text{NH}_4^+ + \text{NH}_4\text{COO}^- \quad (14) \]

\[ m_{CO₂} = \text{CO}_2 + \text{NH}_2\text{COO}^- + \text{HCO}_3^- + \text{CO}_3^{2-} \quad (15) \]

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 CO₂, NH₃ and H₂O 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 NH₃, CO₂ and H₂O 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 NH₃-CO₂-H₂O 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 NH₃-CO₂-H₂O system are shown in Table 6 (Similar results were obtained for RBF model). Comparisons between these values indicate that

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Table 3: Set of the input variables

<table>
<thead>
<tr>
<th>No.</th>
<th>Input scaled variable</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \frac{m_{NH_3} - m_{NH_3_{max}}}{m_{NH_3_{max}} - m_{NH_3_{min}}} )</td>
<td>0-1</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{m_{CO_2} - m_{CO_2_{max}}}{m_{CO_2_{max}} - m_{CO_2_{min}}} )</td>
<td>0-1</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{55.49}{m_{NH_3} + m_{CO_2} + 55.49} )</td>
<td>0.6-1</td>
</tr>
<tr>
<td>4</td>
<td>( \frac{T - T_{min}}{T_{max} - T_{min}} )</td>
<td>0-1</td>
</tr>
</tbody>
</table>

Table 4: Set of the output variables

<table>
<thead>
<tr>
<th>No.</th>
<th>Output scaled variable</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \frac{P_{NH_3} - P_{NH_3_{min}}}{P_{NH_3_{max}} - P_{NH_3_{min}}} )</td>
<td>0-1</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{P_{CO_2} - P_{CO_2_{min}}}{P_{CO_2_{max}} - P_{CO_2_{min}}} )</td>
<td>0-1</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{P_{NH_3} + P_{CO_2}}{P_{NH_3_{max}} + P_{CO_2_{max}}} )</td>
<td>0-1</td>
</tr>
<tr>
<td>4</td>
<td>( \frac{P_{NH_3} + P_{CO_2}}{P_{NH_3_{max}} + P_{CO_2_{max}}} )</td>
<td>0-1</td>
</tr>
</tbody>
</table>

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 NH3-CO2-H2O system

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Data set</th>
<th>MLP</th>
<th>RBF</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>P10</td>
<td>P10</td>
<td>P0.01</td>
<td>P0.01</td>
<td>P0.01</td>
<td>P0.01</td>
</tr>
<tr>
<td>MAE</td>
<td>Training</td>
<td>0.0017</td>
<td>0.0020</td>
<td>0.0018</td>
<td>0.0012</td>
<td>0.0043</td>
<td>0.0033</td>
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<tr>
<td></td>
<td>Validating</td>
<td>4.6e-4</td>
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<td>1.8e-4</td>
<td>1.8e-4</td>
<td>5.9e-5</td>
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<tr>
<td></td>
<td>Testing</td>
<td>9.8e-4</td>
<td>1.6e-4</td>
<td>1.4e-4</td>
<td>5.8e-5</td>
<td>3E-5</td>
<td>1.1e-4</td>
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<tr>
<td></td>
<td>Whole data</td>
<td>0.0037</td>
<td>0.0021</td>
<td>0.0035</td>
<td>0.0013</td>
<td>0.0047</td>
<td>0.0036</td>
</tr>
<tr>
<td>MSE</td>
<td>Training</td>
<td>4.6e-6</td>
<td>5.6e-6</td>
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<td>3.2e-6</td>
<td>7.3e-6</td>
<td>5.6e-6</td>
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<tr>
<td></td>
<td>Validating</td>
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<td>1.4e-4</td>
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<td>7.4e-6</td>
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<tr>
<td></td>
<td>Testing</td>
<td>4.2e-5</td>
<td>7.2e-6</td>
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<td>2.5e-6</td>
<td>1.3e-6</td>
<td>4.7e-6</td>
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<tr>
<td></td>
<td>Whole data</td>
<td>9.5e-6</td>
<td>5.3e-6</td>
<td>9.2e-6</td>
<td>3.2e-6</td>
<td>7.8e-6</td>
<td>5.7e-6</td>
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</table>

Table 6: Comparison between the published experimental data and ANN testing set predictions of NH3-CO2-H2O system

<table>
<thead>
<tr>
<th>No.</th>
<th>T,K</th>
<th>mole</th>
<th>mole</th>
<th>P1</th>
<th>P2</th>
<th>17.7</th>
<th>173</th>
<th>38.5</th>
<th>233.5</th>
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<tbody>
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<td>3.326</td>
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<td>353.15</td>
<td>9.090</td>
<td>5.090</td>
<td>7.31</td>
<td>204</td>
<td>37.4</td>
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<td>25.59</td>
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<td>4</td>
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<td>5</td>
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<td>6</td>
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<td>3.888</td>
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<td>6.163</td>
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<td>1.672</td>
<td>45.3</td>
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<td>851.0</td>
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<tr>
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Table 7: Results of thermodynamic models and ANN models for the NH3-CO2-H2O system

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<td>Kurz et al. (1995)</td>
<td>313-353</td>
<td>P10</td>
<td>18</td>
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<td>12.7</td>
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<td>Moller et al. (1998)</td>
<td>373-433</td>
<td>P10</td>
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<td>48</td>
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<td>104</td>
<td>7.8</td>
<td>20</td>
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<td>Opplert and Maurer (1988)</td>
<td>333-395</td>
<td>P10</td>
<td>214</td>
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<td>32</td>
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<td>6.3</td>
<td>7.9</td>
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<td>347</td>
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<td>144</td>
<td>9.3</td>
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<td>15.9</td>
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</table>

MLP model adequately predicts partial pressure of the system. Table 7 shows the results of neural network and thermodynamic models for ternary NH3-CO2-H2O 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 NH₃-CO₂-H₂O 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 NH₃, CO₂ and H₂O. 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.

REFERENCES


