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Using a Multilayer Perceptron Network for Thermal Conductivity Prediction of Aqueous Electrolyte Solutions

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Supporting Information

ABSTRACT: In this study, a multilayer perceptron (MLP) network is proposed to predict the thermal conductivity (λ) of an electrolyte solution at atmospheric pressure, over a wide range of temperatures (T) and concentrations (x) based on the molecular weight (M) and number of electrons (n) of the solute. The accuracy of the proposed artificial neural network (ANN) was evaluated through performing a regression analysis on the predicted and experimental values of various aqueous solutions, some of which were not used in the network training. The comparison of the developed MLP network to other correlations recommended in the literature indicates that the proposed neural network outperforms other alternative methods, with respect to accuracy as well as extrapolation capabilities. Besides, others' conductivity correlations are usually suggested for a specific electrolyte solution and a limited range of temperatures and concentrations, while such limitations do not exist for the proposed MLP network.

1. INTRODUCTION

Transport properties, particularly the thermal conductivities of aqueous electrolyte solutions, have to be calculated in many industrial and scientific applications such as the chemical industry, desalination processes, geochemistry, the development and utilization of geothermal and ocean thermal energy, geology and mineralogy, and hydrothermal synthesis. The estimation of the thermal conductivities of electrolyte solutions has attracted the attention of many researchers. Theoretical descriptions of such systems are not easy due to long-range electrostatic interactions among ionic species in a solution.

The data available on the thermal conductivities for most electrolyte solutions are quite limited in range and accuracy. The thermal conductivity for a specific aqueous electrolyte solution is, in general, a function of temperature, concentration, and pressure. Some empirical and semiempirical correlations proposed by researchers[1−18] in this field are presented in Table 1 in the Supporting Information. As can be seen from this table, these correlations can cover a limited range of temperatures, concentrations, and electrolyte solutions. The adjusted parameters for many electrolyte solutions are not available. Also, these correlations require a relationship for determining the thermal conductivity of pure water at desired temperatures which can decrease the accuracy of the calculation. Due to aforementioned shortcomings of the correlations of the thermal conductivity of electrolyte solutions, we have suggested a neural network model that tackles the problem of calculating/estimating the thermal conductivity of aqueous solutions over a wide range of temperatures and a vast domain of electrolyte solutions.

In this study, we will develop a neuromorphic formulation for the calculation/estimation of thermal conductivities of aqueous electrolyte solutions. The developed model can be used for a vast variety of salts at different concentrations over a wide range of temperatures. Neural networks have been used for the estimation of physical properties in various fields of chemical engineering. Eslamloueyan and Khademi[19] proposed a feed-forward three-layer neural network to predict the thermal conductivity of pure gases at atmospheric pressure and a wide range of temperatures based on the critical temperature, critical pressure, and molecular weight of the components. They[20] also extended their work to calculate the conductivities of binary gaseous mixtures at atmospheric pressure by using two consecutive multilayer perceptrons (MLPs). The pure component conductivities calculated in the first MLP, and the molecular weights of both substances and the mole fraction of the light component are fed into the second MLP to predict the thermal conductivity of the gaseous mixture. Kauffman and Jurs[21] predicted the surface tension, viscosity, and thermal conductivity for common organic solvents by using multiple linear regression and computational neural networks to train and evaluate models based on statistical indices and overall root-mean-square error. Sablani and Rahman[22] presented an artificial neural network (ANN) model for the prediction of thermal conductivity of food as a function of moisture content, temperature, and apparent porosity. The model was able to predict thermal conductivity with a mean relative error of 12.6%. Kurt and Kayfeci[23] predicted the thermal conductivity of ethylene glycol−water solutions based on the temperature, concentration, and density by using an artificial neural network.

Properties of electrolyte solutions, such as the viscosity, diffusion coefficient, and electrical conductivity, have long been the subject of considerable attention and study. Measurements of the thermal conductivities of electrolyte solutions have so far been restricted to limited ranges of temperature and concentration. For the thermal conductivities of electrolyte solutions there is still a lack of reliable theoretical or semiempirical equations in order to predict this property. The objective of this work is to develop a neural network model for the prediction of thermal

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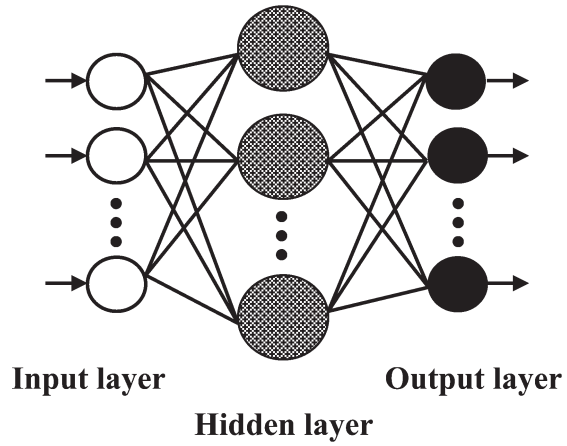

Figure 1. Structure of a feed-forward neural network.

conductivities of aqueous electrolyte solutions at atmospheric pressure over a wide range of temperatures and concentrations. The network inputs are the temperature, concentration of solution, sum of the number of electrons of the anion and cation, and molecular weight of the solute. Section 2 gives a brief overview of the artificial neural network (ANN) used in this study. Then, the proposed method as well as the data used in its development and validation is presented. Section 3 contains the results and discussion about the proposed method.

2. METHODOLOGY

Regarding the inherent capability of artificial neural networks to learn and recognize nonlinear and complex relationships, they can be used to predict conductivities of electrolyte solutions. The method proposed in this study is based on a feed-forward multilayer network. The required steps to develop a neuromorphic model for prediction of electrolyte solution conductivities are described in the following sections.

2.1. Feed-Forward Networks. There are several types of ANNs such as feed-forward networks, recurrent networks, ART networks, and autoassociative networks.[24] Conventional feed-forward networks are the most commonly used one for the function approximation. Hence, in this study a multilayer perceptron (MLP) network is used for the thermal conductivity calculation/estimation of electrolyte solutions. MLP networks consist of groups of interconnected nodes arranged in different layers such as the input layer, hidden layers, and the output layer.

As shown in Figure 1, the input layer receives all input signals and dispatches them to other neurons. Network outputs which are provided by the neurons in the output layer are actually the final results of the neuromorphic model. Consequently, number of nodes for the input and output layers are defined by the number of independent and dependent variables, respectively. The input layer is fed with input variables and passes them into the hidden layer(s) where the mathematical processing task takes place. Finally, the output layer receives the information from the last hidden layer and presents the final results. The network can therefore be interpreted as a form of input/output model, whose parameters are synaptic weights and biases. This type of network is able to approximate almost all types of functions regardless of their complexities.[24]

During the training algorithm, input data are fed to the input layer of the network and the difference between the output layer results and the desired outputs (i.e., network error) is used as a criterion for adjustment of the network's synaptic weights and biases. At the beginning, initial guesses are randomly taken at all synaptic weights and biases. Then, an iterative optimization method trains the network (i.e., its synaptic weights and biases are adjusted) until it correctly simulates the input/output correlation.

Determination of the minimum number of training data is frequently a difficult task. A heuristic guideline states that the number of data points should be 10 times the number of connections in the network. The optimal network architecture for a specific problem can be achieved through using automatic generalization methods that will be described in the next sections. According to Cybenko,[25] a network that has only one hidden layer is able to approximate almost any type of nonlinear mapping. Too few neurons in the hidden layer impair the network, and prevent the network from being trained appropriately. On the other hand, too many neurons cause the network to memorize the training data points without capturing the underlying relationship between the input and output variables. This problem is usually called "overfitting".

2.2. Data Acquisition and Analysis. One of the most essential subjects in the development of a neuromorphic model is the availability of reliable experimental sources of data for the networking training and testing. In this study, 660 experimental data were collected from the literature. These data are divided into three parts: training data set, validation data set, and test data set. Of the total data 60% were chosen for the network training, 20% were chosen for network validating, and the rest were used as the test data set. The training data set has been selected so that it can cover all the temperature and concentration ranges of the experimental data. Table 1 presents the training data set consisting of 389 experimental data points for thermal conductivities of electrolyte solutions.[1,2,26−32] It should be noted that some of the electrolyte solutions existing in the test data set are not used in the training data set (e.g., Na_2CO_3, K_2SO_4, NaBr, and $Ba(NO_3)_2$). This helps us to investigate better the extrapolation capability of the trained MLP network. Table 2 summarizes the overall range of data points used in the development of the multilayer perceptron network proposed in this work.

After providing the required training, validation, and test data sets, the network input variables should be identified. They can be considered as the correlation independent variables. Kapustinskiy and Ruzavin[3] proposed that the thermal conductivity of an electrolyte solution is a function of temperature, concentration, solute molecular weight, and the sum of electrons of the cation and anion as follows:

$$\lambda = f(T, x, M, n) \tag{1}$$

Following this approach, the temperature, concentration, molecular weight, and number of electrons have been used as the inputs of the MLP network developed in this research.

2.3. Neural Network Training. Once the input data have been selected, the next step is to develop the artificial neural network architecture. As mentioned before, a network that has only one hidden layer is capable of approximating almost any type of nonlinear mapping.[25] Hence, a feed-forward network with only one hidden layer has been used in this study. The neural network toolbox of the MATLAB programming language has been used to design the proposed feed-forward MLP network. The MATLAB code of this ANN model is available on request. The proposed multilayer perceptron network was trained by the

Table 1. List of Aqueous Electrolyte Solutions Used in the Development of the Neuromorphic Model (Training Data Set)

no.	electrolyte solution type	no. data points	reference	M	n	temp range (K)	concn range (wt %)
1	$SrCl_2$	25	26	158.527	55	293−473	0.025−0.15
2	BaI_2	31	2	391.136	109	293−473	0.025−0.2
3	$CdCl_2$	30	27	183.317	65	293−473	0.025−0.2
4	KI	33	28	166	72	293−473	0.025−0.25
5	$ZnCl_2$	33	1	136.3	47	293−473	0.025−0.25
6	$CdBr_2$	30	27	272.22	83	293−473	0.025−0.2
7	KBr	35	28	119	54	313−473	0.025−0.25
8	NaCl	36	29	58.443	28	293−473	0.025−0.25
9	$CoCl_2$	35	30	98.92	44	293−473	0.025−0.25
10	$Sr(NO_3)_2$	24	31	211.631	69	293−473	0.025−0.15
11	$LiNO_3$	28	31	68.95	34	293−373	0.0645−0.16
12	KCl	34	29	74.551	36	293−473	0.025−0.25
13	$Mg(NO_3)_2$	10	32	148.315	43	295.98−352.16	0.094−0.3
14	$Ca(NO_3)_2$	5	32	164.088	51	295−347.72	0.1−0.2
total data points		389					

Table 2. Range of Data of Aqueous Electrolyte Solutions

property	minimum	maximum
T (K)	293	473
x (wt %)	2.5	25
M	58.443	391.136
n	28	109
λ ($W \cdot m^{-1} \cdot K^{-1}$)	0.582	0.684

Levenberg−Marquardt algorithm.[33−35] Overfitting is a crucial problem in the design of ANN architecture training. Overfitting can occur in the case where the number of neurons in the hidden layer is too high. In this situation, the ratio of the number of the network adjustable parameters to the number of training data are is such that the network response to training data is very good, but the network results in a poor prediction for new input data. Indeed, the network will memorize the training examples, but it does not generalize to the new experimental conditions. This problem can be prevented through using regularization methods. In the present study, a Bayesian regularization technique in combination with the Levenberg−Marquardt algorithm has been used for training the suggested MLP network. In this method, the input and target data should be normalized within the range −1 to +1.[36] Tan-sigmoid functions (eq 2) have been used in the hidden and output layers of the MLP model proposed in this work.

$$f(a) = \frac{\exp(a) - \exp(-a)}{\exp(a) + \exp(-a)} \quad (2)$$

The Bayesian regularization determines the number of effective parameters used by the network. Therefore, by applying this method the trial-and-error algorithm for specifying the optimum number of hidden layer neurons could be eliminated. The total number of effective parameters calculated by the Bayesian regularization method is independent of the size of hidden layer neurons. The network parameters are adjusted to minimize the sum of the squared errors and the sum of the squared weights, and the network training is finished when these errors remain unchanged over several iterations.

Applying this method to the proposed MLP for estimation of conductivity of electrolyte solution led to (after several trials) an MLP network having 71.3 parameters after 76 epochs. The number of neurons in the hidden layer for a three-layer network can be calculated using the formula[37]

$$N_H = \frac{N_P - N_O}{N_I + 1 + N_O} \quad (3)$$

where N_P, N_I, N_H, and N_O represent the total number of parameters, the number of neurons in the input layer, the number of neurons in the hidden layer, and the number of neurons in the output layer, respectively. Thus, from eq 3, a neural network with approximately 12 neurons in the hidden layer was determined to be successful to model the thermal conductivities of aqueous solutions. Therefore, the designed MLP network has three layers with four neurons in the input layer, 12 neurons in the hidden layer, and one neuron at the output layer.

2.4. ANN Performance. The performance of a trained network can be measured to some extent by the errors in the training and test data sets, but it is often useful to investigate the network response in more detail. Regression analysis was done to assess the network prediction capability. The coefficient of determination, R^2, was used as a measure to evaluate how the trained network results are compatible to the experimental data.

Also, different neural network topologies were compared using their mean relative errors (MREs) and mean square errors (MSEs). The MRE and MSE are defined by the following equations:

$$\mathrm{MRE} = \frac{1}{N}\sum_{i=1}^{N}\frac{|\lambda_{exp} - \lambda_{calc}|}{\lambda_{exp}} \quad (4)$$

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{N}(\lambda_{exp} - \lambda_{calc})^2 \quad (5)$$

3. RESULTS AND DISCUSSION

According to the Bayesian regularization technique, the optimized neural network configuration has one hidden layer with 12 neurons. The parameters (weight and bias values) of the developed MLP network are shown in Table 3. Figure 2 illustrates the correlation between the simulation results of the

Table 3. Parameters (Weight and Bias) of the ANN

	hidden layer					output layer	
	weights					weight	
neuron	T	x	M	n	biases	λ	bias
1	−0.9279	0.0524	−0.2895	0.2043	0.4671	3.7767	−1.2680
2	0.0297	−0.1393	−3.6023	7.5920	4.4359	−5.9036	
3	0.2101	−1.3063	1.0244	−1.0097	−2.1653	0.9335	
4	0.0148	−0.1764	0.3441	4.6739	3.4456	−2.8590	
5	−0.0182	0.4408	−0.4865	0.4633	0.3227	−2.5905	
6	−2.5135	0.1921	0.2075	−0.1881	−1.6609	1.5678	
7	0.0881	0.6129	−3.0056	0.0731	−1.5178	−1.1621	
8	−0.0068	0.6202	−0.7039	−1.9584	−0.5835	1.2138	
9	−0.6613	0.5227	1.4160	−0.4144	−0.2368	0.3480	
10	0.0062	0.0495	0.8031	−3.4949	−2.2540	−6.2244	
11	1.0740	0.1324	−0.6797	0.6293	1.1510	4.2105	
12	−1.9027	0.7006	−0.9234	0.8736	−1.9204	−2.3953	

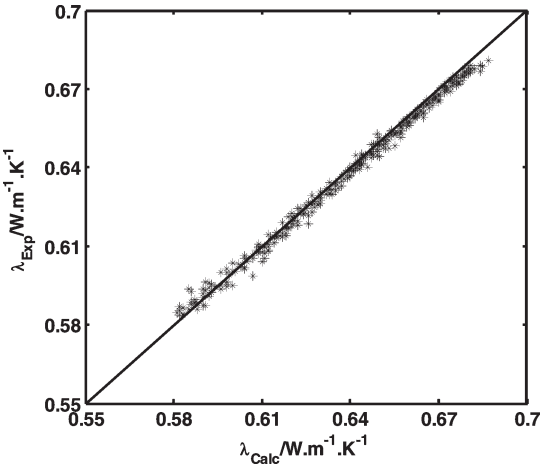

Figure 2. Correlation of experimental data versus neural network predictions for training data set.

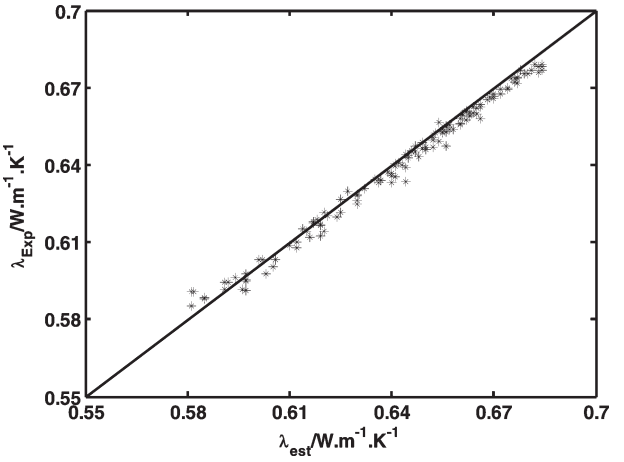

Figure 3. Correlation of experimental data versus neural network predictions for validation data set.

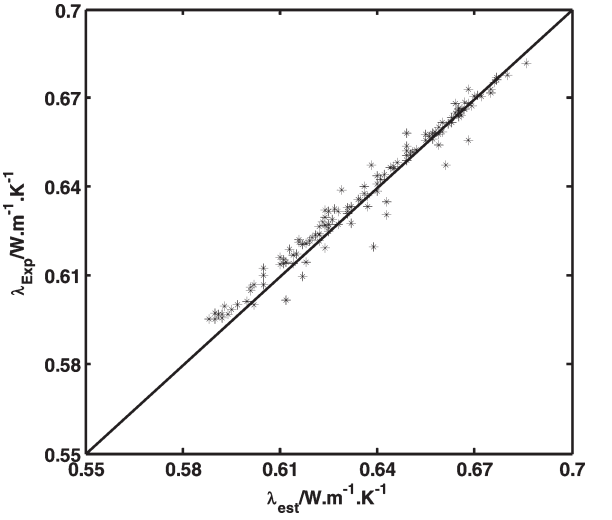

Figure 4. Correlation of experimental data versus neural network values for the test data set.

proposed neural network and the experimental training data points. The perfect fit (output equal to targets) is indicated by the solid line. The close proximity of the best linear fit to the perfect fit, as observed in Figure 2, shows a good correlation among the network predictions and the experimental data. Figure 3 shows the correlation between the calculated results and experimental validation data. The MRE and MSE for this validation data set are 0.486 and 1.369×10^{-5}, respectively.

Also, the performance of the best developed network was tested using another data set consisting of 133 data points not previously used for the network training. The results of the test indicate that the MRE and MSE for the proposed model are about 0.516 and 2.012×10^{-5}, respectively. Figure 4 indicates the correlation between the predicted and experimental test data. In Figure 4, the network outputs for the test data set have been plotted versus the targets and are marked by stars. The perfect fit (output equal to targets) is indicated by the solid line. The slope and the y-intercept of the best linear regression relating targets to the network outputs are respectively 1.0453 and −0.0301, which nearly overlaps the perfect linear fit. The correlation coefficient R^2 between the network predictions and the test data is 0.9862. This shows a very good correlation among the simulated and test data.

Table 2 in the Supporting Information summarizes the results of applying the neural network model and other methods to predict the thermal conductivities of aqueous electrolyte solutions for the test data set. Also, the experimental values of the conductivities are given in the table for comparison. This table shows that the accuracy of the proposed MLP model is better than that of other correlations even though the number of input variables required for the proposed method is the same as that for most other alternative methods. While some of the electrolyte solutions shown in the table were not used in the training, we applied the proposed neural network to them to assess the extrapolation capability of the model. It should be noted that there is no unique correlation to calculate thermal conductivities for the wide range of electrolyte solutions given in Table 2 in the Supporting Information. For example, the adjustable parameters presented in the Abdulagatov and Magomedov,[1,2] Aseyev,[4] and Chiquillo[12] correlations are not available for many electrolyte

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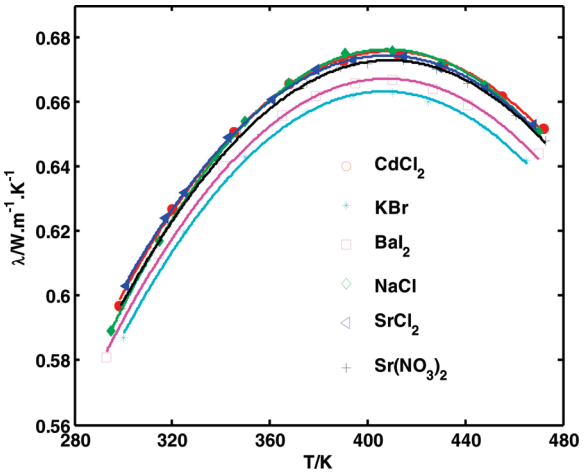

Figure 5. Temperature dependence of thermal conductivities for various electrolyte solutions at fixed concentration of 10 wt %.

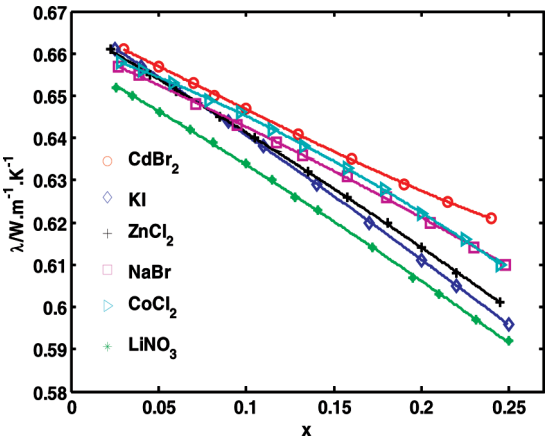

Figure 6. Thermal conductivities of proposed ANN model for various aqueous solutions at constant temperature (350 K) as a function of concentration.

solutions. Based on the type of the electrolyte solution and the desired temperature range, the best correlation has been selected in each case to predict the thermal conductivities to be compared with that of the proposed MLP model.

Indeed, one of the important advantages of the developed neural network model is that it can cover a wide range of temperatures, concentrations, and electrolyte solutions. Other correlations suggested in the literature usually suffer from some limitations with respect to ranges of temperature, concentrations, and type of ionic species. For instance, the correlations proposed by Yusufova et al.[16] and Unterberg[17] are valid for predicting the thermal conductivity of NaCl electrolyte solution and the method of Jamieson and Tudhope[18] can only be used for seawater. To predict the thermal conductivity of electrolyte solution by the Abdulagatov and Magomedov,[1,2] Aseyev,[4] Chiquillo,[12] and Riedel[13] correlations, the adjusted parameters for various solutions are required. Also, the Predvodkelev[14] and Vargaftik and Os'minin[15] correlations for calculating the thermal conductivities of aqueous solutions require accurate values for the heat capacity at constant pressure and also the viscosity of the electrolyte solution which are usually not available at any temperature. The artificial neural network (ANN) model proposed in this article is based on the molecular weight and the number of electrons that can easily be calculated for all electrolyte solutions. This is one of the advantages of the developed MLP network over other correlations.

Figure 5 shows the temperature dependence of the thermal conductivities of $CdCl_2$, KBr, BaI_2, NaCl, $SrCl_2$, and $Sr(NO_3)_2$ electrolyte solutions at a fixed concentration (10 wt %) that have been calculated by the proposed network. As can be observed, the thermal conductivity versus temperature curves go through a maximum between 405 and 415 K. This behavior is analogous to that of the thermal conductivity of pure water in this temperature range, except there is a temperature shift in the location of the maximum.

Figure 6 illustrates the MLP outputs for thermal conductivities of aqueous solutions of $CdBr_2$, KI, $ZnCl_2$, NaBr, $CoCl_2$, and $LiNO_3$ at constant temperature (350 K) as a function of the concentration. According to Figure 6, the intercept of the $\lambda - x$ curve at zero concentration is equal to the thermal conductivity of pure water ($\lambda_{H_2O} = 0.6675\ W \cdot m^{-1} \cdot K^{-1}$). At concentrations up to about 25 wt %, the concentration dependence of the thermal conductivity is linear, as observed by other researchers.[2,26−29,31,32,38−40]

4. CONCLUSION

In this study, an artificial neural network (ANN) has been developed to predict the thermal conductivities of aqueous electrolyte solutions at atmospheric pressure as a function of temperature and concentration. Temperature, concentration, molecular weight, and number of electrons of salt are used as the input variables of the proposed ANN model. The type of ANN used in this study is a multilayer perceptron (MLP) network. A set of 389 experimental data points for thermal conductivities of electrolyte solutions has been used for the network training stage. The best architecture of the MLP network, obtained through a Bayesian regularization technique in combination with the Levenberg−Marquardt algorithm, consists of one hidden layer with 12 neurons. The mean square error (MSE) of the designed network for the training data points is near 7.5×10^{-6}. The performance of the proposed ANN model has also been examined through its application to a test data set consisting of 133 experimental data of thermal conductivities for various aqueous solutions over a wide range of temperatures. The results of this evaluation indicate that the developed ANN model is able to predict thermal conductivities of electrolyte solutions remarkably better than other alternative correlations. The essential advantages of the proposed MLP network against other alternative correlations can be classified into two items: (1) a single neural network model can accurately determine thermal conductivities of various electrolyte solutions over a vast range of temperatures, concentrations, and type of ionic species; (2) the proposed MLP model employs very simple physical parameters as its independent variables that are available for all substances. The thermal conductivity at atmospheric pressure shows a linear dependence on concentration for various electrolyte solutions. For a given concentration, the ANN model results show a thermal conductivity maximum at temperature between 405 and 415 K, as shown in previous literature. The results of applying the trained neural network model to the test data indicate that this method has very good interpolation and extrapolation capabilities with respect to not only the temperature and concentration ranges but also to the kind of electrolyte solution.

■ ASSOCIATED CONTENT

Supporting Information. Table 1, some empirical and semiempirical correlations proposed by researchers for thermal conductivity of aqueous salt solutions; Table 2, comparison of the proposed ANN model with experimental data and other correlations. This material is available free of charge via the Internet at http://pubs.acs.org.

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■ NOMENCLATURE

c_i = electrolyte concentration, mol·L^{-1}
C_p = specific heat capacity
m = molarity
M = molecular weight
n = sum of the numbers of the electrons of anionic and cationic species
N = number of data points
P = pressure, MPa
T = temperature, K
T_c = critical temperature of distilled water, 647 K
x = concentration in mass fraction

Greek Symbols

α_i = ion coefficients
λ = thermal conductivity, W·m^{-1}·K^{-1}
ρ = density
Φ^0_{A-} = apparent thermal conductivity of the anion
Φ^0_{C+} = apparent thermal conductivity of the cation
Φ_λ = apparent molar thermal conductivity

Subscripts

calc = calculated
est = estimated
exp = experimental
H_2O = pure water
sol = aqueous electrolyte solution

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