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Prediction of Kinematic Viscosity of Binary Mixture of Poly (Ethylene Glycol) in Water using Artificial Neural Networks

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Abstract**—**An artificial neural network (ANN) model is presented for the prediction of kinematic viscosity of binary mixtures of poly (ethylene glycol) (PEG) in water as a function of temperature, number-average molecular weight and mass fraction. Kinematic viscosities data of aqueous solutions for PEG (0.55419×10^{-6} – 9.875×10^{-6} m2/s) were obtained from the literature for a wide range of temperatures (277.15 - 338.15 K), number-average molecular weight (200 -10000), and mass fraction (0.0 – 1.0). A three layer feed-forward artificial neural network was employed. This model predicts the kinematic viscosity with a mean square error (MSE) of 0.281 and the coefficient of determination (R^2) of 0.983. The results show that the kinematic viscosity of binary mixture of PEG in water could be successfully predicted using an artificial neural network model.

Keywords**—**Artificial neural network, kinematic viscosity, poly ethylene glycol (PEG)

I. INTRODUCTION

POLY (ethylene glycol) is widely used in cosmetic and pharmaceutical industry. PEG has various characteristics such as water solubility, non-volatility and moderation lubricity. In recent years, great interest has been focused on the prediction of thermodynamic properties of polymers and their mixtures without recourse to experimental measurements [1].

It is common to adopt a linear relationship between the kinematic viscosity of PEG and the mass fraction at each temperature. These types of polynomial correlations of viscosity with temperature and mass fraction suggested in the literature are limited to a narrow range of mass fraction for each temperature and number-average molecular weight, and the correlation parameters vary with the number-average molecular weight at each temperature [1-10].

The artificial neural network (ANN), which has been recognized as a powerful tool capable of performing better than conventional mathematical models particularly for the case of nonlinear and multiple processing systems, is one of widely studied areas within artificial intelligence. The ANN is inspired by biological model and the building blocks are neurons that are combined into layers. The input is received and weighed according to weighting factors, and the resulting quantities are summed up. Without prior and detailed knowledge of the relationship between processing variables, ANN could relate the input to output parameters learning from the provided example and adapting itself through the learning stage [11].

Compared to empirical models, ANN is considered to be more advantageous because it is robust to noise and can accommodate multiple-input and multiple-output systems. In most cases it has been demonstrated that ANN models can perform better than the conventional ones based on regression, statistical or parametric models. Many kinds of networks are developed with different properties and applications. Among these, back propagation (BP) multilayer neural network is the most common and convenient tool. Due to the robustness, fault tolerance, high computational speed and self learning ability, well trained ANN can be employed in many fields [12-15].

The objective of this work was to develop models based on ANN for predicting the kinematic viscosity of binary mixture of PEG in water as a function of mass fraction, temperature and number-average molecular weight. Data needed for the development of ANN model were obtained from the literature.

II. METHODOLOGY

A. Collection of kinematic viscosity data

Kinematic viscosities data set was prepared from literature that included the kinematic viscosity values for given mass fraction, temperature and number-average molecular weight.

B. Training the neural networks

Artificial neural networks were developed using Matlab 7 software. The networks were simulated based on a multi layer feed forward neural network. This type of network is very powerful in function optimization modeling [16]. A three layer feed forward structure with three neurons in the input layer, 20 neurons in the hidden layer and one neuron in the output layer were used in this study as shown in Fig. 1. A back-propagation algorithm was used to implement supervised training of the network. Weights and biases are initialized randomly at the beginning of the training phase, according to the back propagation algorithm.

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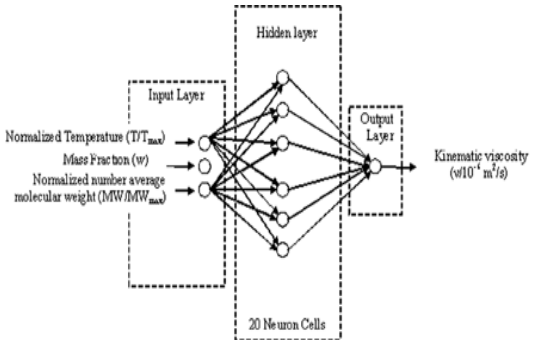

Fig. 1 Selected neural network structure

The inputs included the normalized number-average molecular weight (MW/MW_{max}), normalized temperature (T/T_{max}) and mass fraction. The output layer consisted of kinematic viscosity. The numbers of neurons in hidden layer varied 5 to 25 units (5, 10, 15, 20 and 25). Training was done for trial configuration for each number of hidden units in order to find neurons in hidden layer that produced the minimum error. To avoid the potential problems and over-fitting or memorization while employing the back propagation algorithm two common methods were used [12]. These were (i) early stopping and (ii) minimizing the number of hidden units. The available database was split into three partitions. The first partition was used to perform the training of network. The second partition of the database was used to evaluate the quality of the network during training. In order to estimate the performance of trained network on new database, third test partition was used. The training process was carried out until a minimum of the error was reached in the second (validation) partition. The estimation of the performance of the trained network was based on the accuracy of the network on the test partition. The networks were trained for a fixed number of 1000 cycles.

C. Selection of optimal ANN topology

To achieve the optimum model, several topologies of ANN were evaluated and in each step the mean square error (MSE) was calculated. Furthermore, the coefficient of determination (R^2) of the linear regression line between the predicted value from the ANN model and the desired output were obtained. Error measures used to compare the performance of various ANN models were as follows:

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left(\left|y_{prd,i} - y_{\exp,i}\right|\right)^2 \quad (1)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left(y_{prd,i} - y_{\exp,i}\right)}{\sum_{i=1}^{N}\left(y_{prd,i} - y_{m}\right)} \quad (2)$$

where $y_{prd,i}$ was the predicted value by ANN model, $y_{exp,i}$ was the experimental value, while N was the number of data and y_m was the average of the experimental value.

III. Results and Discussion

The kinematic viscosity data of the 186 cases in our study was divided into three groups. In the first group 130 cases were taken for training, in the second group 28 cases for validation and in the third 28 cases for testing. To achieve the optimal model, several topologies of ANN were evaluated and in each step MSE and R^2 were calculated. The measurement errors and R^2 associated with different ANN topologies for prediction of kinematic viscosity with training data set are presented in table 1. The network topology which has 20 neurons in hidden layer resulted in the best prediction. The MSE and R^2 for this topology were 0.171 and 0.981, respectively. The prediction performances of the optimal models for estimation of kinematic viscosity relative to experimental values are illustrated in Fig. 2. It can be found that a good agreement between the predictive ability of the model and experimental values obtained (R^2= 0.981). In the other steps, the efficiency of the optimum model was evaluated while testing which obtained MSE=0.281and R^2=0.983. The correlation between the predicted and experimental values of kinematic viscosity with validation, testing and total data is shown in Figs. 3-5, respectively.

TABLE I
STATISTICAL RESULTS KINEMATIC VISCOSITY PREDICTION WITH DIFFERENT ANN TOPOLOGY

No. neurons in hidden layer	MSE $(g/cm^3)^2$	R^2
5	0.638	0.934
10	0.396	0.964
15	`0.300	0.971
20	0.171	0.981
25	.0.314	0.963

Fig. 2 Correlation of experimental and predicted values of kinematic viscosity with training data

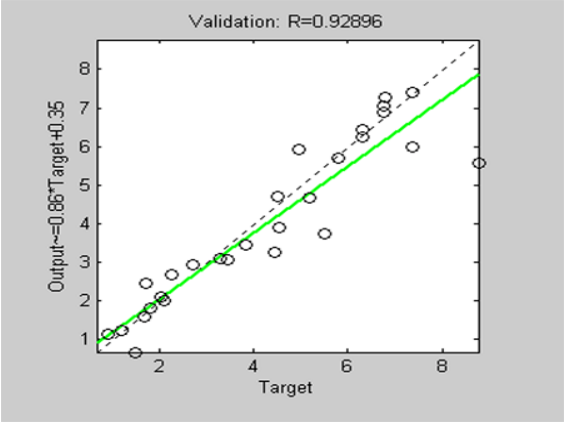

Fig. 3 Correlation of experimental and predicted values of kinematic viscosity with validation data

Fig. 4 Correlation of experimental and predicted values of kinematic viscosity with testing data

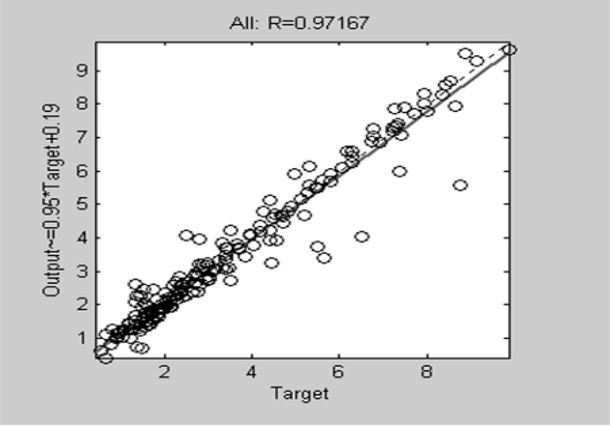

Fig. 5 Correlation of experimental and predicted values of kinematic viscosity with all data

The average percentage of absolute deviation (AAD %) was used for the comparison of experimental and predicted results according to the following equation:

$$AAD(\%) = \left[\left(\sum_{i=1}^{N}\left|\frac{y_{prd,i} - y_{\exp,i}}{y_{\exp,i}}\right|\right)\right] \times \frac{100}{N} \qquad (3)$$

where $y_{exp,i}$, $y_{prd,i}$ and N are the experimental points, predicted points and the number of data points, respectively. The data of AAD was obtained in the literature [10] and was applied for comparison of prediction ability of statistical models and ANN model for kinematic viscosity. The values of AAD were given in Table 2.

TABLE II
THE ADD (%) VALUE FOR KINEMATIC VISCOSITY FROM THE LITERATURE AND THE PRESENT WORK

PEG	AAD (%)	
	statistical	ANN
200	16.7	1.57
300	4.4	0.77
400	5.6	2.25
600	5.2	3.43
1000	6.4	0.84
1500	6.6	1.94
3350	7.6	0.33
6000	6.8	3.97
10000	7.0	4.14

A comparison between values that was obtained in the literature and the values obtained from ANN model shows that the results achieved in the present work are in good agreement with the AAD values presented in the literature and furthermore the ANN model has less error for the kinematic viscosity prediction.Fig. 6 shows the literature viscosity values and those calculated by ANN model at different temperatures and concentrations for PEG 1000.

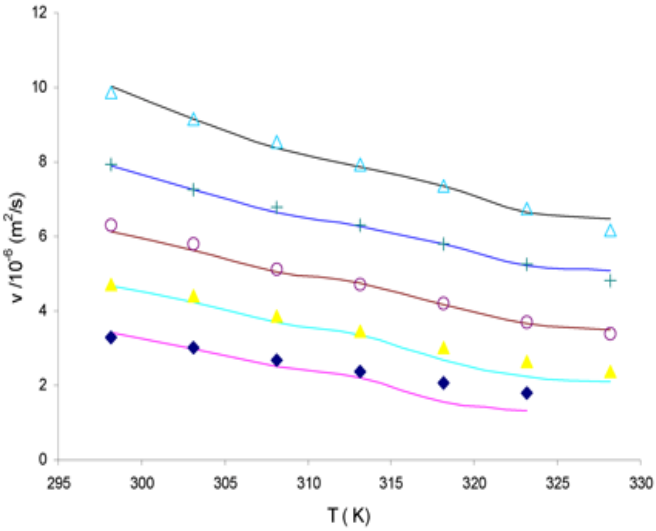

Fig. 6. The literature and calculated viscosities of PEG 1000 at various temperatures and concentrations: ■, w=0.2; ▲, w=0.25; ○, w=0.3; ×, w=0.35; Δ, w=0.4; -, calculated values.

Fig. 7 shows the literature viscosity values and those calculated by ANN model at 293.15 K and various concentrations.

It can be seen that there are good agreements between the results of this work and those reported by others [10]. The advantage of the ANN model presented here, similar to equation reported by Ninni et al. [10], is that it has a generalized form in relation to PEG molecular weight, mass fraction and temperature.

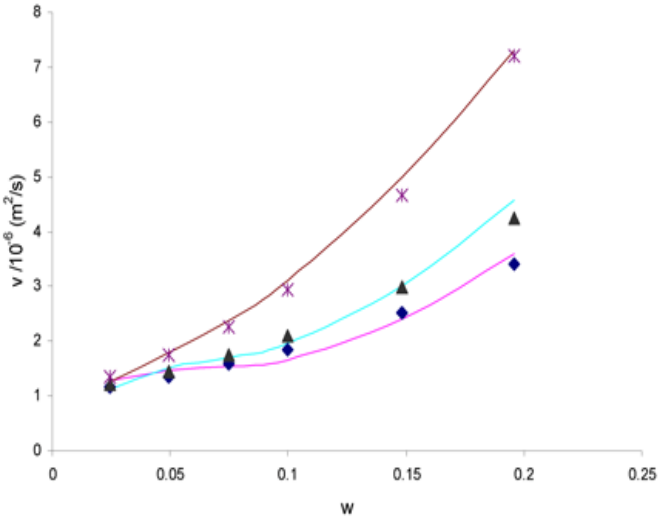

Fig. 7. The literature and calculated viscosities at 293.15 K and various concentrations: ■, PEG 1000; ▲, PEG 1500; *, PEG 3350; -, calculated values.

IV. Conclusion

A neural network based model was developed for the prediction of kinematic viscosity of binary aqueous PEG under a wide range of temperatures, mass fractions, and number average molecular weights. The optimal model, consisting of 20 neurons in the hidden layer, was able to predict viscosity value with an MSE (%) =0.281 and R^2=0.983. The ANN model shows that the error is less than that in statistical models. It is found that the predictive ability of ANN for kinematic viscosity can be used in a wide range of temperatures, mass fractions, and number average molecular weights.

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