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Prediction of density for the mixture of octanol and polyethylene glycol using fuzzy and adaptive neuro-fuzzy systems

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Precise determination of the thermodynamic properties like polymer solutions density is useful for the required polymer processing and polymer equation development. Using fuzzy and neuro-fuzzy systems, this study investigated to present a model to predict the density of the solution of Octanol and Polyethylene Glycol. First, the databank of the dataset collections included 477 data. The data were divided into 120 test data and 357 training data for the fuzzy and neuro-fuzzy systems, and 318 training data and 159 network test data for the neuro-fuzzy system; the training data of both models were used as the inputs to make the related fuzzy inference system. The Gaussian functions were extracted for each input using network segmentation and the optimal parameters were calculated by the neural network with the hybrid algorithm. The comparison of the laboratory results with the predicted amounts by fuzzy and neuro-fuzzy systems indicated that the predicted amounts by these models are in a desirable consistency with the laboratory data and this shows the reliability of these models. The average absolute deviation of the error in fuzzy and neuro-fuzzy systems was 1.1991 and 0.0635, respectively. The results of this prediction indicate a desirable efficiency of neuro-fuzzy modeling for predicting the density of Octanol and Polyethylene Glycol solution.

Keywords: neuro-fuzzy networks, density, octanol, polyethylene glycol, binary solution

INTRODUCTION

The use of polymeric materials is growing in various industries and polymerization processes day by day, and experimental data are less available for polymer systems. Therefore, the issue of process design plays an important role. Obviously, if the thermodynamic properties of polymer mixtures are not recognized, the design of these processes seems impossible. Thermodynamic properties of polymer solutions such as polyethylene glycol and octanol in polymer processing are required and useful for the development of polymer equation of state [1]. Theoretically, the density of physical activity may not be important but economically, it is very significant and is one of the most important factors through which it is possible to determine the behavior of polymer solutions [2]. To calculate the density of polymer solutions, equations of state were used which were dependent on temperature, pressure etc. In fact, the aim of this project is to present a model to address the limitations of existing equations of state and to more accurately predict the density of polymer solution at different pressure and temperature. Given that experimentally measuring the thermodynamic properties is costly and time-consuming process [3], therefore; in this research, to reduce time, cost and to accurately measure density using the fuzzy and neuro-fuzzy network, a model is provided to calculate the density of polyethylene glycol mixture and octanol.

The aim of this paper is to present an appropriate model for predicting the density of octanol mixed with polyethylene glycol in the temperature range of 298 to 338 K and pressure of 0 to 30 MPa to reduce designing cost and synthesis of polymers as well as to save time. This research includes laboratory and field data collection via the Internet; library etc. which examines density of polyethylene glycol and octanol mixture and finally, its modeling is adaptive using fuzzy and neural-fuzzy networks. Input variables of the target model are temperature, pressure, mass fraction and molar fluid composition and the output of the network will be the density of the target mixture. So in this study, the density of polymers using fuzzy and neural-fuzzy systems is simulated and results are compared with experimental data and mathematical and software models.

FUZZY AND NEURO-FUZZY NETWORK

Neuro-fuzzy adaptive inference system was developed by Jung for the first time in 1993. It operates as a fuzzy decision tree to classify data into one of the 2^n or p^n of the linear regression model in a way that it minimizes the sum of squared errors [4]. If there exists knowledge based on fuzzy language rules, we can build a fuzzy inference system and if the data is available, then we can use neural Networks. To build a fuzzy inference system, we need to specify fuzzy sets, fuzzy operators and the basis of existing knowledge and to build a neural network; the user needs to specify the structure and learning algorithm [5].

Research shows that each of these methods has drawbacks by themselves. Therefore, to promote them, it is normal to assimilate these two systems. What fuzzy inference system cannot do, is learning; therefore, the ability to learn is highly significant from the standpoint of fuzzy inference system and neural network structure is interesting from the neural networks point of view. ANN learning algorithms determine parameters of a fuzzy inference system in a neural fuzzy system. In a fuzzy neuro-fuzzy system, structures based on data and on perception cooperate as an input data. A common way to use a learning algorithm in a fuzzy inference system is that the fuzzy inference system is provided through a structure such as neural networks [6-10].

Ming-Jer Lee and colleagues have investigated the properties of a mixture of polyethylene glycol and octanol in the temperature range of 298 to 338 K and pressure of 0 to 30 MPa in 1999 in which the effect of pressure on the density calculated by isothermal compressibility is accurately represented by Tait equation. The overall mean values of absolute deviation percentage are calculated 0/07 and 0/08 respectively by two equations of state FOV and Schotte which then this information was used to calculate the isothermal compressibility [1].

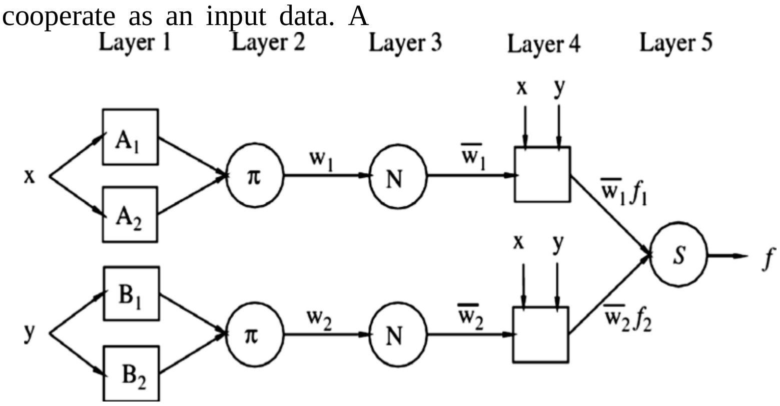

Fig. 1. Structure of an ANFIS network [4].

Hamid Modarres and colleagues attempted to predict the solubility of carbon dioxide in polymers such as polyethylene at a wide range of temperature and pressure using the adaptive neuro-fuzzy system. Their results indicated that adaptive neuro-fuzzy system is an effective method to predict the solubility of carbon dioxide in the polymer which its accuracy and simplicity is more than classic methods [11].

Mohammad Reza Kalaiee and colleagues tried to predict the mechanical properties of reinforced polymeric glass fiber through artificial neural networks and adaptive neuro-fuzzy system in such a way that their results enjoyed small amount of error compared to the experimental values and found that adaptive neuro-fuzzy systems and artificial neural networks are powerful tools to predict the mechanical behavior of multilayer polymeric composites [12].

TRAINING AND NETWORK TEST DATA SELECTION

The main objective of this study was to predict the density of octanol mixed with polyethylene glycol using fuzzy and neuro-fuzzy systems. Data required for network design and training is extracted from the valid papers which have examined the density of octanol mixed with polyethylene glycol with laboratory equipment. After extracting the required data, designing, network training, and testing required fuzzy models are conducted using this experimental data.

Considering modeling done in the areas of density indicates that the parameters of temperature, pressure, the molecular weight of individual molecules in these models are of particular importance.

Because of scattered range of data used for modeling and keeping network training system from sensitization to specific inputs whose numerical values are larger, each of the input data was embedded in a zero to one interval [4].

The data linear normalization in the range of zero and one was done using the equation-1:

$$v_{ronm} = \frac{(v-X_{min})}{(X_{max}-X_{min})} \tag{1}$$

V is the amount of the X variable which is to be normalized and X_{min} and X_{max} are the minimum and maximum amounts among the data.

First, the databank of the dataset collections included 477 data. The data were divided into 318 training data and 159 network test data for the neuro-fuzzy system and 120 test data and 357 training data for the fuzzy system; the training data of both models were used as the inputs to make the related fuzzy inference system.

RESULTS AND DISCUSSION

One of the most effective algorithms in the realm of the automatically law extraction is using observation training and neuro-fuzzy system (ANFIS). As mentioned before, the ANFIS network is a combination of the structure of neural networks and fuzzy logic in which the system uses the training data, extracts the optimal laws, and presents the final model.

To design the adaptive neuro-fuzzy models, the subtractive clustering options in ANFIS tool box within MATLAB software were used. The error back-propagation method and the least squares method were selected as the system optimization criteria in training process. Different parameters like the range of influence, compactness coefficient, acceptance ratio, and rejection ratio need to be set in order to determine the number of clusters and the related membership functions. The characteristic of the best TSK model made by ANFIS is the type of its operators which is presented in the Table 1.

Figure 2 shows the general structure of the fuzzy system network produced for predicting the density of the mixture of Octanol and Polyethylene Glycol. The produced fuzzy system includes four inputs and one output, for each of them, 28 membership functions have been defined.

Table 1. The Type of Operators Used in ANFIS (Genfis2)

Operator Type	Method
AND	prod
OR	probor
Implication	prod
Aggregation	max
Difuzzification	wtaver

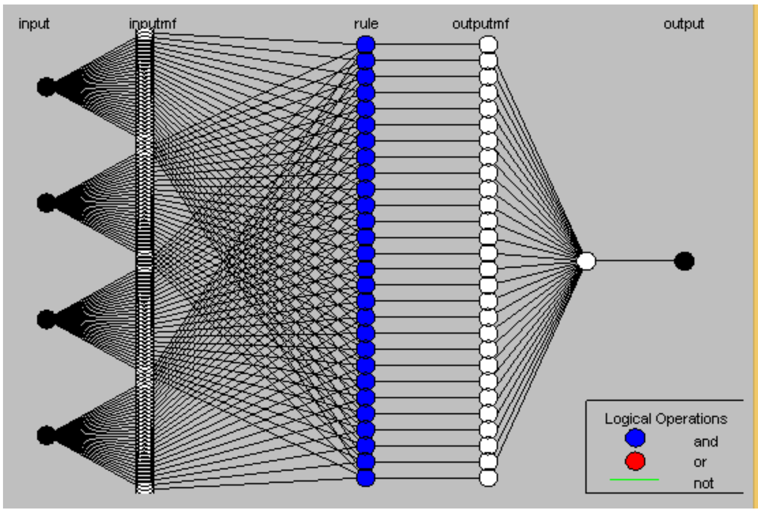

Fig. 2. the general structure of the fuzzy system network ANFIS (Genfis2) produced for predicting the density of the mixture of octanol and polyethylene glycol.

The adaptive neuro-fuzzy inference system has been used in the neuro-fuzzy method. TAE% shows the total mean of error percentage, TAAE% indicates the total mean of absolute error percentage,

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and R is the correlation coefficient for the normalized data. They are calculated based on the following relations, respectively

$$\mathrm{TAE\%} = \left(\frac{100}{n}\right)\sum_{i=1}^{n}\lfloor p_{e,i} - p_{m,i}\rfloor \tag{2}$$

$$\mathrm{TAAE\%} = \left(\frac{100}{n}\right)\sum_{i=1}^{n}\frac{\lfloor p_{e,i} - p_{m,i}\rfloor}{p_{e,i}} \tag{3}$$

$$R = \frac{\sum_{i=1}^{n}[(p_{m,i} - p_{m,av}) * (p_{e,i} - p_{e,av})]}{\sqrt{\sum_{i=1}^{n}[(p_{m,i} - p_{m,av})^2] * \sum_{i=1}^{n}(p_{e,i} - p_{e,av})^2}} \tag{4}$$

In the above relation, $P_{e,i}$, $P_{m,I}$, $P_{e,av}$, and $P_{m,av}$ respectively indicate the desirable output (laboratory), the predicted output by the network, mean of laboratory values, and the mean of the predicted values; n shows the number of data used for training or network test. Tables 2 and 3 show the assessment and performance of the best models made for predicting liquid waste

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Table 2. Comparison of the performance of different models for predicting density in combination

Mixed	MODEL	TAAE%	R
Octanol+PEG200 & Octanol+PEG600	Anfis	0.0635	0.9999
	Fuzzy	1.1991	0.9997
	Fov EOS	0.07	–
	Schotte EOS	0.08	–

Table 3. Comparison of the performance of different models for predicting separate density

Mixed	Model	TAAE%	R
Octanol+PEG200	Anfis	0.1122	0.9998
	Fuzzy	1.639	0.9997
	Fov EOS	0.04	-
	Schotte EOS	0.04	-
Octanol+PEG600	Anfis	0.0399	0.9999
	Fuzzy	0.099	0.9999
	Fov EOS	0.03	-
	Schotte EOS	0.04	-

Figure 3 shows the predicted values for the density of the mixture of octanol and polyethylene glycol by using ANFIS in terms of their real values. They are desirably consistent with each other and it indicates that the results of the presented models by ANFIS are very desirably consistent with the real results, showing the high efficiency of these models.

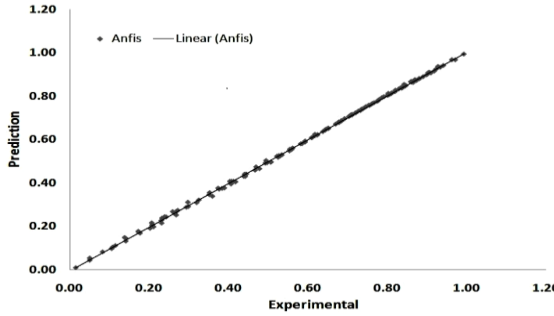

Fig. 3. The correlation between the neuro-fuzzy inference system model and real values.

Figure 4 shows the predicted values for the density of the mixture of Octanol and Polyethylene Glycol by the fuzzy model in terms of their real values.

Figure 6 illustrates the effect of temperature on density. In this figure, density increases when temperature increases and the maximum density is obtained at the temperature unit of 0.22; then, increasing the temperature make the mixture density gradually decrease and reach to a fixed value. As a result, the mixture density is also dependent on temperature.

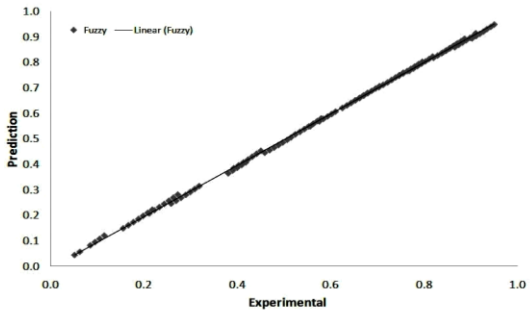

Fig. 4. The correlation between the fuzzy inference system model and real values.

Figures 5 to 7 show the output of the neuro-fuzzy network which demonstrates an important capability compared to the neural network.

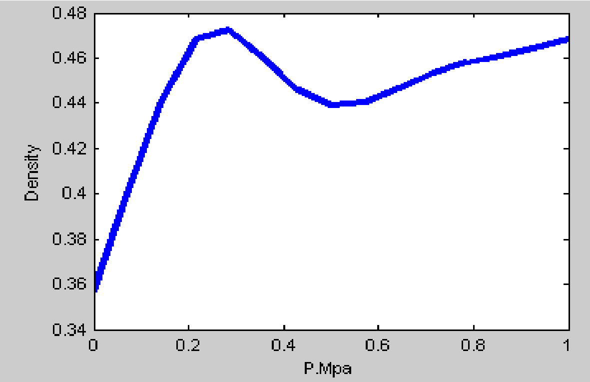

Fig. 5. The effect of pressure on density.

Figure 7 indicates the density changes regarding the mixture pressure and temperature based on the Cartesian coordinate system

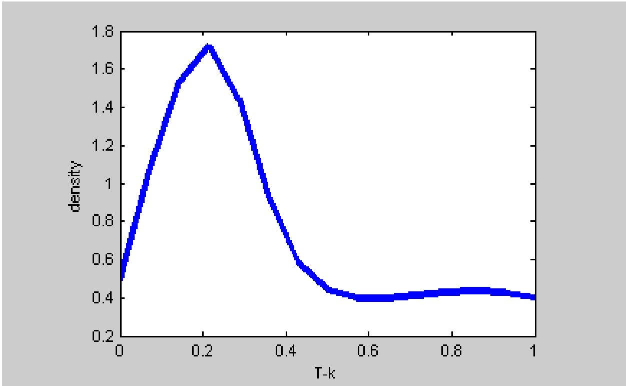

Fig. 6. The effect of temperature on density

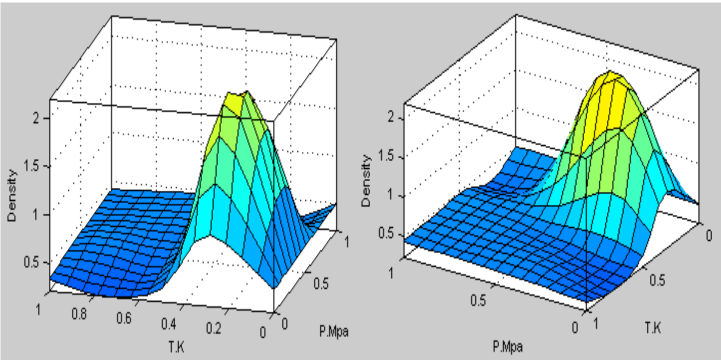

Fig. 7. Density changes regarding pressure and temperature.

Table 4 presents the best parameters related to the developed neuro-fuzzy model.

Table 4. The Parameters Set in ANFIS.

Parameter	Value
Range of effects	0.5
Compression ratio	1.25
Acceptance ratio	0.5
Rejection ratio	0.15
Radius cluster	0.9999

CONCLUSION

This study predicted the density of the mixture of octanol and polyethylene glycol 200 as well as the density of the mixture of octanol and polyethylene glycol 600 both separately and in combination using fuzzy and neuro-fuzzy methods. The amount of the average absolute deviation of the error for these models was calculated as 1.1991 and 0.0635, respectively. In the present study, the efficiency and flexibility of the neuro-fuzzy model in predicting the density of the mixture of octanol and polyethylene glycol were showed. it is obvious that this model is better than the empirical models for predicting the density of the mixture of octanol and polyethylene glycol. Finally, it can be concluded that the presented model eliminated the need to deal with complicated calculations and mathematical models and very precisely was used for density prediction. Therefore, using intelligent systems can be regarded as an appropriate method for density prediction.

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