ARTIFICIAL NEURAL NETWORK MODELING FOR DENSITY OF SOME BINARY SYSTEMS

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Abstract: This paper presents experimental results of density for three binary systems: toluene - n-propanol, toluene - iso-propanol and toluene - propanoic acid. In order to obtain density values at different temperature and concentrations, empirical models were developed using experimental data. Two types of models were built and compared: feedforward neural networks and empirical equations which give the dependence of density on temperature and concentration. Accurate results were obtained in training and validation phases, using neural networks with simple topologies and short training time. In addition, the trend of the predicted densities was qualitatively consistent. The empirical equations also provide good concordance between simulation results and experimental data.

Keywords: *density, empirical models, artificial neural network modeling.*

INTRODUCTION

A rational design or analysis of a chemical process greatly depends on the accurate representation of the thermophysical properties of the process streams. Among these properties, density and liquid viscosity emerges as one of the key transport variables needed in process design and development.

Liquid-liquid extraction, as a separation operation, is based on mass transfer and is largely applied in chemical industry. Different mechanisms and models were proposed to explain the very complex phenomenology of this operation [1].

The mass transfer intensity can be quantified using the individual mass transfer coefficients for each phase. For the liquid-liquid extraction, the determination of these coefficients is a difficult task that was approached by many researchers [2 - 4]. The proposed methods are based on some criterial equations for which the knowledge of viscosity and density of different solutions is necessary. Consequently, the experimental determination of these values, at different concentrations and temperatures, are very useful for the projection of industrial apparatus.

Densities and viscosities of liquid mixtures are important from both practical and theoretical points of view. In the practical aspects, the densities are necessary in a lot of chemical engineering calculations (*i.e.* dimension of storage deposits, design of condensers and boilers) and also in order to determine the dynamic viscosity.

Densities and viscosities for binary mixtures of 1-pentanol with benzene, chlorobenzene, brombenzene, iodobenzene, nitrobenzene, aniline, toluene and p-xylene have been measured over the whole compositions [5]. Nikam, *et al.* and Hasan [6] reported density and viscosity of mixtures of nitrobenzene with methanol, propan-1-ol, propan-2-ol, butan-1-ol, 2-methylpropan-1-ol and 2-methylpropan-2-ol at 298.15 and 303.15 K.

Viscosity and density data are presented by Palepu et. al. [7] for five binary liquid mixtures of acetonitrile with aniline and substituted anilines at five different temperatures and by Villa and co-workers [8] for 1-alkanols and dibutylamine mixtures at 298.15 K.

Taking into account the utility of parameters such as viscosity and density of solutions and the fact that the experiments are very laborious, some mathematical models, which give its variation for different concentration and temperature domains, would by very useful.

In the last decade, neural networks have attracted great interest as predictive models because they have proved to be able to approximate any continuous nonlinear functions [9 - 10] and have been applied widely in process modeling and control [11 - 12]. Neural networks have the ability to learn what happens in the process without actually modeling the physical and chemical laws that govern the system. So they are useful for modeling complex nonlinear processes where process understanding is limited [13].

In this paper, experimental densities for binary mixtures: toluene - iso-propanol, toluene - n-propanol and toluene - propanoic acid over the whole composition range at 19, 26, 32, 38 and 44°C are obtained. From these experimental determinations some mathematical models were established representing empirical relations between density, temperature and concentration. Feedforward neural networks designed to predict density of different binary mixtures as function of temperature and molar fraction represent another type of models. Accurate results are obtained with both types of empirical models: equations relating density of temperature and molar fraction and neural network models.

EXPERIMENTAL

The liquids involved in the experiments, toluene, iso-propanol, n-propanol and propanoic acid, were of analytical purity. A pycnometer equipped with internal thermometer thermostated was used. Preparation of the solutions was performed through weighing using an electronic balance. The molar fractions were known from ±0.0001 to ±0.0005 in all cases. The estimated uncertainty of the measured densities was ±0.0001 g/cm^3.
The experimental values of density for toluene, n-propanol, iso-propanol and propanoic acid, as well as those for toluene - iso-propanol, toluene - n-propanol and toluene - propanoic acid solutions, for different molar fractions (X) and temperatures (t) are given in Tables 1a – 1b.

NEURAL NETWORK MODELING

Multilayer perception (MLP) is the best known and most widely used kind of neural network. It is formed by units (*neurons*), each of them forming a weighted sum of its inputs, to which a constant term is added (*bias*). This sum is then passed through a nonlinearity, called *activation function*. Most often, units are interconnected in a *feedforward manner*, that is, with interconnections that do not form any loops.
A layered topology of a neural network consists in *input, hidden and output layers*. Note that in the multilayer feedforward network there are only interlayer connections. With each connection an *weight* is associated which is a weighted factor that reflects its importance. This weight is a scalar value, positive (excitatory) or negative (inhibitory).
In the *training phase*, the neural network learns the behavior of the process. The *training data set* contains both input patterns and the corresponding output patterns (also called *target patterns*). Neural network training leads to finding values of connection weights that minimize the differences between the network output and the target values. The most extensively adopted algorithm for the learning phase is the *back-propagation algorithm*.
The purpose of developing a neural model is to find a network (set of formulae) that captures the essential relationships in the data. These formulae are then applied to new sets of inputs to produce corresponding outputs. This is called *generalization* and represents subsequent phase after training, *validation* or *testing phase*, respectively. A network is said to generalize well when the input-output relationships, found by the network, is correct for input/output pattern of validation data which were never used in training the network (*unseen data*).
To model the density of the three systems - toluene - n-propanol, toluene - iso-propanol and toluene - propanoic acid - separate neural networks were built. The input variables were temperature and molar fraction of the solution and the output variables was the solution density.
To built an accurate neural network model, a large amount of training data is required. For all three binary systems, experimental data of different temperatures and concentrations were used for building and training the networks. The experiments were conducted in the ranges: t = 19 ÷ 44°C and X = 0 ÷ 1. Randomly, a few experimental data have been extracted to obtain the validation data set and the training was performed without these experimental data.

Table 1a: *Experimental and neural network predicted densities (X)* n- propanol acid molar fraction*

Temperature (t) °C	Toluene - n-propanol		
	Molar fraction (X)* [mol/mol solution]	Experimental density (ρ_{exp}) [kg/m^3]	Neural network density (ρ_{net}) [kg/m^3]
19	0	867.8	865.4
19	0.1238	858.1	859.6
19	0.2459	852.1	853.0
19	0.3657	848.0	846.4
19	0.4954	839.4	838.6
19	0.5832	831.3	833.0
19	0.7513	823.4	822.6
19	0.8755	814.9	814.3
19	1	801.8	802.5
26	0	861.3	860.8
26	0.1238	852.6	853.9
26	0.2459	846.7	847.5
26	0.3657	842.4	841.3
26	0.4954	834.4	833.7
26	0.5832	826.2	828.3
26	0.7513	818.1	818.0
26	0.8755	809.9	809.4
26	1	797.3	797.5
32	0	855.8	855.6
32	0.1238	848.0	848.5
32	0.2459	842.0	842.5
32	0.3657	837.6	836.5
32	0.4954	830.1	829.1
32	0.5832	821.9	823.7
32	0.7513	813.5	813.5
32	0.8755	805.7	804.8
32	1	793.5	793.5
38	0	850.2	849.9
38	0.1238	843.3	843.3
38	0.2459	837.3	837.7
38	0.3657	832.8	831.8
38	0.4954	825.8	824.4
38	0.5832	817.6	819.1
38	0.7513	808.9	809.0
38	0.8755	801.4	800.3
38	1	789.6	790.0
44	0	844.7	844.5
44	0.1238	838.6	838.7
44	0.2459	832.6	833.5
44	0.3657	828.0	827.6
44	0.4954	821.5	820.1
44	0.5832	813.3	814.8
44	0.7513	804.3	804.8
44	0.8755	797.2	796.2
44	1	785.8	787.3

Table 1b: *Experimental and neural network predicted densities $(X)^*$ iso-propanol, propanoic acid molar fraction*

Tempe -rature (t) °C	Toluene - iso-propanol			Toluene - propanoic acid		
	Molar fraction $(X)^*$ mol/mol solution	Experimental density (ρ_{exp}) kg/m^3	Neural network density (ρ_{net}) kg/m^3	Molar fraction $(X)^*$ mol/mol solution	Experimental density (ρ_{exp}) kg/m^3	Neural network density (ρ_{net}) kg/m^3
19	0	867.8	865.6	0	867.8	866.1
19	0.1220	856.3	857.7	0.1290	875.7	876.5
19	0.2459	847.0	847.6	0.2486	887.2	887.3
19	0.3720	838.0	837.6	0.3722	900.1	899.9
19	0.4967	829.3	828.4	0.5082	916.2	915.6
19	0.6200	819.2	819.4	0.6228	931.6	930.6
19	0.7507	808.6	809.1	0.7456	950.0	949.8
19	0.8755	796.8	798.0	0.8724	972.2	973.7
19	1	786.0	785.6	1	995.6	993.1
26	0	861.3	860.8	0	861.3	860.3
26	0.1220	850.2	851.3	0.1290	869.8	870.7
26	0.2459	841.3	841.2	0.2486	881.5	881.9
26	0.3720	832.3	831.8	0.3722	894.4	894.8
26	0.4967	823.4	822.8	0.5082	910.5	910.8
26	0.6200	813.7	813.8	0.6228	925.8	925.7
26	0.7507	802.9	803.2	0.7456	944.3	943.9
26	0.8755	791.2	791.6	0.8724	966.0	967.0
26	1	780.3	779.4	1	989.6	989.0
32	0	855.8	855.6	0	855.8	855.5
32	0.1220	845.0	845.6	0.1290	864.8	865.4
32	0.2459	836.4	836.1	0.2486	876.6	876.6
32	0.3720	827.4	827.0	0.3722	889.6	889.9
32	0.4967	818.4	818.2	0.5082	905.6	906.3
32	0.6200	809.0	809.0	0.6228	920.8	921.3
32	0.7507	797.9	798.0	0.7456	939.3	939.0
32	0.8755	786.4	786.3	0.8724	960.7	961.2
32	1	775.3	774.7	1	984.4	984.6
38	0	850.2	850.0	0	850.2	851.0
38	0.1220	839.7	840.3	0.1290	859.8	860.1
38	0.2459	831.5	831.2	0.2486	871.6	871.0
38	0.3720	822.6	822.4	0.3722	884.7	884.5
38	0.4967	813.4	813.6	0.5082	900.7	901.3
38	0.6200	804.3	804.1	0.6228	915.9	916.6
38	0.7507	793.0	792.9	0.7456	934.4	934.1
38	0.8755	781.6	781.1	0.8724	955.4	955.4
38	1	770.4	770.8	1	979.2	979.5
44	0	844.7	844.4	0	844.7	847.3
44	0.1220	834.5	835.2	0.1290	854.8	855.0
44	0.2459	826.6	826.5	0.2486	866.7	865.1
44	0.3720	817.7	817.9	0.3722	879.9	878.5
44	0.4967	808.3	809.0	0.5082	895.9	895.7
44	0.6200	799.6	799.3	0.6228	910.9	911.4
44	0.7507	788.1	787.7	0.7456	929.5	929.1
44	0.8755	776.8	776.4	0.8724	950.1	949.6
44	1	765.5	767.7	1	974.0	973.9

After the establishing of modeling purpose (input and output variables), one important problem in the developing of a neural network is the determining the network architecture, that is the number of hidden layer and the number of neurons in each hidden layer. It is generally accepted that a large number of hidden layers do not necessarily improve the performance, but increases the difficulties in training [13]. Determining the number of hidden nodes depends on the nonlinearity of the problem and the error tolerance. Too many hidden nodes (an oversized network) cause the network to memorize the training set (*i.e.* over fitting) leading to poor performance of generalization. Too few nodes may not achieve the required error tolerance (*i.e.* under fitting) having difficulties in representing the nonlinear processes.
In our work, the number of hidden layers and units was established by training many networks and selecting the one that balanced generalization performance against network size. The best network topology was determined based upon the mean squared errors (MSE) on the training data. A maximum number of *epochs* (iterations) were fixed. If, after a complete cycle, the overall error is still unacceptable, the neural network would be returned to the beginning of the training patterns and the process would be repeated. So, the training is considered terminated at the point where MSE becomes sufficiently small.
The networks were trained using back-propagation algorithm. Hidden neurons as well as output layer neuron use hyperbolic tangent as nonlinear activation functions. All the network weights were initialized as random numbers in the interval (-0.5, 0.5). Consequently, a configuration of 2 input neurons (for the input variables: temperature and molar fraction), a single hidden layer with 5 neurons and an output layer with 1 output neurons (for the output variable, the solution density) was used. The training errors, mean squared error (MSE) and percent error (E %) are given in Table 2.

Table 2: *The training errors of neural models*

Binary system	Mean Squared Error (MSE)	Percent Error (E %)
Toluene - n-propanol	0.000524	0.104
Toluene - iso-propanol	0.000150	0.0624
Toluene - propanoic acid	0.000106	0.0709

The relative simple structure of the networks, the short training time and the small number of data points needed for training prove that the degree of nonlineraity of the relations between input and output variables is not too high.
A special software application - *NeuroSolutions* - was used in this paper in order to project and obtain predictions of neural networks. In this program, the following specifications are necessary: the network type (MLP), the input and desired output values, the stop condition of the training, the number of hidden layers, the number of processing elements in hidden layers, the activation functions, the learning rule, the maximum number of epochs and some configuration parameters to display the neural model development.

MODELING WITH EMPIRICAL EQUATIONS

Based upon experimental data and using specialized software programs for curve fitting, a series of empirical equations, which compute the density as function of temperature and solution concentration, was determined. Examples of such equations are given in Tables 3a – 3c.
The selection of these equations takes into account the accuracy in experimental data modeling and the simplicity of the equations.
Empirical models presented in Table 3 allowed the determination of density for toluene - n-propanol, toluene - iso-propanol and toluene - propanoic acid solutions at any value of concentration and temperature of the experimental domain. Working with these equations is not difficult, but the introduction of the numerical coefficient for each type of system is necessary. The parameter *correlation*, with values closed to 1, shows the good concordance between experiment and model.

Table 3a: *Empirical equations for density of the binary system toluene – n-propanol*

No. eq.	Equation	Coefficients	Correlation
1.	$\rho = a + b \cdot t + c \cdot X + d \cdot X^2 + e \cdot X^3 + f \cdot X^4 + g \cdot X^5$	a = 880.28181 b = -0.75928 c = -109.07711 d = 470.88307 e = -1323.42784 f = 1504.7769 g = -605.63705	0.998
2.	$\frac{1}{\rho} = a + b \cdot t + c \cdot X + d \cdot X^3 + e \cdot X^{0.5} \cdot \ln X$	a = 0.00113 b = $1.10942 \cdot 10^{-6}$ c = $6.60923 \cdot 10^{-5}$ d = $2.46886 \cdot 10^{-5}$ e = $-3.0811 \cdot 10^{-6}$	0.997
3.	$\frac{1}{\rho} = a + b \cdot t + c \cdot X^{1.5}$	a = 0.00113 b = $1.10984 \cdot 10^{-6}$ c = $8.57292 \cdot 10^{-5}$	0.989
4.	$\rho = a + b \cdot t / \ln t + c \cdot X$	a = 890.96048 b = -3.67159 c = -60.02538	0.989

RESULTS AND DISCUSSION

For modeling the density of the toluene - n-propanol, toluene - iso-propanol and toluene - propanoic acid solutions, three MLP (2:5:1) (2 input neurons for temperature and molar fraction, 5 intermediate neurons in a hidden layer and 1 neuron in output layer for density) were considered.
Firstly, the predictions of neural networks were compared to training (experimental) data to verify how well the networks learned the behavior of the process. Table 1 contains the experimental conditions (temperature and molar fraction), experimental density and neural network predicted densities. A good agreement between the two

categories of data is observed. The parameters average errors and correlations presented in Table 4 show this good concordance.

Table 3b: *Empirical equations for density of the binary system toluene – iso-propanol*

No. eq.	Equation	Coefficients	Correlation
5.	$\ln \rho = a + b \cdot t + c \cdot X^{1.5} + d \cdot X^{0.5}$	a = 6.78462 b = -0.00101 c = -0.07011 d = -0.02855	0.999
6.	$\rho = a + b \cdot t + c \cdot X + d \cdot X^2 + e \cdot X^{2.5} + f \cdot X^3$	a = 882.46790 b = -0.83171 c = -106.69767 d = 283.49991 e = -441.60287 f = 184.26419	0.999
7.	$\rho = a + b \cdot t / \ln t + c \cdot X$	a = 893.13011 b = -4.01949 c = -78.86977	0.997
8.	$\ln \rho = a + b \cdot t + c \cdot X$	a = 6.78559 b = -0.00101 c = -0.0964	0.991

Table 3c: *Empirical equations for density of the binary system toluene – propanoic acid*

No. eq.	Equation	Coefficients	Correlation
9.	$\rho = a + b \cdot t + c \cdot X + d \cdot X^2 + e \cdot X^3 + f \cdot X^4 + g \cdot X^5$	a = 882.81665 b = -0.84337 c = 50.24156 d = 203.84702 e = -388.50794 f = 420.86221 g = -157.8618	0.999
10.	$\rho = a + b \cdot t + c \cdot X + d \cdot X^{2.5} + e \cdot X^{0.5}$	a = 882.80267 b = -0.84337 c = 95.55183 d = 42.10699 e = -9.04571	0.999
11.	$\rho = a + b \cdot t + c \cdot X^{1.5}$	a = 886.1824681 b = -0.84337693 c = 125.419677	0.998
12.	$\rho = a + b \cdot \ln t + c \cdot X^{1.5}$	a = 944.4821636 b = -24.9031149 c = 125.419677	0.998

Table 4: *Average errors and correlations for experimental and predicted densities*

System	Average error	Correlation
Toluene - n-propanol	-0.0003778	0.9987
Toluene - iso-propanol	0.002556	0.9997
Toluene - propanoic acid	0.003603	0.9998

The generalization ability of the artificial neural networks is evaluated using a test dataset distinct from the training data. Consequently, several experimental data were left out the training set, representing validation data set. Tables 5 - 7 show the results of this stage of density modeling. Relative errors were calculated as:

$$Er = \frac{\rho_{net} - \rho_{exp}}{\rho_{exp}} \cdot 100 \qquad (1)$$

where ρ_{net} represent neural network prediction and ρ_{exp} is experimental density.

Table 5: *Validation of neural model for density of toluene - n-propanol solution*

Temperature (t) °C	Molar fraction (X) mol/mol solution	Experimental density (ρ_{exp}) kg/m^3	Neural network density (ρ_{net}) kg/m^3	Relative error (Er)
19	0.7513	823.4	822.869	-0.07516
26	0.4954	834.4	833.569	-0.10538
32	0.2459	842.0	842.494	0.058136
38	0.5832	817.6	819.874	0.270452
44	0.1238	838.6	839.068	0.046776

The relative errors, extremely low, prove the validity of the neural models.
It must be noted that the predictions of the neural models were very good, even for the validation data set, although the number of experimental points used for training was not very large. In this example, it was essential that the limits of experimental domain are large enough, corresponding to the practical purposes. In this way, precautions were taken to ensure that the training set is representative for the process under study. Another idea to emphasize is the importance of the neural network performance in the testing set rather than in the training set. In other words, the network should be design and trained in order to ensure good generalization and not only good performance in the training set.

Table 6: *Validation of neural model for density of toluene - iso-propanol solution*

Temperature (t) °C	Molar fraction (X) mol/mol solution	Experimental density (ρ_{exp}) kg/m^3	Neural network Density (ρ_{net}) kg/m^3	Relative error (Er)
19	0.6200	819.2	819.250	-0.00313
26	0.3720	832.3	831.899	-0.05462
32	0.1220	845.0	845.862	0.09955
38	0.7507	793.0	792.861	-0.02733
44	0.4967	808.3	809.236	0.106063

Table 7: *Validation of neural model for density of toluene – propanoic acid solution*

Temperature (t) °C	Molar fraction (X) mol/mol solution	Experimental density (ρ_{exp}) kg/m^3	Neural network Density (ρ_{net}) kg/m^3	Relative error (Er)
19	0.5082	916.2	915.520	0.076924
26	0.2486	881.5	881.923	0.044811
32	0.7456	939.3	938.946	0.047042
38	0.3722	884.7	884.562	0.025149
44	0.8724	950.1	949.492	0.074229

The main purpose of the neural networks based modeling was to set up the possibility of obtaining the density values at any temperature and concentration from the domain of data used for training. This type of network testing has as results the curves in Figures 1, 2 and 3 (corresponding to the three systems under study) in which density variation with molar fraction is drawn at 22, 29, 35 and 32°C as neural network predictions (curves noted 2, 3 and 4). In these Figures, experimental curves of 19 and 44°C are also presented as limits of experimental domain.

Thus, the neural network predictions make available accurate values of density at any concentration and temperature in 19 - 44°C domain.

Based on the good results obtained in the training and validation of neural models, the predictions of neural networks were extended out of the experimental domain, to higher temperatures (greater than 44°C) and to lower temperature (less than 19°C). Figures 4, 5 and 6 present these results for three values of the molar fractions: 0.2, 0.5 and 0.7 and for the three systems on which this study focuses. In these Figures, the temperatures without experimental domain are marked with circles (10, 15, 45, 50, 55, 60°C). We can appreciate that the trend of the predicted density out of the experimental domain is qualitatively consistent.

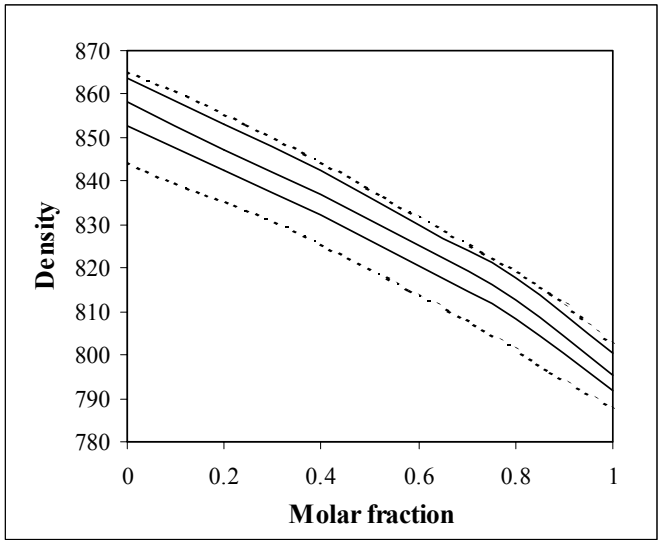

Figure 1: *Density variation with molar fraction for the system toluene - n-propanol obtained as neural network prediction at: 1 - 19℃; 2 - 22℃; 3 - 29℃; 4 - 35℃; 5 - 44℃.*

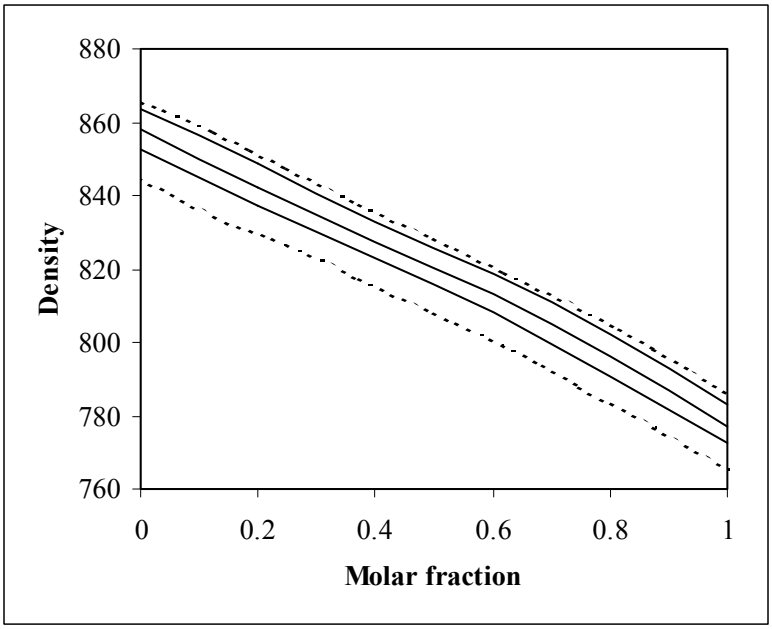

Figure 2: *Density variation with molar fraction for the system toluene - iso-propanol obtained as neural network prediction at: 1 - 19℃; 2 - 22℃; 3 - 29℃; 4 - 35℃; 5 - 44℃.*

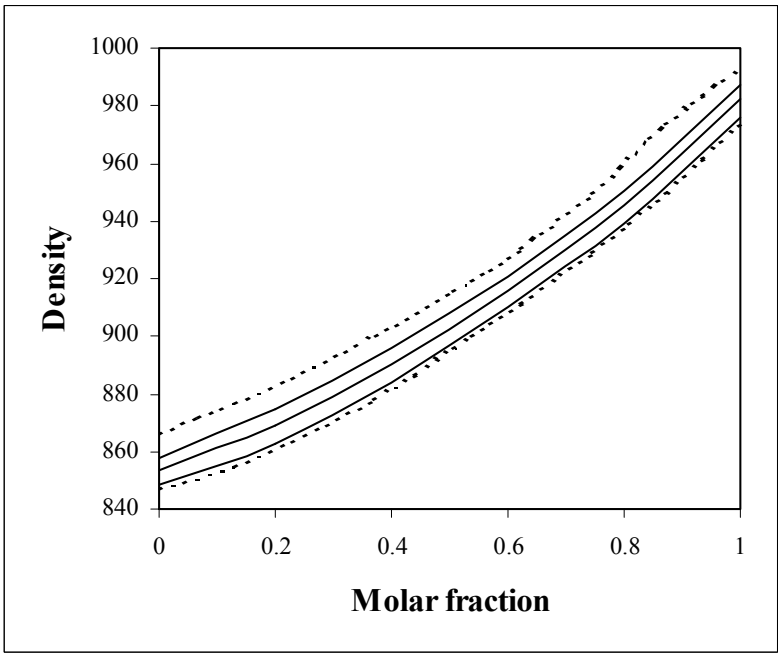

Figure 3: *Density variation with molar fraction for the system toluene - propanoic acid obtained as neural network prediction at: 1 - 19℃; 2 - 29℃; 3 - 35℃; 4 - 42℃; 5 - 44℃.*

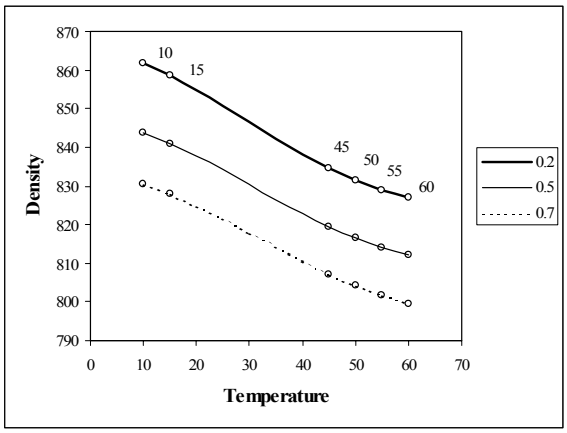

Figure 4: *Neural network predictions out of the temperature experimental domain at different molar fractions (0.2, 0.5 and 0.7) and different temperatures (10, 15, 45, 50, 55, 60 ℃) for the toluene - n-propanol solutions.*

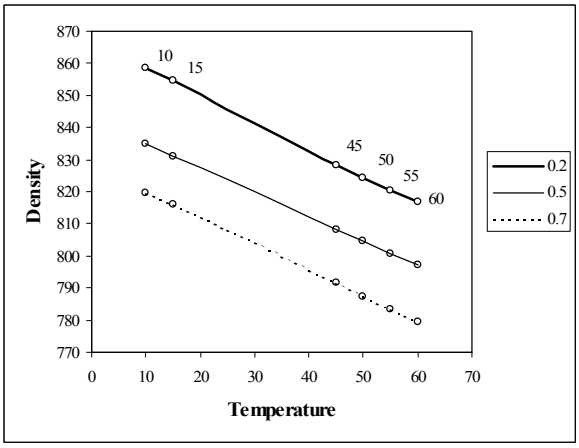

Figure 5: *Neural network predictions out of the temperature experimental domain at different molar fractions (0.2, 0.5 and 0.7) and different temperatures (10, 15, 45, 50, 55, 60 ℃) for the toluene - iso-propanol solutions.*

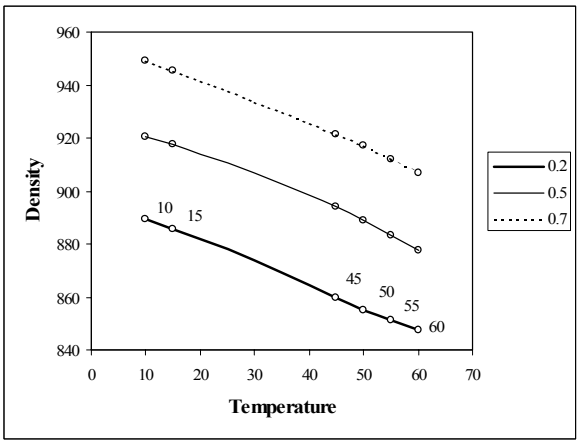

Figure 6: *Neural network predictions out of the temperature experimental domain at different molar fractions (0.2, 0.5 and 0.7) and different temperatures (10, 15, 45, 50, 55, 60 ℃) for the toluene - propanoic acid solutions.*

Another type of empirical modeling is represented by equations from Tables 3 which gives explicitly the dependence of density with temperature and molar fraction. For each of the three systems, the equations with the best correlations (numbered 1, 5 and 10) and the simplest equations (4, 7 and 11) were chosen in order to compare their results with the neural network predictions. The comparisons were made at different temperatures: 26°C for toluene - n-propanol, 38°C for toluene - iso-propanol, 44°C for toluene - propanoic acid. Figures 7 - 9 present these examples.

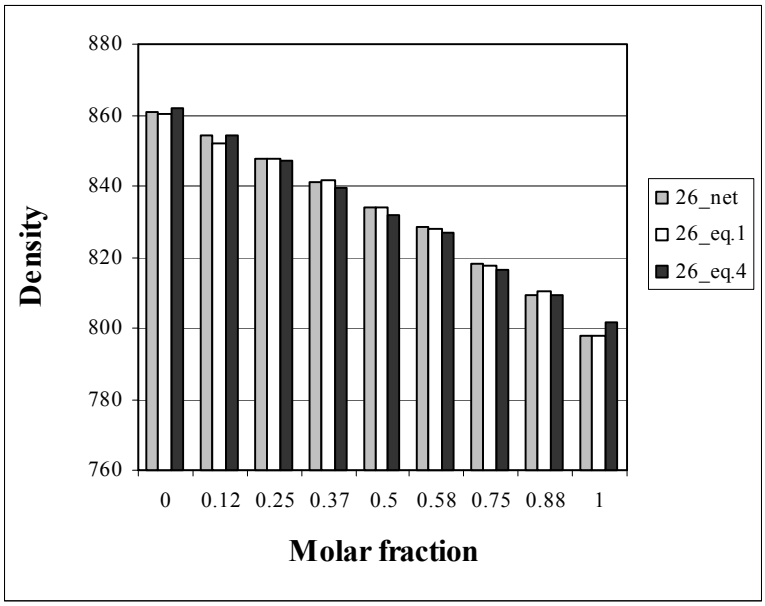

Figure 7: *Density variation with molar fraction for the system toluene - n-propanol obtained at 26°C with neural model and empirical equations 1 and 4.*

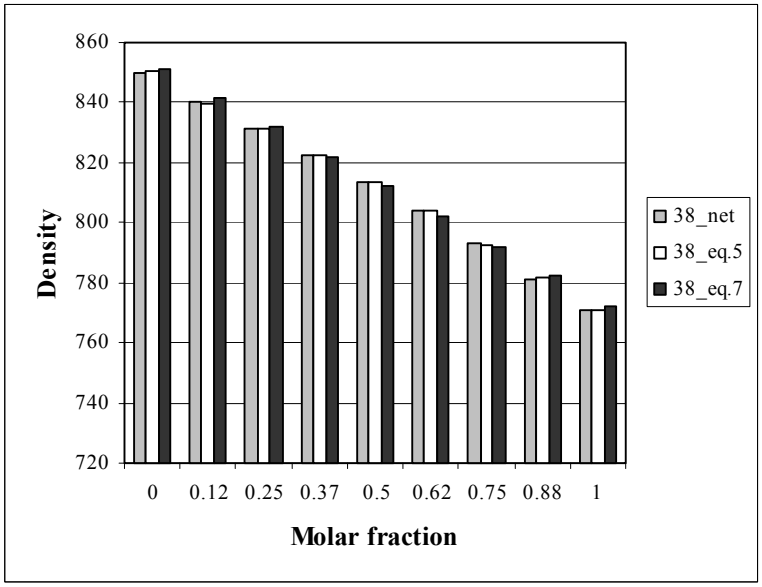

Figure 8: *Density variation with molar fraction for the system toluene - iso-propanol obtained at 38°C with neural model and empirical equations 5 and 7.*

The empirical equations have the advantage of offering an explicit form of viscosity variation with temperature and molar fraction, but they are difficult in handling because of the numerical coefficients which must be replaced for each system. The neural models have also empirical parameters (network weights), but these are available for the whole experimental domain. In addition, the artificial neural networks are easy to build, have a simple topology, a short training time and provide accurate results.

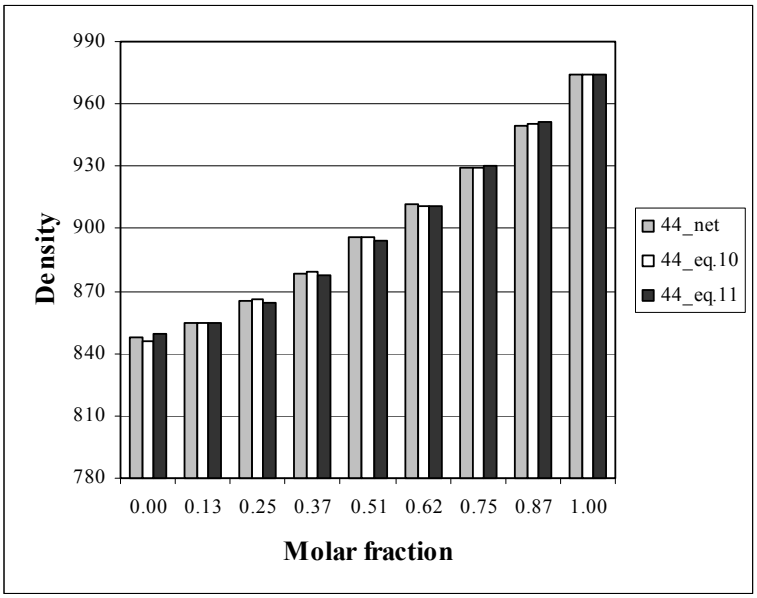

Figure 9: *Density variation with molar fraction for the system toluene - propanoic acid obtained at 44°C with neural model and empirical equations 10 and 11.*

CONCLUSIONS

This paper presents experimental data of density for three binary solutions: toluene - n-propanol, toluene - iso-propanol and toluene - propanoic acid, for different temperatures (19 ÷ 44°C) and molar fractions (X = 0 ÷ 1).

Because the experiments are laborious, mathematical models, which allow calculate the density of the above systems at each temperature and concentration are required.

The neural networks are adequate and recommended instruments for modeling nonlinear processes. The wide use of neural networks is based on their ability of learning from a set of numerical data (corresponding to the input and output desired variables), using an adjustment algorithm for the network' parameters. Once trained, the network will be able to generate predictions faster than any other type of model.

Three neural networks were built to predict the density of the toluene - n-propanol, toluene - iso-propanol and toluene - propanoic acid solutions. These MLP (2:5:1) work with temperature and molar fraction as input variables and have 5 neurons in a single hidden layer. Errors smaller than 0.4 % have been obtained in training and testing phases. The neural models make available accurate values of density at any molar fraction and temperature in the experimental domain used for network training (19 ÷ 44°C) and replace, in this way, experiments. Qualitatively, we can appreciate that the

predictions of the neural models outside the temperature experimental domain are precise, as show the trend curves.
Explicit correlations between density and temperature and molar fraction are given by empirical equations obtained with a curve fitting procedure starting from experimental data.
A comparison between the empirical equations and neural models shows the advantages and disadvantages of the two modeling techniques. The empirical equations offer an explicit form of viscosity variation with molar fraction, but they are difficult to handle due to the numerical coefficients. The neural models are easy to design and provide in a simple and fast manner accurate results, but they work like a black box.
One should note that both types of models are easy to obtain and provide good concordance with experimental data.

Acknowledgements

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