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# Experimental Studies of Surface Tensions for Binary and Ternary Systems of Benzyl Alcohol, N-Hexanol and Water. Modeling with Neural Networks

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**ABSTRACT**

*The design of installations in the chemical industry requires the knowledge of the thermodynamic properties of liquid mixtures. In the absence of experimental data, accurate predictive methods are needed. In this work, refractive index and surface tension, at different temperatures and atmospheric pressure, are experimentally determined for the binary and ternary systems of benzyl alcohol, n-hexanol and water, which are studied less in literatures.. Two models were developed to have excess surface tension corelate composition, normalized temperature and refractive index. The statistical processing of the experimental data with the multiple linear regression method allowed the development of a model of which, in the validation stage, the correlation coefficient was 0.9086 and the standard deviation was 4.36. With the best performing neural model, a correlation coefficient of 0.9727 and a standard deviation of 2.14 were obtained in the validation stage.*

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## 1. Introduction

A good knowledge of the thermodynamic properties of liquid systems [1-14] is very important in engineering, as they lead to obtaining important experimental data for the design of distillation separation plants [15, 16]. The specialized literature reveal the fact that there is no data on the surface tension and refractive index of the binary systems of benzyl alcohol - n-hexanol, benzyl alcohol - water and the ternary system of benzyl alcohol - n-hexanol - water. Azizian and Bashavard [7] experimentally determined the surface tension for binary mixtures of benzyl alcohol - linear alcohols (1-propanol, 2-propanol, 1-butanol, 2-butanol, 1-pentanol, and 2-pentanol) at the

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temperatures of 293.15 to 323.15 K. They observed negative deviations from the ideal behavior in the case of these binary mixtures and highlighted the fact that linear alcohols that have a lower surface tension tend to migrate to the surface so that they will have higher concentrations on the surface than in the mass of the mixture. Negative deviations from the ideal behavior for binary mixtures of dimethyl sulphoxide with linear alcohols (1-propanol, 1-butanol, and 1-hexanol) were also reported by Bagheri and others [4]. Surface tension is an important property that can influence heat and mass transfer processes in distillation and extraction plants. It is known that the surface tension for pure liquids and for most liquid mixtures decreases by increasing temperature. However, there is a different behaviour that occurs in the case of mixtures of liquids containing water and alcohols with the number of carbon atoms ≥4. In this situation – the solutions of alcohol diluted in water – the increase of surface tension with the increase of temperature has been reported in literatures [17-19]. Thermodynamic properties (surface tension, refractive index, density, viscosity, etc.) can correlate with the variation of composition and temperature using different types of models [20-24]. Several groups of researchers have used various artificial intelligence tools to predict the surface tension for pure components, binary or ternary systems [25-28]. Refractive index is determined easily and accurately, using a small amount of substance. Members of our research group used MLR models to predict excess molar volume based on experimentally determiningrefractive index [16]. They also used different types of neural networks to predict excess molar volume [29, 30] and excess refractive index [31].

In this paper, it is analyzed the influence of temperature and composition on excess surface tension for binary and ternary systems of benzyl alcohol, n-hexanol and water, which has almost not been studied in literatures. Surface tension and refractive index in an area of composition influenced by the miscibility of the components, different temperatures and atmospheric pressure are determined experimentally. The increase of surface tension with the increase of the temperature is highlighted for both the binary system n-hexanol-water, and the ternary system benzyl alcohol-n-hexanol-water. MLR models obtained by processing experimental data using the multiple linear regression method and also neural models with multilayer perceptron (MLP) are proposed. These models make excess surface tension correlate with refractive index, molar fractions, and normalized temperature. MLR models obtained by statistical processing of the experimental data with the multiple linear regression method and also multilayer perceptron (MLP) neural models having excess surface tension correlate refractive index, mole fractions and normalized temperature are proposed.

## 2. Experimental

### 2.1. Liquid materials

The experiments were performed using double-distilled water, benzyl alcohol (Purity 99.5%, Merck) and n-hexanol (Purity 99%, Sigma-Aldrich).

Table 1 compares the experimental values of the refractive index and surface tension for pure liquids with the data from literatures.

**Table 1**
Thermodynamic properties of pure compounds at atmospheric pressure (0.1 MPa).

| Liquid | Temperature (K) | Refractive index | | Surface tension mN/m | |
|---|---|---|---|---|---|
| | | Exp*. | Literature | Exp. | Literature |
| benzyl alcohol | 293.15 | 1.5427 | 1.5400[8] | 39.484 | 39.05[7]<br>38.58 at 298.15 K[7]<br>35.90[8] |
| | 303.15 | 1.5398 | | 38.598 | 39.03 at 298.15 K[9]<br>38.81[9] |
| | 313.15 | 1.5386 | | 37.712 | 36.63 at 318.15 K[7]<br>38.31[9] |
| | 323.15 | 1.5361 | | 36.826 | |
| n-hexanol | 293.15 | 1.4212 | 1.4163 at 298.15 K[11]<br>1.41775 at 298.15 K [12]<br>1.4180[13] | 24.137 | 24.511 at 298.15 K [4]<br>25.39 at 298.15 K [6] |
| | 303.15 | 1.4193 | 1.4140[13]<br>1.4149[11]<br>1.41409[14] | 23.361 | 23.861 at 308.15 K[4]<br>25.27[17] |
| | 313.15 | 1.4111 | 1.4110[11]<br>1.41005[14] | 22.585 | 23.018 at 318.15 K[4]<br>24.58[17] |
| | 323.15 | 1.4067 | 1.40608[14]<br>1.4067[12] | 21.809 | 22.331 at 328.15K[7]<br>23.44[17] |

* Experimental
Standard uncertainties u are u(T) = ±0.01 K for surface tension and u(T) = ±0.1 K for refractive index , u(γ) = ±0.25 mN/m, u(n) = ±0.0002 and u(P) = ±0.001MPa

The preparation of binary and ternary solutions using the mentioned liquids was performed by weighing samples on an Mettler Toledo XP105 analytical balance., which ensures a measurement accuracy of ± 0.01 mg. The estimation of molar fractions was thus performed with an accuracy of ± 0.0001. The liquid mixtures were made in sealed vials to avoid preferential evaporation, and then refractive index and surface tension were measured.

### 2.2. Measuring refractive index

The refractive index for pure liquids and binary and ternary mixtures was measured with an Abbe refractometer with a corresponding Na wavelength (589.3 nm) and a Lauda E100 thermostat to maintain a constant temperature with an accuracy of 0.1 K. The refractometer was calibrated using double-distilled water. Based on the line of reflection of Na, this type of refractometer has a standard uncertainty of ± 0.0002 of reading refractive index.

### 2.3. Measuring surface tension

The surface tension for pure liquids and binary and ternary mixtures was measured using the Wilhelmy plate method with a KSV Sigma 700 automatic tensiometer. Each obtained value is an average of at least 6 measurements. The maximum standard deviation is ± 0.25 mN/m. A recirculating thermostat was used to keep the temperature constant. It kept the temperature constant with an accuracy of 0.1 K.

### 2.4. Modeling the excess surface tension

The modelling of excess surface tension was performed by statistically processingthe experimental data with multiple linear regression method (MLR). The Sigmaplot 11 software was used to determine the dependence between excess surface tension (dependent variable) and composition ($X_1$ and $X_2$), normalized temperature (T/273.15) and refractive index (independent variables).

The modelling with the help of neural networks (Figure 1) was done with the Neurosolutions commercial simulator produced by the Neurodimension company. 50,000 training epochs were used for testing all neuronal models. The used transfer functions were of the TanhAxon type. The duration of the training process was less than 3 minutes, and the applied learning algorithm was Momentum.

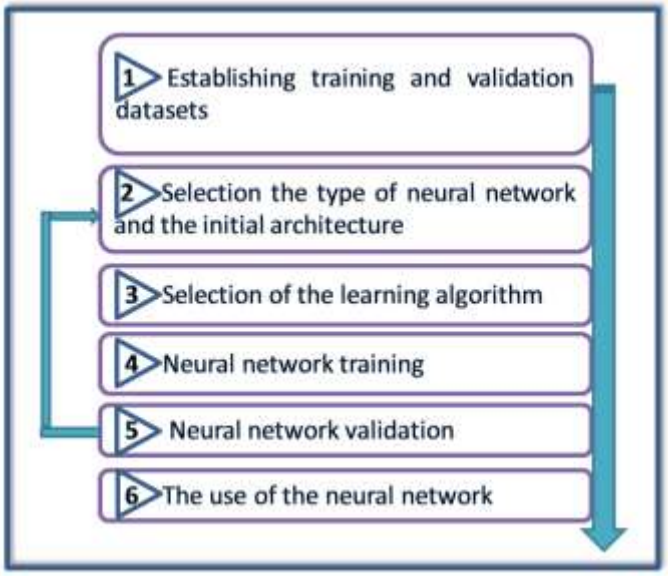


**Figure 1.** Methodology of modeling excess surface tension .

## 3. Results and discussions

The refractive index and surface tension for binary and ternary liquid mixtures were determined experimentally at the following temperatures: 293.15, 303.15, 313.15 and 323.15 K and the pressure of 0.1 MPa. The results are presented in table 2.

The experimental results indicate that refractive index decreases by increasing temperature for the binary systems benzyl alcohol-water and benzyl alcohol-n-hexanol. For the n-hexanol-water binary system and benzyl-n-hexanol-water alcohol ternary system (with $0.0033 < X_2 < 0.0059$), surface tension increases by increasing temperature. A first considered hypothesis was the change of the composition of liquid mixtures by evaporation at higher temperatures. This hypothesis was not confirmed because the refractive indices for the mentioned binary and ternary mixtures used in the surface tension tests were measured and it was found that they kept their values. The review of literatures indicated that other researchers also reported higher values of surface tension for the dilute solutions of alcohols with a number of carbon atoms ≥4 by increasing temperature [17-19]. Another hypothesis would be the accumulation of surface active components at the air/water interface which lowers surface tension. Thus, an increase in surface tension by increasing temperature indicates that the concentration of surface excess of the surface active compound decreases as the temperature increases. This is consistent with the increased solvation of the solute at higher temperatures. Cheng and Park [17] found that the surface tension for the n-hexanol - water binary system remains approximately constant or increases by increasing temperature. Also, Ono et al. [18] presented the results obtained for the surface tension of the binary systems butanol-water and pentanol-water by two methods: the maximum bubble pressure method and Wilhelmy's method. By both methods a tendency to increase surface tension was

observed for these binary mixtures at temperatures above a critical temperature. The increase in surface tension by increasing temperature is more pronounced when Wilhelmy's method is used. It was also observed that the onset of the increase in surface tension with temperature occurs at lower temperatures for pentanol compared to butanol and is more intense for the binary system containing the alcohol with a higher number of carbon atoms. Romero et al. [32] used a LAUDA TVT1 drop volume tensiometer to measure the surface tension of 1-hexanol-water binary systems with the mole fractions between 0.00025 and 0.00093 at the temperatures between 288.15 and 308.15K. In the mentioned temperature range the authors found that regardless of the mole fraction of 1-hexanol, surface tension decreased by increasing temperature and the magnitude of the slopes became less negative as the temperature increased. If we compare the results obtained in our study with those reported by Romero et al. [32], for approximately the same mole fractions and temperatures, we find a good agreement, although two very different methods were used to determine surface tension.. For example, in our study of the surface tension for a mixture with the n-hexanol mole fraction of 0.0003, the surface tension is 48.01 mN/m at 293.15K and 49.05 mN/m at 303.15K. For a molar fraction of 1-hexanol of 0.00025, Romero et al. [32] obtained 47.94 mN/m of n-hexanol at the temperature of 293.15K and 46.91 mN/m at 303.15K.

Based on the experimentally determining the surface tension for binary and ternary mixtures, as well as for pure components, the excess surface tension of which the values are reported in Table 2 was calculated with equation (1).

$$\gamma^{exc} = \gamma - X_1\gamma_1 - X_2\gamma_2 - (1 - X_1 - X_2)\gamma_3 \quad (1)$$

where $\gamma$ is the experimental value of the surface tension of binary and ternary mixtures, $X_1$ – the molar fraction of benzyl alcohol, $X_2$ – the molar fraction of n-hexanol, and $\gamma_1$, $\gamma_2$ and $\gamma_3$ represent the experimental surface tension for pure compounds.

For both binary and ternary mixtures, deviations from the ideal behaviour are negative and more pronounced in the case of binary systems containing double-distilled water and in the case of the ternary system (table 2). This behaviour is due to the the mixture, for these systems, including small amounts of n-hexanol and benzyl alcohol which have lower surface tension and tend to migrate to the phase separation interface so that the concentration in the surface layer will be higher than that in the main mass of the mixture. [7, 8] In the case of the benzyl alcohol-n-hexanol alcohol binary system, we also have negative but smaller deviations (Figure 2). In this system, the composition of the mixture varies in a wide range, with molar fractions being between 0.1 and 0.9. The predominant interactions between benzyl alcohol and n-hexanol molecules are of the (O ... H - O) type, but also of weaker dipole-dipole interactions [19].

The excess thermodynamic properties are most often correlated in the literature [20, 33-36] with the molar fractions, with the empirical model proposed by Redlich-Kister. [37]. Since it is easy to measure refractive index and with fairly good accuracy and due to the low consumption of material,researchers [38-40] have been interested in finding models that correlate other thermodynamic properties that are more difficult to experimentally measure (surface tension, viscosity, density, etc.) with this parameter. The best-known model of this kind, that has surface tension correlate refractive index, is the one proposed by Sugden [41].

The Multiple linear regression module of the Sigma Plot 11.2 program was used in this study to have excess surface tension correlate refractive index, molar fraction and normalized temperature:

$$\gamma^{exc} = 478.5 + 101.514\,X_1 + 58.389\,X_2 + 47.083\,(T/273.15) - 416.897\,n \quad (2)$$

The correlation coefficient for the model that has the excess surface tension correlate molar fraction, normalized temperature and refractive index is 0.9086 (Figure 3), and the standard deviation is 4.36. Equation (2) is valid for: the binary system of benzyl alcohol – water for $X_1 \leq 0.0059$; binary system of n-hexanol – water for $X_2 \leq 0.0011$; and ternary systems of benzyl alcohol - n-hexanol-water for $X_1 \leq 0.0006$ and $X_2 \leq 0.0059$.

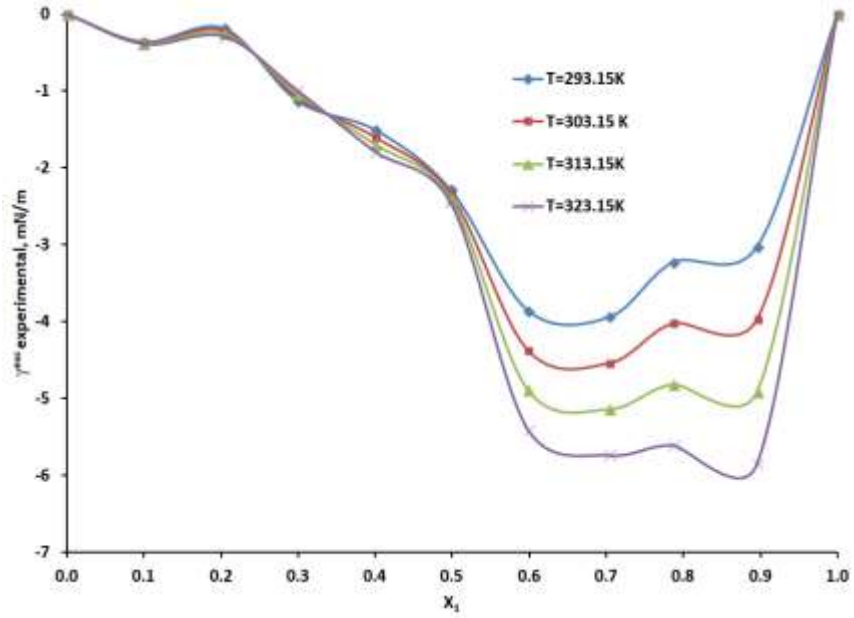


**Figure 2.** Excess surface tension of the binary system of benzyl alcohol-n-hexanol alcohol.

**Table 2**

Experimental values of surface tension for binary and ternary liquid mixtures at different temperatures and atmospheric pressure (0.1 MPa)

| System | $X_1$ | $X_2$ | 293.15 K | | | 303.15 K | | | 313.15 K | | | 323.15 K | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | n | $\gamma$ (mN/m) | $\gamma^{exc}$ (mN/m) | n | $\gamma$ (mN/m) | $\gamma^{exc}$ (mN/m) | n | $\gamma$ (mN/m) | $\gamma^{exc}$ (mN/m) | n | $\gamma$ (mN/m) | $\gamma^{exc}$ (mN/m) |
| benzyl alcohol – water | 0.0012 | 0 | 1.3391 | 48.16 | -23.99 | 1.3387 | 44.53 | -25.31 | 1.3379 | 40.90 | -26.63 | 1.3371 | 37.26 | -27.95 |
| | 0.0023 | 0 | 1.3408 | 46.37 | -25.75 | 1.3393 | 42.26 | -27.55 | 1.3388 | 38.14 | -29.36 | 1.3379 | 34.03 | -31.16 |
| | 0.0031 | 0 | 1.3412 | 43.15 | -28.94 | 1.3404 | 40.31 | -29.47 | 1.3398 | 37.47 | -30.00 | 1.3391 | 34.63 | -30.53 |
| | 0.0040 | 0 | 1.3429 | 44.52 | -27.54 | 1.3412 | 42.62 | -27.13 | 1.3407 | 40.72 | -26.73 | 1.3402 | 38.82 | -26.32 |
| | 0.0051 | 0 | 1.3439 | 40.96 | -31.07 | 1.3426 | 39.95 | -29.77 | 1.3420 | 38.93 | -28.48 | 1.3408 | 37.92 | -27.19 |
| | 0.0059 | 0 | 1.3446 | 41.29 | -30.70 | 1.3433 | 40.75 | -28.94 | 1.3424 | 40.20 | -27.18 | 1.3419 | 39.66 | -25.42 |
| benzyl alcohol - n-hexanol | 0.0989 | 0.9011 | 1.4317 | 25.30 | -0.36 | 1.4289 | 24.50 | -0.37 | 1.4278 | 23.70 | -0.38 | 1.4221 | 22.91 | -0.39 |
| | 0.2037 | 0.7963 | 1.4432 | 27.08 | -0.18 | 1.4396 | 26.25 | -0.22 | 1.4373 | 25.41 | -0.25 | 1.4334 | 24.58 | -0.29 |
| | 0.2991 | 0.7009 | 1.4528 | 27.60 | -1.13 | 1.4502 | 26.83 | -1.08 | 1.4484 | 26.07 | -1.04 | 1.4456 | 25.31 | -0.99 |
| | 0.3997 | 0.6003 | 1.4646 | 28.77 | -1.50 | 1.4617 | 27.85 | -1.60 | 1.4593 | 26.94 | -1.69 | 1.4551 | 26.02 | -1.79 |
| | 0.4978 | 0.5022 | 1.4758 | 29.50 | -2.28 | 1.4726 | 28.61 | -2.34 | 1.4711 | 27.72 | -2.39 | 1.4668 | 26.84 | -2.45 |
| | 0.5985 | 0.4015 | 1.4874 | 29.47 | -3.86 | 1.4848 | 28.11 | -4.37 | 1.4825 | 26.75 | -4.89 | 1.4796 | 25.39 | -5.41 |
| | 0.7036 | 0.2964 | 1.5015 | 31.00 | -3.94 | 1.4987 | 29.54 | -4.54 | 1.4948 | 28.09 | -5.14 | 1.4927 | 26.64 | -5.74 |
| | 0.7869 | 0.2131 | 1.5127 | 32.99 | -3.22 | 1.5093 | 31.33 | -4.02 | 1.5068 | 29.67 | -4.81 | 1.5046 | 28.02 | -5.61 |
| | 0.8958 | 0.1042 | 1.5267 | 34.86 | -3.02 | 1.5232 | 33.05 | -3.96 | 1.5215 | 31.23 | -4.91 | 1.5198 | 29.41 | -5.85 |
| n-hexanol – water | 0 | 0.0011 | 1.3383 | 20.99 | -51.15 | 1.3376 | 33.75 | -36.08 | 1.3362 | 46.52 | -21.00 | 1.3359 | 59.29 | -5.92 |
| | 0 | 0.0009 | 1.3377 | 25.70 | -46.45 | 1.3367 | 34.95 | -34.89 | 1.3356 | 44.20 | -23.33 | 1.3352 | 53.45 | -11.76 |
| | 0 | 0.0007 | 1.3374 | 34.60 | -38.46 | 1.3365 | 39.54 | -30.02 | 1.3355 | 44.48 | -21.58 | 1.3349 | 49.42 | -13.14 |
| | 0 | 0.0005 | 1.3372 | 39.08 | -33.09 | 1.3364 | 45.00 | -24.86 | 1.3352 | 50.91 | -16.64 | 1.3346 | 56.82 | -8.41 |
| | 0 | 0.0003 | 1.3370 | 48.01 | -24.17 | 1.3362 | 49.05 | -20.81 | 1.3349 | 50.10 | -17.45 | 1.3344 | 51.15 | -14.09 |
| | 0 | 0.0001 | 1.3369 | 57.86 | -14.32 | 1.3357 | 55.93 | -13.94 | 1.3347 | 54.00 | -13.55 | 1.3344 | 52.07 | -13.18 |
| benzyl alcohol - n-hexanol-water | 0.0003 | 0.0033 | 1.3410 | 40.29 | -31.73 | 1.3407 | 42.15 | -27.57 | 1.3392 | 44.00 | -23.41 | 1.3382 | 45.85 | -19.25 |
| | 0.0002 | 0.0013 | 1.3389 | 50.39 | -21.74 | 1.3387 | 48.09 | -21.73 | 1.3372 | 45.79 | -21.71 | 1.3360 | 43.50 | -21.70 |
| | 0.0003 | 0.0059 | 1.3436 | 37.85 | -34.05 | 1.3434 | 38.58 | -31.02 | 1.3420 | 39.31 | -27.98 | 1.3406 | 40.04 | -24.95 |
| | 0.0003 | 0.0053 | 1.3429 | 37.19 | -34.74 | 1.3426 | 38.81 | -30.82 | 1.3409 | 40.43 | -26.89 | 1.3399 | 42.05 | -22.97 |
| | 0.0004 | 0.0043 | 1.3419 | 35.72 | -36.25 | 1.3414 | 37.56 | -32.10 | 1.3397 | 39.41 | -27.96 | 1.3383 | 41.25 | -23.81 |
| | 0.0006 | 0.0038 | 1.3412 | 31.23 | -40.76 | 1.3410 | 34.91 | -34.78 | 1.3395 | 38.59 | -28.79 | 1.3376 | 42.27 | -22.81 |

$X_1$ – molar fraction of benzyl alcohol, $X_2$ –molar fraction of n-hexanol

Standard uncertainties u are u(T) = ±0.01 K for surface tension and u(T) = ±0.1 K for refractive index , u(γ) = ±0.8 mN/m, u(n) = ±0.0002 and u(P) = ±0.001MPa

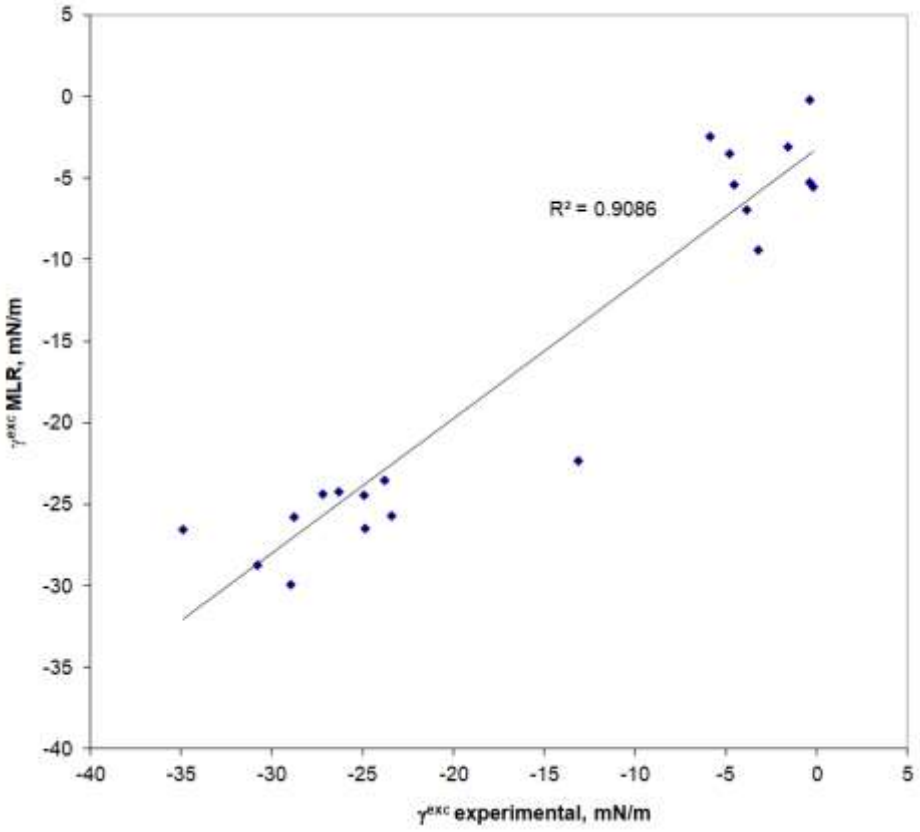


**Figure 3.** Excess surface tension values calculated with the MLR model and compared to the experimental ones.

An alternative to this type of modeling is the use of artificial intelligence tools such as Multilayer perceptrons (MLP) which represent the simplest form of Feedforward Neural Networks where information flows in a single direction, from input to output, and there are no cycles or loops in the network architecture. To obtain the neural models, the 108 experimental data related to composition, normalized temperature, refractive index and excess surface tension were divided as follows: 88 were used in the training stage of the constructed neural models and 20 were kept for the validation stage.

Neural models were constructed with one or two layers of hidden neurons of which the numbers ranged from 4 to 36. Performance in the training stage was evaluated based on the mean square error (MSE), the correlation coefficient ($r^2$) and the percentage errors (Ep):

$$MSE = \frac{\sum_{j=1}^{P}\sum_{i=1}^{N}(D_{ij} - O_{ij})^2}{N \cdot P} \quad (3)$$

where P represents the number of output quantities (in this case, P = 1), N the number of data, $O_{ij}$ is the output value for element i with the processing of element j and $D_{ij}$ is the desired output for i with the processing of element j;

$$r^2 = \frac{\Sigma\left(O_{exp_i} - \overline{O}_{exp}\right)\cdot\left(O_{net_i} - \overline{O}_{net}\right)}{\sqrt{\Sigma\left(O_{exp_i} - \overline{O}_{exp}\right)^2 \cdot \left(O_{net_i} - \overline{O}_{net}\right)^2}} \quad (4)$$

$$E_p = \frac{O_{exp} - O_{net}}{O_{exp}} \cdot 100 \quad (5)$$

where O's are the values of the output data, exp and net respectively denote the experimental values and those obtained from the neural models.

The structure of the neural models and the performances obtained in the training stage are presented in Table 3.

**Table 3**
Structure of the neural models and performance obtained in the training stage

| No. | Network topology | MSE | $r^2$ | $E_p$ (%) |
|---|---|---|---|---|
| 1. | MLP(4:4:1) | 0.030001 | 0.926009 | 20.659 |
| 2. | MLP(4:8:1) | 0.026452 | 0.935079 | 23.604 |
| 3. | MLP(4:16:1) | 0.027475 | 0.933262 | 24.074 |
| 4. | MLP(4:20:1) | 0.026666 | 0.934535 | 23.030 |
| 5. | MLP(4:24:1) | 0.027890 | 0.932594 | 20.464 |
| 6. | MLP(4:28:1) | 0.028091 | 0.932381 | 22.164 |
| 7. | MLP(4:32:1) | 0.028305 | 0.931914 | 19.642 |
| 8. | MLP(4:36:1) | 0.028037 | 0.932323 | 23.886 |
| 9. | MLP(4:8:4:1) | 0.025795 | 0.936733 | 22.344 |
| 10. | MLP(4:16:8:1) | 0.023165 | 0.944421 | 17.426 |
| ***11.*** | ***MLP(4:20:12:1)*** | ***0.019218*** | ***0.954051*** | ***14.110*** |
| 12. | MLP(4:24:16:1) | 0.021031 | 0.948870 | 18.020 |
| 13. | MLP(4:28:20:1) | 0.018359 | 0.955420 | 15.420 |
| 14. | MLP(4:32:24:1) | 0.019814 | 0.951758 | 20.050 |
| 15. | MLP(4:36:28:1) | 0.019851 | 0.952253 | 15.156 |
| 16. | MLP(4:36:18:1) | 0.020560 | 0.950284 | 15.290 |
| 17. | MLP(4:32:16:1) | 0.019133 | 0.953488 | 14.160 |

In the validation stage, the standard deviation calculated for the best performing MLP neuronal model (4:20:12:1) was 2.14. Figure 4 compares the values calculated with the mentioned neural model to the experimental ones for the 20 data kept for the validation stage. The correlation coefficient for the model is 0.9727 and the standard deviation is 2.14.

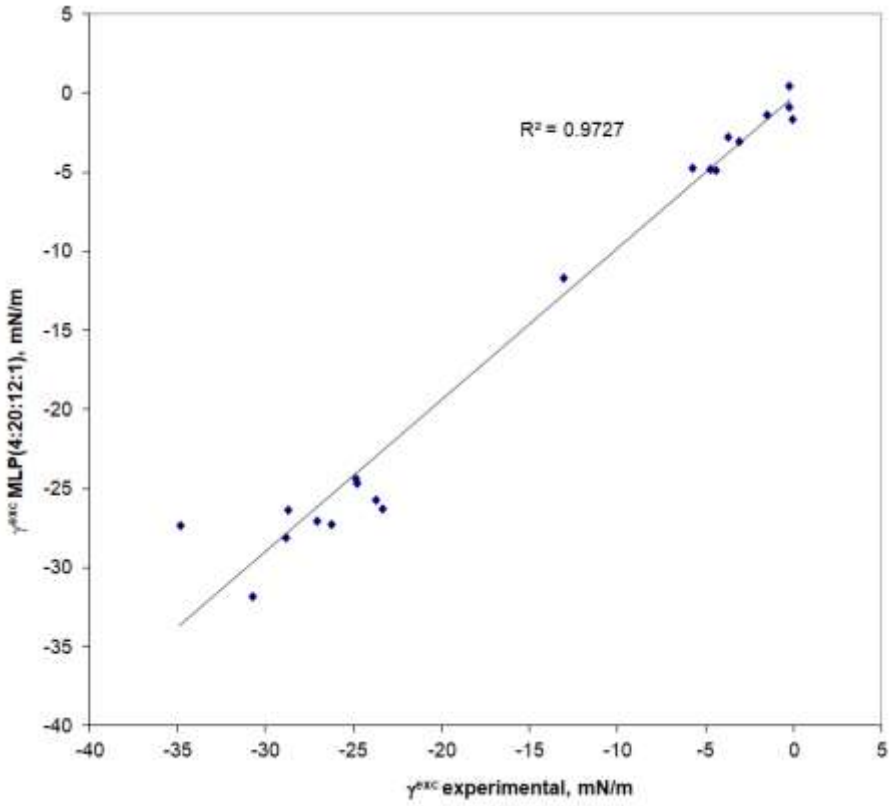


**Figure 4**. Excess surface tension values calculated with the MLP (4:20:12:1) model and compared to the experimental ones.

The neural model performs better than the MLR model, but the advantage of the latter is that it provides a mathematical expression that can be more easily used by chemical engineers to predict excess surface tension based on the experimental measurements of refractive index.

## 4. Conclusion

The influence of temperature and composition on surface tension for binary and ternary systems containing water, n-hexanol and benzyl alcohol was evaluated. The increase in surface tension was found with the increase in temperature for the binary system of n-hexanol-water and the ternary system of benzyl alcohol-n-hexanol-water alcohol (except for the mixture containing a smaller n-hexanol molar fraction). The increase in surface tension can be explained by the increase in the solvation of the solute at higher temperatures, which causes the concentration of the excess surface of the active compound to decrease as the temperature increases.

Negative values for excess surface tension were obtained for all types of analysed mixtures. Deviation from the ideal behavior is more pronounced in the case of binary systems containing double distilled water and in the case of the ternary system.. This behaviour is due to the presence of small amounts of n-hexanol and benzyl alcohol, in the mixture for these systems, which have lower surface tension and tend to migrate to the phase separation interface so that the concentration in the surface layer will be higher than in the main mass of the mixture.

An MLR model was proposed to have excess surface tension correlate refractive index (which is much easier to determine

experimentally), molar fraction and normalized temperature. The correlation coefficient for the data from the validation stage of this model is 0.9086, and the standard deviation is 4.36.

Modelling with neural networks with forward propagation error - Multilayer perceptrons (MLP) was also used to have excess surface tension correlaterefractive index (which is much easier to determine experimentally), molar fraction and normalized temperature. In the validation stage for the MLP neuronal model with the best performance (4:20:12:1) the correlation coefficient is 0.9727, and the standard deviation is 2.14.

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**Declaration of Competing Interest**

The authors declare that they have no known competing financial interest or personal relationship that could have appeared to influence the work reported in this paper.

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