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Prediction of surface tension of alcohol + water solutions using artificial neural networks

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Abstract: Different Artificial Neural Network architectures have been implemented to predict Surface Tension of aqueous solutions of methanol, ethanol, 1-propanol and 2-propanol in range temperatures of 293.15-323.15 K. Artificial Neural Networks with four entrance variables, Critical Volume, log *P*, Mole Fraction and Temperature, were used. Best ANN architecture was formed by four input neurons, two middle layers (with eleven and three neurons respectively) and one output neuron. Root Mean Square Errors (*RMSE*s) are 0.34 $mN \cdot m^{-1}$ (R^2= 0.9995) for the training set and 1.31 $mN \cdot m^{-1}$ (R^2= 0.9955) for the validation set. Those errors correspond with a 0.62% error and 4.37% of error for training and validation set, respectively. For the full data set the Root Mean Square Error is 0.72 $mN \cdot m^{-1}$ (R^2= 0.9976) with a 1.56% error.

Keywords: Surface Tension, Alcohol, Prediction, Artificial Neural Network.

Introduction

It is well known that most of the chemical processes occur in aqueous media. The study of the physical properties of these solutions gave birth to a bulk of valuable data useful in the design and control of these chemical processes. Surface Tension (σ) of mixtures of alcohols with water is of particular interest for physics and chemistry[1]. Surface tension is a physical property of capital importance in mass transfer processes such as distillation, extraction, absorption, chemical and biochemical engineering, environmental protection and in reservoir studies[2-6].

Vázquez et al. provided data of Surface Tension over the entire concentration range of 293.15-323.15 K for different solutions of methanol, ethanol, 1-propanol and 2-propanol in water[2]. These measurement techniques are expensive as in time as in resources, and also they do not lack of errors, so that is the reason that makes simulation and prediction techniques of interest. Other methodologies have been used to forecast Tension[2] such as Gibbs method[7,8], perturbed-chain statistical associating fluid theory[9,10], density functional theory (DFT)[11-13] and quantitative structure–property relationship (QSPR)[14-16].

In this article we are going to implement a system to predict the Surface Tension of water solutions of alcohols. The procedure used is to develop Artificial Neural Networks (ANNs) to relate the different variables involved with Surface Tension.

ANNs are used successfully in different fields such as: Biology[17-20], Soil Science[21,22], Medicine[23-25], Industry[26,27], Food Technology[28], Hydrology[29-31], Energy[32], Chemistry[33-39], etc.

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They are mathematical models inspired by the structure of biological neural networks, which try to reproduce the human ability of taking decisions. An ANN is a flexible structure, which is able to make a non-linear mapping between input and output spaces[40]. The main feature of ANNs is that they can learn from real cases and re-learn when new data are introduced in the case of study.

Results and discussion

Once trained the ANN, its correct operation was tested with the validation data corresponding to 98 aqueous solutions of 2-Propanol. In Table 1 training *RMSE* ($RMSE_T$) and validation *RMSE* ($RMSE_V$) values for each implemented ANN are shown. To evaluate the accuracy of the ANN model, the root mean square errors in validation ($RMSE_V$) were calculated.

Table 1. Adjustment parameters R^2, Root mean square errors (*RMSE*) and % error of training and validation phases for different ANN architectures.

	Training			Validation		
Topology	R_T^2	$RMSE_T$	% $Error_T$	R_V^2	$RMSE_V$	% $Error_V$
4-11-3-1	0.9995	0.3421	0.6204	0.9955	1.3055	4.3679
4-9-7-1	0.9997	0.2331	0.4908	0.9947	1.4177	4.9524
4-13-3-1	0.9997	0.2334	0.4674	0.9963	1.4290	4.7599
4-11-3-1*	0.9995	0.3178	0.5872	0.9959	1.3672	4.6290
4-11-9-1	0.9997	0.2443	0.5103	0.9912	1.5278	4.9268
4-11-3-1**	0.9996	0.2992	0.5863	0.9967	1.4820	5.0261
4-9-5-1	0.9997	0.2949	0.6434	0.9960	1.5015	4.6251
4-11-3-1***	0.9995	0.3089	0.6137	0.9959	1.5181	5.0723
4-7-7-1	0.9997	0.2330	0.4715	0.9884	1.6460	5.0349
4-9-1	0.9996	0.2950	0.6136	0.9976	1.6072	5.1896

*, **, *** Indicate that networks were checked with different operation times

It can be seen that the network with the best fit according to $RMSE_V$ value is 4-11-3-1. We want to remark that in training we implemented networks with a better $RMSE_T$ value than this one, but it is clearly better forecasting Surface Tension with cases not used in training (2-Propanol). Figures 1 and 2 shows training and validation fits and the satisfactory results obtained.

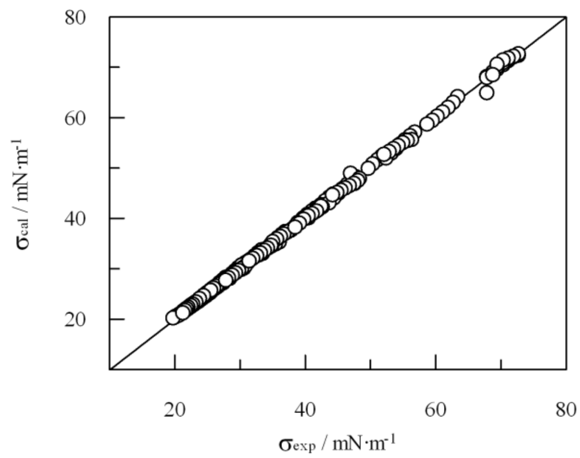

Figure 1. Experimental (σ_{exp}) vs. calculated (σ_{cal}) value of Surface Tension for training phase (Methanol +

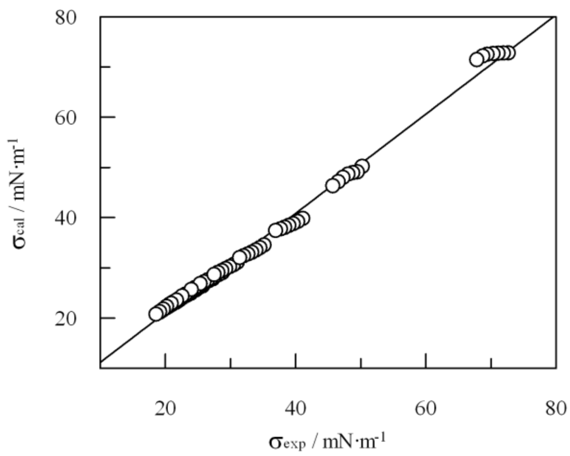

Figure 2. Experimental (σ_{exp}) vs. calculated (σ_{cal}) value of Surface Tension for validation phase (2-

Water, Ethanol + Water and 1-Propanol + Water). Propanol + Water).

The importance of every connection between neurons is denoted by a non-dimensional value so-called weight (presented in Table 2 as a matrix). They represent the synaptic strength of every connection in the way that every time weight exceed a pre-set value neuron is fired.

Table 2. Weight matrix of the ANN.

CV	**Log *P***	***X***	***T***							
1.076	-0.024	-16.167	-0.324							
1.107	-0.014	-16.060	-0.383							
0.621	-0.704	-15.021	-1.571							
0.160	-1.662	-3.684	0.193							
0.324	-1.744	-10.136	-0.508							
1.179	0.610	-16.973	0.001							
1.312	0.679	-5.497	-2.473							
1.155	-3.687	-1.734	0.201							
0.950	-0.011	-16.449	-0.106							
0.676	-0.766	-13.799	0.132							
-0.057	0.673	-0.339	-0.565							
-5.629	-5.565	-5.014	-0.730	1.139	-5.308	1.576	-4.242	-5.824	-2.612	-1.337
0.194	0.320	-0.820	-0.769	-3.577	-1.920	-0.040	-0.837	-0.458	-3.331	-0.992
0.453	0.324	-0.593	-2.654	-2.607	1.261	-2.615	-2.344	0.820	-1.523	-3.870
-4.649	-2.351	-4.320								

If we take a look to the weight matrix, we find that the most important variable in order to predict Surface Tension is the Molar Fraction of alcohol (115.858). Other variables used shows low importance when comparing with Molar Fraction; log *P* (10.574), Critical Volume (8.618) and finally Temperature (6.455). Importance results from the sum of weight in the input layer.

Conclusion

In sum, Perceptron Multilayer ANN with four entrance variables Critical Volume (*CV*), log *P*, Mole Fraction of alcohol (*X*) and Temperature (*T*), has been implemented to predict Surface Tension of alcohol aqueous solutions. The best ANN architecture obtained consists in four input neurons, two middle layers (with eleven and three neurons respectively) and one output neuron. This ANN presents Root Mean Square Errors (*RMSEs*) of 0.34 $mN \cdot m^{-1}$ (R^2= 0.9995) for the training set and 1.31 $mN \cdot m^{-1}$ (R^2= 0.9955) for the validation set. Average percentage error for training and validation set is 1.56%. With these results, we can recommend ANNs as a suitable forecasting method for Surface Tension determination.

On the other hand, the fact that testing were done with 2-propanol instead of choosing random data proves that our ANN will predict the effect of the position of hydroxyl group in the alcohol carbon chain. However, it would be wise to improve the quality of predictions adding new cases for training.

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Experimental Section

Surface Tension Determination

For the implementation of different ANNs, we used the Surface Tension data of 392 alcohols that were collected from Vázquez *et al*[2]. The data set was divided in two groups: one group for training of 294 compounds and another group for validation of 98 compounds. The training set was used to implement the ANN. The prediction capability or the ANN was evaluated with the validation set. Artificial Neural Networks are often validated with similar cases to the training but in this case a compound not used in training was chosen to test the network (2-propanol). This was done in order to see if the network is able to extrapolate learning out of the training set compounds.

Descriptors

To predict the value of Surface Tension of different aqueous solutions of alcohols the variables Critical Volume (*CV*), log *P*, Mole Fraction of alcohol (*X*) and Temperature (*T*) were selected. Critical Volume and log *P* were chosen in order to introduce some characteristic inherent to every alcohol and were obtained from Chemdraw Ultra software. The remaining variables, Surface Tension, Mole Fraction of alcohol and Temperature were obtained from Vázquez *et al*[2].

Table 3. Surface Tensions (σ) of aqueous solutions of Methanol, Ethanol, 1-Propanol and 2-Propanol for different temperatures[2]. Input variables are: i) Critical Volume (*CV*), ii) log *P*, iii) Mole Fraction of alcohol (*X*) and iv) Temperature (*T*).

Compound	*CV*	log *P*	*X*	*T*	σ	Compound	*CV*	log *P*	*X*	*T*	σ
					Training						
Methanol	110.50	-0.27	0.000	293.15	72.75	Methanol	110.50	-0.27	0.273	308.15	35.36
Methanol	110.50	-0.27	0.029	293.15	63.46	Methanol	110.50	-0.27	0.360	308.15	31.85
Methanol	110.50	-0.27	0.059	293.15	56.87	Methanol	110.50	-0.27	0.458	308.15	28.86
Methanol	110.50	-0.27	0.090	293.15	51.83	Methanol	110.50	-0.27	0.568	308.15	26.56
Methanol	110.50	-0.27	0.123	293.15	47.86	Methanol	110.50	-0.27	0.692	308.15	24.60
Methanol	110.50	-0.27	0.158	293.15	44.38	Methanol	110.50	-0.27	0.835	308.15	22.95
Methanol	110.50	-0.27	0.194	293.15	41.67	Methanol	110.50	-0.27	1.000	308.15	21.52
Methanol	110.50	-0.27	0.273	293.15	37.02	Methanol	110.50	-0.27	0.000	313.15	69.52
Methanol	110.50	-0.27	0.360	293.15	33.37	Methanol	110.50	-0.27	0.029	313.15	60.32
Methanol	110.50	-0.27	0.458	293.15	30.32	Methanol	110.50	-0.27	0.059	313.15	54.01
Methanol	110.50	-0.27	0.568	293.15	27.91	Methanol	110.50	-0.27	0.090	313.15	47.04
Methanol	110.50	-0.27	0.692	293.15	25.98	Methanol	110.50	-0.27	0.123	313.15	45.17
Methanol	110.50	-0.27	0.835	293.15	24.37	Methanol	110.50	-0.27	0.158	313.15	41.82
Methanol	110.50	-0.27	1.000	293.15	22.95	Methanol	110.50	-0.27	0.194	313.15	39.14
Methanol	110.50	-0.27	0.000	298.15	72.01	Methanol	110.50	-0.27	0.273	313.15	34.79
Methanol	110.50	-0.27	0.029	298.15	62.77	Methanol	110.50	-0.27	0.360	313.15	31.26
Methanol	110.50	-0.27	0.059	298.15	56.18	Methanol	110.50	-0.27	0.458	313.15	28.44
Methanol	110.50	-0.27	0.090	298.15	51.17	Methanol	110.50	-0.27	0.568	313.15	26.12
Methanol	110.50	-0.27	0.123	298.15	47.21	Methanol	110.50	-0.27	0.692	313.15	24.21

Methanol	110.50	-0.27	0.158	298.15	43.78
Methanol	110.50	-0.27	0.194	298.15	41.09
Methanol	110.50	-0.27	0.273	298.15	36.51
Methanol	110.50	-0.27	0.360	298.15	32.86
Methanol	110.50	-0.27	0.458	298.15	29.83
Methanol	110.50	-0.27	0.568	298.15	27.48
Methanol	110.50	-0.27	0.692	298.15	25.54
Methanol	110.50	-0.27	0.835	298.15	23.93
Methanol	110.50	-0.27	1.000	298.15	22.51
Methanol	110.50	-0.27	0.000	303.15	71.21
Methanol	110.50	-0.27	0.029	303.15	61.98
Methanol	110.50	-0.27	0.059	303.15	55.41
Methanol	110.50	-0.27	0.090	303.15	50.43
Methanol	110.50	-0.27	0.123	303.15	46.56
Methanol	110.50	-0.27	0.158	303.15	43.14
Methanol	110.50	-0.27	0.194	303.15	40.43
Methanol	110.50	-0.27	0.273	303.15	35.90
Methanol	110.50	-0.27	0.360	303.15	32.33
Methanol	110.50	-0.27	0.458	303.15	29.34
Methanol	110.50	-0.27	0.568	303.15	26.99
Methanol	110.50	-0.27	0.692	303.15	25.06
Methanol	110.50	-0.27	0.835	303.15	23.43
Methanol	110.50	-0.27	1.000	303.15	22.01
Methanol	110.50	-0.27	0.000	308.15	70.42
Methanol	110.50	-0.27	0.029	308.15	61.14
Methanol	110.50	-0.27	0.059	308.15	54.67
Methanol	110.50	-0.27	0.090	308.15	49.76
Methanol	110.50	-0.27	0.123	308.15	45.84
Methanol	110.50	-0.27	0.158	308.15	42.51
Methanol	110.50	-0.27	0.194	308.15	39.77
Ethanol	166.50	0.07	0.000	293.15	72.75
Ethanol	166.50	0.07	0.020	293.15	56.41
Ethanol	166.50	0.07	0.042	293.15	48.14
Ethanol	166.50	0.07	0.065	293.15	42.72
Ethanol	166.50	0.07	0.089	293.15	38.56
Ethanol	166.50	0.07	0.115	293.15	36.09
Ethanol	166.50	0.07	0.144	293.15	33.53
Ethanol	166.50	0.07	0.207	293.15	30.69
Ethanol	166.50	0.07	0.281	293.15	28.51
Ethanol	166.50	0.07	0.370	293.15	26.72
Ethanol	166.50	0.07	0.477	293.15	25.48
Ethanol	166.50	0.07	0.610	293.15	24.32
Ethanol	166.50	0.07	0.779	293.15	23.23
Ethanol	166.50	0.07	1.000	293.15	22.31
Ethanol	166.50	0.07	0.000	298.15	72.01
Ethanol	166.50	0.07	0.020	298.15	55.73
Ethanol	166.50	0.07	0.042	298.15	47.53
Methanol	110.50	-0.27	0.835	313.15	22.57
Methanol	110.50	-0.27	1.000	313.15	21.13
Methanol	110.50	-0.27	0.000	318.15	68.84
Methanol	110.50	-0.27	0.029	318.15	59.58
Methanol	110.50	-0.27	0.059	318.15	53.27
Methanol	110.50	-0.27	0.090	318.15	48.39
Methanol	110.50	-0.27	0.123	318.15	44.48
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Methanol	110.50	-0.27	0.692	318.15	23.72
Methanol	110.50	-0.27	0.835	318.15	22.06
Methanol	110.50	-0.27	1.000	318.15	20.61
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Methanol	110.50	-0.27	1.000	323.15	20.21
Ethanol	166.50	0.07	0.207	308.15	29.27
Ethanol	166.50	0.07	0.281	308.15	27.11
Ethanol	166.50	0.07	0.370	308.15	25.43
Ethanol	166.50	0.07	0.477	308.15	24.21
Ethanol	166.50	0.07	0.610	308.15	23.01
Ethanol	166.50	0.07	0.779	308.15	21.94
Ethanol	166.50	0.07	1.000	308.15	21.04
Ethanol	166.50	0.07	0.000	313.15	69.52
Ethanol	166.50	0.07	0.020	313.15	53.63
Ethanol	166.50	0.07	0.042	313.15	45.58
Ethanol	166.50	0.07	0.065	313.15	40.27
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Ethanol	166.50	0.07	0.144	298.15	32.98	Ethanol	166.50	0.07	1.000	313.15	20.62
Ethanol	166.50	0.07	0.207	298.15	30.16	Ethanol	166.50	0.07	0.000	318.15	68.84
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Ethanol	166.50	0.07	1.000	298.15	21.82	Ethanol	166.50	0.07	0.144	318.15	30.89
Ethanol	166.50	0.07	0.000	303.15	71.21	Ethanol	166.50	0.07	0.207	318.15	28.28
Ethanol	166.50	0.07	0.020	303.15	55.04	Ethanol	166.50	0.07	0.281	318.15	26.21
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Ethanol	166.50	0.07	0.207	303.15	29.68	Ethanol	166.50	0.07	0.000	323.15	67.92
Ethanol	166.50	0.07	0.281	303.15	27.53	Ethanol	166.50	0.07	0.020	323.15	52.16
Ethanol	166.50	0.07	0.370	303.15	25.81	Ethanol	166.50	0.07	0.042	323.15	44.26
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Ethanol	166.50	0.07	0.115	308.15	34.41	Ethanol	166.50	0.07	0.779	323.15	20.71
Ethanol	166.50	0.07	0.144	308.15	31.94	Ethanol	166.50	0.07	1.000	323.15	19.82
1-Propanol	222.50	0.55	0.000	293.15	72.75	1-Propanol	222.50	0.55	0.167	308.15	24.51
1-Propanol	222.50	0.55	0.016	293.15	42.51	1-Propanol	222.50	0.55	0.231	308.15	24.02
1-Propanol	222.50	0.55	0.032	293.15	34.86	1-Propanol	222.50	0.55	0.310	308.15	23.73
1-Propanol	222.50	0.55	0.050	293.15	30.87	1-Propanol	222.50	0.55	0.412	308.15	23.31
1-Propanol	222.50	0.55	0.070	293.15	28.31	1-Propanol	222.50	0.55	0.545	308.15	23.09
1-Propanol	222.50	0.55	0.091	293.15	27.08	1-Propanol	222.50	0.55	0.730	308.15	22.84
1-Propanol	222.50	0.55	0.114	293.15	26.41	1-Propanol	222.50	0.55	1.000	308.15	22.51
1-Propanol	222.50	0.55	0.167	293.15	25.68	1-Propanol	222.50	0.55	0.000	313.15	69.52
1-Propanol	222.50	0.55	0.231	293.15	25.18	1-Propanol	222.50	0.55	0.016	313.15	39.86
1-Propanol	222.50	0.55	0.310	293.15	24.89	1-Propanol	222.50	0.55	0.032	313.15	32.69
1-Propanol	222.50	0.55	0.412	293.15	24.47	1-Propanol	222.50	0.55	0.050	313.15	28.89
1-Propanol	222.50	0.55	0.545	293.15	24.23	1-Propanol	222.50	0.55	0.070	313.15	26.51
1-Propanol	222.50	0.55	0.730	293.15	23.98	1-Propanol	222.50	0.55	0.091	313.15	25.36
1-Propanol	222.50	0.55	1.000	293.15	23.69	1-Propanol	222.50	0.55	0.114	313.15	24.74
1-Propanol	222.50	0.55	0.000	298.15	72.01	1-Propanol	222.50	0.55	0.167	313.15	24.09

1-Propanol	222.50	0.55	0.016	298.15	41.83	1-Propanol	222.50	0.55	0.231	313.15	23.64
1-Propanol	222.50	0.55	0.032	298.15	34.32	1-Propanol	222.50	0.55	0.310	313.15	23.33
1-Propanol	222.50	0.55	0.050	298.15	30.36	1-Propanol	222.50	0.55	0.412	313.15	22.93
1-Propanol	222.50	0.55	0.070	298.15	27.84	1-Propanol	222.50	0.55	0.545	313.15	22.68
1-Propanol	222.50	0.55	0.091	298.15	26.64	1-Propanol	222.50	0.55	0.730	313.15	22.44
1-Propanol	222.50	0.55	0.114	298.15	25.98	1-Propanol	222.50	0.55	1.000	313.15	22.11
1-Propanol	222.50	0.55	0.167	298.15	25.26	1-Propanol	222.50	0.55	0.000	318.15	68.84
1-Propanol	222.50	0.55	0.231	298.15	24.80	1-Propanol	222.50	0.55	0.016	318.15	39.22
1-Propanol	222.50	0.55	0.310	298.15	24.49	1-Propanol	222.50	0.55	0.032	318.15	32.08
1-Propanol	222.50	0.55	0.412	298.15	24.08	1-Propanol	222.50	0.55	0.050	318.15	28.36
1-Propanol	222.50	0.55	0.545	298.15	23.86	1-Propanol	222.50	0.55	0.070	318.15	26.03
1-Propanol	222.50	0.55	0.730	298.15	23.59	1-Propanol	222.50	0.55	0.091	318.15	24.91
1-Propanol	222.50	0.55	1.000	298.15	23.28	1-Propanol	222.50	0.55	0.114	318.15	24.29
1-Propanol	222.50	0.55	0.000	303.15	71.21	1-Propanol	222.50	0.55	0.167	318.15	23.69
1-Propanol	222.50	0.55	0.016	303.15	41.16	1-Propanol	222.50	0.55	0.231	318.15	23.24
1-Propanol	222.50	0.55	0.032	303.15	33.81	1-Propanol	222.50	0.55	0.310	318.15	22.92
1-Propanol	222.50	0.55	0.050	303.15	29.88	1-Propanol	222.50	0.55	0.412	318.15	22.54
1-Propanol	222.50	0.55	0.070	303.15	27.41	1-Propanol	222.50	0.55	0.545	318.15	22.28
1-Propanol	222.50	0.55	0.091	303.15	26.22	1-Propanol	222.50	0.55	0.730	318.15	22.04
1-Propanol	222.50	0.55	0.114	303.15	25.56	1-Propanol	222.50	0.55	1.000	318.15	21.69
1-Propanol	222.50	0.55	0.167	303.15	24.88	1-Propanol	222.50	0.55	0.000	323.15	67.92
1-Propanol	222.50	0.55	0.231	303.15	24.42	1-Propanol	222.50	0.55	0.016	323.15	38.54
1-Propanol	222.50	0.55	0.310	303.15	24.11	1-Propanol	222.50	0.55	0.032	323.15	31.48
1-Propanol	222.50	0.55	0.412	303.15	23.69	1-Propanol	222.50	0.55	0.050	323.15	27.90
1-Propanol	222.50	0.55	0.545	303.15	23.48	1-Propanol	222.50	0.55	0.070	323.15	25.59
1-Propanol	222.50	0.55	0.730	303.15	23.21	1-Propanol	222.50	0.55	0.091	323.15	24.49
1-Propanol	222.50	0.55	1.000	303.15	22.89	1-Propanol	222.50	0.55	0.114	323.15	23.88
1-Propanol	222.50	0.55	0.000	308.15	70.42	1-Propanol	222.50	0.55	0.167	323.15	23.32
1-Propanol	222.50	0.55	0.016	308.15	40.53	1-Propanol	222.50	0.55	0.231	323.15	22.86
1-Propanol	222.50	0.55	0.032	308.15	33.26	1-Propanol	222.50	0.55	0.310	323.15	22.54
1-Propanol	222.50	0.55	0.050	308.15	29.39	1-Propanol	222.50	0.55	0.412	323.15	22.14
1-Propanol	222.50	0.55	0.070	308.15	26.96	1-Propanol	222.50	0.55	0.545	323.15	21.91
1-Propanol	222.50	0.55	0.091	308.15	25.79	1-Propanol	222.50	0.55	0.730	323.15	21.66
1-Propanol	222.50	0.55	0.114	308.15	25.16	1-Propanol	222.50	0.55	1.000	323.15	21.31
Validation											
2-Propanol	216.50	0.38	0.000	293.15	72.75	2-Propanol	216.50	0.38	0.167	308.15	24.23
2-Propanol	216.50	0.38	0.016	293.15	50.32	2-Propanol	216.50	0.38	0.231	308.15	23.27
2-Propanol	216.50	0.38	0.032	293.15	41.21	2-Propanol	216.50	0.38	0.310	308.15	22.54
2-Propanol	216.50	0.38	0.050	293.15	35.27	2-Propanol	216.50	0.38	0.412	308.15	21.71
2-Propanol	216.50	0.38	0.070	293.15	31.16	2-Propanol	216.50	0.38	0.545	308.15	21.18
2-Propanol	216.50	0.38	0.091	293.15	28.88	2-Propanol	216.50	0.38	0.730	308.15	20.66
2-Propanol	216.50	0.38	0.114	293.15	27.38	2-Propanol	216.50	0.38	1.000	308.15	20.23
2-Propanol	216.50	0.38	0.167	293.15	25.81	2-Propanol	216.50	0.38	0.000	313.15	69.52
2-Propanol	216.50	0.38	0.231	293.15	24.78	2-Propanol	216.50	0.38	0.016	313.15	47.37
2-Propanol	216.50	0.38	0.310	293.15	24.05	2-Propanol	216.50	0.38	0.032	313.15	38.43
2-Propanol	216.50	0.38	0.412	293.15	23.17	2-Propanol	216.50	0.38	0.050	313.15	32.76
2-Propanol	216.50	0.38	0.545	293.15	22.62	2-Propanol	216.50	0.38	0.070	313.15	28.79

2-Propanol	216.50	0.38	0.730	293.15	22.21	2-Propanol	216.50	0.38	0.091	313.15	26.58
2-Propanol	216.50	0.38	1.000	293.15	21.74	2-Propanol	216.50	0.38	0.114	313.15	25.18
2-Propanol	216.50	0.38	0.000	298.15	72.01	2-Propanol	216.50	0.38	0.167	313.15	23.72
2-Propanol	216.50	0.38	0.016	298.15	49.58	2-Propanol	216.50	0.38	0.231	313.15	22.78
2-Propanol	216.50	0.38	0.032	298.15	40.42	2-Propanol	216.50	0.38	0.310	313.15	22.03
2-Propanol	216.50	0.38	0.050	298.15	34.63	2-Propanol	216.50	0.38	0.412	313.15	21.22
2-Propanol	216.50	0.38	0.070	298.15	30.57	2-Propanol	216.50	0.38	0.545	313.15	20.71
2-Propanol	216.50	0.38	0.091	298.15	28.28	2-Propanol	216.50	0.38	0.730	313.15	20.16
2-Propanol	216.50	0.38	0.114	298.15	26.82	2-Propanol	216.50	0.38	1.000	313.15	19.71
2-Propanol	216.50	0.38	0.167	298.15	25.27	2-Propanol	216.50	0.38	0.000	318.15	68.84
2-Propanol	216.50	0.38	0.231	298.15	24.26	2-Propanol	216.50	0.38	0.016	318.15	46.66
2-Propanol	216.50	0.38	0.310	298.15	23.51	2-Propanol	216.50	0.38	0.032	318.15	37.78
2-Propanol	216.50	0.38	0.412	298.15	22.68	2-Propanol	216.50	0.38	0.050	318.15	32.13
2-Propanol	216.50	0.38	0.545	298.15	22.14	2-Propanol	216.50	0.38	0.070	318.15	28.18
2-Propanol	216.50	0.38	0.730	298.15	21.69	2-Propanol	216.50	0.38	0.091	318.15	26.04
2-Propanol	216.50	0.38	1.000	298.15	21.22	2-Propanol	216.50	0.38	0.114	318.15	24.66
2-Propanol	216.50	0.38	0.000	303.15	71.21	2-Propanol	216.50	0.38	0.167	318.15	23.21
2-Propanol	216.50	0.38	0.016	303.15	48.88	2-Propanol	216.50	0.38	0.231	318.15	22.29
2-Propanol	216.50	0.38	0.032	303.15	39.73	2-Propanol	216.50	0.38	0.310	318.15	21.52
2-Propanol	216.50	0.38	0.050	303.15	34.01	2-Propanol	216.50	0.38	0.412	318.15	20.76
2-Propanol	216.50	0.38	0.070	303.15	29.98	2-Propanol	216.50	0.38	0.545	318.15	20.23
2-Propanol	216.50	0.38	0.091	303.15	27.71	2-Propanol	216.50	0.38	0.730	318.15	19.74
2-Propanol	216.50	0.38	0.114	303.15	26.26	2-Propanol	216.50	0.38	1.000	318.15	19.21
2-Propanol	216.50	0.38	0.167	303.15	24.74	2-Propanol	216.50	0.38	0.000	323.15	67.92
2-Propanol	216.50	0.38	0.231	303.15	23.76	2-Propanol	216.50	0.38	0.016	323.15	45.82
2-Propanol	216.50	0.38	0.310	303.15	22.97	2-Propanol	216.50	0.38	0.032	323.15	37.04
2-Propanol	216.50	0.38	0.412	303.15	22.18	2-Propanol	216.50	0.38	0.050	323.15	31.51
2-Propanol	216.50	0.38	0.545	303.15	21.66	2-Propanol	216.50	0.38	0.070	323.15	27.59
2-Propanol	216.50	0.38	0.730	303.15	21.18	2-Propanol	216.50	0.38	0.091	323.15	25.47
2-Propanol	216.50	0.38	1.000	303.15	20.72	2-Propanol	216.50	0.38	0.114	323.15	24.11
2-Propanol	216.50	0.38	0.000	308.15	70.42	2-Propanol	216.50	0.38	0.167	323.15	22.69
2-Propanol	216.50	0.38	0.016	308.15	48.16	2-Propanol	216.50	0.38	0.231	323.15	21.81
2-Propanol	216.50	0.38	0.032	308.15	39.06	2-Propanol	216.50	0.38	0.310	323.15	21.01
2-Propanol	216.50	0.38	0.050	308.15	33.38	2-Propanol	216.50	0.38	0.412	323.15	20.28
2-Propanol	216.50	0.38	0.070	308.15	29.37	2-Propanol	216.50	0.38	0.545	323.15	19.78
2-Propanol	216.50	0.38	0.091	308.15	27.14	2-Propanol	216.50	0.38	0.730	323.15	19.23
2-Propanol	216.50	0.38	0.114	308.15	25.73	2-Propanol	216.50	0.38	1.000	323.15	18.69

Artificial Neural Network

The ANN can be understood as a collecting of information by neurons in the input layer. This information, collected by a vector (eq. 1) is propagated to the first intermediate layer by the so-called spread function whose mission is to add all the excitatory signals that reach neuron (eq. 2). In this equation N is the number of neurons of the input layer, w_{ji} is the value of the weight between the input neuron i and the intermediate neuron j and b_j is the value of the bias neuron associated to the neuron j of the intermediate layer.

$$x = (x_1, x_2, ..., x_n) \quad (1)$$

$$s_j = \sum_{i=1}^{N} w_{ji} x_i + b_j \quad (2)$$

Generated value is treated by the activation function, which generates an excitatory response to signals received (eq. 3). In our case the activation function chosen is the sigmoidal (eq. 4).

$$y_j = F_j(s_j) \quad (3)$$

$$F(z) = \frac{1}{1+e^{-z}} \quad (4)$$

When the information reaches last neuron, the value generated is compared with the experimental value (eq. 5) to establish an error value. This error is used in order to establish the moment training ends.

$$E = \frac{1}{2} \sum_{k=1}^{P} (d_k - y_k)^2 \quad (5)$$

All neural networks were implemented with an input layer, an output layer and a variable number of intermediate layers that was tested taking into account the number of neurons distributed in these layers by the equation 6.

$$\frac{M}{2N} < n < \frac{2M}{N} \quad (6)$$

M corresponds with the number of training cases, N is the number of input variables and n corresponds with the number of neurons in the intermediate layers[41,42].

To clearly differentiate all neural networks will be named using the following notation; N_{in}-$[N_{int1}$-N_{int2}-$N_{int3}]_e$-N_{out} where N_{in} is the number of neurons in the input layer and N_{out} corresponds with the number of neurons in the output layer respectively. N_{int1}, N_{int2} and N_{int3} correspond with the number of neurons in the intermediate layers if they were implemented (Figure 3).

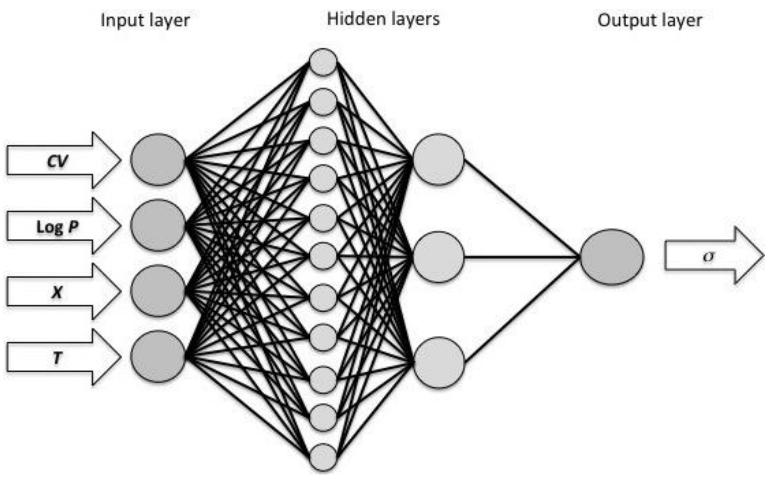

Figure 3. Diagram of the implemented perceptron network, were variables are Critical Volume (*CV*), log *P*, Mole Fraction of alcohol (*X*), Temperature (*T*).

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