

Application of Neural Networks for the Prediction of Surface Tension in Pure and Binary Solutions

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In this work, ANN was utilized to model and predict surface tension in pure and binary solution for selected systems. The results obtained illustrate the possibilities of an alternative and less cumbersome prediction approach relying on the application of artificial neural networks (ANN) for correlating and predicting the surface tension. It is also shown that a multi-layer perceptron network (MLP) can be trained better than other neural network types and can be used as a predictive model in thermodynamics. The AARD (Absolute Average Relative Deviation) of the best neural network that it designed for prediction of the surface tension is about 1 % . More than 200 binary and pure solutions were modeled with an ANN. The trained network was compared with available correlation and thermodynamics models, it was shown that ANN correlated data fairly; meanwhile the number of adjustable parameters in the usual correlations is much more than for an artificial neural network. In the modeling procedure 70 % of the database was selected as a training set and the remaining data were used for testing of the network to prevent memorizing. After the training and testing procedures, ANN was used for the prediction of new solutions. Fortunately ANN could predict with 5 % accuracy.