Application of Neural Network in Prediction of Activity Coefficient in Single and Mixed Electrolyte Solution

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In this work ANN was utilized to model and predict the mean ionic activity coefficient single and mixed electrolyte in all available systems. The results obtained illustrates the possibilities of an alternative and less cumbersome modeling approach relying on the application of artificial neural networks (ANN) for correlating and predicting the activity coefficient. 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 of amino acid electrolyte solution. The RMSD (root mean square deviation) of the best neural network that it designed for prediction of the activity coefficient of electrolytes is 0.005. More than 100 aqueous electrolyte solution was modeled with an ANN. the trained network was compared with mean spherical approximation and pitzer models, it was shown that ANN correlated data as well as MSA and pitzer method, meanwhile the number of adjustable parameter in MSA and pitzer is much more than artificial neural network. In modeling procedure 70 % of database selected as training set and remaining data used for testing of network to prevent memorizing. After training and testing procedure ANN used for prediction of 10 new aqueous electrolyte solutions. Fortunately ANN could predict with 5% accuracy. Trained MLP network has 7 input, 2 hidden layer with 7 and 10 neuron in first and second layer respectively.