Applicability of ANN technique in predicting the molecular weight and acentric factor of pure components

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Abstract

In the present study, the intelligent, prompt, and robust techniques are introduced to predict the physical properties including molecular weight, and acentric factor. This methods are developed based on feed forward artificial neural networks (ANNs) with back propagation algorithm that is non-group contribution techniques. The input parameters for estimation of molecular weight are specific gravity and acentric factor and for the latter, critical pressure, critical temperature, and normal boiling point are selected as input variables. To develop the models, experimental data of 563 pure components are selected from the literature. The results of this study are compared to previously developed methods for estimation of molecular weight and acentric factor. The statistical and graphical error analyses are applied for survey of the results. Applying these techniques reveal that the proposed techniques are more accurate than previously provided methods. Using the relevancy factor, the impact of each input parameter on the output results is proposed. Additionally, to discover the applicability region of the developed techniques, and to demonstrate the reliability of the model, Leverage method is used. There are few data out of the applicability domain of the provided techniques. The values of average absolute percent relative error for ANN models in prediction of molecular weight is reported 6.52%. Furthermore, the stated parameter for prediction of acentric factor using ANN technique is assessed 2.74%. These values are less than the previous models for both of the stated properties. All the statistical and graphical resolutions, demonstrate the trustworthy applicability of ANN technique in predicting the molecular weight and acentric factor.

Key words: molecular weight; acentric factor; non-group contribution; artificial neural network

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