

ABSTRACT

The need for a mathematical relationship between carbon nanotube (CNT) concentration and hydrophilicity of nanocomposites (during the purification process of water-oil mixture) is essential for research in the area of membrane separation. In this study, the effect of CNT concentration on hydrophilicity of functionalized CNT-infused polymeric membrane was reviewed and a mathematical model that can effectively predict the contact angle of functionalized CNT-infused polysulfone membrane for water-oil treatment was developed. Hydrophilicity tests were performed on the functionalized CNT-infused polysulfone membrane by sessile drop method using Goniometer at CNT concentration of 0%; 0.04%; 0.08%; 0.1%; 0.2%; 0.3% and 0.4 wt%. The results showed that the contact angle of the synthesized membrane decreased with increase in CNT content. This confirmed that the hydrophilicity of the membrane was enhanced by the addition of functionalized CNTs. A symbolic regression model was then used to predict correlations between the CNT concentration and the contact angle of the nanocomposite membrane using EureqaTM (desktop version 0.99.9) software.

The Nutonian models using EureqaTM software were then subjected to verification to select the best model based on complexity-to-accuracy Pareto, error metrics and sensitivity tests. The selected model was adjusted based on the underlying model assumptions. The final model was tested for adequacy by means of standard deviation, σ and percentage absolute average relative error, %AARE using a new set of experimental data outside the region of data space used for the model development. The results showed that standard deviation, σ and %AARE of the model output against the validating experimental data are 0.017 and 2.09%, respectively. This indicates that the model is adequate to predict hydrophilicity of functionalized CNT-infused polysulfone membrane (irrespective of the method of functionalizing CNT and the polysulfone membrane base solvent used).