Feedforward Artificial Neural Network-Based Model for Predicting the Removal of Phenolic Compounds from Water by Using Deep Eutectic Solvent-Functionalized CNTs

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Academic Editors: Mert Atilhan and Santiago Aparicio
Received: 9 July 2019; Accepted: 25 August 2019; Published: 26 March 2020

Abstract: In the recent decade, deep eutectic solvents (DESs) have occupied a strategic place in green chemistry research. This paper discusses the application of DESs as functionalization agents for multi-walled carbon nanotubes (CNTs) to produce novel adsorbents for the removal of 2,4-dichlorophenol (2,4-DCP) from aqueous solution. Also, it focuses on the application of the feedforward backpropagation neural network (FBPNN) technique to predict the adsorption capacity of DES-functionalized CNTs. The optimum adsorption conditions that are required for the maximum removal of 2,4-DCP were determined by studying the impact of the operational parameters (i.e., the solution pH, adsorbent dosage, and contact time) on the adsorption capacity of the produced adsorbents. Two kinetic models were applied to describe the adsorption rate and mechanism. Based on the correlation coefficient ($R^2$) value, the adsorption kinetic data were well defined by the pseudo second-order model. The precision and efficiency of the FBPNN model was approved by calculating four statistical indicators, with the smallest value of the mean square error being $5.01 \times 10^{-5}$. Moreover, further accuracy checking was implemented through the sensitivity study of the experimental parameters. The competence of the model for prediction of 2,4-DCP removal was confirmed with an $R^2$ of 0.99.

Keywords: water quality; deep eutectic solvents; carbon nanotubes; feedforward back propagation neural network; adsorption