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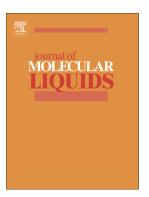
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ACCEPTED MANUSCRIPT

INSIGHTS AND PITFALLS OF ARTIFICIAL NEURAL NETWORK MODELING OF COMPETITIVE MULTI-METALLIC ADSORPTION DATA

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ABSTRACT: This manuscript discusses the advantages and limitations of ANNs models for modeling and predicting multi-component adsorption of heavy metal ions on bone char. In particular, the simultaneous adsorption of cadmium, nickel, zinc and copper ions in binary, ternary and quaternary mixtures on bone char has been used as a case study to analyze the problems associated with the training variables, activation function and architecture used in the ANNs modeling of multi-metallic adsorption data. The results of this study demonstrated that a proper ANNs training variable was fundamental for a reliable fitting and for the prediction of the complex adsorption behavior of metallic mixtures. In particular, the use of equilibrium concentrations as output data for the training of ANNs model may cause incorrect predictions of the multi-metallic adsorption on bone char. These pitfalls of ANNs models could prevail for multi-component systems with an antagonistic adsorption if extensive variables, such as equilibrium concentrations or removal percentages, were used in the training stage. These findings are valuable and can be used as guidelines for the application of ANNs models in the simulation and prediction of multi-component adsorption systems involved in water treatment and purification.

Keywords: Artificial neural networks, Adsorption, Heavy metals, Water Treatment, Modeling

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