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Enhancing selenium removal using pre-treated natural clay: experimental investigation and predictive modeling

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Abstract

A heat treatment methodology was adopted as a pretreatment strategy, altering the porous structure of the clay to minimize leaching for selenium adsorption in an aqueous system. Rigorous experiments were carried out in batch mode to determine optimal parameters across various variables, including contact time, adsorbent dosages, selenium concentrations, pH, temperature, and stirring speed during selenium removal using natural clay. Investigating several kinetic and isotherm models revealed the best fitting for the pseudo-second-order and the Langmuir isotherm. Endothermic and spontaneous characteristics of the adsorption process were shown during thermodynamic analysis. In this study, a predictive model for the efficiency of selenium separation was established using Response Surface Methodology (RSM). Additionally, an Artificial Neural Network (ANN), a data-driven model, was employed for comparative analysis. The predictive model exhibited a high degree of agreement with experimental data, demonstrated by a low relative error of <0.10 , a high regression coefficient of >0.97 , and a substantial Willmott-d index of >0.95 . Moreover, the efficacy of pre-activated clay in selenium removal was assessed, revealing the superior performance of ANN models over RSM models in forecasting the efficiency of the adsorption process. This research significantly advances an effective and sustainable material for selenium removal, providing valuable insights into predictive modeling techniques applicable to similar contexts to boost scale-up confidence during industrial implementation in affected regions.

1. Introduction

The concentration of selenium in water plays a crucial role in determining whether it serves as a vital element or poses a risk of toxicity (Janz 2011, Pommier *et al* 2019). In the realm of water quality regulations, divergent standards exist for selenium concentration. The United States mandates a permissible limit of $50 \mu\text{g l}^{-1}$ in drinking water, while the European Union enforces a more stringent maximum threshold of $10 \mu\text{g l}^{-1}$ (He *et al* 2018). Meanwhile, the World Health Organization (WHO) suggests a daily intake of 40 to 400 μg of selenium, stipulating a maximum allowable concentration of $40 \mu\text{g l}^{-1}$ in drinking water (World Health Organization 2011). The escalating concern over selenium contamination in groundwater and wastewater has spurred the development of diverse removal methodologies. These encompass membrane-based processes, reduction techniques, adsorption, electrocoagulation, coagulation-flocculation, phytoremediation, co-precipitation, electrochemical approaches, chemical precipitation, and biological remediation strategies (Zheng *et al* 2014, Kalaitzidou *et al* 2020, Mora *et al* 2020, Malhotra *et al* 2020,