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Mathematical Modeling of Sorption on Novel Sorbent Materials

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The emission of metal ions in the environment has increased in recent times and since metal ions are not biodegradable, they belong to the cumulative toxins. Contamination of the environment with metal ions poses a serious danger to the entire ecosystem, agricultural production, quality of food and water, as well as to the health of humans and animals. This study investigates sorption as one of the processes which can be used for pollutants removal and efficiency of certain sorbent materials. Specifically, we focus on development and validation of non-linear Langmuir model and non-linear Freundlich model. Their application in sorption experiments is examined by applying different error functions and statistical methods which are employed to calculate the error divergence between observed data and predicted data of sorbate-sorbent system. Presented non-linear sorption models are developed by using programming language Fortran, and the data analysis is obtained by using different tools and packages in programming language R. Many authors are using linear sorption models in the way that they would linearize non-linear sorption models. It is evident that linear sorption models are used due to their simplicity in parameters estimation. We use approach of trying different algorithms and tools in programming language R in order to find the best objective function. This study shows that both non-linear Langmuir model and non-linear Freundlich model can be used for experimental data representation. The results also denote that better estimation and the better fit is given by Langmuir model due to divergence in error functions and graphical representation itself. The choice of sorption model has a great influence on the prediction of solute transfer and great care should be taken in selection of convenient approach.