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Sensitivity analysis and modeling of 4-chlorophenol degradation in aqueous solutions by an nZVI-sodium persulfate system

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ABSTRACT

In the present study, an artificial neural network (ANN) and response surface methodology (RSM) were used to model the 4-chlorophenol (4-CP) removal in a nanoscale zero-valent iron (nZVI)/persulfate/water system. The impacts of experimental parameters, including persulfate, nZVI, reaction time, pH, and initial 4-CP concentration were considered as input variables in the models. The experiments were conducted based on the central composite design (CCD). The CCD of experiments was also employed as the training set for ANN models. The results of nZVI/persulfate system on removal of 4-CP indicated that the process was directly influenced by the extent of generated sulfate free radicals for the initiation of the oxidative degradation of 4-CP. With increasing the persulfate concentration to 2 mM and nZVI dosage to 1 g/L in the system, the removal percentage of 4-CP was increased. In addition, the acidic condition (pH = 3) turned out to be more favorable than alkaline and neutral conditions for 4-CP elimination. The modeling results showed that ANN with an R^2 value of 0.992 can be more reliable than the RSM model with an R^2 value of 0.9245. A sensitivity analysis was conducted to determine the relative importance of each variable on the ANN model output. The results of the sensitivity analysis showed that all factors were important for model output. However, pH was the most influencing factor.

Keywords: Persulfate; nZVI; ANN; RSM; Sensitivity analysis

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