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QSAR modeling of VOCs degradation by ferrous-activated persulfate oxidation

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ABSTRACT

The objective of the study is to evaluate the degradability of volatile organic compounds (VOCs, in mixture) by sodium persulfate (SPS) with Fe(II) activation. Degradation of 51 VOCs by SPS alone and with 3 Fe(II)-based activators (i.e. ferrous ion, citric acid-chelated Fe(II), and EDTA-chelated Fe(II)) was investigated in batch experiments. In 48 h, 16 VOCs degraded over 90% with non-activated SPS, and 31 VOCs degraded over 90% with Fe(II) activation. The reaction rate constants of VOC degradation were also analyzed by quantitative structure-activity relationship (QSAR) model. Genetic algorithm and multiple linear regression analysis were applied to select the descriptors to build QSAR model. The main contribution to the degradation rate was given by energy level of highest occupied molecular orbital (E_{HOMO}), double bond equivalent, and the largest negative partial net charge on a carbon atom (Q_c^-). Based on cluster analysis of degradation rates and main descriptors, the degradability of target VOCs were classified into three classes—rapid, moderate, and slow. The obtained statistically robust QSAR model can be used to estimate the removal efficiency of VOCs by persulfate radicals.

Keywords: Persulfate oxidation; VOCs; QSAR model; Ferrous; Kinetics

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