Quantitative structure-activity relationship (QSAR) for the adsorption of organic contaminants by nascent state manganese dioxide

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ABSTRACT

Nascent state manganese dioxide exhibits promising adsorptive capacity as it has large surface area with many water molecules and hydroxyls on. Therefore it has been applied as a treatment of organic pollution. The experimental removal rates ($R_{exp}$) under 3 different pH conditions and 18 quantum descriptors of 29 organic contaminants were used to construct quantitative structure-activity relationship (QSAR) models to predict the removal rate at a certain pH. The optimum models at pH 3, 7, 10 are listed as follows respectively, $R_{pre} = 1.437 - 5.627f(+) x + 1.018q(C--) x + 0.099E_{HOMO} (R^2 = 0.9273, pH = 3)$; $R_{pre} = -4.153 + 2.632BO x + 0.688BO n - 0.696q(C--) n (R^2 = 0.7459, pH = 7)$; $R_{pre} = -0.057 + 0.031\mu + 0.243BO n + 4.976f(0) n - 3.938f(+) x (R^2 = 0.9213, pH = 10)$. All of the optimum models show satisfactory stability, evident reliability and powerful predictability. Furthermore, they have no possibility of chance correlation. The results presented that affinity with solvent, charge distribution and stability of a molecule were main molecular characters influencing removal effect.

Keywords: QSAR; Organic contaminants; Adsorption; Nascent state manganese dioxide; Quantum descriptors