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Screening of commercial sorbents for the removal of phosphates from water and modeling by molecular simulation

Lorena Delgadillo-Velasco^a, Virginia Hernández-Montoya^{a,*}, Norma A. Rangel-Vázquez^a,

Francisco J. Cervantes^b, Miguel A. Montes-Morán^c, Ma del Rosario Moreno-Virgen^a

^aTecNM/Instituto Tecnológico de Aguascalientes, Av. Adolfo López Mateos No. 1801 Ote. C.P. 20256, Aguascalientes, Ags., México.

^bDivisión de Ciencias Ambientales, Instituto Potosino de Investigación Científica y Tecnológica (IPICYT), Camino a la Presa San José 2055, Col. Lomas 4^a. Sección, San Luis Potosí, SLP, 78216 México.

^cInstituto Nacional del Carbón, INCAR-CSIC, Apartado 73 E-33080, Oviedo, Spain.

Abstract

Eight commercial sorbents of different origin and nature were studied in the present work for the removal of phosphate from water using synthetic solutions and a wastewater from an anodizing company. The materials included activated carbons, bone char, catalytic carbon, natural silica, natural zeolite, a manganese(II) oxide composite and iron(III) hydroxide. These materials were characterized with different analytical techniques such as nitrogen adsorption isotherms at -196 °C, FT-IR spectroscopy, SEM/EDX analysis and X-ray diffraction. The adsorption studies were performed in batch systems. Iron(III) hydroxide was found the best sorbent, showing a maximum adsorption capacity of 193.75 mg/g at pH 7 in contrast with natural zeolite and silica, which registered very low adsorption values (2.92 and 4.17 mg/g, respectively). According to molecular simulation studies, the adsorption of phosphates from water on iron(III) hydroxide allowed the formation of the complex $\equiv\text{FePO}_4\text{H}_2$, with a Gibbs free energy of -21.38 kcal/mol, showing that it is possible to recover

*Corresponding author. Tel.: +52 449 9105002 Ext. 137

E-mail address: virginia.hernandez@yahoo.com.mx (Virginia Hernández-Montoya)

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