
Title

Removal of two carbamate pesticides from aqueous solutions using an adsorbent material based on poly(vinyl alcohol) and malic acid hydrogels

Abstract

This study describes through Molecular dynamics simulations the interactions between two carbamate pesticides, Carbofuran (CFN) and Methomyl (MML), with PVA hydrogels, crosslinked with malic acid (CLPHMAs), for the quantitative capture of these insecticides and the remediation of aqueous solutions. The crosslinked hydrogels were prepared and characterized by FTIR, SEM, TGA, and equilibrium swelling ratio. The FTIR spectra revealed the presence of a peak around ~ 1719 attributed to the ester group (C-O-C), which resulted from the esterification reaction between PVA and the crosslinker. The simulations correlate with experimental trials based on the Design of Experiments (DoE), allowing the capture of CFN and MML in aqueous solutions of 500 mg L^{-1} , using a capture time of 10 min. In conclusion, both tools enhance each other, demonstrating that CLPHMAs can remove these pesticides, constituting a technological alternative for treating contaminated water.

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