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ORIGINAL PAPER

Mathematical modeling studies for the adsorptive removal of ciprofloxacin drug from water samples using functionalized silica resin

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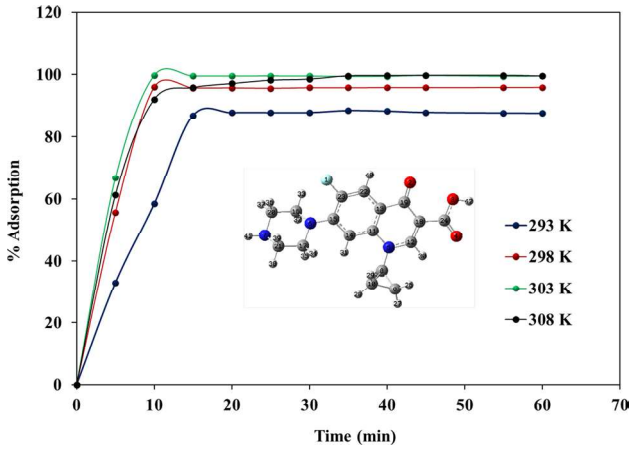
Abstract

The current research demonstrates the adsorptive removal of ciprofloxacin antibiotic drug from pharmaceutical wastewater samples using functionalized silica (FS) resin through batch adsorption experiments. The adsorption experiments were performed under the optimized parameters such as pH effect, FS-resin amount, ciprofloxacin concentration, equilibrium time and temperature. Results demonstrate that the maximum adsorption of ciprofloxacin was achieved at pH (6.5), while the effective resin dose was 20 mg L^{-1}. The Langmuir and Freundlich models were applied on equilibrium data, and it has been observed that the adsorption was best fit to the Freundlich model with a good correlation coefficient ($R^2 = 0.999$). Moreover, the thermodynamic and kinetic parameters show that the adsorption of ciprofloxacin is endothermic and spontaneous in nature followed by pseudo-second-order kinetic model. To explore the efficiency of resin, the real wastewater samples were collected and it has been observed that resin has better potential to treat pharmaceutical effluents. Furthermore, the FS-resin and ciprofloxacin interaction were analyzed at a molecular level through quantum chemical calculation.

Graphical abstract



Keywords Adsorption · Antibiotic ciprofloxacin · Equilibrium modeling · Silica-based adsorbent · DFT calculations · Thermodynamic and kinetic studies

Introduction

The antibiotics in pharmaceutical effluents, discharged into fresh water, cause adverse effects on human as well as aquatic life (Rik et al. 2019). However, the sewage water

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