



# Mechanistic study of diclofenac and carbamazepine adsorption on functionalized silica-based porous materials

Nakorn Suriyanon<sup>a,b</sup>, Patiparn Punyapalakul<sup>b,c</sup>, Chawalit Ngamcharussrivichai<sup>d,\*</sup>

<sup>a</sup> International Postgraduate Programs in Environmental Management, Graduate School, Chulalongkorn University, Bangkok 10330, Thailand

<sup>b</sup> Center of Excellence for Environmental and Hazardous Waste Management (EHWM), Bangkok 10330, Thailand

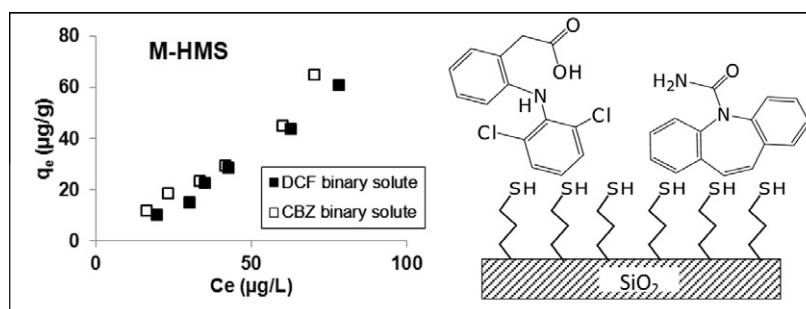
<sup>c</sup> Department of Environmental Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok 10330, Thailand

<sup>d</sup> Fuels Research Center, Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

## HIGHLIGHTS

- ▶ Adsorption of DCF and CBZ onto all adsorbents reached equilibrium within 4 h.
- ▶ Film diffusion was the likely rate-limiting step in the adsorption process.
- ▶ Addition of mercapto-functional group to HMS increased its adsorption capacity.
- ▶ The adsorption capacities of M-HMS, A-HMS and HMS were dependent on the pH.
- ▶ The adsorption capacity might be related to the molecular size of the adsorbate.

## GRAPHICAL ABSTRACT



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## ABSTRACT

Adsorption of diclofenac and carbamazepine by hexagonal mesoporous silicate (HMS), and the amine- and mercapto-functionalized HMS derivatives (A-HMS and M-HMS, respectively), were evaluated in comparison to that for the mesoporous silicates SBA-15 and MCM-41 plus powdered activated carbon, so as to evaluate the adsorption mechanism, effects of surface functional groups, pH and temperature on the adsorption capacity of these adsorbents. The adsorption of diclofenac and carbamazepine onto all adsorbents was found to decrease rapidly in the first 30 min and reach equilibrium within 4 h. The adsorption kinetics and isotherm data obtained were best described by a pseudo-second-order kinetic rate model and linear isotherm model, respectively. Comparison of the adsorption capacities of HMS, A-HMS and M-HMS suggested that the addition of a mercapto functional group to HMS, increased its adsorption capacity, most likely through increased hydrogen bonding and hydrophobic interactions. The adsorption capacities of these adsorbents were dependent on the pH, being highest at pH 5 due to the optimal electrostatic interactions and hydrogen bonding at this pH. Thermodynamic analysis indicated that the adsorption process was endothermic for all adsorbents. The adsorption capacity of the adsorbent for each solute might be related to the molecular size of the adsorbate.

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## 1. Introduction

In this last decade, pharmaceutical residues have grown in interest and importance to environmental scientists, as well as basic and pharmaceutical researchers. A large and increasing number of pharmaceutical compounds have been used for the treatment of

\* Corresponding author. Tel.: +66 2 218 7528x2325; fax: +66 2 255 5831.

E-mail address: [chawalit.ng@chula.ac.th](mailto:chawalit.ng@chula.ac.th) (C. Ngamcharussrivichai).