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Experimental and Theoretical Thermodynamic Studies of the Adsorption of Polyhalogenated Organic Compounds from Aqueous Solution by Chemically Modified Multi-walled Carbon Nanotubes

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Abstract Multi-walled carbon nanotubes (MWCNTs) were chemically modified with octadecyl amine or polyethyleneglycol and then used as solid phase adsorbents for the adsorption from aqueous solution of different polyhalogenated organic pollutants: pentachlorophenol, 2,4,5-trichlorophenol, 3,3′,4,4′-tetrachlorobiphenyl and 2,2′,5,5′-tetrabromobiphenyl from model aqueous solutions. The effects of temperature were measured and thus the Gibbs energy, enthalpy, and entropy of adsorption were calculated. In general, the Gibbs energy of adsorption was negative for the target analytes, indicating that adsorption was spontaneous at all temperatures. On the other hand, the values of the enthalpy and entropy of adsorption were significantly dependent on the type of modified MWCNTs as well as the analytes used. Computer modeling was used to simulate the adsorption process and calculate the Gibbs energies of adsorption. The results showed moderate agreement with the experimentally determined values.

Keywords Multi-walled carbon nanotubes · Modification · Polyhalogenated organic pollutants · Adsorption · Thermodynamics · Computer modeling

1 Introduction

Recently, releases of different pollutants to the water environment have drawn the attention of scientists due to their toxic effects. Most of these pollutants have limited solubility in

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