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Theoretical and experimental studies of benzoic acid batch adsorption dynamics using vermiculite-based adsorbent

Ehsan Sadeghi Pouya^a, Hossein Abolghasemi^{a,b,*}, Moein Assar^a,
Seyed Jalaledin Hashemi^{a,c}, Alireza Salehpour^d,
Mohammad Foroughi-dahr^a

^a Center for Separation Processes Modeling and Nano-Computations, School of Chemical Engineering, College of Engineering, University of Tehran, P.O. Box 11365-4563, Tehran, Iran

^b Oil and Gas Center of Excellence, University of Tehran, Tehran, Iran

^c Pulp and Paper Research Center, Department of Chemical Engineering, McGill University, Montreal, Canada

^d Laboratory for Instrumental Analysis, School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran

Dedicated to the memory of our dear colleague Seyed Jalaledin Hashemi, who passed away a few days ago.

A B S T R A C T

In this article, the batch adsorption of benzoic acid from aqueous solution onto modified vermiculite was both experimentally and theoretically investigated. Mechanical modification of raw vermiculite was carried out by means of a laboratory vibratory disk mill. In addition, an organic modification was performed by cetyltrimethylammonium bromide. A set of experiments were conducted in order to optimize the adsorbent dosage, initial pH value and contact time and to evaluate the batch kinetics and the equilibrium isotherm. The Freundlich and the Toth isotherms best fitted our experimental data. A mathematical model was developed for the investigation of the adsorptive dynamic characteristics, thereby estimating the pore diffusivity based on the experimental results. The model showed a good agreement with the experiments and the effective diffusivity, the model adjustment parameter, was estimated as $0.33 \times 10^{-9} \text{ m}^2 \text{ s}^{-1}$.

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1. Introduction

Industrial effluents containing many organic and inorganic components are the main source of drinking water contamination. Benzoic acid (BA), an aromatic organic compound with an electron-withdrawing carboxyl group, is not decomposed biologically and consequently, it must be removed from wastewaters at high concentrations in accordance with the instructions of World Health Organization (WHO) (Huang et al., 2011; Wibbertmann et al., 2005). Adsorption is a cost-effective, simple and common method for eliminating BA from aqueous solution (Ayrançi et al., 2005; Xin et al., 2011; Yıldız et al., 2005;

Yan et al., 2007). Activated carbons are classic adsorbents to remove a variety of impurities (Ahmad et al., 2012; Lo et al., 2012; Mohanty et al., 2005). The disadvantages of the activated carbons such as high cost of production and the necessity for regeneration have caused a growing attempt for use of other effective adsorbents (Foroughi-dahr et al., 2014). Today, natural minerals are widely used due to their low cost, abundance, high potential for ion-exchange, mechanical and chemical stability and high surface area (Ahmaruzzaman, 2008; Kim et al., 2014). Vermiculite is one of the most known aluminosilicate clay minerals, which has a hydrophilic, negatively charged and layered crystalline structure (Tang et al., 2012; Pérez-Rodríguez et al., 2002). As an organic

* Corresponding author. Tel.: +98 21 61112186; fax: +98 21 66954051.

E-mail addresses: ehsan.sadeghipouya@gmail.com (E. Sadeghi Pouya), hoab@ut.ac.ir, Abolghasemi.ha@gmail.com (H. Abolghasemi), assar.engbox@gmail.com (M. Assar), sj.hashemi@mcgill.ca, jhashemi@ut.ac.ir (S.J. Hashemi), asalehpour@ut.ac.ir (A. Salehpour), mfd.foroughi@ut.ac.ir (M. Foroughi-dahr).

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Nomenclature

A	external area of a grain
C	adsorbate concentration
D_e	effective macropore diffusivity
D_{AB}	diffusivity of A in pure B
I	number of the discretized nodes
i	node identifier
N	number of adsorbent grains
Q	nonlinear term
q	adsorption capacity
r	radial coordinate for the grain
R	average radius of the grain
t	time
V	liquid solution volume
W	adsorbent weight
N	number of experimental data
C_C	carbon content in weight percentage
n_C	number of carbon atoms in surfactant
M_C	molecular weight of carbon
K	Scherrer constant

Greek letters

ε_p	adsorbent porosity
δr	increment in r -direction
δt	time increment
ρ_s	skeletal density
μ	arithmetic mean of experimental data
λ	Cu $K\alpha$ wavelength
β	full width at half-maximum intensity
θ	Bragg's diffraction angle

Subscripts

0	at initial condition
b	bulk phase
e	at equilibrium state
p	pore liquid phase
exp	experimental value
cal	calculated value

modification, applying cationic surfactants like cetyltrimethylammonium bromide (CTAB) with concentrations above the critical micelle concentration, about 0.9 mM at 25 °C for CTAB, reverses the structure of raw vermiculite from hydrophilic to hydrophobic and from negative to positive by forming a patchy bilayer of the surfactant on the surface (Yu et al., 2010; Medeiros et al., 2009; Guan et al., 2010; Anirudhan and Ramachandran, 2006; Simpson and Bowman, 2009). Grinding by a vibratory disk mill as a mechanical modification can improve the factors of porosity of raw vermiculite as well as its surface energy and reactivity (Maqueda et al., 2009; Hongo et al., 2012).

A number of mathematical models namely the external film diffusion model, the intraparticle diffusion model, the film-surface diffusion model and the film-pore diffusion model have been developed and adopted by different researchers to predict the adsorption characteristics of such processes (Crank, 1979; Perry and Green, 1997). These models usually lead to highly nonlinear differential equations except for special cases such as linear isotherms (Hsu and Chen, 1987; Lapidus and Amundson, 1952; Park, 2005; Rasmuson, 1981). For the case of the stirred tank batch adsorption process, several numerical solution methods such as the collocation algorithm, the finite difference

algorithm, the matrix multiplicative weights algorithm, the integral formulation method and the weighted arithmetic mean method have been applied to solve the resultant mathematical equations (Lee and McKay, 2004; McKay, 2001).

Recently, the density functional theory (DFT) has been employed to provide mechanistic and structural insights into the adsorptive behavior of BA, particularly the interaction mechanism and configuration of the adsorbate species on the surface of different adsorbents (Gao et al., 2013; Lozzi and Cossi, 2007; Zhao and Fang, 2006).

The purpose of this research was twofold. Firstly, the modification of raw vermiculite both mechanically and organically was investigated for the batch adsorption of BA adsorbate in an aqueous solution. Afterwards, the kinetics and the equilibrium isotherm of the process at the optimized values of initial solution pH and adsorbent dosage were obtained at a constant temperature of 30 °C. The experimental equilibrium isotherm was modeled employing the Langmuir, the Freundlich, the Sips and the Toth models. Secondly, a pore diffusion-based model was developed to investigate the batch adsorption characteristics of the mentioned system. Implicit finite difference method of line was adopted to discrete and solve the governing equations. The model was successfully exploited to evaluate the effective diffusivity of BA in the adsorbent.

2. Mathematical modeling

The proposed model is based on the pore diffusion theory. The following assumptions are to develop the model:

- The isothermal condition prevails as the temperature is kept constant throughout the adsorption process.
- The external mass transfer coefficient is assumed negligible comparing to the pore diffusion resistance since a well mixing was established.
- At every single point of the adsorbent, the pore concentration is at equilibrium with the solid concentration. This assumption is not inaccurate because regarding the extremely small ratio of the mean pore diameter relative to the system dimensions, it is clear that the certain packs of the adsorbate solution reside inside the pores for relatively long periods of time. Such periods last sufficiently enough to ensure the establishment of local concentration equilibria between the pore and the solid phases.

It is one of the simplifying assumptions which has been commonly used in the literature; for example see (Choy et al., 2004; Firouztale et al., 1994; McKay, 2001; Maekawa et al., 1995; Quek and Al-Duri, 2007; Tao et al., 2012; Webber and Miller, 1988).

2.1. Equilibrium condition

The adsorbent ultimately reaches an equilibrium concentration with the solution. The overall mass balance at the equilibrium state is expressed by

$$C_{b,0}V = C_eV + q_eW. \quad (1)$$

The equilibrium concentration can be calculated using the above equation together with an equilibrium isotherm. The following equation can be obtained by means of the Langmuir isotherm:

$$C_e = \frac{V(C_{b,0}K_L - 1) - Q_0K_LW + \sqrt{(V(1 + C_{b,0}K_L) + K_LWQ_0)^2 - 4b^2WQ_0VC_{b,0}}}{2K_LV}. \quad (2)$$

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