



A new simplified method for estimating film mass transfer and surface diffusion coefficients from batch adsorption kinetic data



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HIGHLIGHTS

- The film mass transfer coefficient is related to the initial adsorption rate.
- The initial adsorption rate is estimated from the early-stage kinetic data.
- The surface diffusion coefficient is related to the late-stage rate constant.
- The late-stage rate constant is estimated from the late-stage kinetic data.
- The method is applied to four adsorption systems.

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ABSTRACT

A new simplified method is presented for estimating the film mass transfer and the surface diffusion coefficients from batch adsorption kinetic data without solving partial differential equations. The film mass transfer coefficient is determined from the initial adsorption rate which is estimated by fitting the kinetic data in the early adsorption stage to the early-stage kinetic equation. The surface diffusion coefficient is related to the late-stage adsorption rate constant which is estimated by fitting the late-stage kinetic data to the late-stage kinetic equation. The method is applied to four different adsorption systems in the literature. The predicted kinetics obtained with the estimated film mass transfer and surface diffusion coefficients shows a reasonable agreement with the experimental kinetics.

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1. Introduction

Adsorption is an effective and widely used method for the removal of pollutants from water and wastewater. The adsorption of an adsorbate from a liquid solution by a particulate adsorbent is generally viewed as a three-step process [1–6]: (1) diffusion across the liquid film surrounding the adsorbent particle (film diffusion or mass transfer); (2) diffusion inside the adsorbent particle (intraparticle diffusion or mass transfer) which may be due to pore diffusion or surface diffusion or a combination of both; (3) adsorption on the pore surface of the adsorbent (surface reaction). Depending on whether the diffusion steps or the reaction step are taken as the controlling step, adsorption kinetics is often treated in one of two methods: (1) the reaction method and (2) the diffusion (mass transfer) method. To the first method belong the pseudo-first-order kinetic model, the pseudo-second-order

kinetic model and the Langmuir kinetic model [7–12]. This method enjoys wide popularity because of its simplicity and the model parameters such as the adsorption rate constants are usually obtained by linear or nonlinear regression of batch adsorption kinetic data. But the method takes no consideration of the diffusion steps which are unneglectable in many (perhaps most) adsorption processes. The diffusion method includes the film–pore diffusion model, the film–surface diffusion (or the film–solid diffusion or the homogeneous surface diffusion) model and the film–parallel pore and surface diffusion model [1–6]. This method is less used because it usually involves partial differential equations. But diffusion (film diffusion, pore diffusion, surface diffusion or a combination of them) is often controlling [6] and the diffusion or mass transfer parameters (such as the film mass transfer coefficient, the pore and the surface diffusion coefficients) are fundamental parameters needed for the design of an adsorption process (batch, fixed-bed, etc.). The usual method for obtaining the diffusion parameters is to match the solution of the film–intraparticle diffusion model equations to experimental kinetic data [1–6,13,14]. This method is not convenient in that the film–intraparticle

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Nomenclature

a	a constant in Eq. (18)	n	Freundlich isotherm parameter
b	a constant in Eq. (33)	n_T	Toth isotherm parameter
c	bulk phase concentration in equilibrium with q	q	adsorbed phase concentration in equilibrium with c
c_0	initial bulk phase concentration	q_e	equilibrium value of q_t
c_b	bulk phase concentration at time t	q_m	Langmuir isotherm parameter
c_e	equilibrium value of c_b	q_r	adsorbed phase concentration at r
c_s	liquid phase concentration at adsorbent surface	q_s	adsorbed phase concentration at adsorbent surface
D_s	surface diffusion coefficient	q_t	adsorbed phase concentration or amount adsorbed by unit mass of adsorbent at time t
k_1	pseudo-first-order rate constant	q_T	Toth isotherm parameter
k_2	pseudo-second-order rate constant	r	radial coordinate
k_e	near-equilibrium- or late-stage rate constant defined by Eq. (29)	r_0	initial adsorption rate defined by Eq. (16)
k_f	film mass transfer coefficient	R	adsorbent radius
K_F	Freundlich isotherm parameter	t	time
K_L	Langmuir isotherm parameter	V	volume of bulk liquid solution
K_T	Toth isotherm parameter	ρ_p	adsorbent particle density
m	adsorbent mass		

diffusion equations have in general to be solved numerically except in some special and simplified cases.

The purpose of this study is to present a new simplified method for estimating the film mass transfer and the surface diffusion coefficients in the film–surface diffusion model from batch adsorption kinetic data without solving partial differential equations. The method is first developed and then applied to four adsorption systems taken from the literature to demonstrate its usage.

2. Theory

2.1. Bulk phase mass balance for batch adsorption

For a batch adsorption process the bulk (liquid) phase mass balance can be expressed as

$$V(c_0 - c_b) = mq_t \quad (1)$$

where c_0 and c_b are respectively the initial and instantaneous (at time t) adsorbate concentration in the bulk solution, V the volume of the bulk solution, m the adsorbent mass, q_t the instantaneous amount adsorbed by unit mass of adsorbent or the adsorbed phase concentration at time t . When adsorption reaches equilibrium, Eq. (1) becomes

$$V(c_0 - c_e) = mq_e \quad (2)$$

where c_e and q_e are respectively the equilibrium bulk and adsorbed phase concentrations.

2.2. Adsorption equilibrium

Adsorption equilibrium is often expressed by the Langmuir isotherm equation

$$q = \frac{q_m K_L c}{1 + K_L c} \quad (3)$$

or the Freundlich isotherm equation

$$q = K_F c^{1/n} \quad (4)$$

where q is the adsorbed phase concentration in equilibrium with the bulk phase concentration c , q_m and K_L the Langmuir isotherm parameters, and K_F and n the Freundlich isotherm parameters. These parameters are generally obtained by fitting experimental equilibrium data to the respective equations. When the two-parameter equations (3) and (4) do not fit well, a three-parameter

equilibrium equation may be used, one of which is the Toth isotherm equation [14]

$$q = \frac{q_T K_T c}{[1 + (K_T c)^{n_T}]^{1/n_T}} \quad (5)$$

where q_T , K_T and n_T are the Toth isotherm parameters.

It is noted that for a batch adsorption process the equilibrium values c_e and q_e can be determined by solving simultaneously the bulk phase mass balance equation and the adsorption isotherm equation.

2.3. Adsorption kinetics

2.3.1. Pseudo-first-order kinetic model

The pseudo-first-order kinetic model is usually written as

$$\frac{dq_t}{dt} = k_1(q_e - q_t) \quad (6)$$

where k_1 is the pseudo-first-order rate constant. Integration of Eq. (6) with the initial condition $q_t = 0$ at $t = 0$ gives

$$-\ln\left(1 - \frac{q_t}{q_e}\right) = k_1 t \quad (7)$$

The pseudo-first-order rate constant k_1 and the equilibrium adsorbed amount q_e are usually obtained by fitting kinetic data according to Eq. (7).

2.3.2. Pseudo-second-order kinetic model

The pseudo-second-order kinetic model is generally expressed as

$$\frac{dq_t}{dt} = k_2(q_e - q_t)^2 \quad (8)$$

where k_2 is the pseudo-second-order rate constant. Integration of Eq. (8) with the initial condition $q_t = 0$ at $t = 0$ gives

$$q_t = \frac{k_2 q_e^2 t}{1 + k_2 q_e t} \quad (9)$$

k_2 and q_e are usually obtained by fitting kinetic data according to Eq. (9) or its linear forms [8].

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