



Further verification of adsorption dynamic intraparticle model (ADIM) for fluid–solid adsorption kinetics in batch reactors



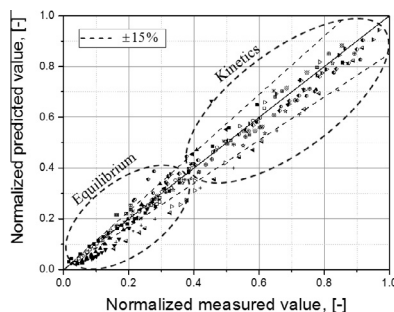
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HIGHLIGHTS

- Transient intraparticle model for fluid–solid adsorption kinetics.
- The PDEs system solved with method of lines.
- Literature datasets tested with the proposed model obtaining good results.
- Physical parameters fitted on the experimental data.
- The model is a starting point to design adsorption columns.

GRAPHICAL ABSTRACT



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ABSTRACT

Recently, a diffusive intraparticle dynamic model has been published by the authors and applied for describing few systems in order to check its validity. The aim of the present paper is to improve its validity in describing different kind of systems. At this purpose, adsorption data have been taken from literature, in which different adsorbate/adsorbent systems have been considered. In every case, the surface diffusivity of the pollutant (D_s) has been fitted on the experimental data. The obtained parameters fall within reasonable ranges and a good fitting has been obtained for each case, demonstrating the generality of the adopted model.

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1. Introduction

Fluid–solid adsorption is a separation technique very commonly adopted in the industries to solve different problems. In particular, it can be used for different applications: (i) the purification of industrial waste waters coming out from chemical plants [1]; (ii) the separation of products/by-products after synthesis routes [2];

(iii) in biotechnological processes where added value products must be removed from complex matrixes [3]. This technique is based on the transfer of one or more components from a fluid mixture to a solid surface, with which they establish chemical or physical interactions, thus causing an interfacial concentration variation with respect to the adjacent phases. Since the XVIII century, a systematic study of this phenomenon has been developed bringing to the derivation of equations for interpreting adsorption kinetics data collected in batch reactors and a huge number of models have been proposed for investigating both the equilibrium [4–6] and the kinetics of fluid–solid adsorption [7–10]. By considering the kinetic models, they can be roughly divided in two

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Nomenclature

a_{sp}	geometrical specific surface area, $m^2 m^{-3}$	N_{DATA}	number of parameters, –
b	Langmuir adsorption constant, $m_{liq,P}^3 mol^{-1}$	n_+, n_-	valences of respectively cation and anion, –
C_B	solute bulk concentration, $mol m_{BULK}^{-3}$	R	ideal gas constant, $J mol^{-1} K^{-1}$
C_L	solute concentration in the liquid of the pores, $mol m_{liq,P}^{-3}$	r_p	particle radial direction, m
C_S	solute concentration in the solid, $mol m_{sol,P}^{-3}$	R_p	particle radius, m
$C_{S,*}$	saturation solute solid concentration, $mol m_{sol,P}^{-3}$	s	shape factor, –
D	impeller diameter, m	t	time, s
D^0	molecular diffusivity, $m^2 s^{-1}$	T	temperature, K
d_p	particle diameter, m	V_A	solute molar volume, $cm^3 mol^{-1}$
D_p	pore diffusivity based on the cross sectional area, $m^2 s^{-1}$		
D_S	surface diffusivity, $m^2 s^{-1}$		
D_S^0	pre-exponential term in surface diffusivity temperature dependence, $m^2 s^{-1}$		
E_S	surface diffusion activation energy, $J mol^{-1}$		
F	Faraday, $96.5 C/g^{-1}$ -equiv		
K_F	Freundlich adsorption constant, $(mol m^{-3}) \cdot (mol m^{-3})^{-n}$		
k_m	mass transfer coefficient, $m s^{-1}$		
M_B	solvent molecular mass, $g mol^{-1}$		
N	impeller rounds per minutes, –		
n	adsorption intensity, –		
N_{PAR}	number of experimental data, –		
		Greek symbols	
		ΔH	adsorption molar enthalpy, $kJ mol^{-1}$
		ε	particle porosity, $m_{liq,P}^3 m_P^{-3}$
		ε'	volumetric ratio between the bulk volume and the overall particle volume, $m_{BULK}^3 m_P^{-3}$
		λ_+^0, λ_-^0	limiting zero concentration ionic conductances, $(A m^{-2}) (V m^{-1}) (g\text{-equiv } m^{-3})$
		μ_B, μ_L	solvent viscosity, cP
		ρ_L	solvent density, $g m^{-3}$
		τ	tortuosity factor, –
		φ_B	Wilke–Chang association factor, –

classes: (i) empirical or semi-empirical, considering the adsorption as a reaction kinetics [11–13]; (ii) diffusive models, derived from mechanism considerations on the adsorption phenomenon, such as the definition of a rate-determining step in the adsorption kinetics [14,15]. In the recent years, many researchers have put particular attention on the last ones, due to their interesting characteristic of involving parameters that can be correlated to properties with a precise physical meaning. Moreover, some specific journals in the adsorption technology, such as Journal of Hazardous Materials and Separation and Purification Technology, are rejecting papers in which a data interpretation is presented by using the simple kinetic models [7,16].

Recently, Russo et al. [17] tested a diffusive model proposed by Do [5], applied for gas–solid systems, for liquid–solid adsorption kinetics based on both film and intraparticle mass transfer. Cu(II) and Pb(II), adsorption batch experiments onto various kind of silica were interpreted obtaining good results in terms of data fitting [17]. However, in order to demonstrate that the model can be considered general, so independent on the adsorbate/absorbent couple, it is necessary to test it on a wider number of cases, including adsorbents and pollutants/products/by-products of different chemical nature. With this perspective, in the present manuscript data from three batch adsorption systems have been interpreted with the mentioned model. A summary of all the investigated cases is here reported:

- (1) Organic molecule in organic media on inorganic adsorbent: *p*-xylene in isooctane over Faujasite.
- (2) Ions in inorganic media on organic adsorbent: Cu(II) in water over active carbons.
- (3) Ions in inorganic media on organic adsorbent: Cd(II) in water over chitosan.

2. Theory

The kinetic data interpretation reported in this manuscript have been performed with the dynamic model recently published by Russo et al. [17]. The main points are here summarized to make the reader friendly with the topic. The system is conceptually divided into three domains: a bulk liquid phase in which the pol-

lutant concentration changes with time, a liquid intraparticle phase and the solid intraparticle phase, where the concentration depends on time and radius of the particle. Conceptually, the pollutant is transferred from the bulk phase to the particle through the liquid film and then it diffuses along the particle radius in the pore, in which the mass transfer is divided into the two parallel contributions of liquid porous diffusion and surface diffusion. Another important assumption is the intraparticle local equilibrium between surface and liquid phases expressed in terms of the adopted equilibrium isotherm. With these assumptions, the adsorption kinetics can be described by writing the mass balances constituted by two partial differential equations, one considering the bulk/film mass transfer (Eq. (1)) and one the intraparticle diffusion (Eq. (2)):

$$\varepsilon' \cdot \frac{\partial C_B}{\partial t} = -k_m \cdot a_{sp} \cdot (C_B - C_L|_{R_p}) \quad (1)$$

$$\begin{aligned} \varepsilon \cdot \frac{\partial C_L}{\partial t} + (1 - \varepsilon) \cdot \frac{\partial C_S}{\partial t} = \varepsilon \cdot \frac{D_p}{r_p^s} \cdot \frac{\partial}{\partial r_p} \left(r_p^s \cdot \frac{\partial C_L}{\partial r_p} \right) \\ + (1 - \varepsilon) \cdot \frac{1}{r_p^s} \cdot \frac{\partial}{\partial r_p} \left(r_p^s \cdot \frac{D_S}{1 - C_S/C_{S,*}} \cdot \frac{\partial C_S}{\partial r_p} \right) \end{aligned} \quad (2)$$

In Eq. (1), the bulk accumulation is equal to the film mass transfer, while in Eq. (2) the overall accumulation term (liquid and solid) is set equal to the sum of both the pore and the surface intraparticle diffusion terms.

Such a system needs a set of boundary conditions to be solved. A fundamental boundary condition is represented by the adsorption isotherm and is necessary to establish the local equilibrium condition, for example the Langmuir isotherm (Eq. (3)). Then, further boundary conditions are expressed by the particle symmetry (Eq. (4)) and surface steady-state hypothesis (Eq. (5)).

$$C_S = C_{S,*} \cdot b \cdot \frac{C_L}{1 + b \cdot C_L} \quad (3)$$

$$\left. \frac{\partial C_L}{\partial r_p} \right|_{r_p=0} = 0, \quad \left. \frac{\partial C_S}{\partial r_p} \right|_{r_p=0} = 0 \quad (4)$$

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