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Modeling of Batch and Continuous Adsorption Systems by Kinetic Mechanisms

Alice F. Souza[1], Leôncio Diógenes T. Câmara[2] and Antônio J. Silva Neto[2]
[1]Universidade Federal do Rio de Janeiro-UFRJ, Rio de Janeiro-RJ,
[2]Instituto Politécnico da Universidade do Estado do Rio de Janeiro, IPRJ-UERJ
Dep. Mechanical Eng. Energy - DEMEC, Nova Friburgo-RJ,
Brazil

1. Introduction

This chapter is related to the main aspects of the kinetic adsorption models by heterogeneous mechanisms applied in the studies of mass transfer in chromatography. The kinetic adsorption models are implemented and described according to the adsorption mechanisms as in the next Figure 1. The illustrations as in Fig. 1 are a good way to show the steps in the determination of the final models that represent the mass transfer between the solid and liquid phase.
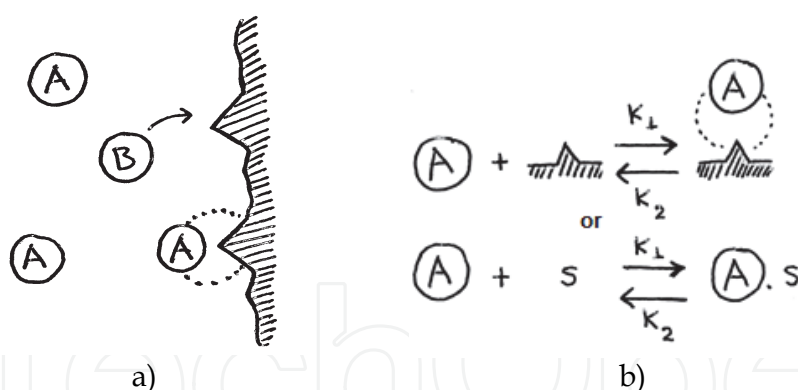

Fig. 1. Mechanisms of heterogeneous kinetic adsorption of molecules A on sites s.

From Fig. 1a) can be observed that the mass transfer of molecules A and B between the liquid (left) and solid (right) phase is related to the surface of the solid phase, so it depends on number of active sites on the surface and the number of molecules in the liquid phase. Such surface mechanism is called adsorption and it is represented in the Fig. 1b). In Fig. 1b) the adsorption is related to a kinetic constant k_1 and the desorption is related to a kinetic constant k_2. The adsorption is the main phenomenology present in the chromatography which provides different affinities of the molecules with the adsorbent phase leading to the separation.

The kinetic modeling approach utilized in this work considers the total sum of the adsorption sites which can be located on the internal and external active surface. The

modeling routines were implemented in Fortran 90 and the equations solved numerically applying the 4th order Runge-Kutta method (time step of 10^{-4}).

The rate of consumption of the molecules A ($-r_A$) can be written as follow in terms of the mass balance between the adsorbent solid phase and the liquid phase.

$$(-r_A) = k_1.C_A.C_S - k_2.C_{AS} = k_1.C_A.C_S - k_2.q_A \qquad (1)$$

in which C_A, C_S and q_A corresponds, respectively, to the concentration of solute A in the liquid phase, the concentration of active sites on the adsorbent phase and the concentration of solute A in the solid phase.

Different types of adsorption processes can be considered in the separation as can be seen in the Fig. 2. In the batch adsorption process (Fig. 2a) there is no flow entering and exiting the system; In the continuous (Fig. 2b) there is flow entering and exiting and it is considered perfect mixture (CSTR) inside the system in which the concentration inside is the same at the exit; and in the plug flow (PFR) also there is flow entering and exiting and it is considered an axial variation of concentration along the system.
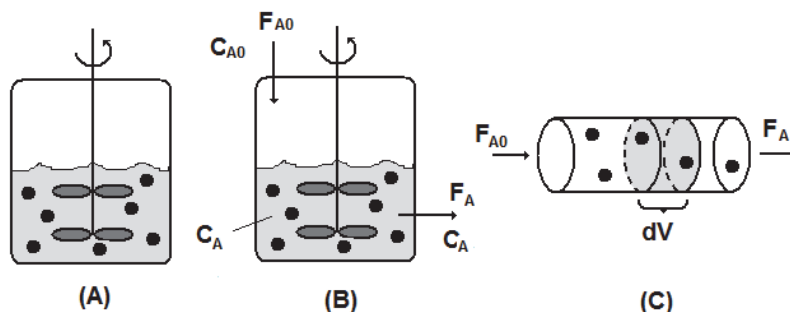

Fig. 2. Types of adsorption processes: a) batch; b) continuous (CSTR) and c) plug flow (PFR).

In the case of batch adsorption process (Fig. 2a) the moles balance (N moles per time) equation is applied without the terms of flow entering and exiting,

$$\frac{dN_j}{dt} = F_{j0} - F_{j0} + r_j.V \qquad \frac{dN_j}{dt} = r_j.V \qquad (2)$$

leading to a final expression of rate of adsorption that can be substituted into Eq. 1.

$$r_j = \frac{dN_j}{V.dt} \qquad r_j = \frac{dC_j}{dt} \qquad (3)$$

The following final expression (Eq. 4) shows that the concentration of solute A in the liquid phase decreases with the adsorption and increases with the desorption.

$$-\frac{dC_A}{dt} = k_1.C_A.C_S. - k_2.q_A \qquad (4)$$

2. Continuous separation by reversible kinetic adsorption models

The chromatographic separation processes, which are involved by the adsorption phenomena, correspond to a very important field for separating substances with high

aggregated value utilized mainly by the chemical and pharmaceutical industry. The application of the modeling and simulation to study such separation mechanisms is a key factor for the comprehension and therefore the improvement of the performance of the chromatographic systems.

The modeling of the chromatographic separation processes can be done applying different mathematical approaches, with advantages and limitations according to the method assumed. A revision of the dynamic and mathematical modeling of the adsorption isotherms and chromatography can be seen in the work of Ruthven, 1984. Among the models of mass transfer kinetics in chromatography, the LDF and the Langmuir, are the most utilized, being both related to a first order kinetic of mass transfer (Guiochon and Lin, 2003). The publication of Thomas (1944) corresponds to a precursor work following the simple adsorption kinetic of Langmuir (kinetic of first order), which derived a solution for the Riemann problem (i.e, for the breakthrough curve) of a model of chromatography combined with the mass balance equation of an ideal model (no axial diffusion). Later, Goldstein (1953) derived a solution of the Thomas model that is valid in the case of a rectangular pulse injection. Wade et al. (1987) obtained a simple solution of the Thomas model that is valid in the case of a Dirac injection. Following the same consideration of adsorption order (kinetic of first order), Chase (1984) derived an analytical form for the breakthrough curve, being it identical to the Thomas's model.

The assumption of LDF or adsorption kinetic of first order is a way to reduce the complexity of the chromatographic systems, being possible through this procedure achieve analytical expressions that can represent the dynamic behavior of these processes as obtained by Thomas (1944) and Chase (1984). The study of the chromatographic continuous systems by the consideration of others adsorption orders is a possibility to understand the separation mechanisms by adsorption, although this procedure can lead to more complex mathematical models. The application of the continuous mass balance models of perfect mixture with the kinetic mechanisms of adsorption with superior orders is an opportunity to analyze the equations terms and parameters that are relevant to the adsorption mechanism involved with the separation processes.

In this work different configurations of adsorption mechanisms combined with mixture mass balance models of the chromatographic columns are analyzed to determine the influence of the equation terms and parameters on the dynamic and equilibrium behavior of the separation processes.

2.1 Modeling approach

The modeling of the chromatographic separation process was based on the adsorption kinetic mechanisms over a solid surface as represented in the Fig. 3.

From the Fig. 3 it can be observed that the adsorption phenomena can follow different mechanisms, as verified from the cases (a) to (c).From it, the rate of consumption of solute A, represented by ($-r_A$), is determined by the following expression

$$(-r_A) = k_1.C_A{}^{\alpha}.C_S{}^{\beta} - k_2.q_A{}^{\gamma} \tag{5}$$

in which C_A, C_S and q_A represent the concentration of solute in the liquid phase, the concentration of active sites of the adsorbent and the concentration of solute A adsorbed in the solid phase, respectively. The parameters α, β and γ represent the stoichiometric coefficients of the adsorption mechanism (See Fig. 3 case (a)).
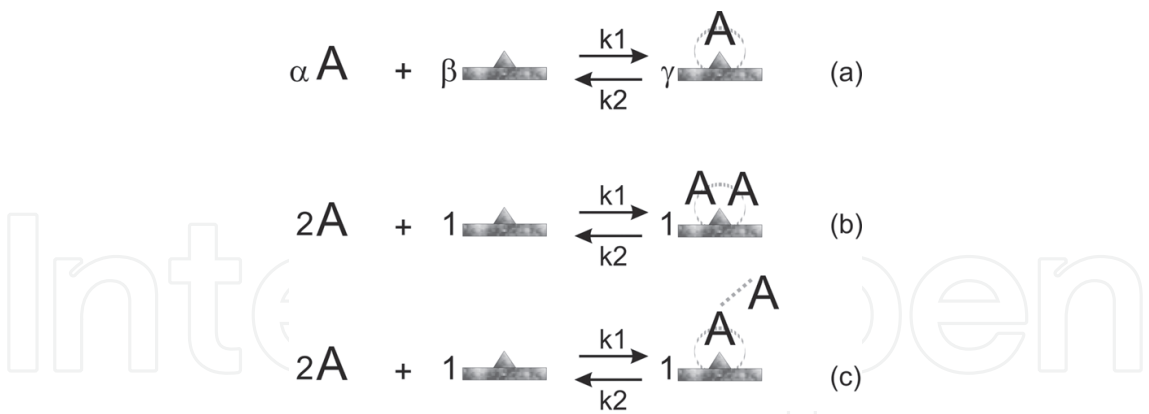
Fig. 3. Mechanisms of adsorption of solute (A) on the adsorbent surface

The active sites concentration are obtained by the mass balance in the adsorbent

$$C_s = (q_m - q_A) \tag{6}$$

with the parameter q_m representing the maximum capacity of adsorption or the maximum concentration of active sites on the surface of the adsorbent.

From the mass transfer of the solute A from the liquid phase to the solid phase can be established that $(-r_A = r_{SA})$, where $(-r_A)$ and (r_{SA}), represent the rate of consumption of the solute A in the liquid phase and the rate of adsorption of the solute A on the solid surface, respectively. Figure 4a presents the chromatographic column configuration assumed in the modeling, in which C_{A0} and C_A represent the initial concentration of solute (A) at the entrance of the column and the solute concentration at the column exit, respectively. Figure 4b presents a typical experimental curve of rupture or breakthrough curve for a chromatographic system, which was adapted from the experimental work of Cruz (1997), which studied the adsorption of insulin by the resin Accel Plus QMA.
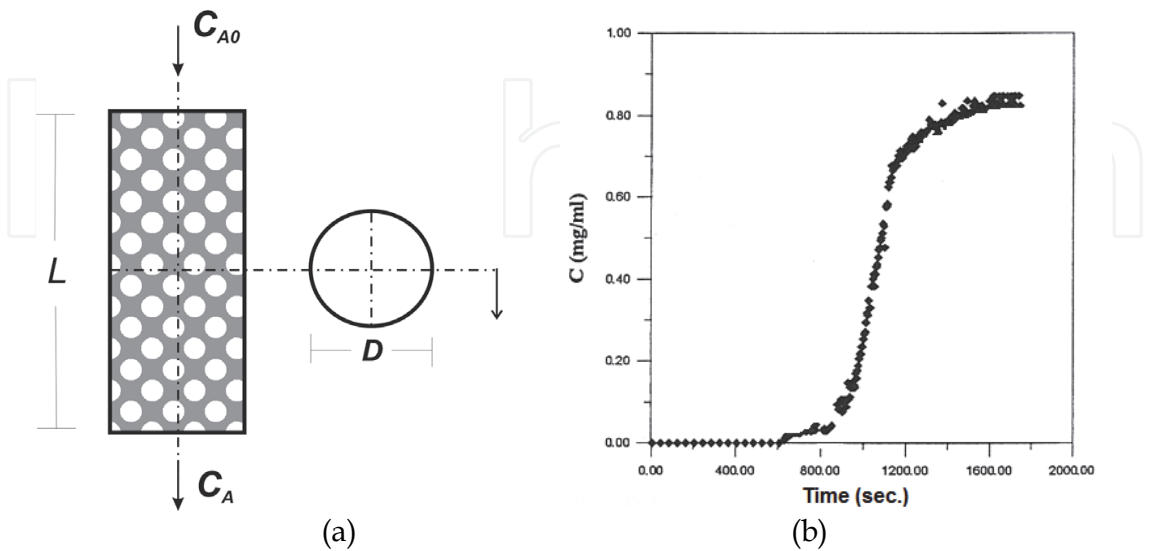

(a)   (b)

Fig. 4. (a) Representation of the chromatographic column modeled; (b) typical curve of rupture or breakthrough (adapted from Cruz, 1997).

Applying the mass balances in the chromatography column, according to the column configuration presented in Fig. 4, we obtain the following expressions for the mass balance of the solute in the liquid phase,

$$\varepsilon.V.\frac{dC_A}{dt} = Q.C_{A0} - Q.C_A - r_A.\varepsilon.V \tag{7}$$

and in the solid phase,

$$\varepsilon.V.\frac{dq_A}{dt} = r_{S.A}.\varepsilon.V \tag{8}$$

in which the parameters ε, V and Q correspond to the porosity, the volume and the volumetric flow, respectively. The first term of Eq. 7 corresponds to the accumulation, being the second, third and fourth the terms of solute entering, the solute exiting and the consumption rate, respectively. The accumulation term of the Eq. 7 is proportional to the rate of solute adsorption. These expressions correspond to mass balance models of perfect mixture, in which the solute concentration is the same in all the positions of the system.

Assuming $\varepsilon=1$, for a practical consideration, and substituting the Eqs. 5-6 into the Eqs. 7 and 8 we obtain

$$\frac{dC_A}{dt} = c_1.C_{A0} - c_1.C_A - [k_1.C_A{}^\alpha.(q_m - q_A)^\beta - k_2.q_A{}^\gamma] \tag{9}$$

$$\frac{dq_A}{dt} = k_1.C_A{}^\alpha.(q_m - q_A)^\beta - k_2.q_A{}^\gamma \tag{10}$$

In which the parameter c_1 is equals to Q/V.

The system of Eqs. 9 and 10, which represents, respectively, the mass balance of solute in the liquid and solid phase, was solved numerically, applying a routine according to the 4th order Runge-Kutta method (time step of 10-4) for different considerations of the separation process.

2.2 Results and discussion
2.2.1 Analysis of the separation process only by adsorption

In a first step the calculations were done assuming only the adsorption term of Eqs. 9 and 10, i.e. not considering the desorption term (k_2=0). The stoichiometric coefficients were also considered equal to the unit ($\alpha=\beta=1$). For the above considerations Eqs. 9 and 10 are transformed into

$$\frac{dC_A}{dt} = c_1.C_{A0} - c_1.C_A - k_1.C_A.(q_m - q_A) \tag{11}$$

$$\frac{dq_A}{dt} = k_1.C_A.(q_m - q_A) \tag{12}$$

Figure 5 presents the simulation results of the numerical solutions of the previous system of ordinary differential equations (Eqs. 11 and 12). From Fig. 5 it can be observed that the solute concentration in the liquid phase (C_A) presented a different behavior if compared to the concentration of solute adsorbed in the solid phase (q_A). The solute concentration (C_A)

showed a behavior similar to that for the chromatographic systems as can be verified by the typical result of the experimental curve in Fig. 4b. This characteristical aspect ("s" profile) for the chromatographic answer is called the rupture or breakthrough curve. From Fig. 5 it can also be seen that the concentration on the solid surface (q_A) is almost linear, presenting a significant variation at the same time as the inflexion point of the breakthrough curve. Note that the solute adsorption (q_A) is higher at initial times, leading to a high consumption of the solute in the liquid phase (the later appearance of solute at the column exit).
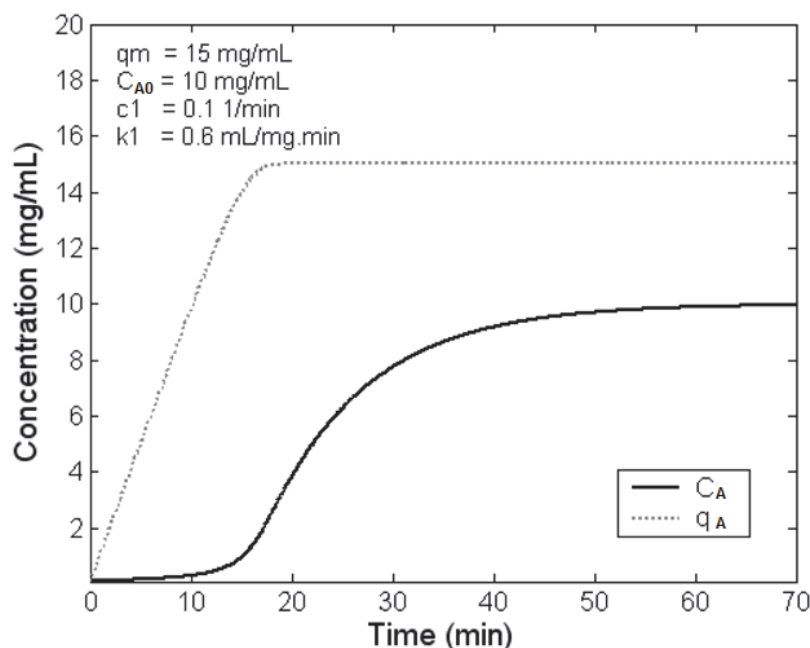

Fig. 5. Profiles of the solute concentration in the liquid (C_A) and solid phase (q_A)

Simulation results with a similar behavior as that obtained in Fig. 4b were obtained from conditions in which either the maximum capacity of adsorption (q_m) was greater than the initial concentration of solute at the entrance (C_{A0}) and the kinetic constant of adsorption was high. These parameters conditions led to higher values of the consumption term of Eq. 11. This observation is coherent with the real processes of chromatographic separation, which in general present high capacity of adsorption.

Figure 6 presents a result with the same behavior as that one observed in Fig. 4b. For this case, the high adsorption rate is attributed to the high kinetic constant of adsorption. From Fig. 6 it can be seen also the great variation of the solute concentration on the solid phase (q_A) at the same time of the inflexion point of the solute concentration in the liquid phase (C_A).

Simulation results showing the increase in the consumption rate of solute due to the increase in the maximum capacity of adsorption (q_m) are presented through the Fig. 7. The rate of adsorption was increased increasing the capacity of adsorption of the adsorbent from $q_m = 10$ mg/mL (Fig. 7a) to $q_m = 40$ mg/mL (Fig. 7b). From the case of low adsorption capacity (Fig. 7a) it can be observed that the concentration of solute in the solid phase increases slowly, allowing the appearance of solute in the liquid phase at initial times. For a high capacity of adsorption (Fig. 7b), the concentration of solute in the

solid phase increases fast, allowing a latter appearance of solute at the column exit (around 20 min).
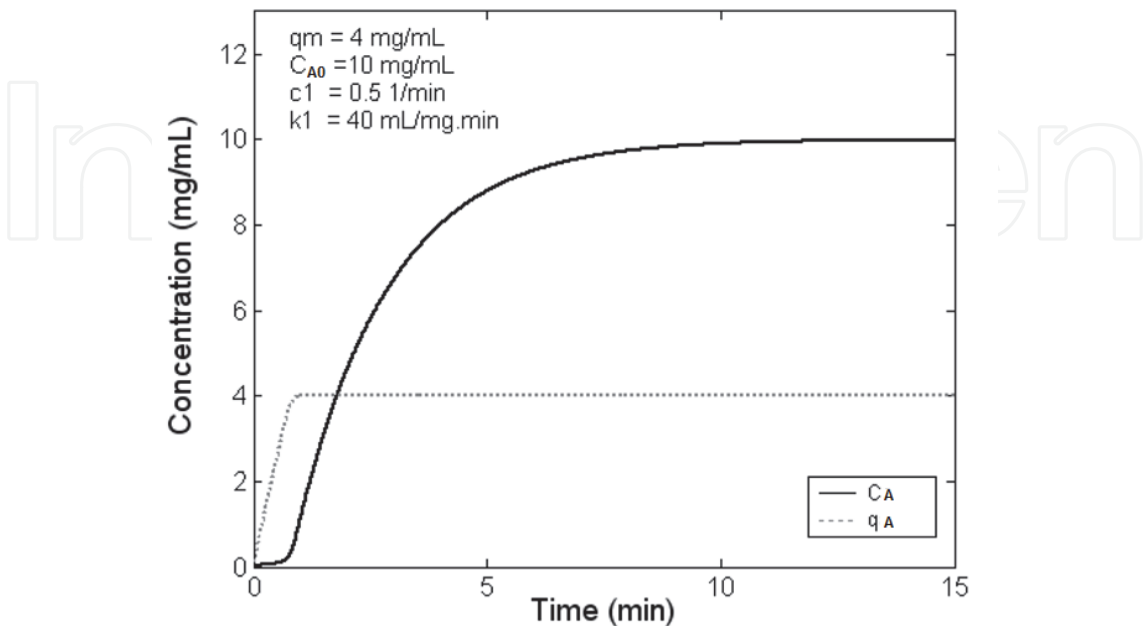

Fig. 6. Profiles of C_A and q_A for a high value of the kinetic constant of adsorption
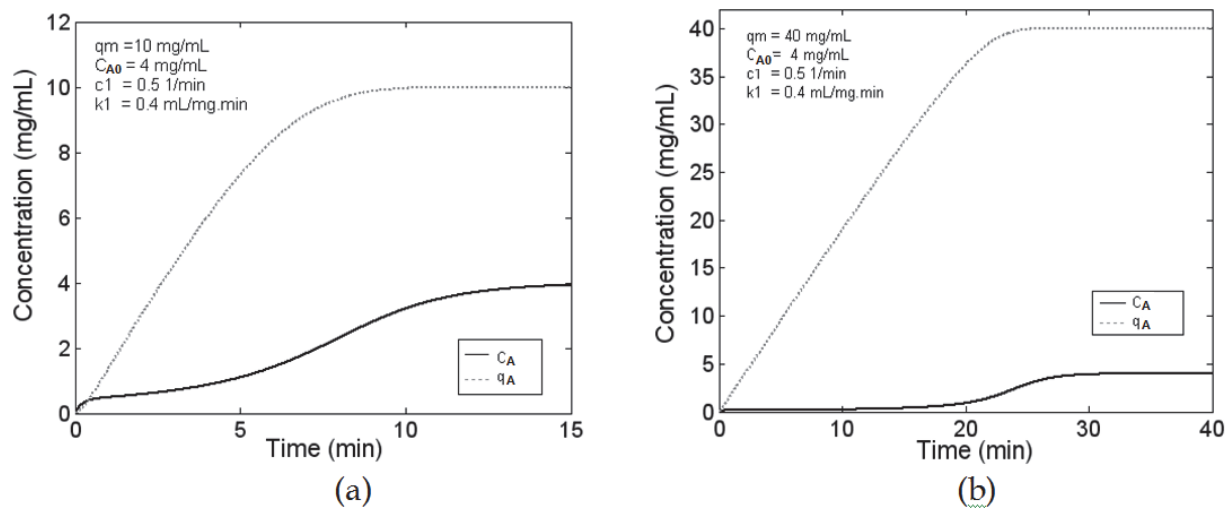

Fig. 7. Influence of q_m in the profile of C_A and q_A

2.2.2 Effects of the adsorption order

In this section, the effects of the stoichiometric coefficients or the order of adsorption on the dynamic behavior were analyzed. From Eqs. 9 and 10 it was assumed, in a first case, only the adsorption term ($k_2=0$) with the following stoichiometric coefficients ($\alpha=1$, $\beta=5$) which lead to the next expressions

$$\frac{dC_A}{dt} = c_1.C_{A0} - c_1.C_A - k_1.C_A.(q_m - q_A)^5 \qquad (13)$$

$$\frac{dq_A}{dt} = k_1.C_A.(q_m - q_A)^5 \qquad (14)$$

A comparison is presented through Figs. 8a and 8b, which shows the simulation results from the adsorption kinetic of first ($\alpha=1$, $\beta=1$) and fifth ($\alpha=1$, $\beta=5$) order, respectively, with respect to the active sites concentration (solid phase). As can be seen from Fig. 8 the increase in the adsorption order of the active sites increases the rate of adsorption, leading to a steeper breakthrough curve. Another remark is the decrease in the capacity of adsorption as the final concentration of solute A (q_A) in the solid phase decreases. The decrease in the final amount of solute adsorbed can be attributed to the number of active sites that is necessary for the adsorption. From the adsorption kinetic of fifth order ($\alpha=1$, $\beta=5$) is necessary the presence of 5 (five) adsorption sites to interact and adsorb the solute. At the end of the adsorption process the quantity of available sites is small and they must be close to each other to promote the adsorption of the molecule (for example, by the mechanism of fifth order, for five isolated sites it is not possible to have the adsorption of one solute molecule). The condition of close sites becomes more important as the order of adsorption increases, being necessary a higher quantity of close sites to promote the adsorption of the molecule.
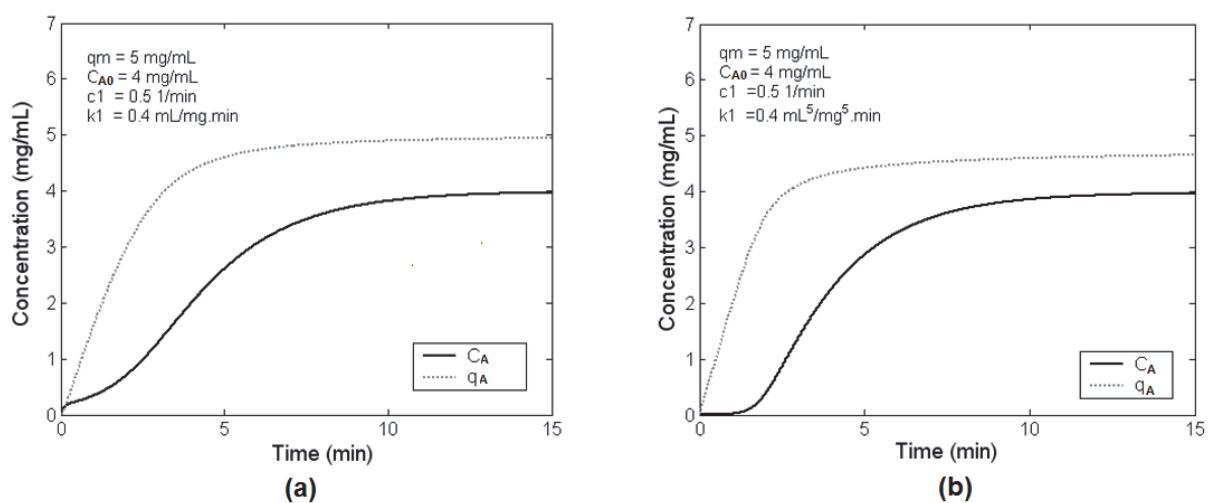

Fig. 8. Influence of the stoichiometric coefficients in the profile of C_A and q_A

2.2.3 Analysis of the separation process by adsorption and desorption

In this part of the work, the desorption term of Eqs. 5 and 6 are considered, with the stoichiometric coefficients equal to the unity (α, β and $\gamma=1$) Taking into account these considerations Eqs. 9 and 10 are transformed into

$$\frac{dC_A}{dt} = c_1.C_{A0} - c_1.C_A - k_1.C_A.(q_m - q_A) + k_2.q_A \qquad (15)$$

$$\frac{dq_A}{dt} = k_1.C_A.(q_m - q_A) - k_2.q_A \tag{16}$$

The simulations from Eqs. 15 and 16 provided results with behavior equivalent to those obtained by the previous condition without the desorption term.

The Fig. 9 shows the simulation results of the adsorbed phase (q_A) varying the kinetic constant of desorption (k_2). From these results it can be observed that the higher the kinetic constant of desorption the lower the real capacity of adsorption as the final amount of solute adsorbed decreases. This information shows that although the adsorption can reach a maximum capacity (q_m), the real amount adsorbed will be determined by some parameters like the kinetic constant of desorption (k_2).
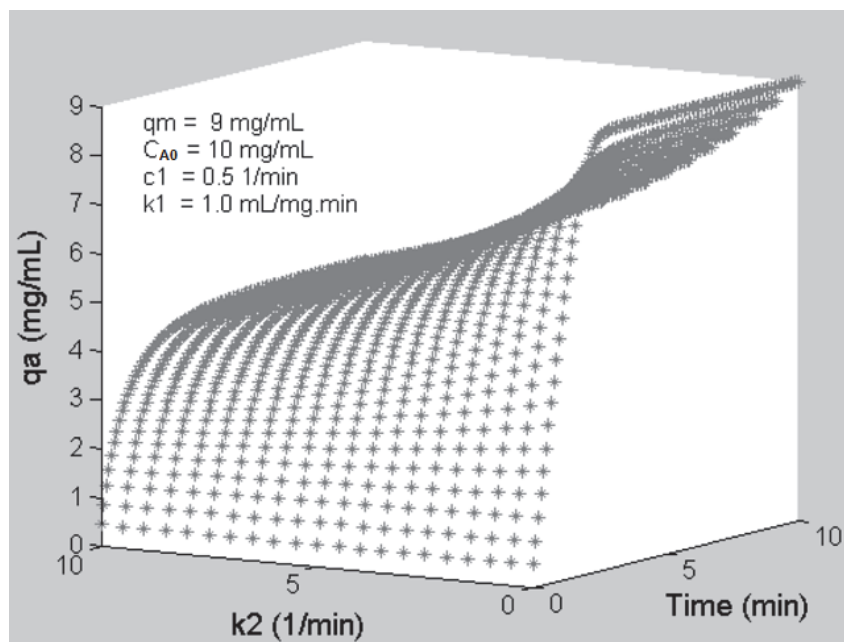

Fig. 9. Effect of the desorption parameter (k_2) over the amount of solute adsorbed (q_A)

Calculations using different adsorption and desorption orders were also performed, showing a great influence of these parameters on the dynamic answer of the chromatographic system. It is important to notice that higher values of the order of desorption ($\gamma > 1$) significantly decreases the final amount of solute adsorbed with the increase in the kinetic constant of desorption (k_2).

2.2.4 Protein chromatography by steps of adsorption and desorption

Simulations results obtained for a continuous feed for a time period into the protein chromatography are shown in this part of the work. It is considered a flow of solute with a specific concentration being introduced into the column over an initial period of time. Figure 10 presents a typical result obtained with Eqs. 15 and 16, which correspond to a system with a rate of solute adsorption and desorption, for a feed over a time period of 10 min. After the time of feed (10 min), the initial concentration of solute was considered null ($C_{A0}=0$), which led the system to decrease exponentially the solute concentration of the liquid phase inside the column. Note that the concentration of solute adsorbed starts to

decrease after this point, although the kinetic constant of adsorption is higher than the kinetic constant of desorption (the same parameters for the adsorption and desorption steps). This is attributed to the solute concentration that becomes low, leading to a decrease in the term of adsorption, which is not compensated by the high kinetic constant of adsorption.
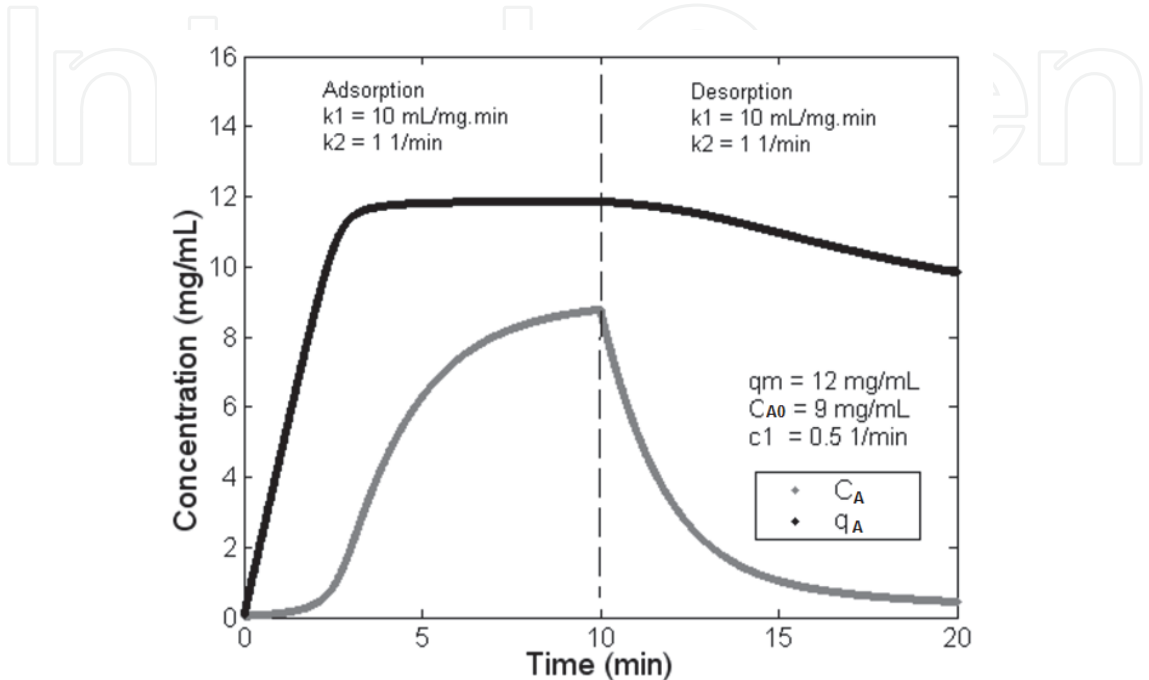

Fig. 10. Influence of feed in the steps of adsorption and desorption

A comparison between the simulation results and the experimental data from a chromatographic procedure of protein separation is presented in Fig. 11. Figures 11a and 11b present the calculations and the experimental data from Silva (2000), respectively.
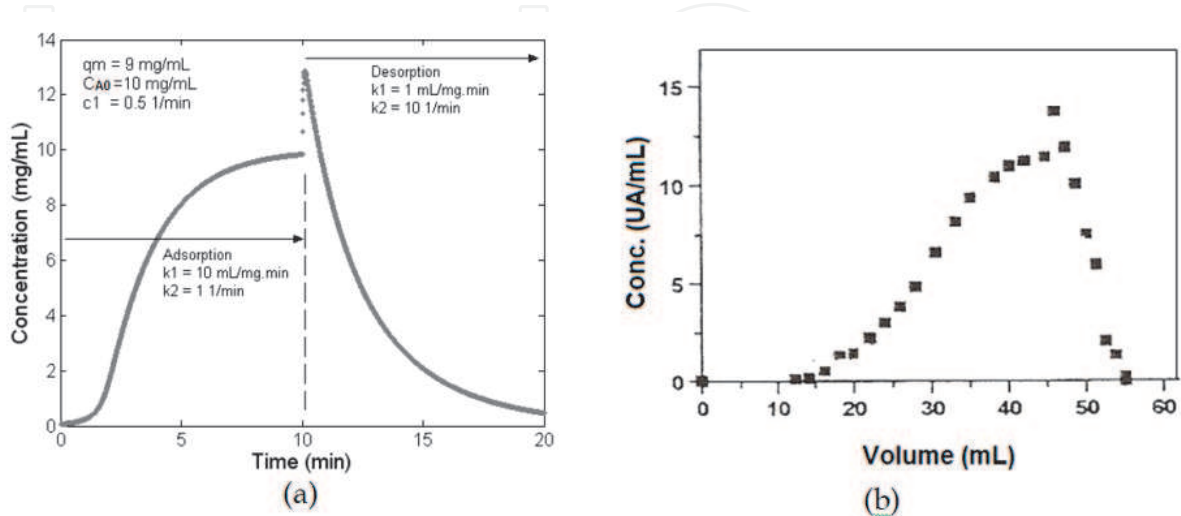

Fig. 11. Adsorption and desorption steps from simulation results (a) and experiments (b)

From the experiments, it can be observed that there is an increase in the solute concentration in the desorption procedure or wash, which corresponds to a volume higher than 45 ml. The wash procedure leads the solute concentration to a value that is higher than the initial concentration (C_{A0}=11.5 UA/mL; UA- enzymatic activity unit). From the simulations (Fig. 11a) it can be seen that an increase in the solute concentration can be reached by the increase in the kinetic parameter of desorption in the step of desorption. This fact is coherent once in the wash procedure the solvent is utilized to promote the desorption of the molecules adsorbed in the solid surface.

3. Irreversible kinetic model with batch adsorption

The agitated batch process of adsorption is an important method used for equilibrium parameters estimation, which are applied in the processes modeling such as chromatography and simulated moving bed (SMB) separation. The hydrodynamic aspects of these processes become the kinetic modeling an interesting tool for the process modeling in obtaining parameters that will be incorporated in the equipment design.

Some contributions in the application of adsorption kinetic models for the liquid phase can be encountered through the following publications: Thomas (1944), Chase (1984), Sarkar and Chattoraj (1993), Hamadi et al. (2001, 2004), Otero et al.(2004), Gulen et al.(2005) and Aroguz (2006). An important contribution comes from the work of Chase (1984), which implemented semi-analytical expressions to model the adsorption phenomenon in agitated tanks and chromatographic columns. He considered the kinetic concepts to model the adsorption process as a reversible system with an overall rate of second-order. In a general point of view, the above publications, with exception of the Chase model (Chase, 1984), use simplified or empiric expressions for the kinetic models. The advantage of utilizing the concepts of kinetic theory to develop new models is that the stoichiometric and order, related to the compounds in the adsorption system considered, can be varied and analyzed independently, leading to a better comprehension of the evolved kinetic phenomenology.

In this work was implemented an irreversible kinetic model of adsorption being it applied in the modeling of salicylic acid adsorption onto different adsorbents as the activated carbon (F400) in three different temperature conditions. The model adjustment through the experimental data is done with the application of an inverse problem approach that minimize the square residues of a cost function.

3.1 Formulation of the adsorption kinetic model

The agitated adsorption techniques to measure adsorption properties are modeled with the following expression for batch processes

$$r_j = \frac{1}{V}\frac{dN_j}{dt} \tag{17}$$

in which r_j, that corresponds to the adsorption rate of component j, is proportional to the variation of the moles number of solute j (N_j) with time. The tank volume (V) is assumed to be constant.

The adsorption stoichiometry considered is represented in Fig. 12. It is related to an irreversible kinetic of adsorption with a kinetic constant k_i. This adsorption mechanism depends both on the solute concentration (liquid phase) and the active surface concentration on the solid phase (site concentration on solid phase).
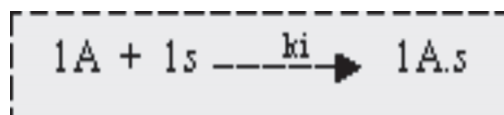
Fig. 12. Representation of the adsorption mechanism assumed.

The adsorption mechanism of Fig. 12 considers the adsorption of 1 (one) mol of solute A on 1 (one) mol of active site (s). The kinetic modeling, in terms of consumption rate of solute j (r_j), is written in the following form.

$$(-r_j) = k_i C_j{}^n . C_s{}^m \qquad (18)$$

where k_i, C_j and C_s represent the kinetic constant, the concentration of solute j in the liquid phase and the concentration of sites of adsorption in the solid phase, respectively. For a first order elementary adsorption, the exponents n and m are equal to 1, which corresponds to an overall rate of second order. The irreversible adsorption is an adequate hypothesis, since in the experimental studies (Pereira, 1999 and Silva, 2000) the desorption procedures are necessary to return the original adsorbent properties, without solute traces. This is done with elution and washing steps.

With the considerations just described, Eq. (18) can be solved analytically through expression (17), applying a balance in the moles number of active sites of adsorption, i.e.

$$C_t = C_s + C_{A.s} \qquad (19)$$

in which C_t corresponds to the maximum concentration of adsorption sites, that is the sum between the concentration of vacant sites (C_S) and occupied sites by solute A (C_{AS}). Another important balance is related to the concentration of solute A. In the balance of solute A, the initial concentration in the solution (C_{A0}) corresponds to the sum of the final solute concentration in the solution (C_A) and the adsorbed solute concentration in the solid phase (C_{AS}), i.e.

$$C_{A0} = C_A + C_{A.s} \qquad (20)$$

The combination of Eqs. (17-20) leads to

$$\int \frac{dC_A}{C_A(a + C_A)} = \int -k_i dt \qquad (21)$$

in which $a = C_t - C_{A0}$. Performing the integrations in Eq. (21) and utilizing the initial and equilibrium conditions lead to the final expressions for the time dependent concentration of solute A (Eq. 22) as a function of C_t, C_{A0} and k_i.

$$\frac{C_A}{a + C_A} = \left(\frac{C_{A0}}{a + C_A} \right) e^{-a.k_i.t} \quad \text{or} \quad C_A = \frac{a.C_{A0}}{(a + C_{A0})e^{-a.k_i.t} - C_{A0}} \qquad (22)$$

Note that the implemented IKM2 (irreversible kinetic model of second order) expression comes from the balance of moles following the moles relation shown in Fig. 12, which can be calculated independently of the volume of each phase. The parameter a in the IKM2 (Eq. 22)

can be replaced by the term $-C_{eq}$ (equilibrium concentration of solute A in the liquid phase) becoming the model only dependent on the liquid phase parameters.

The Fig. 13 presents the correlation results between the IKM2 model and the experimental data from Otero *et al.* (2004). As can be observed from the Fig. 13 the IKM2 model showed high fit correlating the experimental points over all temperature conditions.

The IKM2 model was highly satisfactory correlating the experimental data both at the initial period of time and at long times. It provided better correlation results, according to best fits, than those obtained by Otero *et al.*, 2004, which applied a linear driving force (LDF) model for the adsorption kinetic.

An interesting characteristic of the implemented model (IKM2) is the very small computational effort in obtaining the simulation results. It is related to the analytical form of the mathematical expression (Eq. 22). Besides the good agreement with the real experimental data, the kinetic model described (IKM2) requires only two parameters (C_{A0} and C_t or C_{eq}) to obtain the rate kinetic constant (k_i).
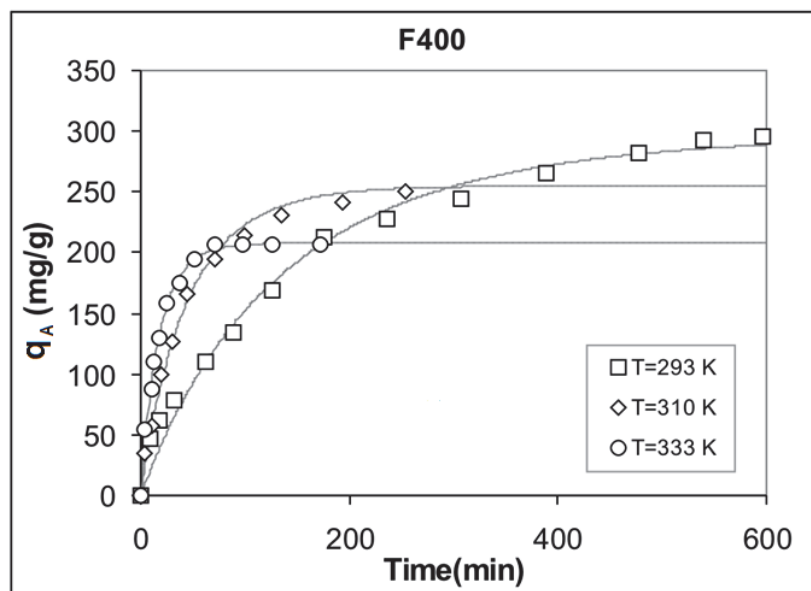

Fig. 13. IKM2 fit with experimental adsorption data of salicylic acid on F400 adsorbent.

4. Acknowledgment

5. Conclusions

The kinetic mechanisms presented showed potential in the representation of different adsorption systems involved with mass transfer in the chromatographic separation processes.

The modeling of the chromatographic column by the mass balance models of perfect mixture with the concepts of heterogeneous adsorption mechanisms showed to represent the behavior of the chromatographic processes of adsorption. The simulation results

showed that either the maximum capacity of the adsorbent and the kinetic constant of adsorption and desorption influenced significantly the dynamic behavior of the system. The stoichiometric parameters, related to the order of adsorption and desorption, showed to be also very important for the dynamic of the separation process, being a crucial tool for the comprehension about the dominant mechanism of adsorption. The stoichiometric parameters showed to influence the equilibrium amount of solute adsorbed. This fact was also observed for the reversible mechanism, in which the higher the kinetic constant of desorption the lower the final amount of solute adsorbed. The closer behavior to the chromatographic answer was obtained by the models with higher orders related to the adsorption term. This observation direct to mechanisms of adsorption that the number of sites necessary to promote the solute adsorption is great, which indicate that more than one site participate in the adsorption process.

The analytical kinetic model of adsorption implemented (IKM2) has proved to be satisfactory due to a number of aspects. Firstly, it provided better agreements with experimental data when compared to other kinetic models, such as the kinetic model of linear driving force (Otero *et al.*, 2004). Other relevant aspects are related to the necessity of a small number of parameters in the model and the straightforward procedure obtaining the solution. The consideration of an acceptable error domain for the equilibrium concentration (C_{eq}) provided good results by reductions in the residues cost function, which led to a better experimental correlation with an increase in the accuracy of the parameters estimated.

6. Nomenclature

k_1 Kinetic constant of adsorption
k_2 Kinetic constant of desorption
k_i Irreversible kinetic constant of adsorption
$(-r_A)$ Rate of consumption of molecules A in the liquid phase
(r_{SA}) Rate of adsorption of molecules A in the solid phase
C_A Solute concentration in the liquid phase
C_s Vacant active sites of adsorption in the solid phase
q_A Solute concentration in the solid phase
C_t Maximum concentration of adsorption sites in a kinetic experiment
q_m Absolute maximum concentration from isotherm data
F_j Molar flow of the molecules j
N_j Number of moles of the molecules j
V Volume of the column
Q Volumetric flow
ε Column bed porosity
α, β, γ Stoichiometric coefficients of the adsorption

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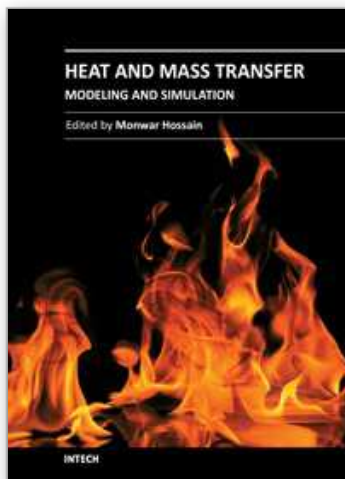
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