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## **Influence of the adsorbent particle size distribution on the adsorption parameters from stirred tank dynamic experiments**

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### **Abstract**

The parameters that affect the separation of n-heptane from a binary mixture conformed of n-heptane and iso-octane, by adsorption in a microporous material called IMP-C12 are presented in this paper. The procedure involves a mass transfer model that considers a mean particle size calculated from the particle diameter distribution. Experimental adsorption curves of n-heptane were determined in a stirred tank by previously probed that iso-octane is not adsorbed by the IMP-C12. The system of nonlinear differential equations was solved by the finite differences method. The model reproduced with good accuracy ( $R=0.99$ ) the experimental adsorption kinetics with a determined mean particle size obtaining a Biot number and an intraparticle diffusivity coefficient. In order to predict the n-heptane adsorption kinetics and validate the model, solute transfer simulations were performed. The results (simulations and experimental kinetics test) were in good agreement provided that the process uses the same particle diameters distribution. The influence of the mean particle size in the adsorption kinetics was studied considering different particle diameters distribution. The results showed that particle size is essential to predict with good accuracy the adsorption curves, therefore it is extremely important to have a homogeneous (size and shape) particle distribution to determine adsorption kinetics.

Keywords: Modelling; mass transfer; adsorption kinetics; particle size distribution

### **1. Introduction**

Today, adsorption process plays a key role in modern industries especially in the field of environmental protection engineering, and is applied widely in chemical, biochemical and agro-alimentary industries (Hui et al., 2003, Montesinos et al., 2001, Viard, 1991). In order to predict or evaluate the performance of an industrial separation procedure involving

adsorption, the mathematical description of the dynamic process is required. The packed column with porous particles as adsorbent is a conventional operation in the industries for mixture separation. Normally, in the common operation, for modeling adsorption kinetics it is necessary to know the model parameters (i.e. adsorption equilibrium parameters and effective intraparticle diffusivity). Experimental data from tank systems are used to obtain equilibrium parameters and transport parameters for adsorbents. Although, while performing batch adsorption experiments, the estimation of the intraparticle diffusivity becomes more difficult when the stirring speed is slow, in which the liquid-solid interface mass transfer resistance is not negligible.

In the other hand, the separation of linear and branched alkanes present in hydrocarbons mixtures is a challenge for the petroleum industry. However, the microporous materials have attracted the attention in the field of environmental protection engineering (Do and Do 2002, Chuang et al. 2003), as a valuable adsorbent medium for removing numerous unnecessary substances from the gas-liquid phase. Consequently, the microporous materials may be used in the separation of hydrocarbons mixtures.

Mathematical modeling of adsorption kinetics has been reported by a number of researchers who consider the phenomenon as a diffusive transport from liquid/gas phase to solid phase into adsorbent particle volume (Qinglin et al., 2003, Li et al., 2003, Kaczmarski and Bellot, 2003, Alpay et al., 2003, Hui et al., 2003, Lee et al., 2003, Yang et al., 2003, Marroquin et al., 2002, Montesinos et al., 2001, Reid and Thomas, 2001). This phenomenon has been modeled with different levels of complexity considering two different ways for solving the nonlinear equation system: analytical and numerical solution. Usually adsorption model in the batch system considers two coupled simultaneous nonlinear differential equations, one for the liquid phase and another for the solid phase. Normally most systems under investigation behave as complex phenomena, where the effect of nonlinearity of the equilibrium isotherm is represented by assuming that the effective diffusivity coefficient depends on the concentration. The only way to solve such models is by numerical methods as finite differences or finite elements (Alpay et al., 2003, Kaczmarski and Bellot, 2003, Lee et al., 2003, Yang et al., 2003, Montesinos et al., 2001). These models are of great importance in the scientific study of adsorption kinetics mainly to determine non-easy-measured parameters. However, the nonlinear equations system can be simplified and solved analytically and therefore, the most common assumptions are the following: the equilibrium isotherm is linear, there is no particle volume change, there is no suspension volume variation in the batch system, and the effective intraparticle diffusivity is considered as independent of the solute concentration. Marroquin et al., (2002) reported an analytical solution of the equations that govern the reactant transport in a well stirred tank that contains particles where diffusion and first-order reaction occur. A Laplace transform method was used to solve the reactant transport equations in the fluid and particle. They concluded that these equations can be used to determine the effect of mass transfer resistances on transient experiments and to obtain a mapping of situations when these kinds of effects are important.

Recently, Kaczmarski and Bellot (2003) have evaluated the effect of particle size distribution and the variation of particle porosity on the mass transfer kinetics. The authors concluded that the error in the prediction of uptake curves decreases when the particle diameters distribution (obtained approximated by mean particle diameters) is reduced. However, a detailed analysis is necessary to indicate precisely the acceptable intervals of the particle size distribution.

The objective of the present work was to evaluate the importance of the particles size distribution on the adsorption parameters (equilibrium parameters and effective intraparticle

diffusivity) of n-heptane from binary mixtures (n-heptane/isooctane) into IMP-C12 in a stirred tank. Additionally, an analysis was made to test the efficiency of the mathematic model to predict the adsorption process in a batch system. The validation of the model was made with experimental data obtained by the stirred tank.

## 2. Materials and methods

### Theoretical part

In Fig. 1 the system is shown. For the molecules it is assumed that the suspension is well mixed. The porous particles of different size are considered spherical and suspended in the fluid; therefore, only radial transport takes place through the porous particles. We assumed that the transport and adsorption in all different size particles is represented by the mean diameter (see Eq. 13).

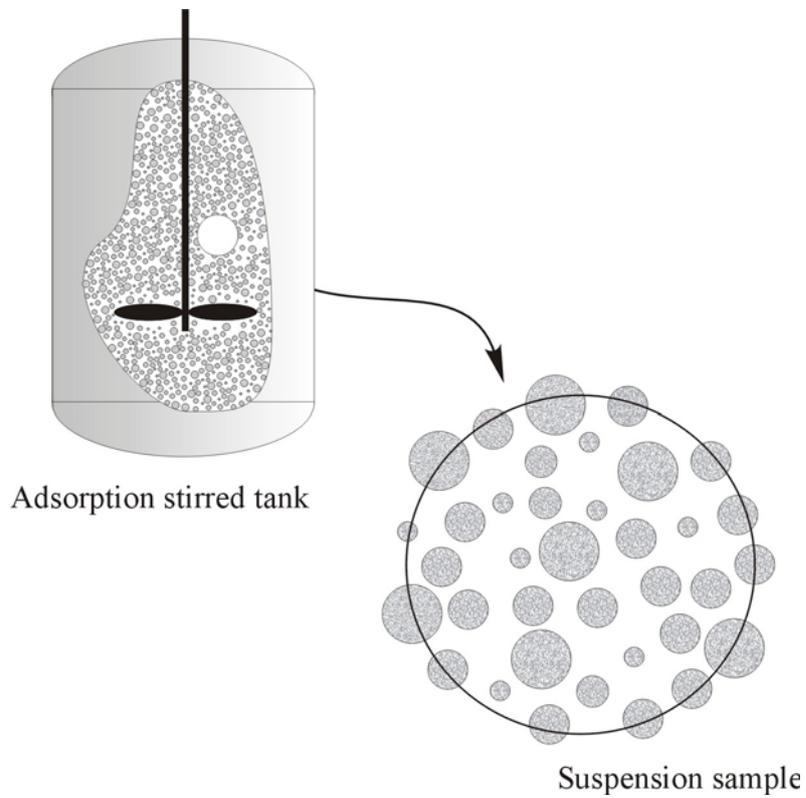


Figure 1. Experimental stirred tank and fluid sample with porous suspended particles.

According to Li, et al., (2003), Qinglin, et al., (2003), Marroquin, et al., (2002), Do, (1998), Viard, (1991), and Ruthven, (1984) the mass transport equations that govern the adsorption kinetics in a well mixed batch system that contains spherical porous particles where the interparticle diffusion is considered, the solute concentration variation in the adsorbent porous particle is described by the following equation:

$$\varepsilon_{\gamma} \frac{\partial C_{\gamma}}{\partial t} + (1 - \varepsilon_{\gamma}) \frac{\partial C_{\kappa}}{\partial t} = \varepsilon_{\gamma} \frac{1}{r^2} \frac{\partial}{\partial r} \left( D_{\gamma} r^2 \frac{\partial C_{\gamma}}{\partial r} \right) \quad 0 \leq r \leq r_p \quad (1)$$

and to describe the solute concentration change in the bulk fluid when there is change of volume:

$$\varepsilon_{\beta} \frac{dC_{\beta}}{dt} + C_{\beta} \frac{d\varepsilon_{\beta}}{dt} = \frac{A_{fp}}{V} k_f \left( C_{\beta} \Big|_{r=r_p} - C_{\beta} \right) \quad (2)$$

In Eq. (1),  $\varepsilon_{\gamma}$  is the particle void fraction,  $C_{\gamma}$  and  $C_{\kappa}$  are the solute volume average concentrations in the fluid and adsorbent in the porous particles respectively,  $D_{\gamma}$  represents the intra-particle effective diffusivity and  $r$  is the radial coordinated spherical in the particles.

In Eq. (2),  $\varepsilon_{\beta}$  is the fluid volume fraction of the suspension,  $C_{\beta}$  represent the solute concentration in the well mixed fluid,  $A_{fp}$  is the particle-fluid interfacial area,  $V$  represent the volume occupied by the suspension,  $k_f$  is the film mass transfer coefficient of the fluid around the particle and  $r_p$  is the particle radius.

In terms of the adsorption capacity, the equilibrium relationship between fluid phase and adsorbent or adsorbed phase concentrations may well be represent by linear isotherms (Viard, V., 1991, Ruthven, D. M., 1994), nonlinear isotherms (Li et al., 2003, Yang et al., 2003, Kaczmariski and Bellot, 2003) or irreversible isotherms (Montesinos R. M., 2001). The experimental equilibrium data represented by nonlinear expression complicates the mathematical representation of the separation process since the particle diffusivity is dependent of the intra-particle concentration. However, sometimes in the nonlinear phenomenon a linear isotherm equation can be assumed in the model in order to predict the adsorption kinetics giving acceptable predictions (Viard, V., 1991). Therefore to simplify the solution of the complex equations, the micro-pore diffusivity has been assumed as independent of the intraparticle concentration, which is generally a good approximation (Ruthven 1984, Viard 1991). The Eq. (1) can be re-written as (Ruthvem 1984):

$$\frac{\partial C_{\gamma}}{\partial t} = \frac{\varepsilon_{\gamma} D_{\gamma}}{\varepsilon_{\gamma} + (1 - \varepsilon_{\gamma}) K} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial C_{\gamma}}{\partial r} \right) \quad 0 \leq r \leq r_p \quad (3)$$

where:

$$D_{ay} = \frac{\varepsilon_{\gamma} D_{\gamma}}{\varepsilon_{\gamma} + (1 - \varepsilon_{\gamma}) K} \quad (4)$$

This Eq. 4 is reported as the apparent diffusivity by different authors (Ruthven, D. M., 1984, Viard, V. 1991).

Eqs. (2) and (3) are coupled by the following interfacial boundary conditions:

$$\text{at } r = r_p, \quad -\varepsilon_{\gamma} D_{\gamma} \frac{\partial C_{\gamma}}{\partial r} = k_f \left( C_{\beta} \Big|_{r=r_p} - C_{\beta} \right) \quad (5)$$

$$\text{at } r = r_p, \quad C_{\beta} = C_{\gamma} \quad (6)$$

In Eq. (5),  $C_{\beta} \Big|_{r=r_p}$  is the solute concentration in the fluid at the surface particle. The initial conditions, for equations (2) and (3), are taken to be:

$$\text{for } t = 0, \quad C_{\beta} = C_{\beta 0} \quad \text{and} \quad C_{\gamma} = C_{\gamma 0} \quad \text{for} \quad 0 \leq r \leq r_p \quad (7a-b)$$

Eqs. (2-7) were rewritten in terms of the following dimensionless variables:

$$U_p = \frac{C_{\gamma}}{C_{\gamma 0}}, \quad U_f = \frac{C_{\beta}}{C_{\beta 0}}, \quad \tau = t \frac{D_{ay}}{r_p^2}, \quad \xi = \frac{r}{r_p}, \quad (8a-d)$$

where  $C_{\gamma 0}$  and  $C_{\beta 0}$  represent initial solute concentration for the solid and fluid phase, respectively.

Thus, the corresponding mass balances Eqs. (2-3) are given by:

In the particle

$$\frac{\partial U_p}{\partial \tau} = \frac{1}{\xi^2} \frac{\partial}{\partial \xi} \left( \xi^2 \frac{\partial U_p}{\partial \xi} \right) \quad (9)$$

In the fluid

$$\frac{dU_f}{d\tau} = \frac{r_p^2}{\varepsilon_\beta D_{ay}} \left[ \frac{A_{fp} K_f}{V} (U_p|_{\xi=1} - U_f) - \frac{U_f d\varepsilon_\beta}{dt} \right] \quad (10)$$

Those are subjected to the interfacial boundary condition and initial condition given by

$$\text{at } \xi = 1, \quad -\frac{\partial U_p}{\partial \xi} = B_i (U_p|_{\xi=1} - U_f) \quad (11)$$

$$\text{for } \tau = 0, \quad U_f = U_{f0} \quad \text{and} \quad U_p = U_{p0} \quad \text{for} \quad 0 \leq \xi \leq 1 \quad (12a-b)$$

### **Model solution**

Eqs. (9-12) represent the complete mass transport model for describing the adsorption kinetics in the batch system. This nonlinear equations system of mass transfer was discretized and solved for the well known method of explicit finite differences. This explicit method is very easy to program but fails to give a correct solution when  $\Delta \xi$  is too small. However, in this solution, we have carefully taken in account the particularity of the method. To describe an adsorption process where variations of bed fluid volume caused by the extraction of samples for analysis during the process are presented, the mechanism of numerical solution was preferred.

### **Experimental part**

The IMP-C12 used as adsorbent for this study was produced in IMP (patent in step). This material adsorbent is obtained of a modification from the method described by Dacey and Thomas (1954).

#### **Adsorption kinetics**

The IMP-C12 was previously sieved to obtain a fraction named A, with particle sizes within 106 and 180  $\mu\text{m}$  and a second one named B, with particles smaller than 106  $\mu\text{m}$ . One gram of the IMP-C12 (sample A or B) was placed into a stirred tank microreactor (50 mL volume) and 10 mL of a mixture of n-heptane and isooctane (v/v) were added. The mixture was prepared with 10% (v/v) of n-heptane. Assays were performed at constant temperature (30  $^\circ\text{C}$ ), with mechanical agitation at 300 and 450 rpm. A star-shaped magnetic stir bar (2 cm diameter) was used. Samples were taken at different times from the microreactor with a constant volume (200  $\mu\text{L}$ ) and the liquid was placed into chromatographic vials for GC analysis. The number of samples taken from the microreactor was typically seven for each experiment which means a reduction of 1.4 mL of the n-heptane and iso-octane mixture. Liquid phase aliquots were withdrawn avoiding the removal of adsorbent. This decrease in the volume of the liquid phase involves a variation of the adsorbent volumetric fraction inside the reactor that must be taken into account in the model to predict the adsorption kinetics.

### **Properties estimation**

Porosity (micropore volume,  $\varepsilon_v$ ). The porosity of the IMP-C12 was estimated from a nitrogen gas adsorption quantification using Micromeritics ASAP 2405 equipment (Micromeritics Inc., USA).

Density. The density of IMP-C12 was quantified by using a calibrated volumetric tube where 1 mL of the adsorbent was placed and weighed afterwards. The material was previously sieved to obtain particles with diameters within 106 and 180  $\mu\text{m}$ .

Particle size distribution. It was estimated by laser ray dispersion technique using Horiba LA500 equipment (Horiba, USA).

Adsorption Isotherm. Adsorption of n-heptane for the isotherm was quantified once the thermodynamic equilibrium was reached, typically after 150 minutes. This is when no more changes in n-heptane adsorption were observed as a function of time. These experiments were conducted at constant temperature 30 °C, mechanical agitation at 300 rpm, an adsorbent load of 100 g of material per liter of solution. The adsorption isotherms experimental data are analyzed and fitted to simple mathematic models. The method of optimization used to fit the equilibrium constant is the Nelder-Mead simplex method of the Optimization Toolbox of Matlab (Demuth and Beale, 2000).

### **3. Results and discussion**

A mass transfer model is used to evaluate the importance of the adsorbent particle size distribution on the adsorption parameters. The effective intraparticle diffusivity of n-heptane on IMP-C12 and Biot number were estimated for a stirred microreactor at two different speeds of agitation (300 and 450 rpm). The model considers a mean particle size calculated from the broad diameter size distribution. In addition, a volume variation of the suspension is considered in the mass transfer model due to the extraction of samples for analysis during the process. This model was solved using the well known method of explicit finite differences. However, in order to obtain the solution of the transport model, it was necessary to determine some properties of the adsorbent. These properties are displayed below.

#### **Properties estimated of the adsorbent IMP-C12**

Porosity (micropore volume,  $\varepsilon_v$ ), Values of micropore area (1048.23  $\text{m}^2/\text{g}$ ) and porosity (0.38  $\text{cm}^3/\text{g}$ ) were estimated by the t-plot method reported by Do (1998).

Density, A density of the IMP-C12 of 0.5  $\text{g}/\text{mL}$  was obtained by weighing the samples in a volumetric tube.

Particle size, Figure 2 shows the particle diameters distribution obtained for two samples: Sample A, material with particle diameters of 106-180  $\mu\text{m}$  and Sample B, material with particle diameters smaller than 106  $\mu\text{m}$ . A unimodal distribution was found in each case with a broad distribution due to an inefficient sieving procedure. For the A sample (106-180  $\mu\text{m}$ ), a particle diameter distribution presents a peak at 152.4  $\mu\text{m}$  (18.6%) with 0.2% of particles smaller than 6.2  $\mu\text{m}$  and 7.1 % of particles bigger than 200  $\mu\text{m}$ . For the B sample (<106  $\mu\text{m}$ ), the maxim (19.5%) was found at particle diameter of 67.5  $\mu\text{m}$ . The particle size distribution ranges from 6.7 to 116  $\mu\text{m}$ . Particles smaller than 34.2  $\mu\text{m}$  accounts for the 11.1% of the population. This broad distribution of particle diameter has influenced the adsorption as it depends on the particle surface area and hence on the particle diameter. Therefore to consider

this broad particle size distribution, we assumed that the equation of average diameter reported by Morales et al., (2003) could be used:

$$d_{pm} = \frac{\sum_{i=1}^{i=N_i} X_i d_{pi}^3}{\sum_{i=1}^{i=N_i} X_i d_{pi}^2} \quad (13)$$

where  $X_i$  is the size distribution in particle number and  $d_{pi}$  represent the particle diameter for  $i$ -th particle size.

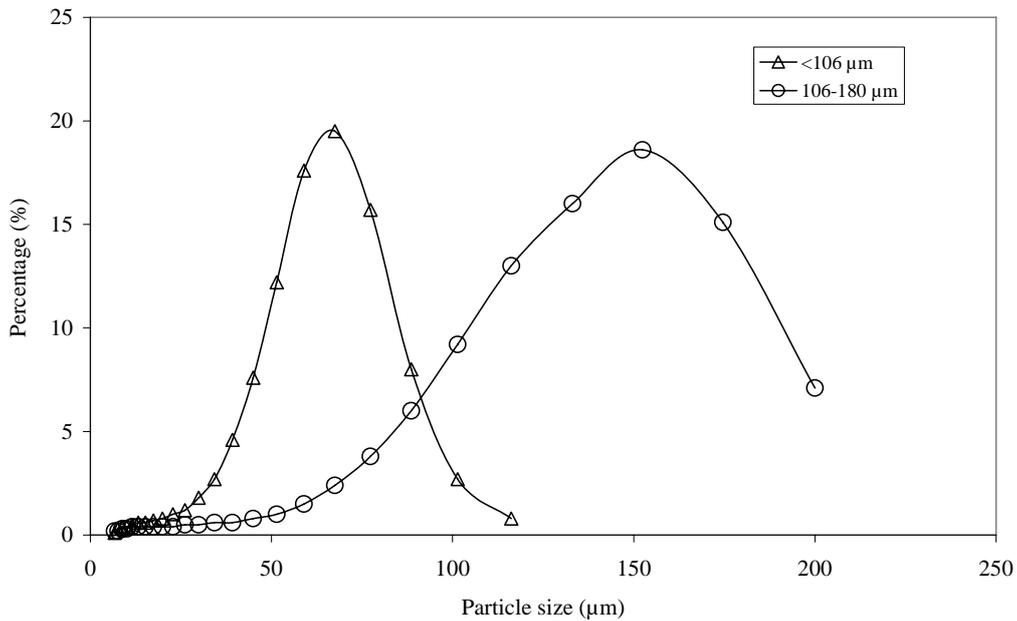


Figure 2. Broad particle diameters distribution (106-180 and <106μm).

Adsorption Equilibrium Isotherm of n-heptane in IMP-C12. This isotherm was quantified after reaching equilibrium (150 min, Figure 3). The experimental data, were analyzed and fitted to linear and Langmuir type-equations. The best fit values of the equilibrium constant were determined by linear regression. For the linear model, the ratio of n-heptane adsorbed by the IMP-C12 and n-heptane concentration in the fluid is 0.6775 ( $R = 0.9803$ ) and for the Langmuir model, the constant is 0.0159 ( $R = 0.9810$ ). The two models show satisfactory results to predict the equilibrium isotherm. However, in order to simplify the solution of the equations, the simple linear model was used.

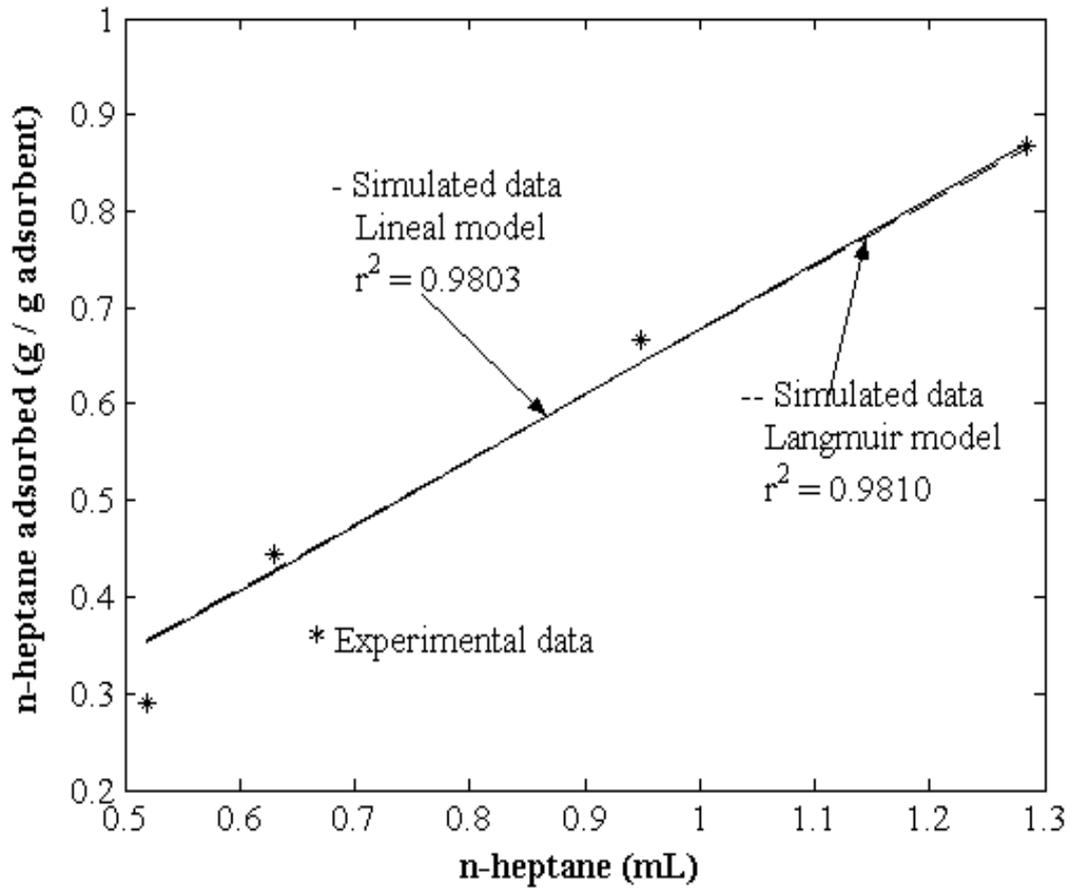


Figure 3. Adsorption isotherm data and models fitting of n-heptane.

The Table 1 summarizes the results obtained and used in the mathematical model to predict the adsorption kinetics for a stirred tank.

TABLE I. Estimated data for the mathematical model of mass transfer.

Parameter	Value
Particle porosity	$\epsilon_{\gamma} = 0.38$
Equilibrium constant	$K = 0.67$
Density of IMP-C12	$\rho = 0.5 \text{ g/ml}$
Mean particle size diameter	152.47 $\mu\text{m}$ to 106-180 $\mu\text{m}$ and 72.06 $\mu\text{m}$ to <106 $\mu\text{m}$

### Prediction adsorption kinetics

For the IMP-C12 adsorption experiments in a stirred tank (Fig. 1) a binary mixture of n-heptane and iso-octane was used. Preliminary experimentation showed that the iso-octane was not adsorbed by the IMP-C12, therefore it was used as a solvent. The nonlinear equations

system (Eqs. 9-12) for the n-heptane mass transfer, includes an equation for the variations of the suspension due to the aliquots required to experimentally determine the adsorption kinetics. Figure 4 shows the volume variation of the suspension versus time. In order to predict the experimental data of the volume variation, we proposed an accuracy exponential type-model ( $r^2 = 0.9891$ ) which contains four fitted parameters. This exponential type-model is presented in Figure 4. The method of optimization used to fit the parameters was the Nelder-Mead simplex method of the Optimization Toolbox of Matlab (Demuth and Beale, 2000). This fit was made for each one of the experiments.

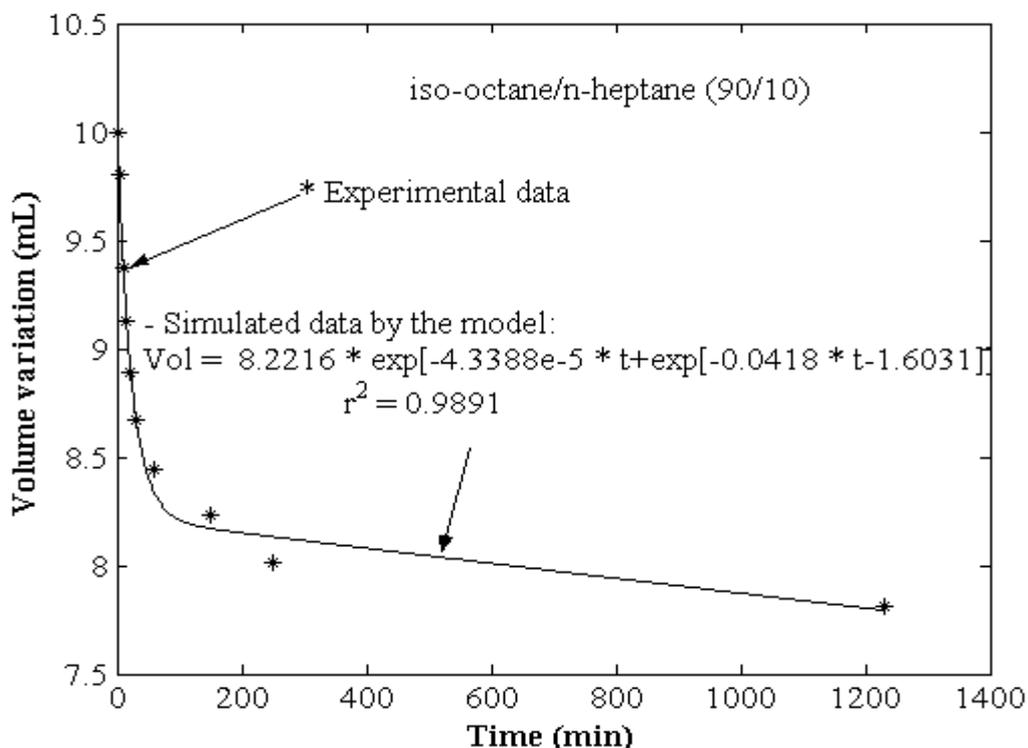


Figure 4. Volume variation against time of the binary mixture (iso-octane/n-heptane, 90/10).

To the A sample, the Figure 5 [A] presents the n-heptane adsorbed values (experimental and simulated) versus time for the binary mixture (iso-octane/n-heptane, 90/10) in IMP-C12 in a stirred tank (450 rpm). Figure 5[A] and [B] show that the prediction of adsorbed n-heptane in the particle is correct ( $r^2 = 0.995$ ), considering an effective intraparticle diffusivity coefficient of  $D_\gamma = 1.76 \times 10^{-9} \text{ cm}^2\text{s}^{-1}$ , with a Biot number of 5.3 and a mean particle size of 152.47  $\mu\text{m}$  calculated from the particle diameters distribution range (106-180  $\mu\text{m}$ ). The effective intraparticle diffusivity coefficient is comparable to the reported by Kaczmariski and Bellot, 2003, and Montesinos et al., 2001. However, it is interesting to mention that if the mean particle diameters is different of 152.47, the parameters calculated (effective intraparticle diffusivity coefficient and Biot number) are also different, therefore this confirms that the parameters obtained are dependent of the mean particle diameters calculated. Figure 5 [C] gives the prediction of n-heptane concentrations in liquid phase from Eq. (2). This result presents an acceptable behavior of n-heptane in the binary solution. It is evident that the concentration of n-heptane in the liquid suspension into the stirred tank diminishes when the n-heptane is adsorbed by the IMP-C12.

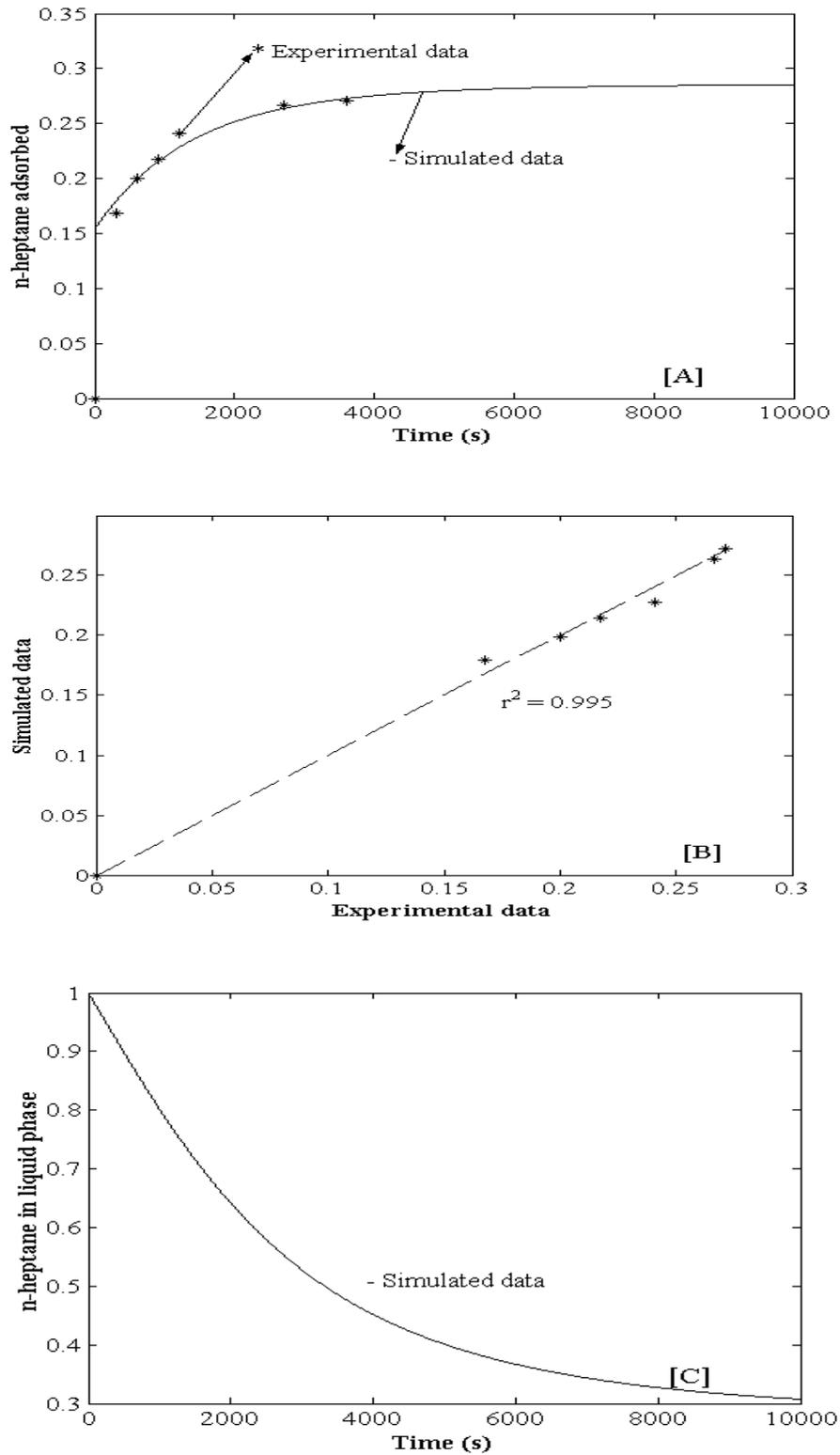


Figure 5. Experimental and simulated curves for the adsorption kinetics of n-heptane in IMP-C12.

### Validation of the proposed model

Figure 6 depicts the ability of the model to predict adsorption kinetics for the A sample. This Fig. 6 presents the simulated adsorption uptake curves and adsorption kinetic experimental data against time at two different stirring velocities (300 and 450 rpm) with the same intraparticle diffusivity coefficient obtained and mean particle diameter calculated from the A sample ( $1.76 \times 10^{-9} \text{ cm}^2\text{s}^{-1}$  and  $152.47 \text{ }\mu\text{m}$ ). A very good agreement between calculated and experimental adsorption curves is observed ( $r^2 = 0.995$  at 450 rpm and  $r^2 = 0.99$  at 300 rpm) with Biot numbers of 5.3 and 4.4 respectively. It is evident that the model was successful in predicting experimental adsorption kinetics because the same broad particle size distribution was used. It is clear that the adsorption curve present a minor adsorption capacity at 300 rpm, compared to the values obtained at 450 rpm, due to the interfacial resistance in the solid-liquid phase. Consequently, It will be very interesting to study the influence of the particle size distribution on the parameters in the adsorption kinetics.

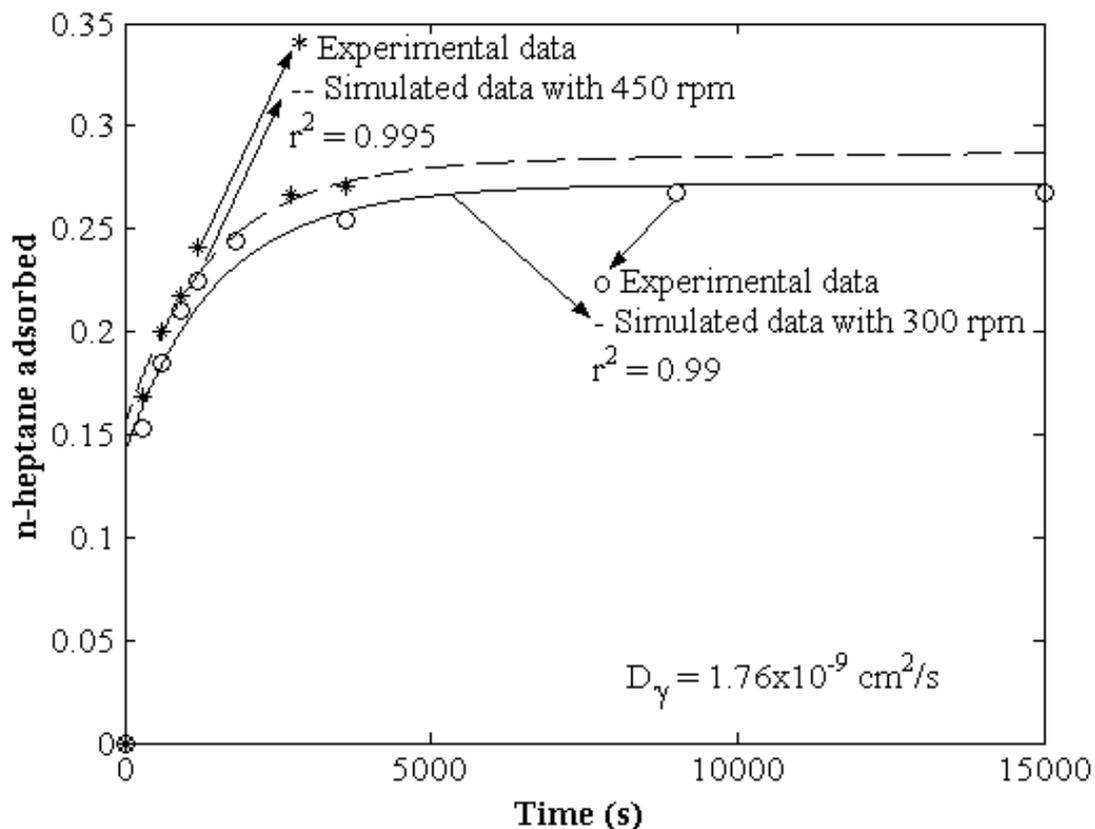


Figure 6. Validation of the proposed model to predict adsorption kinetics of n-heptane in a stirred tank with 300 and 450 rpm.

### Effect of the adsorbent particle size distribution on the development of the adsorption kinetics

In this section, an analysis of the mean particle diameter on the evolution of the adsorption kinetics was made to test the importance of the particle size distribution during the process. The parameters calculated from the A sample are used to predict the adsorption kinetics with different particle size distribution (B sample). The Biot number calculated in the A sample was employed to estimate the Biot number for the B sample in the adsorption kinetics

prediction. Figure 7 present the experimental and simulated data of adsorption curves for the B Sample. In Fig. 7[A], the discontinuous line represents the simulated data obtained by the model considering a mean particle diameter of 72.06  $\mu\text{m}$ , with an estimated Biot number of 2.5 from the two mean particle diameters (152.47 and 72.06  $\mu\text{m}$ ) and the Biot number of 5.3. The discontinuous line does not predict the experimental adsorption curves probably due to the inefficient values calculated: mean particle diameter, effective intraparticle diffusivity coefficient and Biot number obtained; as a result of the broad particle size distribution. In order to confirm the importance of the mean particle diameter in the simulation of the adsorption kinetics, Figure 7 [B] shows simulated data at different mean particle diameters (73, 90, 120 and 150  $\mu\text{m}$ ). This Fig. 7 [B] demonstrates that the mean particle diameter is strongly critical since from 73  $\mu\text{m}$  to 150  $\mu\text{m}$ , the adsorption kinetic changed almost 42 %. A good agreement is observed between the predicted and the experimental adsorption curve ( $R = 0.89$ ) in the B sample with mean particle diameter of 150  $\mu\text{m}$ . It is important to remark that in each adsorption kinetics prediction the Biot number was different because the Biot number is function of the particle size. However, in Figure 7[C], the mean particle diameter is considered constant and only the Biot number is modified (2.5 to 0.4). This Figure 7[C] shows that if the Biot number decreases the adsorption curve also decreases, which is normal since great resistance exist in the interface liquid-solid. Nevertheless, a Biot number of 0.4 does not predict satisfactory the results. Therefore, in order to predict with good accuracy the adsorption kinetics, a mean particle diameter is required in all samples. Consequently, a homogeneous particle size distribution with same diameter is indispensable to obtained the parameters corrects. Finally, the particle size, effective intraparticle diffusivity coefficient and Biot number (when there is small mechanic agitation) are very important parameters in the simulation of adsorption kinetics. The numeric solution of the model shows the importance to predict the adsorption kinetics in a wide range of operations conditions.

#### **4. Conclusions**

This study shows that the particle size distribution is strongly important to predict the adsorption kinetics when the mass transfer type-model is used. Therefore if the particle size diameter is homogeneous and with a same particle size, it is possible to estimate the effective intraparticle diffusivity of the n-heptane into IMP-C12 in batch system and predict with good accuracy the adsorption kinetics. Particle size diameter, intraparticle diffusivity and Biot number (at low stirring rates) are significant factors for the simulation of the adsorption process. Volume variation predictions were well represented by the proposed model.

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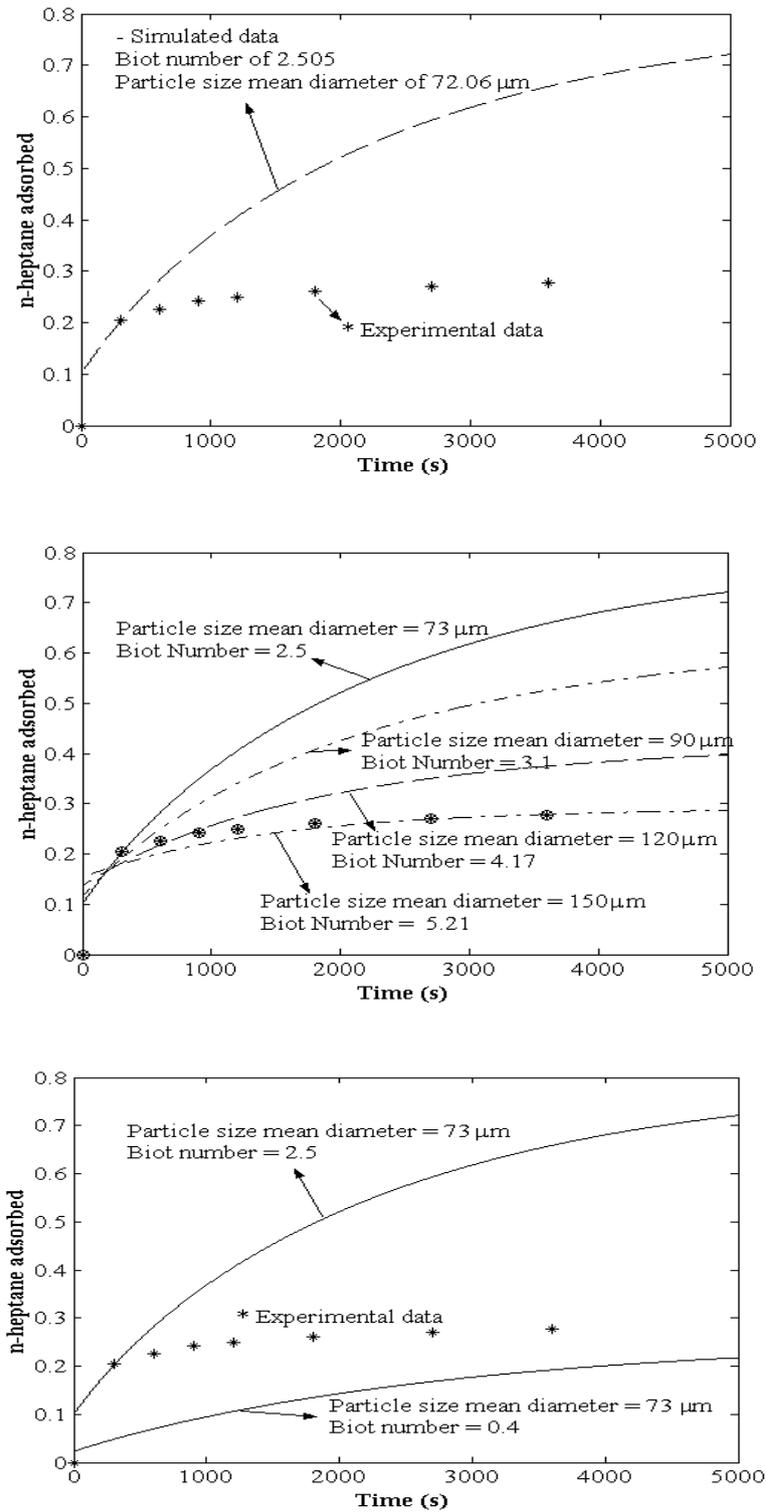


Figure 7. Comparison between experimental and simulated data of n-heptane adsorption kinetics for the B sample (particle diameters distribution  $<106 \mu\text{m}$ ) considering  $D_\gamma = 3.6 \times 10^{-9} \text{ cm}^2 \text{ s}^{-1}$ .

## **Nomenclature**

$A_{fp}$	particle fluid interfacial area, cm <sup>2</sup>
$B_i = \frac{K_f r_p}{D_\gamma}$	Biot number
$C_\gamma, C_\kappa$ and $C_\beta$	solute concentration in the fluid porous particle, in the particle and in the fluid, gcm <sup>-3</sup> respectively
$C_{\gamma 0}$ and $C_{\beta 0}$	initial solute concentration in the fluid of the adsorbent microporous and in the fluid, gcm <sup>-3</sup>
$D_{a\gamma}$	micro-pore particle apparent diffusivity, cm <sup>2</sup> s <sup>-1</sup>
$D_\gamma$	micro-pore particle diffusivity, cm <sup>2</sup> s <sup>-1</sup>
$K$	equilibrium constant
$K_f$	particle liquid film mass transfer coefficient, cms <sup>-1</sup>
$r$	radial distance in the adsorbent particle, cm
$r_p$	particle radius, cm
$U_p$ and $U_f$	solute dimensionless concentration in particle and fluid phase, respectively
$V$	volume occupied by particle and fluid, cm <sup>3</sup>
Greek letters	
$\varepsilon_\gamma$	particle void fraction
$\varepsilon_\beta$	fraction of volume occupied by the fluid
$\tau$	dimensionless time
$\xi$	dimensionless radial position
Subscripts	
f	fluid
p	particle

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