CMNE/CILAMCE 2007
Porto, 13-15 Junho, 2007

MODELING AND SIMULATION OF FIXED-BED AND SIMULATED MOVING BED CHROMATOGRAPHIC PROCESSES USING PDECOL, EPDCOL, BACOL AND BACOLR SOFTWARE PACKAGES

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Key words: Modeling and Simulation, Numerical Methods, Nonlinear Partial Differential Equations, Fixed-bed Chromatography, Simulated Moving Bed.

Summary: *The objective of this work is to compare different software packages for the numerical solution of mathematical models of fixed bed (FB) and simulated moving bed (SMB) chromatography. The FB and SMB models assume axial dispersion flow for the liquid phase; SMB model assumes plug flow for the solid phase, through the equivalence with the true moving bed (TMB) model. Mass transfer is described by the linear driving force (LDF) model. The different software packages (PDECOL, EPDCOL, BACOL and BACOLR) are compared in terms of accuracy of the numerical solutions obtained and CPU times.*

1. INTRODUCTION

The preparative liquid chromatography is an important separation process with a large number of applications, namely in general chemical industrial processes, pharmaceutical drugs and biotechnology. In order to reduce the cost associated with the development of chromatographic processes, modelling and computational simulation have been intensely used. The simulation of fixed-bed and simulated moving bed chromatographic models allows the prediction and optimization of the performance of several separation processes with industrial applications.

The problem of modeling a simulated moving bed (SMB) separation process can be analyzed by two different strategies: one, by simulating the system directly, as a set of fixed-bed chromatographic columns and taking into account its intermittent behavior; other by representing its operation in terms of a true counter current system. The first model represents the real SMB and considers the periodic switch of the injection and collection points. The second is developed by assuming the equivalence with the ideal true moving bed (TMB), where solid and fluid phases flow in opposite directions [1].

The FB and TMB models must be numerically solved, using software packages for nonlinear partial differential equations (PDEs) in one space and one time dimension. The objective of this work is to compare related software packages, such as PDECOL [2], EPDCOL [3], BACOL [4] and BACOLR [5], to solve these kind of separation processes. PDECOL software, still widely used in Chemical Engineering problems, is based on the method of lines (MOL) and uses a finite element collocation procedure for the discretization of the spatial variable. The collocation procedure reduces the PDE system to an initial-value ODE system, which then depends only on the time variable. BACOL is an adaptive method of lines software package, developed for solving one dimensional parabolic partial differential equations. Contrary to PDECOL, BACOL has the ability to change the number of mesh points and thus control the spatial error. In this way, the remeshing strategy of BACOL software allows it to control both the spatial error and the temporal error. Computational results presented by Wang *et al.* [6] indicate that BACOL is reliable and extremely efficient in dealing with problems having solutions with rapid variation. EPDCOL and BACOLR are modifications of PDECOL and BACOL, respectively, developed to improve the performance of the former software packages.

The objective of this work is to evaluate the potentiality of BACOL and BACOLR software packages to simulate FB and SMB chromatographic processes, which are also characterized by moving concentration fronts.

2. MATHEMATICAL MODELS

The mathematical models for the fixed bed (FB) and simulated moving bed (SMB) processes are established with the following assumptions: (i) axial dispersion for the liquid phase; (ii) plug flow for the solid phase in SMB process (TMB equivalence); (iii) the adsorbent particles are considered as homogeneous material and the mass transfer between fluid and solid is described by the linear driving force (LDF) model. Both models can handle with any kind of adsorption equilibrium isotherm.

2.1. FIXED BED MODEL

Mass balances:

$$\frac{\partial C_i}{\partial \theta} = \frac{1}{Pe}\frac{\partial^2 C_i}{\partial x^2} - \frac{\partial C_i}{\partial x} - \frac{1-\varepsilon}{\varepsilon}\alpha(q_i^* - q_i)$$
$$\frac{\partial q_i}{\partial \theta} = \alpha(q_i^* - q_i) \tag{1}$$

Initial and boundary conditions (feed step inlet, breakthrough experiment):

$$\theta = 0, \forall x : C_i = 0, q_i = 0$$
$$x = 0 : C_i - \frac{1}{Pe}\frac{dC_i}{dx}\bigg|_{x=0} = C_{i0} \tag{2}$$
$$x = 1 : \frac{dC_i}{dx}\bigg|_{x=1} = 0$$

where: i is for species (two components, A and B); θ is the dimensionless time variable; x is the dimensionless axial coordinate; C_i is the liquid phase concentration of species i; C_{i0} is the feed concentration of species i (known); q_i is the average adsorbed phase concentration of species i; q_i^* is the adsorbed phase concentration in equilibrium with C_i; ε is the bed porosity; Pe is the Peclet number; α is the number of mass transfer units.

2.2. SIMULATED MOVING BED MODEL (THROUGH THE EQUIVALENCE WITH TRUE MOVING BED)

The model used for the SMB process is based on the analogy with the TMB process, which considers the real movement of the solid phase in the opposite direction to the liquid phase.

Mass balances:

$$\frac{\partial C_{ij}}{\partial \theta} = \gamma_i\left\{\frac{1}{Pe}\frac{\partial^2 C_{ij}}{\partial x^2} - \frac{\partial C_{ij}}{\partial x}\right\} - \frac{(1-\varepsilon)}{\varepsilon}\alpha_j(q_{ij}^* - q_{ij})$$
$$\frac{\partial q_{ij}}{\partial \theta} = \frac{\partial q_{ij}}{\partial x} + \alpha_j(q_{ij}^* - q_{ij}) \tag{3}$$

Initial and boundary conditions:

$$\theta = 0, \forall x : C_{ij} = 0, q_{ij} = 0$$
$$x = 0 : C_{ij} - \frac{1}{Pe}\frac{dC_{ij}}{dx}\bigg|_{x=0} = C_{ij0} \quad ; \quad \frac{dq_{ij}}{dx}\bigg|_{x=0} = 0 \tag{4}$$
$$x = 1 : \frac{dC_{ij}}{dx}\bigg|_{x=1} = 0$$

where: j is for section (four SMB/TMB sections: I, II, III, IV); C_{ij} is the liquid phase concentration of species i in section j; q_{ij} is the average adsorbed phase concentration of species i in section j; q_{ij}^* is the adsorbed phase concentration in equilibrium with C_{ij}; α_j is the number of mass transfer units in section j; γ_j is the ratio between fluid and solid velocities in section j of the TMB system; C_{ij0} is the inlet concentration of species i in section j and takes into account the inlet and outlet lines of the TMB system. For more detailed information about the Simulated Moving Bed principles and SMB and TMB models, see Pais *et al.* [1].

3. NUMERICAL ASPECTS

The FB and TMB models, defined by a set of partial differential equations, were numerically solved by using four different software packages (PDECOL, EPDECOL, BACOL and BACOLR). For the FB model, there are four PDEs: for each component there is a PDE resulting from the mass balance in a volume element of the bed, and other resulting from mass balance in the particle. For the same reasons, the SMB (or TMB) model has four PDEs in each section. Since the SMB (or TMB) is composed by four sections, and considering a binary separation, the SMB (or TMB) model is defined by a set of 16 PDEs. All of the used software packages employ collocation in finite elements for spatial discretization. However, BACOL and BACOLR have the capacity to change the number and the location of the mesh points. This can bring great advantages when faced with problems having solutions with rapid variation.

3.1. PDECOL

PDECOL is a software package developed for solving systems of nonlinear partial differential equations (PDEs) in one space and one time dimension. The solution of the PDEs system is based on the method of lines (MOL) approach and uses a finite element collocation process for the spatial discretization. After spatial discretization, the original PDE system becomes an ODE system which is only time dependent. The time integration is then accomplished by using the ODE solver STIFIB, which is a modified version of the GEARIB ODE package developed by Hindmarsh [7].

The user must specify the piecewise polynomial space which is used to compute the approximate solution. This space is specified by defining the polynomial order (KORD = polynomial degree +1), the number intervals (NINT) into which the spatial domain is divided, and the number of continuity conditions (NCC). The dimension of piecewise polynomial space is then NPTS=KORD*NINT-NCC*(NINT-1). At any given time t, each component of the approximate solution is a piecewise polynomial in the user specified space and, hence, can be written in terms of the B-spline basis function as:

$$u_k(t,x) = \sum_{i=1}^{NCPTS} C_{i,k}(t)\Phi_i(x) \qquad k = 1,2,\ldots,NPDE$$

where the $C_{i,k}$ coefficients are unknown and time depend and Φ_i are the known basis functions which only depend on spatial variable. To know the approximate solution is necessary to determine the $C_{i,k}$ coefficients.

3.2. BACOL

BACOL is a software package based on the method of lines (MOL), developed for solving systems of parabolic PDEs in one spatial and one temporal dimension. The BACOL software employs collocation in finite elements with a B-spline base for the spatial discretization, and a modification of the widely used differential algebraic equation (DAE) solver, DASSL [8], for the time integration.

The BACOL package provides both time and spatial error control. At each time step, two approximate solutions are computed; one solution for the piecewise polynomial subspace p, and another for the piecewise polynomial subspace p+1. With these two solutions, a spatial error estimate is obtained. If the spatial error estimated is greater than an error tolerance, BACOL uses an equidistribution principle to redistribute the mesh and change the number of mesh points if necessary.

3.3. BACOLR

As it was said before, BACOL uses the DAE solver DASSL. Because DASSL employs backward differential formulas (BDFs), two problems appear when BACOL software package is used. The first problem is related with the fact that a multi-step method requires the solution approximations from previous time steps, evaluated at the current spatial mesh. The problem arises when BACOL refine and redistribute the spatial mesh. When this happens, BACOL must to compute the solution approximations for the new mesh, at the current time and for several previous time steps. The approximate solution values in previous time steps must be interpolated on the new mesh. This results in an increase of the computational effort. The second problem arises when DASSL is used to solve a DAE system characterized by Jacobian eingenvalues purely imaginary [5].

The solution for these problems is addressed by using implicit Runge-Kutta methods. These are one-step methods and do not need previous time steps solutions. BACOLR was developed from BACOL, through a substantial modification process, which involved replacing DASSL with a significantly modified version of RADAU5 [9].

4. SIMULATION RESULTS

The chromatographic resolution of bi-naphthol enantiomers was used as a case study in both FB and SMB simulations. The adsorption equilibrium isotherms are described by a bi-Langmuir model, through the following equations [1]:

$$q_A^* = \frac{2.69C_A}{1+0.0336C_A+0.0466C_B} + \frac{0.10C_A}{1+C_A+3C_B}$$
$$q_B^* = \frac{3.73C_B}{1+0.0336C_A+0.0466C_B} + \frac{0.30C_B}{1+C_A+3C_B} \qquad (5)$$

For all software packages, it must be set some numerical parameters that influence the software performance and results accuracy. Tables 1 and 2 describe the main numerical parameters that can be manipulated by the user. All software packages used a polynomial degree of 3 (KORD=4 for PDECOL/EPDCOL and KCOL=2 for BACOL/BACOLR).

Contrary to BACOL and BACOLR, PDECOL and EPDCOL do not have the ability to change the number and position of mesh points. For these software packages, the fixed mesh points were distributed along the column or section, preferentially near its boundaries.

NINT	Number of intervals in which spatial domain is divided.
KORD	Polynomials order (KORD = polynomial degree +1)
EPS	Relative error limit

Table 1. PDECOL/EPDECOL numerical parameters.

NINT	Number of intervals in which spatial domain is divided.
KCOL	Number of collocation points to be used in each subinterval (KCOL = polynomial degree -1)
ATOL	Absolute error tolerance

Table 2. BACOL/BACOLR numerical parameters.

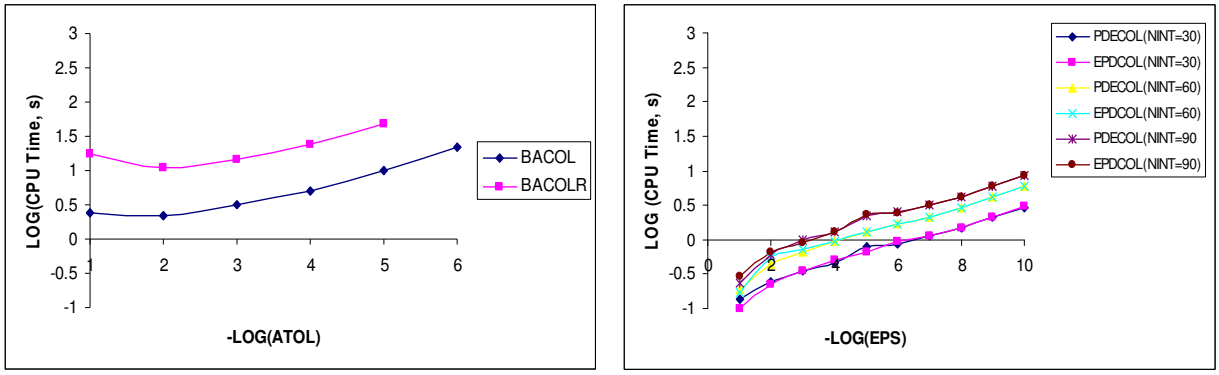
Beyond the numerical parameters, it is also necessary to define the model parameters. An important model parameter is the mass transfer coefficient. In this work, two different values were used: k=0.1 s^{-1} (α=144), which represents significant mass transfer resistances, and k=1 s^{-1} (α=1440), which represents negligible mass transfer resistances.
Numerical simulations were carried out in a Personal Computer AMD Athlon (tm) XP 1600+ 1,40 GHz, 256 kB Cache, 512 MB RAM.

4.1. FIXED-BED PROCESS SIMULATION

The FB performance was simulated for a feed step inlet (breakthrough experiment) using the model equations presented before (Equations (1) and (2)) and the operating conditions and model parameters presented in Table 3. The four software packages were compared in terms of CPU time (Figures 1 and 4) and quality (accuracy) of the numerical solutions obtained for the chromatographic FB response (Figures 2 and 5) and FB internal concentration profiles (Figures 3 and 6). Figures 7 and 8 present the evolution of the number of intervals (NINT) and the position of mesh points for FB simulation, using the BACOL and BACOLR software packages.

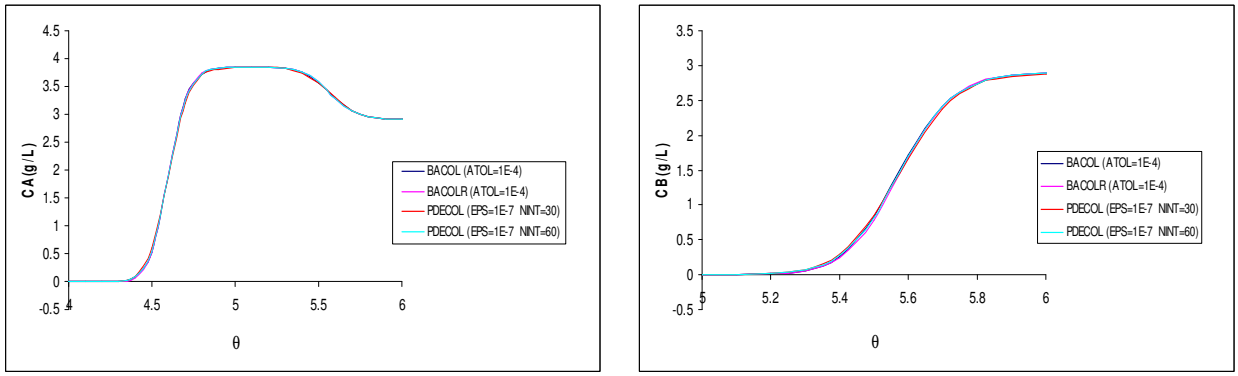
Column:	Model parameters:
Diameter, D_C=2.6 cm	Peclet number, Pe= 8000
Length, L=84 cm	Solid/fluid Volumes, (1-ε)/ ε =1.5
	Number of mass transfer units:
Operating conditions:	Significant mass transfer resistance; α=144 (k=0.1 s^{-1})
Feed concentration = 2.9 g/l each	Negligible mass transfer resistance; α=1440 (k=1 s^{-1})
Holdup time, τ = 1440 s	

Table 3. Operating conditions and model parameters for FB process simulation.



(a) (b)

Figure 1. CPU time as function of: (a) ATOL (for BACOL and BACOLR); (b) EPS (for PDECOL and EPDCOL); FB performance under significant mass transfer resistance (k=0.1 s^{-1}, α=144)



(a) (b)

Figure 2. Chromatographic FB response to a feed step inlet (breakthrough curves) under significant mass transfer resistance (k=0.1 s^{-1}, α=144) for different software packages and numerical parameters.

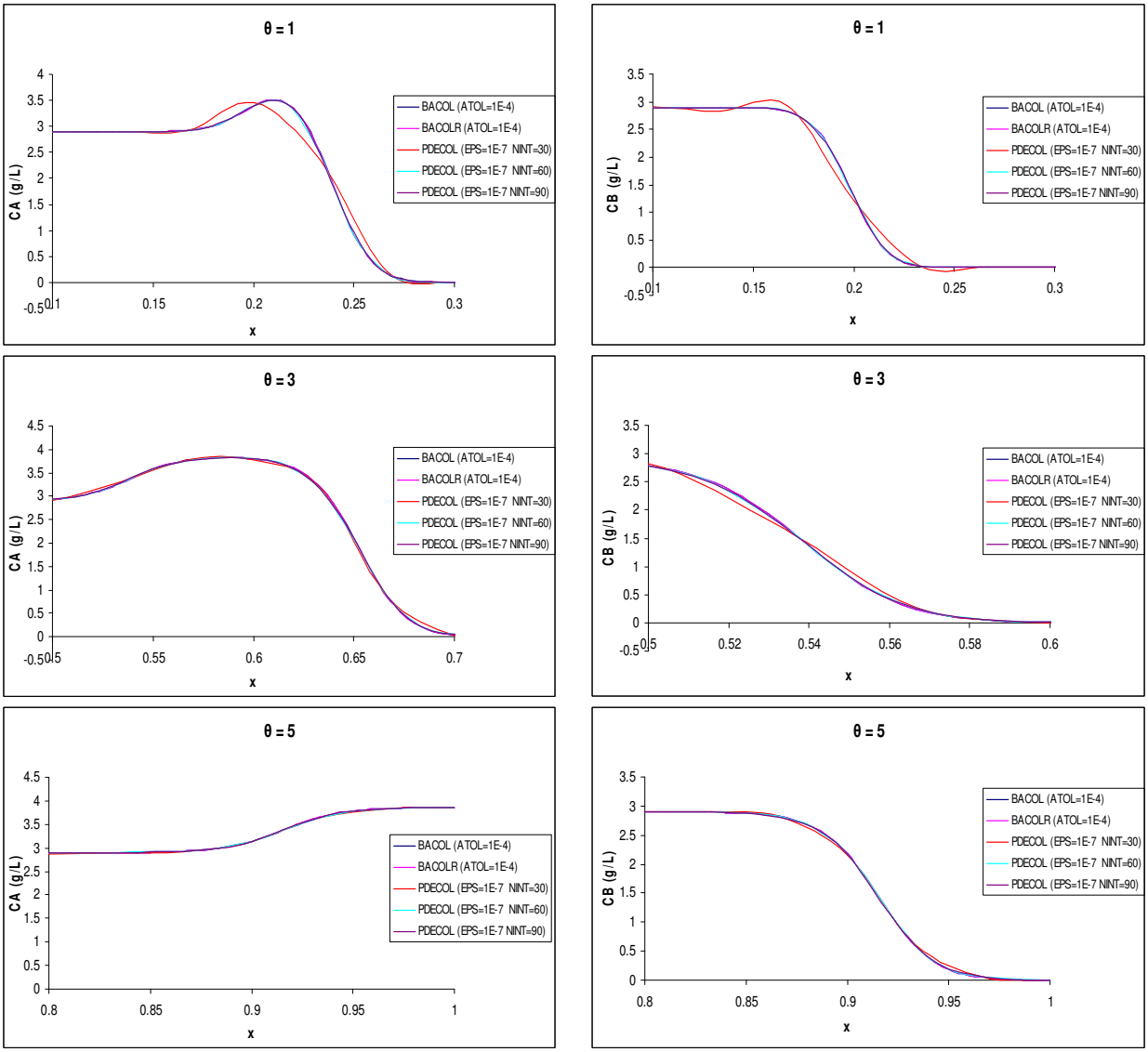
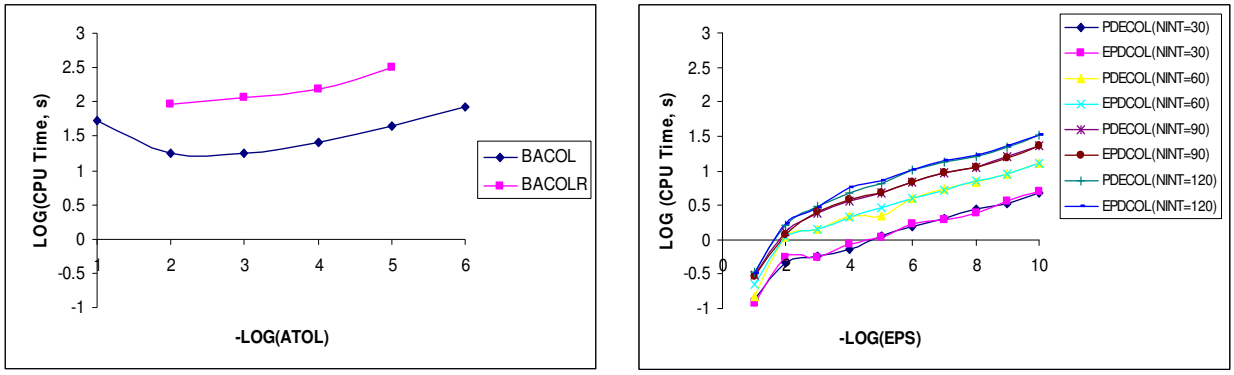


Figure 3. FB internal concentration profiles at different operation times (θ=1, θ=3, and θ=5) under significant mass transfer resistance (k=0.1 s^{-1}, α=144) for different software packages and numerical parameters.



(a) (b)

Figure 4. CPU time as function of: (a) ATOL (for BACOL and BACOLR); (b) EPS (for PDECOL and EPDCOL); FB performance under negligible mass transfer resistance (k=1 s^{-1}, α=1440)

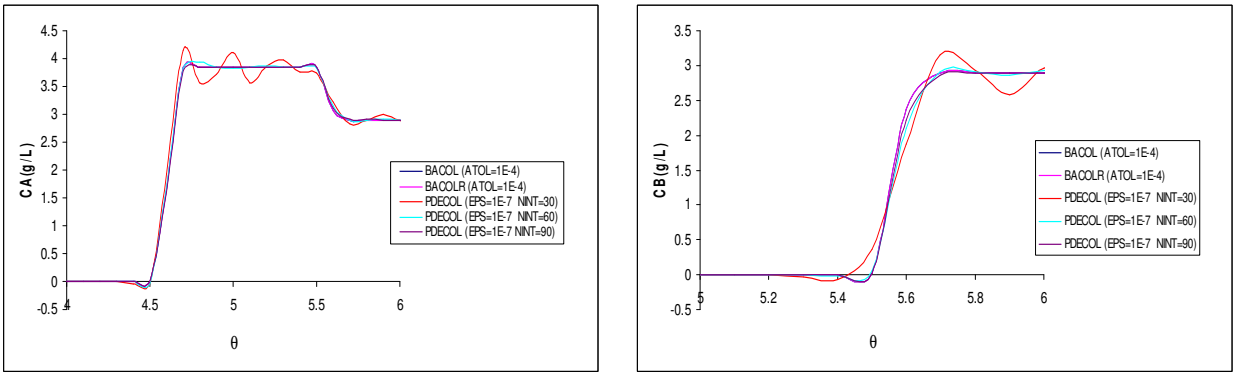


Figure 5. Chromatographic FB response to a feed step inlet (breakthrough curves) under negligible mass transfer resistance (k=1 s^{-1}, α=1440) for different software packages and numerical parameters.

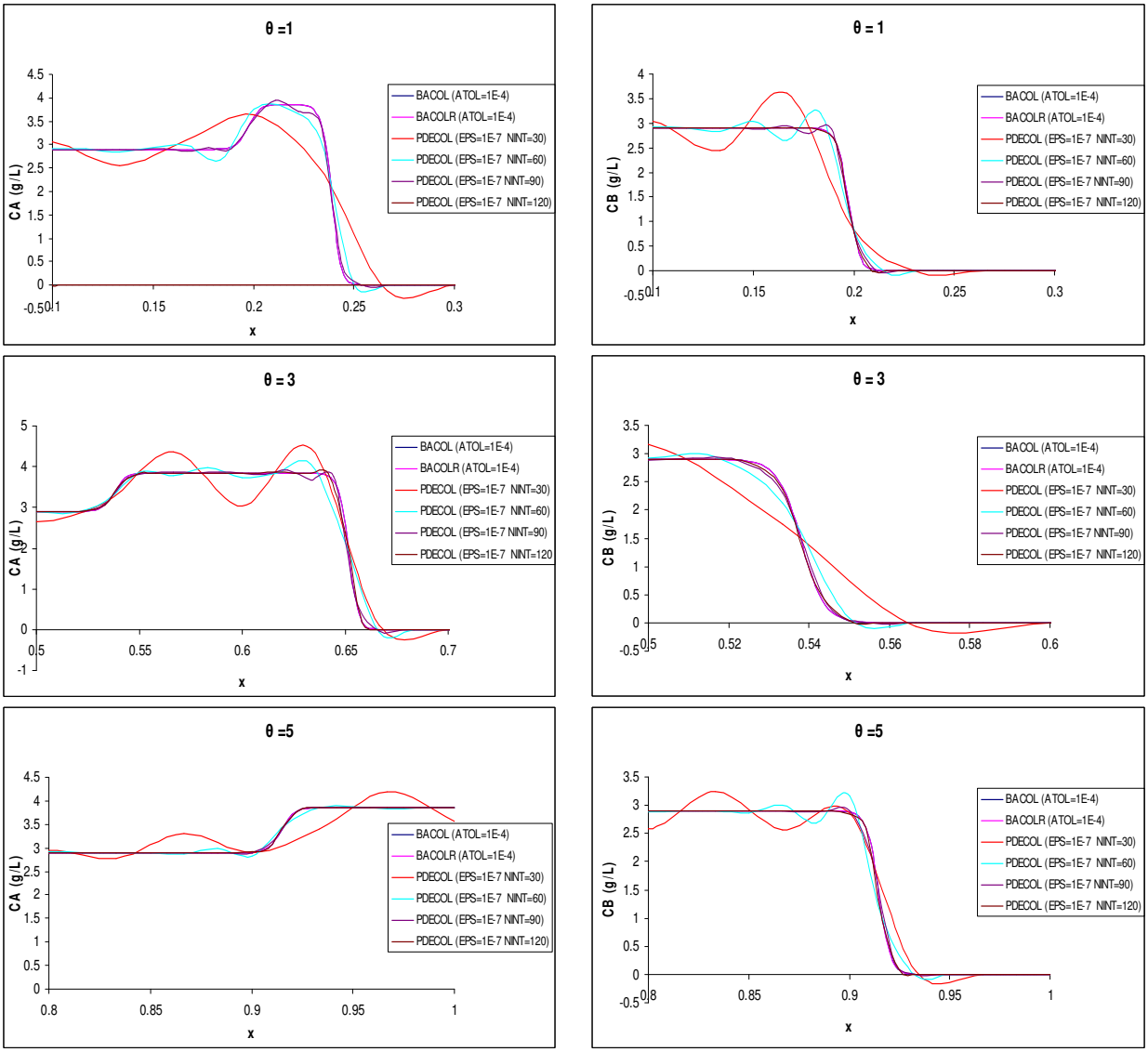
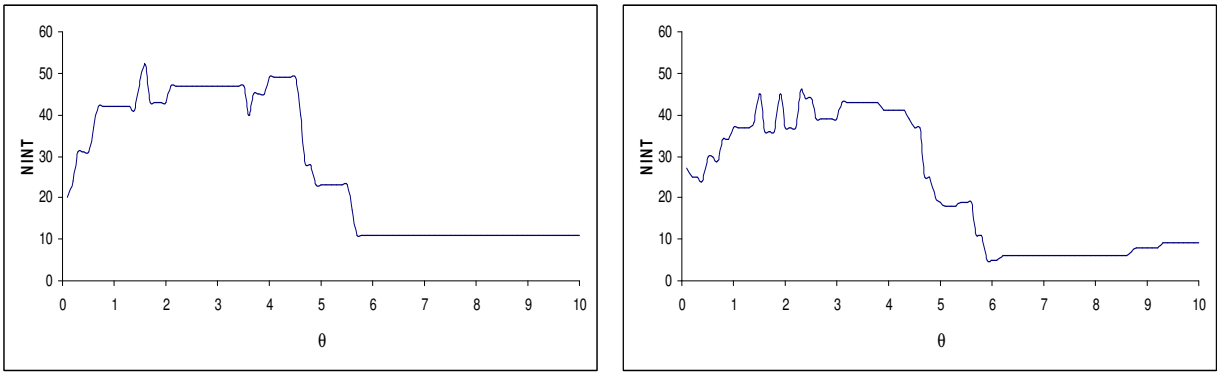
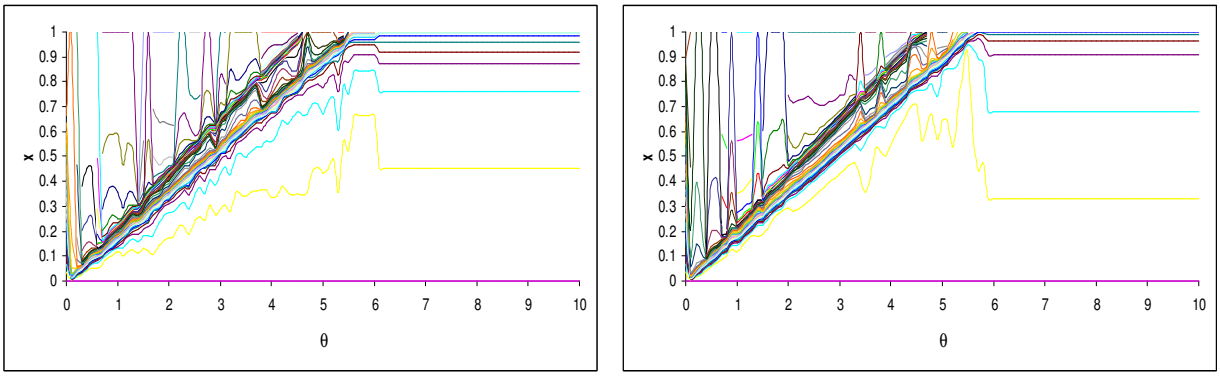


Figure 6. FB internal concentration profiles at different operation times (θ=1, θ=3, and θ=5) under negligible mass transfer resistance (k=1 s^{-1}, α=1440) for different software packages and numerical parameters.



(a) (b)

Figure 7. Evolution of the number of intervals (NINT) during the FB simulation, under negligible mass transfer resistance (k=1 s^{-1}, α=1440): (a) BACOL (ATOL=1E-4); (b) BACOLR (ATOL=1E-4).



(a) (b)

Figure 8. Evolution of the position of mesh points during the FB simulation, under negligible mass transfer resistance (k=1 s^{-1}, α=1440): (a) BACOL (ATOL=1E-4); (b) BACOLR (ATOL=1E-4).

From Figures 1 to 8, it can be concluded that:

(a) The decrease of mass transfer resistances (increase of k and α) demands for more accurate numerical parameters (higher number of intervals and lower ATOL/EPS values) and higher CPU times, since the resulting concentration moving fronts are sharper;

(b) For FB simulations, PDECOL and EPDCOL present similar CPU times and numerical solutions. BACOLR presents higher CPU times than BACOL, with no increase on the accuracy of the numerical solution;

(c) PDECOL and EPDCOL present, in most situations, lower CPU times than BACOL and BACOLR. However, these last group of software packages present more accurate numerical solutions, particularly under negligible mass transfer resistance (when k and α are higher; that is, sharper concentration moving fronts).

(d) Through the simulation of the FB process, BACOL and BACOLR significantly change the number of intervals (see Figure 7) and the position of mesh points (see Figure 8).

Figure 8 also clearly shows that the position of mesh points follows the concentration moving fronts of the FB process.

4.2. SIMULATED MOVING BED PROCESS SIMULATION (THROUGH THE EQUIVALENCE WITH TRUE MOVING BED)

The simulation of SMB process is carried out by solving an equivalent TMB model. The equivalence between TMB and SMB models can be made by keeping constant the liquid velocity relative to the solid velocity, i.e, the liquid velocity in the TMB is:

$$v_j = v_j^* - u_s \tag{6}$$

where v_j^* and v_j are the interstitial liquid velocities in SMB and TMB, respectively, and u_s is the interstitial solid velocity. Also, the solid velocity in TMB model must be evaluated from the value of switch time interval (t^*) of the SMB model, as:

$$u_s = L_C / t^* \tag{7}$$

where L_C is the length of one SMB column.
Alternatively, the equivalence can be made in terms of flow-rates:

$$Q_j = Q_j^* - \frac{\varepsilon}{1-\varepsilon} Q_S \tag{8}$$

with:

$$Q_S = \frac{(1-\varepsilon)V_C}{t^*} \tag{9}$$

where Q_j^* and Q_j are the volumetric liquid flow-rates in section j of a SMB and TMB, respectively, Q_S is the solid flow-rate in the equivalent TMB model, and V_C is the volume of one SMB column [1].
The TMB process simulations were carried out, from an initial condition where just eluent exists in the whole system ($\theta = 0, \forall x : C_{ij} = 0, q_{ij} = 0$), until steady-state is reached. For the TMB simulation the steady-state is considered to be achieved when:

i. The absolute errors between the average concentrations (evaluated during a full cycle for SMB operation; that is, during a solid space time interval, for the TMB equivalent model) of each component in the extract and raffinate outlet streams for two successive iterations are less than a maximum error defined by the user.
ii. The relative errors between the total amount of each component that enters (in the feed stream) and leaves (in extract and raffinate streams) the system (evaluated during a full cycle for SMB operation; that is, during a solid space time interval, for the TMB equivalent model) are less than a maximum error defined by the user.

In this way, it can be defined two types of errors: one related with the absolute differences of concentrations in the extract and raffinate streams for two successive iterations (Equation

(10); in steady-state, they must be zero); other related with the global mass balances (Equation (11); in steady-state, what enters must be equal to what leaves the system);

$$e_1 = e_X + e_R \tag{10}$$

$$e_2 = e_A + e_B \tag{11}$$

where:

e_X is the absolute error of the average concentration of the two components in the extract for two successive iterations:

$$e_X = \left|\overline{C}^{A}_{X[i]} - \overline{C}^{A}_{X[i-1]}\right| + \left|\overline{C}^{B}_{X[i]} - \overline{C}^{B}_{X[i-1]}\right| \tag{12}$$

e_R is the absolute error of the average concentration of the two components in the raffinate for two successive iterations:

$$e_R = \left|\overline{C}^{A}_{R[i]} - \overline{C}^{A}_{R[i-1]}\right| + \left|\overline{C}^{B}_{R[i]} - \overline{C}^{B}_{R[i-1]}\right| \tag{13}$$

e_A is the relative error between the amount of the less retained component (A) that enters (in the feed stream) and leaves (in extract and raffinate streams) the system:

$$e_A = \frac{\left|Q_F C_F^A - (Q_X \overline{C}_X^A + Q_R \overline{C}_R^A)\right|}{Q_F C_F^A} \tag{14}$$

e_B is the relative error between the amount of the more retained component (B) that enters (in the feed stream) and leaves (in extract and raffinate streams) the system:

$$e_B = \frac{\left|Q_F C_F^B - (Q_X \overline{C}_X^B + Q_R \overline{C}_R^B)\right|}{Q_F C_F^B} \tag{14}$$

where Q_F, Q_X, and Q_R are the flow-rates of feed, extract, and raffinate, respectively. The numerical steady-state can be considered to be achieved when both e_1 and e_2 are less than a maximum error defined by the user, δ (for example, $\delta = 0.001$).

The SMB process was simulated by numerically solving the TMB model equations presented before (Equations (3) and (4)) and the operating conditions and model parameters presented in Tables 4 to 6. Note that, since a SMB or TMB system is composed by four sections, the total length of all columns is 84 cm and the total number of mass transfer units is 144 (for $k=0.1\ s^{-1}$) or 1440 (for $k=1\ s^{-1}$).

The four software packages were compared in terms of errors obtained (Figures 9 and 10), quality (accuracy) of the numerical solutions obtained for TMB internal concentration profiles (Figures 11 and 12) and CPU times (Figure 13). Figures 14 and 15 present the evolution of

the number of intervals (NINT) and the position of mesh points for TMB simulation, using the BACOL and BACOLR software packages.

Column Diameter, D_C=2.6 cm	Model parameters:
Section Length, L_j=21 cm	Peclet number, Pe_j= 2000
Feed concentration = 2.9 g/l each	Solid/fluid Volumes, (1-ε)/ ε =1.5
SMB switch time interval, t^* = 360 s	Number of mass transfer units in each section:
(if one column per section)	Significant mass transfer resistance; α_{ij}=36 (k=0.1 s^{-1})
TMB solid flow-rate, Q_S=11.15 ml/min	Negligible mass transfer resistance; α_{ij}=360 (k=1 s^{-1})
Liquid flow-rates: see Tables 5 and 6	

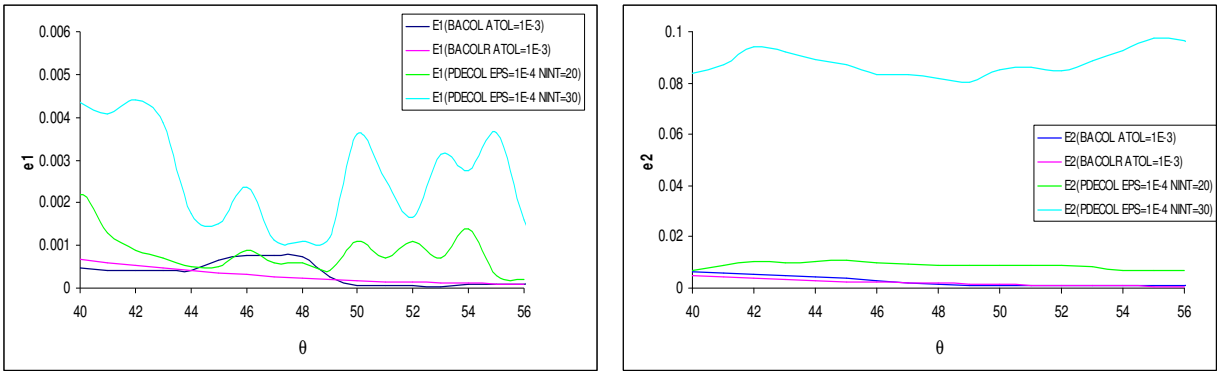
Table 4. Operating conditions and model parameters for TMB process simulation.

Section	SMB		Equivalent TMB	
	Q_j^* (ml/min)	γ_j^*	Q_j (ml/min)	γ_j
I	56.83	7.65	49.40	6.65
II	38.85	5.23	31.42	4.23
III	42.49	5.72	35.06	4.72
IV	35.38	4.76	27.95	3.76

Table 5. Equivalence between TMB and SMB internal flow-rates.

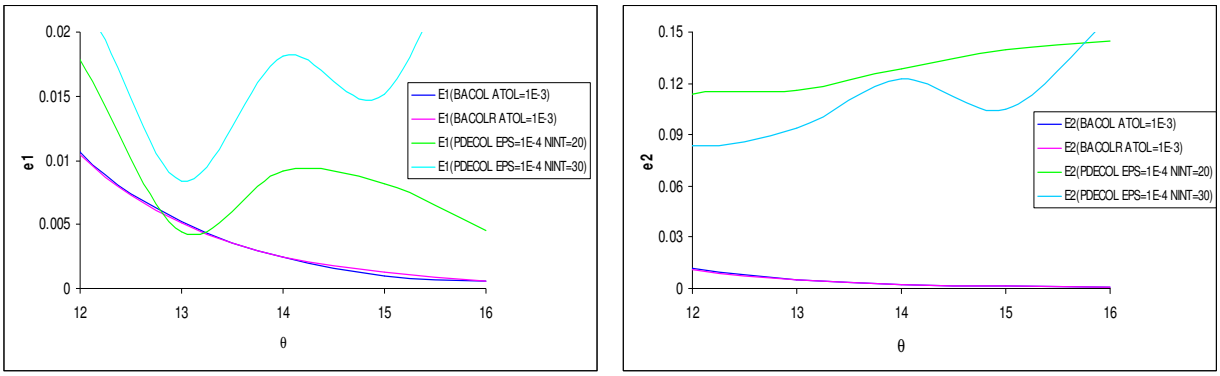
Inlet and outlet line	TMB or SMB inlet/outlet flow-rates (ml/min)
Eluent	$Q_E = Q_I - Q_{IV} = 21.45$
Extract	$Q_X = Q_I - Q_{II} = 17.98$
Feed	$Q_F = Q_{III} - Q_{II} = 3.64$
Raffinate	$Q_R = Q_{III} - Q_{IV} = 7.11$

Table 6. Inlet and outlet flow-rates.



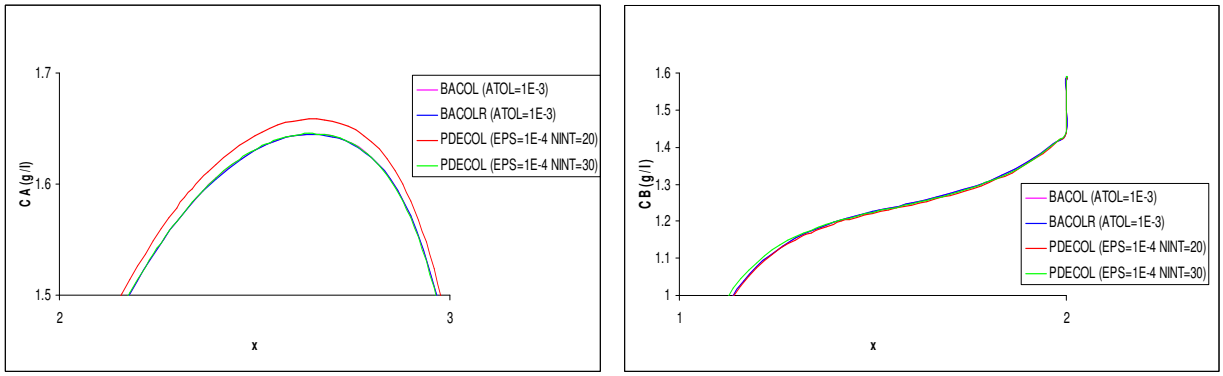
(a) (b)

Figure 9. Errors obtained for PDECOL, BACOL and BACOLR software packages, under significant mass transfer resistance (k=0.1 s^{-1}): (a) absolute errors, e_1; (b) relative errors, e_2.



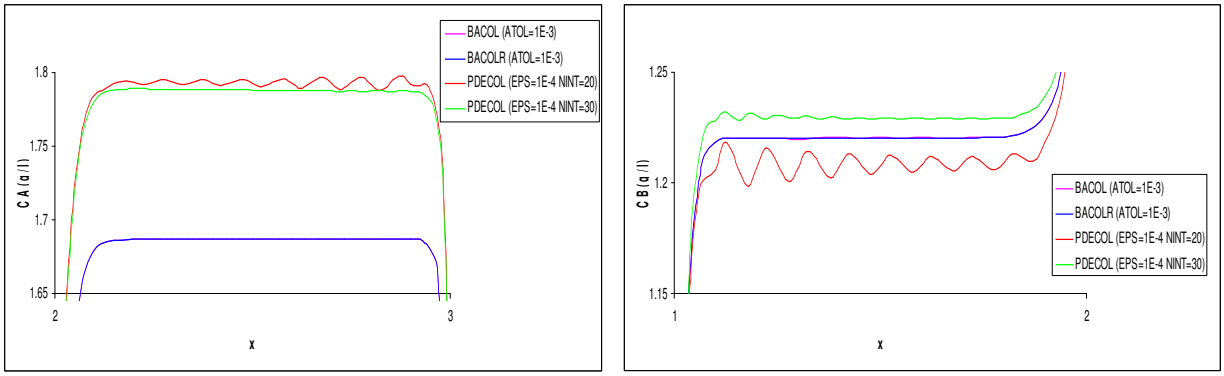
(a) (b)

Figure 10. Errors obtained for PDECOL, BACOL and BACOLR software packages, under negligible mass transfer resistance (k=1 s^{-1}): (a) absolute errors, e_1; (b) relative errors, e_2.



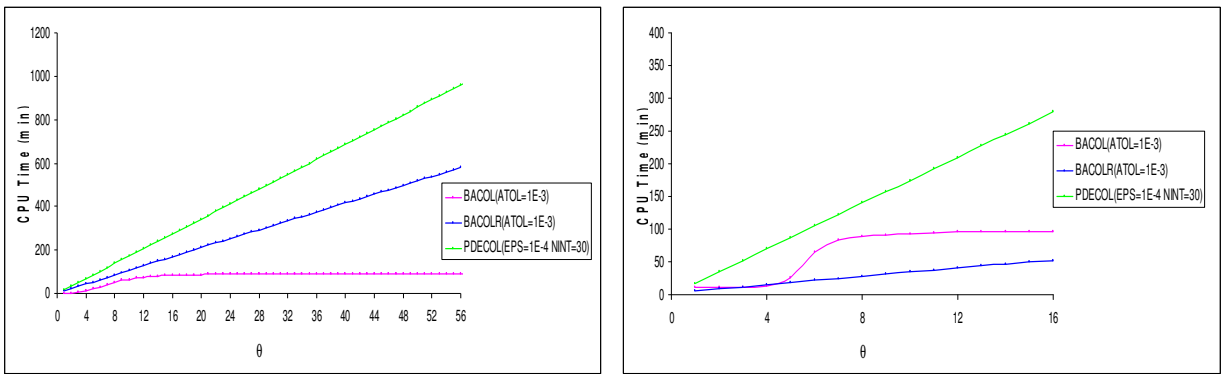
(a) (b)

Figure 11. Detail of the internal concentration profiles obtained under significant mass transfer resistance (k=0.1 s^{-1}) at θ=56 (considered steady-state): (a) component A in section III; (b) component B in section II.



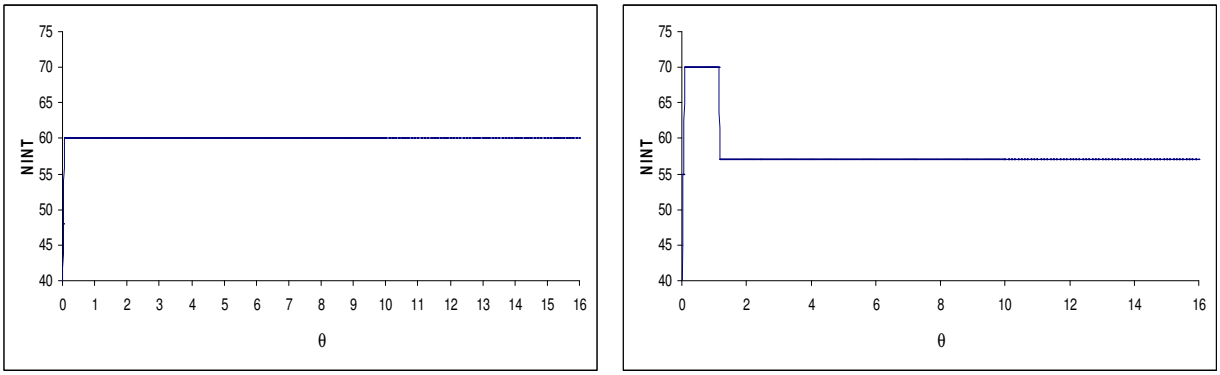
(a) (b)

Figure 12. Detail of the internal concentration profiles obtained under negligible mass transfer resistance (k=1 s^{-1}) at θ=16 (considered steady-state): (a) component A in section III; (b) component B in section II.



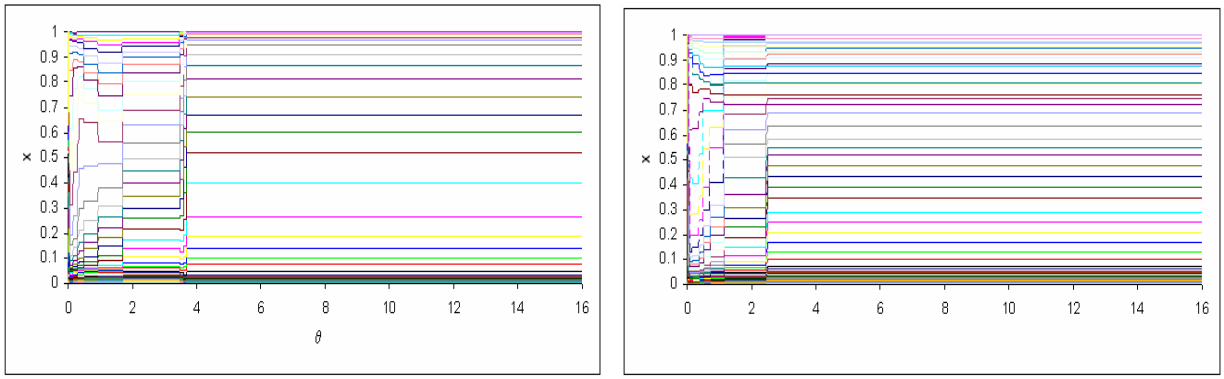
(a) (b)

Figure 13. CPU times for PDECOL, BACOL and BACOLR software packages:
(a) significant mass transfer resistance case (k=0.1 s^{-1}); (b) negligible mass transfer resistance case (k=1 s^{-1}).



(a) (b)

Figure 14. Evolution of the number of intervals (NINT) during the TMB simulation, under negligible mass transfer resistance (k=1 s^{-1}): (a) BACOL (ATOL=1E-3); (b) BACOLR (ATOL=1E-3).



(a) (b)

Figure 15. Evolution of the position of mesh points during the TMB simulation, under negligible mass transfer resistance (k=1 s^{-1}): (a) BACOL (ATOL=1E-3); (b) BACOLR (ATOL=1E-3).

From figures 9 to 15, it can be concluded that:

(a) BACOLR presents lower errors (e_1 and e_2) than BACOL. These two software packages are both much better than PDECOL (see Figures 9 and 10). PDECOL presents difficulties to reach the numerical steady-state, particularly for negligible mass transfer resistances and with respect to the global mass balances (e_2 error);

(b) BACOL and BACOLR present similar internal concentration profiles. PDECOL presents some discrepancies, more pronounced under negligible mass transfer resistances; that is, for high values of k and α (see Figures 11 and 12);

(c) BACOL and BACOLR needs lower CPU times than PDECOL, since this last software package needs more than 30 intervals to obtain an accurate numerical solution (or even considerable higher values, depending on the k value). BACOLR, besides presenting more accurate numerical solutions than BACOL (lower errors), also needs lower CPU times under negligible mass transfer resistances (see Figure 13);

(d) Through the simulation of the TMB process, BACOL and BACOLR do not significantly change the number of intervals (if compared with the FB simulation). For both software packages, the mesh points are preferentially fixed near the boundaries of sections, particularly, near its inlet.

5. CONCLUSIONS

The BACOL and BACOLR software packages provide both time and spatial error control by redistributing the mesh and change the number of mesh points. This ability presents clear benefits in the simulation of Simulated Moving Bed processes, characterized by moving concentration fronts. BACOLR presents more accurate numerical solutions and lower CPU times, particularly under negligible mass transfer resistances.

ACKNOWLEDGEMENTS

Financial support by the Portuguese R&D foundation FCT (Fundação para a Ciência e a Tecnologia) and European Community through FEDER (project POCI/EQU/59738/2004), is gratefully acknowledged.

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