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Design Methodology and Performance Analysis of a Pseudo-Simulated Moving Bed for Ternary Separation

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Abstract: This paper presents design equations for ternary separation using a pseudo-simulated moving bed unit. The analysis of the dynamics of separation as well as the positioning of the concentration waves of species into units is addressed. The derived equations in the frame of the equilibrium theory for linear adsorption provide constraints on the position of the species, which allow the determination of operational conditions for a required separation performance. A flow chart is tested with a pseudo-SMB applied to the separation of two ternary mixtures of sugars. It is shown how strongly the positioning of concentration waves and then the operational parameters can affect the unit performance. Mass transfer effects play an important role on the decision of using SMBs in cascade or pseudo-SMB unit in ternary separations.

Keywords: Chromatography, separation, moving bed, design, JO technology, ternary mixture

INTRODUCTION

Some different Simulated Moving Bed (SMB) configurations have been proposed to achieve the separation of multicomponent mixtures. The use of

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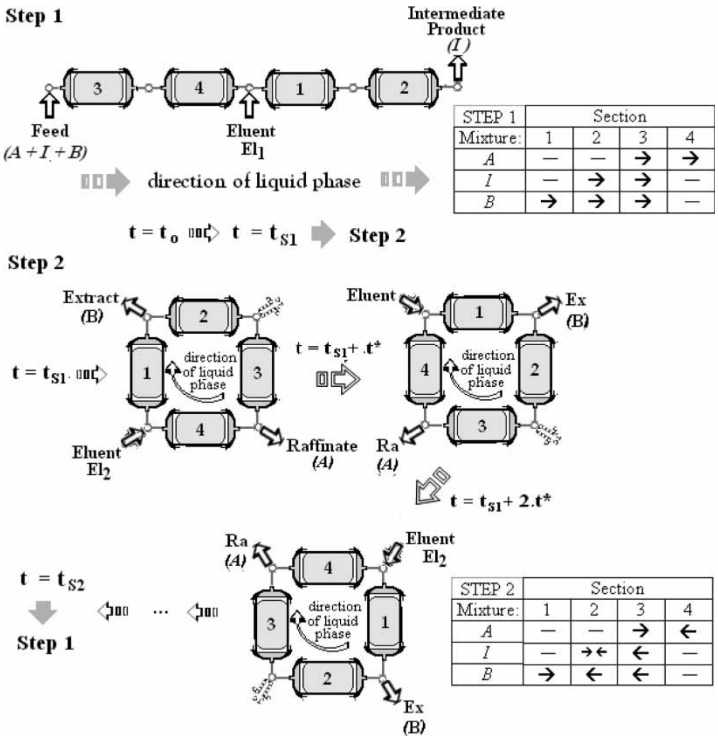
two SMB in series, which can be either separated or combined in a single device (eight zone SMB or nine zone SMB) has been discussed for ternary separation (1–5). Cascade of different SMB systems has been reported for ternary and quaternary separation (6–10). A five zone SMB system was also investigated, with an additional side-stream besides products of extract or raffinate, for some ternary separations of sugar alcohols (11), chirals (12), and biomolecules where different solvent strength are used in different sections (13).

Commercially, ternary separations have been carried out with two SMB cascades using direct or indirect connections (6). Another alternative technology for ternary separation is a device called JO chromatographic separator commercialized by Organo Corporation (previously known as the Japan Organo Corporation) (14). In this technique, there is a switch in the operating mode throughout a process cycle: the system operates in batch chromatography mode alternating with SMB mode with no feed (15, 16). The JO system (pseudo-simulated moving bed) concept has been discussed in a number of publications: Mata and Rodrigues (17) have developed a pseudo-SMB model for such process, Kurup et al. (18) have considered multi-objective optimization of these units, Borges da Silva and Rodrigues (19) analyzed JO performance and suggested an extended JO for the quaternary separation; and Sayama et al. (20) have experimentally tested this technology for the separation of raffinose from beet molasses.

In this study, we develop a design algorithm to set the operating conditions for ternary separation in JO system according to a required unit performance. Equilibrium theory and a detailed process model taking into account axial dispersion and mass transfer resistance are used in the design methodology of JO systems. In the previous work (19), a method for calculating the flow rates required for both steps in JO operation was established; however, little attention was given to the p_i parameters that are associated with the positioning of the species concentration waves at the end of a step of a JO cycle. Since the selection of these parameters has a strong impact on the JO system performance, this subject is addressed in this paper. With regard to step 2, in which the JO system works as SMB unit without feed, the application of the strategies for the determination of the key flow rates in section 2 (and 3) and switching time is now based on set of the (p_A; p_B; p_C) and is not limited to ternary mixtures with a maximum Henry constant for the strongly or the weakly adsorbed compound (19).

The principle of a JO system has been described elsewhere (15, 17, 19). It usually consists of four sections (Fig. 1), which have identical fixed bed columns connected in series (here called 4-section JO). The process using this technology is cyclic with two steps: in step 1, the system works as a series of chromatographic columns, and in step 2, the system is a SMB unit without feed with a periodic shift of inlet/outlet ports in direction of the liquid flow.

A ternary mixture including species A, I, and B is introduced at the feed port during the time corresponding to the step 1 (t_{S1}). The order of species affinity is: $A < I < B$ (from less to more adsorbed on solid phase). In step 1,



STEP 1	Section			
Mixture:	1	2	3	4
A	—	—	→	→
I	—	→	→	—
B	→	→	→	—

STEP 2	Section			
Mixture:	1	2	3	4
A	—	—	→	←
I	—	→←	←	—
B	→	←	←	—

Figure 1. Four section JO system for ternary separation. Direction of the movement of components in each section of the system.

all species migrate in the direction of the liquid phase. In this step the system is loaded and the intermediate species is collected. An eluent stream allows the withdrawal of compound *I* in the intermediate port (*Int*). After step 1, the system starts to operate according to the SMB technology without feed during the time of the step 2 (t_{S2}). The JO process retains the concept of operation with partial feed (21, 22). There are two withdrawal points: raffinate (collection of species *A*) and extract (collection of species *B*). The adsorption wave of *I* and *B* must propagate in the direction of the solid phase, and at the end of step 2 must be:

i. for species *I*, positioned in some place into section 2;
ii. for species *B*, positioned nearby the extract port. The less retained compound must move in the direction of the liquid flow to be recovered in the raffinate port.

Section 1 allows desorption of species *B* and recycling of the solid; and in section 4 the adsorption of species *A* takes place to enable the recycling the liquid phase.

One cycle of operation is finished at the end of step 2. For the recovery of the high-purity products, some important aspects must be taken into account in the design of these systems, particularly the choice of the duration of the steps, flow rates in each section in both steps, and switching time that directly affects the separation efficiency. An analysis of design objectives (higher purity and productivity of the compounds in outlet streams or lower eluent consumption) lead us to the scheme of an hypothetical optimized behavior of the concentration profiles of the species in system, at the end of the two steps of a JO cycle (in cyclic steady state), as illustrated in Fig. 2. The profiles are based on the idea that each concentration wave of the components should be located in specific positions in each section to guarantee the purity of the compounds. The intermediate species should remain between section 2 and 3. If the concentration front of component *A* does not go beyond the end of section 4 at the end of step 2, there is no contamination of *B* by species *A* and the eluent recycle stream is clean. The concentration tail of *B* should not spread for section 4, at the end of step 2, and its concentration front

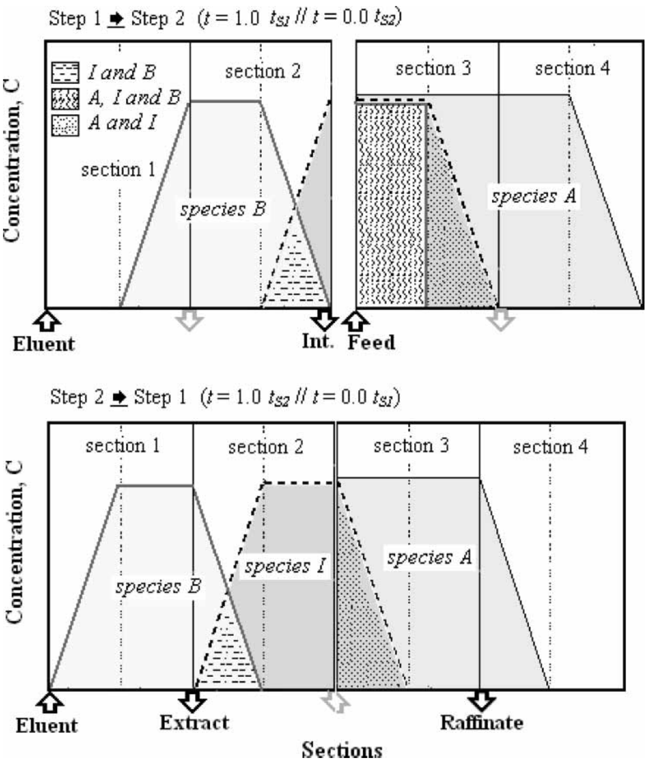


Figure 2. Scheme of a hypothetical optimized behavior of the concentration profiles of species in 4-section JO, at the end of the two steps of a JO cycle (in cyclic steady state).

should not go beyond the collect point of the intermediate species at the end of step 1 in order to avoid contaminations in the enriched streams of compounds *A* and *I*. Hence, these situations should be avoided to achieve a successful separation and a set of operating conditions must be determined to operate a JO system properly. This is addressed as follows.

CHOICE OF JO OPERATING CONDITIONS

In Table 1, we summarized a procedure of our previous work (19) to determine the operating conditions of 4-section JO in order to separate compounds characterized by linear adsorption isotherms. However, some new approaches are introduced (particularly new restrictions are given considering step 2). The optimum operating condition giving high-purity products, highest productivity and lowest eluent consumption is linked with the correct migration rates of the compounds in both liquid and solid flow directions. The required separation is achieved if each species migrates through each section to the respective product outlet. In Fig. 1, the net-flow directions of the species either in step 1 as in step 2 in each JO section for a desired separation are indicated. The continuous countercurrent process in step 2 is represented by an equivalent true moving bed (TMB).

Step 1

The duration of step 1(t_{S1})in Table 1 is based on the retention time of *I*, because this compound should not enter into section 4. Mass transfer resistance should be taken into account (17, 23). The variable $\bar{t}_I$ is the first moment of the pulse response after p_{tS1} columns length in section 3, where the parameter p_{tS1} has values between zero and the number of columns in section 3 (n_{Se3}).

If the feed flow rate is known, the liquid flow rates in sections 3 and 4 are defined automatically. The flow rate in sections 1 and 2 is such that the intermediate compound is eluted from section 2 during step 1. In Eq. (T2), the p_{Qs1} parameter assumes values that allow elution of a desired quantity of compound *I* from the unit during step 1.

Step 2

In step 2, the JO system works as a continuous counter-current process. In order to achieve the ternary mixture separation, the species have to migrate either with the liquid phase or with the solid phase depending on the given section. Concerning the migration of species in step 2 and assuming an ideal counter-current column, the differential mass balance equations of

Table 1. Operating conditions of 4-section JO for a ternary separation (case of linear adsorption isotherms)

	Step 2	
Step 1	Strategy 1	Strategy 2
$t_{S1} = \bar{t}_I - 2\left(\frac{2\bar{t}_I^2}{Pe} + \frac{2}{k_I}(\bar{t}_I - p_{tS1}\frac{\varepsilon L_C A_C}{Q_f})\right)^{1/2}$ $(0 < p_{tS1} < n_{Se3})$ (T1)	$Q_{2,S2} = \frac{\varepsilon A_c}{t_{S2}}\left(\frac{K_B}{K_B - K_I}\right)\left[\phi_I x_{I,2/3,S2} - \phi_B \frac{K_I}{K_B} x_{B,2/3,S2}\right]$ (T5)	$Q_{2,S2} = \frac{\varepsilon A_C}{t_{S2}}\left(\frac{K_I}{K_I - K_A}\right)\left[\phi_A x_{A,2/3,S2} - \phi_I \frac{K_A}{K_I} x_{I,2/3,S2}\right]$ (T7)
$Q_{1,S1} = p_{QS1}\varepsilon\frac{L_C A_C}{t_{S1}}\left(1 + \frac{1-\varepsilon}{\varepsilon}K_I\right)$ $(0 < p_{QS1} < n_{Se2})$ (T2)	$Q_S = \frac{\varepsilon A_c}{t_{S2}}\left(\frac{1}{K_B - K_I}\right)\left[\phi_I x_{I,2/3,S2} - \phi_B x_{B,2/3,S2}\right]$ (T6)	$Q_S = \frac{\varepsilon A_C}{t_{S2}}\left(\frac{1}{K_I - K_A}\right)\left[\phi_A x_{A,2/3,S2} - \phi_I x_{I,2/3,S2}\right]$ (T8)
$Q_f = Q_{3,S1} = Q_{4,S1};\ Q_{El1} + Q_f = Q_{1,S1} = Q_{2,S1}$ (T3)/(T4)	$Q_{1,S2} = \beta_1\ Q_S K_B - \frac{t_{S1}}{t_{S2}} Q_{Int}(\text{with}\ \ \beta_1 > 1\ \ \text{and}\ \ \beta_1 > \frac{t_{S1}\ Q_{Int}}{t_{S2}\ Q_S K_B})$ (T9)	
	$Q_{4,S2} = \beta_4\ Q_S K_A - \frac{t_{S1}}{t_{S2}} Q_f(\text{with}\ \ \frac{t_{S1}\ Q_f}{t_{S2}\ Q_S K_A} < \beta_4 < 1)$ (T10)	

[a] The parameter β represents a "safety margin" (27).

species using the local equilibrium assumption and linear case allow us to write,

$$\begin{aligned} x_{A,2/3,S2} &= p_A L_C - x_{A,3,S1} \\ &= \frac{t_{S2}}{\varepsilon A_C \phi_A}(Q_{2/3,S2} - Q_S K_A) \quad (\text{with } p_A \geq \frac{x_{A,3,S1}}{L_C}) \end{aligned} \tag{1}$$

$$\begin{aligned} x_{I,2/3,S2} &= -(x_{I,3,S1} + p_I L_C) \\ &= \frac{t_{S2}}{\varepsilon A_C \phi_I}(Q_{2/3,S2} - Q_S K_I) \quad (\text{with } 0 < p_I < n_{c,2}) \end{aligned} \tag{2}$$

$$\begin{aligned} x_{B,2/3,S2} &= -(x_{B,3,S1} + p_B L_C) \\ &= \frac{t_{S2}}{\varepsilon A_c \phi_B}(Q_{2/3,S2} - Q_S K_B) \quad (\text{with } p_B > 0) \end{aligned} \tag{3}$$

with $\phi_i = 1 + (1 - \varepsilon)/(\varepsilon)K_i$. The variable $x_{i,\ j,\ Sn}$ is the distance travelled by species i in section j during step n $(=1, 2)$, $Q_{j,S2}$ and Q_S $(=(1 - \varepsilon)A_C\, u_S$; where u_s is the solid velocity) are the liquid flow rate in section j of the unit and the solid flow rate, respectively, in step 2. The p_i parameters are the key for a successful separation and assume different values for each species. The range for the parameters are shown in Eqs. (1–3) and they will be the basis of the upcoming discussion. The liquid flow rate in section 2 (with $Q_{2,S2} = Q_{3,S2} = Q_{2/3,S2}$) and solid flow rate ($Q_S$) can be determined through Eqs. 1–3 in such a way that the concentration waves of species are at specific positions at the end of step 2 to achieve an adequate operation.

In Table 1, we presented two strategies to find these flow rates (strategy 1 and strategy 2). Strategy 1 is to be used for a ternary mixture when the "harder" separation is between the intermediate (I) and strongly adsorbed (B) components and strategy 2 is for a ternary mixture when the "harder" separation is between the intermediate (I) and weakly adsorbed (A) components.

Strategy 1 considers Eqs. (2–3) to define the liquid flow rate in section 2 ($Q_{2,S2}$) and the solid flow rate (Q_S), which, in terms of concentration wave velocity, leads species B to the extract and species I travel to section 2. However, the constraint for the migration of species A should also be satisfied. Species A must travel with liquid phase to be recovered in the raffinate stream. If the equations of $Q_{2/3,S2}$ and Q_S are used in Eq. (1), a relation between p_{I} and p_B parameters will be obtained which has to be verified so that the operation occurs adequately. The following relation is obtained for p_B by combining Eqs. (1), (T5) and (T6):

$$\begin{aligned} p_B \geq{} & \left(\frac{K_B - K_A}{K_I - K_A}\right)\frac{\phi_I}{\phi_B}\left(p_I + \frac{x_{I,3,S1}}{L_C}\right) - \frac{x_{B,3,S1}}{L_C} \\ & + \left(\frac{K_B - K_I}{K_I - K_A}\right)\frac{(p_A L_C - x_{A,3,S1})}{L_C}\frac{\phi_A}{\phi_B} \end{aligned} \tag{4}$$

If the above inequality is satisfied, the flow rates calculated by Eqs. (T5) and (T6) will allow the displacement of species A in the direction of the raffinate port. On the other hand, the strategy 2 considers Eqs. (1–2) to define the $Q_{2,S2}$ and Q_S, which, in terms of concentration wave velocity, leads species A to the raffinate port and species I travel to section 2. The flow rates given by Eqs. (T7) and (T8) did not consider the constraint of the displacement of B for the extract port. At the end of step 2, species B should be located at $x_{B,2/3,S2}$ which depends on the p_B value. Therefore, Eq. (3) is used to determine a relation between p_I and p_B in such way that species B can be directed to the extract port. Now, the relation is,

$$p_B \leq \left(\frac{K_B - K_A}{K_I - K_A}\right)\frac{\phi_I}{\phi_B}\left(p_I + \frac{x_{I,3,S1}}{L_C}\right) - \frac{x_{B,3,S1}}{L_C} + \left(\frac{K_B - K_I}{K_I - K_A}\right)\frac{\left(p_A L_C - x_{A,3,S1}\right)}{L_C}\frac{\phi_A}{\phi_B} \tag{5}$$

One can note that Eq. (4) and Eq. (5) differ only by the sign of the inequality. When the equality is established, the calculated operating conditions by either strategy 1 or strategy 2 are equal.

Analysis on the p_i parameters

A procedure to find the operating conditions in a given JO system configuration has been presented. However, some open questions still remain unsolved such as which values should be assigned to p_i parameters (p_{tS1} and p_{QS1} in step 1; p_A, p_B and p_I in step 2) in order to achieve a required separation performance.

Due to the counter-current movement of phases during step 2, the separation occurs mainly in sections 2 and 3 and then the $Q_{2/3,S2}$ and Q_S flow rates are the key operating parameters for the separation. Thus, the knowledge of the limiting values of p_i parameters and the strategy that should be adopted becomes important. In our previous work (19), it has been discussed the JO performance for the separation of ternary mixtures with different "degrees of difficulty". We have explained the 4-section JO behavior in terms of performance variables (purity, productivity, and eluent consumption) using operating conditions calculated by the described procedure for some pairs (α_{IA}; α_{BI}) – where α is the separation factor between the species ($\alpha_{IA} = K_I/K_A$; $\alpha_{BI} = K_B/K_I$). The analysis was based on fixed p_i parameters: $p_I = 1$ and $p_B = 3$ for the strategy 1 and $p_A = 3$ and $p_I = 1$ for strategy 2. Therefore, since the JO system configuration had three columns per section, concentration waves of the stronger and the weaker adsorbable compound were directed exactly to their respective enriched outlets when any strategy was applied. In this work, the implications of using different positioning of the concentration waves of species of the mixture into JO system must be studied. The limitation of the application of one or another strategy is carried out by the p_i parameters – in Eqs. (1) to (3) – and not through the analysis of the adsorption constants of the species, as shown before in (19). The focus of our discussion is on which values of p_i must be selected for the different cases of separation, i.e., degrees of separation difficulty.

Let us keep the classification of the "degree of separation difficulty" based on the separation factor. It is assumed easy separations when $\alpha > 2.5$, moderate separations for $\alpha \approx 1.5$, and hard separations for $\alpha \approx 1.1$. A ternary mixture is characterized by a pair (α_{IA}; α_{BI}), which represents the separation factor between the species *I* and *A* and the separation factor between species *B* and *I*, respectively. A mixture can have several combinations of the degree of separation difficulty, as for example a hard separation for species *A* and *I* and easy separation for *I* and *B*.

Some properties of the 4-section JO used in these analyses are described in Table 2. Since the p_i parameters are necessary for the determination of the operating conditions of the step 2 and, according to the Eqs. (1–3), some variables from the step 1 are needed, operating conditions of the step 1 in the system are also listed in Table 2. We have arbitrarily chosen the adsorption equilibrium constant (K_I) and the mass transfer coefficient (k_I) for species *I* as 0.39 and 0.5 s^{-1}, respectively.

Once the conditions in step 1 are defined, one of the strategies for determining the flow rates $Q_{2/3,S2}$ and Q_S in step 2 should be used to allow the separation of the ternary mixture indicated by (α_{IA}; α_{BI}). Nevertheless, before evaluating some particular mixture of industrial interest, let us consider both possible alternatives for any mixture.

When applying the strategy 1, $Q_{2/3,S2}$ and Q_S are calculated in such a way that for the chosen value of p_I (which defines the positioning for the peak of the intermediate species in section 2 at the end of step 2) and p_A, the value of p_B must satisfy the Eq. (4). When strategy 2 is applied, the same can be said with p_B satisfying the Eq. (5). Therefore, diagrams can be constructed

Table 2. Properties and operational variables of the 4-section JO

Column length, L_C	1.20 m
Column diameter, d_C	0.1084 m
Porosity, ε	0.4
N° Peclet	2000
System configuration	3/3/3/3
Step 1	
Q_f	$5.83\ 10^{-6}\ m^3/s$
Q_{Int}	$1.29\ 10^{-5}\ m^3/s$
t_{S1}	1090.1 s
p_{tS1}; p_{QS1}	1; 2

$^a x_{A,3,S1}/L_C = 0.516$; $\beta_I = 1.03$; $\beta_4 = 0.97$.

to show the limits of applicability of both strategies for the choice of operating conditions in step 2 of a 4-section JO. As the application of these strategies depends also on the adsorption equilibrium of the components of the ternary mixture, their limits of application are constructed according to the pairs of separation factors α_{IA} and α_{BI} of a given mixture.

Figure 3 shows some graphs in $\alpha_{IA} \times \alpha_{BI}$ plan, which were built using the minimum value of p_A ($=x_{A,3,S1}/L_C$); it means that there is no propagation of the concentration wave of species A during step 2 in section 3. This component will only be conveyed along with the liquid phase during the operation of the step 1. Each line in this diagram will separate regions in which the application of one strategy can be made to obtain an adequate separation.

Figure 3 illustrates the cases of p_I equal to 1 and 1.5; and of p_B equal to 2.5, 3, and 4 that means to locate the concentration wave of the species B nearby the extract port. In order to analyse this plot, let us use the notation (p_A; p_I; p_B). Each point on this figure represents a ternary mixture with "degree of separation difficulty" defined by the pair (α_{IA}; α_{BI}). In those ternary mixtures in which the linear adsorption constants of the components define points (α_{IA}; α_{BI}) positioned to the left of the separative line of (p_A; p_I; p_B), the strategy 1 can be applied. On the other hand, for those mixtures in which the linear adsorption constants of the three components define points (α_{IA}; α_{BI}) to the right of the separative line, it is possible to use the strategy 2 for the determination of the operating conditions in step 2. As an example, in order to set the flow rates $Q_{2,S2}$ and Q_S using strategy 1 for the ternary mixture ($\alpha_{IA} = 1.6$; $\alpha_{BI} = 1.2$), one can use Fig. 3 and verify the possibility of using all shown combinations of p_i parameters – ($p_A = x_{A,3,S1}/L_C$; p_I; p_B) – with $x_{A,3,S1}/L_C$ =0.516 (according to the conditions in Table 2) and different values of p_I and p_B. But, in the case of a mixture ($\alpha_{IA} = 1.6$;

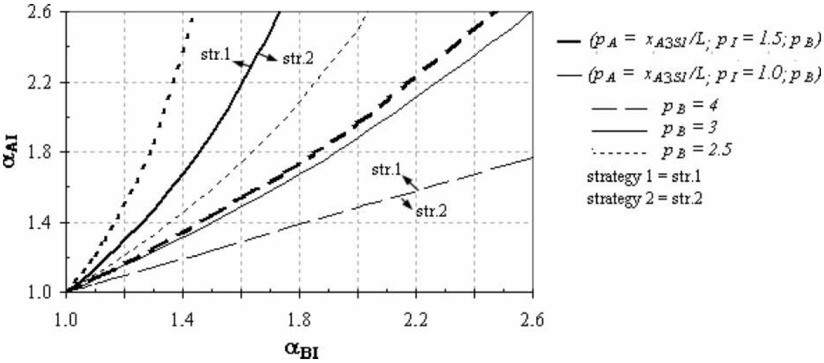


Figure 3. Separative lines for strategies 1 and 2 in the plan (α_{IA}; α_{BI}). Value of the parameters: $p_A = x_{A,3,S1}/L_C$ (=0.516; for the conditions in Table 2)//(thin lines) $p_I = 1$; (thick lines) $p_I = 1.5$//(----) $p_B = 2.5$, (—) $p_B = 3$ and (– – –) $p_B = 4$. (strategy 1 = str.1; strategy 2 = str.2).

$\alpha_{BI} = 1.6$), the option to use the combination ($x_{A,3,S1}/L_C$; 1; 2.5) would not allow the application of strategy 1, because the maximum value of p_B calculated from Eq. (4) is 2.72. The application of strategy 1 would provide conditions such that the peaks of concentration of the species A move in the direction of the solid phase during step 2 and it could contaminate the collection outlet of the species I.

It is observed that the region for the application of strategy 1 is expanded when the value of p_I parameter decreases. This means that the region of application of strategy 1 is smaller when the concentration wave of I is required to be closer to the extract outlet (i.e., larger values of p_I). It can be also seen that the region for the application of strategy 1 for a given p_I becomes larger when p_B is higher.

Figure 4 shows the regions for the application of both strategies when different values of p_A parameters are fixed. The value of p_A establishes the positioning of the concentration wave of the species A at the end of t_{S2}. The p_A parameters are written in a way to allow an idea on the displacement of the concentration wave of the species A in the system during step 2. If, for example, p_A is equal to $(3.6 + x_{A,3,S1})/L_C$, it means that the wave travels a distance of 3.6 m during step 2 (or $x_{A,3,S2} = 3.6$). Larger values of p_A, minor regions for the application of strategy 1.

The choice of the set of parameters (p_A; p_I; p_B) and therefore the use of strategy 1 or strategy 2 has an impact on the JO system performance. In order to analyze the effect of p_i parameters and to understand the JO system behavior and performance, simulation studies have been performed for the system described in Table 2.

The process simulation, either for the first part of a JO cycle (system represented by a fixed bed column) or for the second part (system in SMB

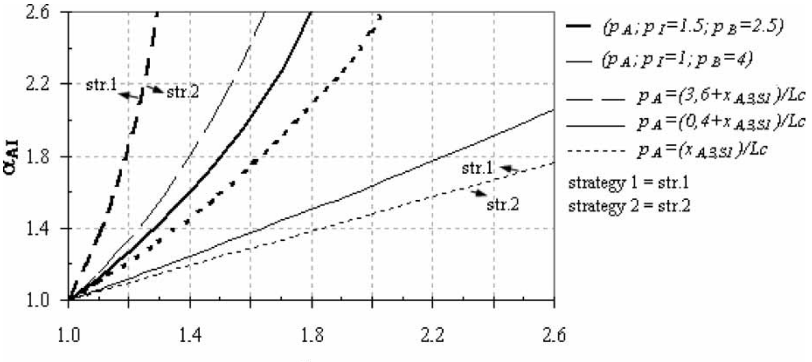


Figure 4. Separative lines for strategies 1 and 2 in the plan (α_{IA}; α_{BI}).Value of the parameters: (– – –) $p_A = x_{A,3,S1}/L_C$; (—) $p_A = (0.4 + x_{A,3,S1})/L_C$ (=0.85, for the conditions on Table 2); (– – –) $p_A = (3.6 + x_{A,3,S1})/L_C$ (=3.52, for the conditions on Table 2)// $p_I = 1$//(thick lines) $p_B = 2.5$; (thin lines) $p_B = 4$. (strategy 1 = str.1; strategy 2 = str.2)

operation, here represented by a equivalent true moving bed), is based upon a model where axial dispersion, mass transfer resistance within the liquid and solid phase as well as the periodic change of the operation in a JO cycle are accounted for. Mass balance equations referring to the concentrations of components *i* in JO column k in the liquid and stationary phases are:
– Liquid phase,

$$\frac{\partial(C_{ik})}{\partial t}+\frac{(1-\varepsilon)}{\varepsilon}\left[\frac{\partial(\bar{q}_{ik})}{\partial t}-u_s\frac{\partial(\bar{q}_{ik})}{\partial z}\right]+v_k\frac{\partial(C_{ik})}{\partial z}-D_a\frac{\partial^2(C_{ik})}{\partial z^2}=0 \qquad (6)$$

–Stationary phase (*Linear Driving Force* approximation):

$$\frac{\partial(\bar{q}_{ik})}{\partial t}=u_s\frac{\partial(\bar{q}_{ik})}{\partial z}+k_i(q_i^*-\bar{q}_{ik}) \qquad (7)$$

When the system operates in step 1, the velocity of the solid is zero in Eqs. (6) and (7). Initial and Danckwerts boundary conditions as well as global mass balances in inlet and outlet nodes are complementary equations to the model. The mathematical model is described in detail elsewhere (19). With regard to step 2, the true moving bed equivalent model has been used because lower computing times are required and their results are suitable for this analysis. The simulations are performed for a SMB unit (without feed) with numerous columns (i.e., 12 columns in system) and, for these cases, one can expect that TMB equivalent simulations agree with the SMB intermittent model (24, 25). Certainly, in the case of few columns and extreme operating conditions, the TMB model loses accuracy and the SMB model must be used.

A periodic steady state corresponding to a given cycle of the JO system is reached. This means that for a given cycle the concentration profiles in sections of the JO system vary with time in its both operation modes, but such profiles are repeated in each new cycle.

Some performance parameters are used in the analysis of the p_i parameters for the positioning of the concentration peaks of the components of a mixture into JO system. The definition of the average concentration ($\bar{C}$) and the purity (*Pu*) of the components in the respective enrichment stream, and the average eluent consumption ($\bar{E}_C$) of the unit for the recovery of the species are in Table 3.

RESULTS AND DISCUSSION

Performance Analysis

The effect of the positioning of the concentration waves of species at the end of step 2 on the process performance for a 4-section JO is presented. Simulations are performed for ternary mixtures characterized by the pair (1.5;

Table 3. Performance parameters for the analysis of the positioning of concentration waves of the components of a mixture in the 4-section JO

Average conc. (g/L)	Purity (%)	Eluent consumption (L/g)	Average El. consumption (L/g)
$\bar{C}_{i,m,n} = \frac{\int_0^{t_{Sn}} C_{i,m,n}\,dt}{t_{Sn}}$	$Pu_{i,m,n} = \frac{\bar{C}_{i,m,n}}{\sum_{c=A,I,B} \bar{C}_{c,m,n}} 100$	$EC_{i,m,n} = \frac{Q_{El11} t_{S1} + Q_{El21} t_{S2}}{Q_m \bar{C}_{i,m,n} t_{Sn}}$	$\bar{E}_C = \frac{\sum_{i,m,n} E_{C_{i,m,n}}}{3}$

[a] In performance parameters, index i,m,n refers to A,Ra,2; I,Int,1 and B,Ex,2.

α_{BI}) that means a moderate separation between the species *A* and *I* and a separation that can vary from easy to hard between species *B* and *I*. The system and operating parameters of step 1 are those described in Table 2. The operating parameters of the step 2 depend on the values of p_i parameters and the adsorption constants of the components in the mixture (1.5; α_{BI}). Very rapid mass transfer is assumed, with global mass transfer coefficient equal to 0.5 s^{-1} for all species. The effect of lower mass transfer rates is considered in Mata and Rodrigues (17). The feed composition is 100 g/L for each component. The duration of the step 2 (t_{S2}) is chosen as 200 min to perform this analysis.

Figure 5 shows the average concentration of each species in its enrichment stream obtained from the separation of ternary mixture (1.5; α_{BI}). For each mixture, the operating conditions for step 2 are calculated following the discussed procedure in the previous item. This performance variable of separation is showed for combinations of p_i parameters. Each combination (p_A; p_I; p_B) presents a vertical line that separates the regions of application of the strategy 1 and strategy 2. As can be observed in Fig. 3, when α_{IA} is equal to 1.5, the curve (p_A; $p_I = 1$; $p_B = 2.5$) has a limit of application of strategy 1 (following from the left to the right) in which the value of α_{BI}

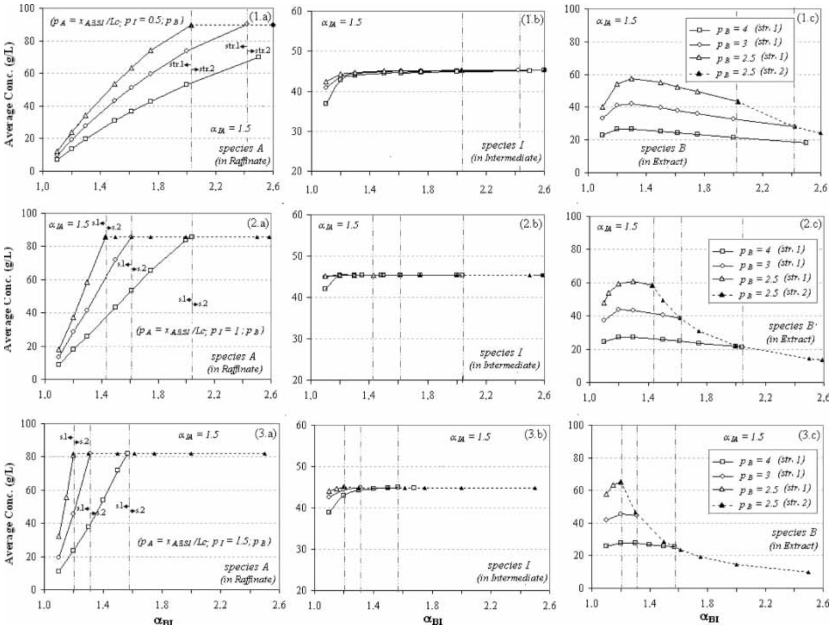


Figure 5. Average concentration of the species in enrichment streams of the 4-section JO as function of separation factor α_{BI} ($\alpha_{IA} = 1.5$). Operational conditions: Step 1 from Table 2 and Step 2 from strategy 1 and 2 for the combinations: $p_A = x_{A,3,S1}/L_C$//(1a–c) $p_I = 0.5$; (2a–c) $p_I = 1.0$; (3a–c) $p_I = 1.5$//$p_B = 2.5$, 3, 4.

comes to 1.435. Therefore, this point is the limit that establishes the use of the first or second strategy.

For each vertical line (line of delimitation of strategy), its left side is the area for the application of the strategy 1 and on the right side strategy 2 can be used. The operational conditions defined by using strategy 2 are not modified with the change of the p_B parameter. This means that the performance achieved for (p_A; p_I; $p_B = 2.5$) with the application of strategy 2 will correspond to the performance obtained by strategy 2 with other different values of p_B, from its respective line of delimitation of strategy. A similar statement can be made for the determination of operational parameters using the strategy 1 when the p_A parameter is changed, i.e, the performance remains unchanged with the variation of this parameter.

Dilution of the Products

First, let us analyze the Fig. 5 to show the JO performance according to average concentration of the species (or the degree of dilution) in their respective collection outlets for different values of p_B and fixed p_I – for example ($p_A = x_{A,3,S1}/L_C$; $p_I = 1$; $p_B = 2.5$, 3 and 4) – in the region of application of the strategy 1. One can verify that the combination of parameters with lower value of p_B provides the more concentrated products for a pair (α_{IA}; α_{BI}). However, when smaller values of p_B are used, the area for the application of strategy 1 becomes narrower; as an example, it is not possible to apply the combination (p_A; 1; 2.5) for a mixture (1.5; $\alpha_{BI} > 1.435$).

For combinations of parameters where there are different values of p_I and fixed p_B, it can be seen that larger values of p_I also lead to a higher average concentration of products, but the area of application of strategy 1 is reduced when larger values of p_I are applied. Utilizing a combination ($x_{A,3,S1}/L_C$; 1; 3), strategy 1 could be used in the case of ternary mixtures (1.5; $\alpha_{BI} < 1.6$); however, if the set ($x_{A,3,S1}/L_C$; 1.5; 3) is to be used, the application of strategy 1 would be limited for mixtures (1.5; $\alpha_{BI} < 1.3$).

The maximum concentration of species A and I is always achieved when the value of α_{BI} in mixture (α_{IA}; α_{BI}) is on the line of delimitation of the strategies of a certain combination of p_i parameters, despite the variation of the concentration of I is not so large in these studied cases. For species B, the plots of average concentration as a function of the separation factor α_{BI} have a maximum point when the strategy 1 is applied; however, the concavity of curves is not so sharp when larger values of p_I and p_B are used. The explanation for the behavior of the graphs has been detailed in previous work (19).

The application of strategy 2 when the value of p_A leads to a stationary wave of concentration of the species A in section 3 shows a peculiar situation. Since both strategies have the same operational conditions on the lines of limitation of strategy, the performance achieved by strategy 2 can be predicted connecting the points where the curves of performance of the unit obtained from strategy 1 cross the vertical lines for each one of the combinations of the p_i parameters.

The application of strategy 2 for any mixture, when it is feasible, would lead to a better performance regarding the dilution of the species than the application of the strategy 1, for which a combination of p_i parameters with larger values of p_B would be necessary. As an example, for mixtures (1.5; $1.6 < \alpha_{BI} < 2.05$) in Fig. 5, the use of strategy 2 for the combination (p_A; $p_I = 1$; $p_B = 2.5$ or 3) provides products with higher average concentrations than the use of the strategy 1 using the combination (p_A; $p_I = 1$; $p_B = 4$).

If some combinations of p_i parameters are selected for a mixture (α_{IA}; α_{BI}) corresponding to the delimitation line, another aspect can be observed. As an example the mixture (1.5; 2.0) is considered and the combination (p_A, 1; 4) leads the limit of application of the strategies approximately to the point of $\alpha_{BI} = 2.0$. Regarding the dilution of the products, with the comparison between the obtained performance with that reached by combination (p_A; 0.5; 2.5), which the line of delimitation is also in $\alpha_{BI} = 2.0$, one can verify that the first one is lower and a inferior value of p_I was applied. However, a lower value of p_B has also been used.

In order to decide which values of the p_i parameters will be more adequate for these ternary separations in the 4-section JO, other performance variables must be taken into account. The purity of the collected species and eluent consumption can disclose important information in search of a required separation.

Purity of Outlet Streams

For a ternary separation in a JO system, the effect of the p_i parameters on the purity of the species at the outlet ports is illustrated in Fig. 6. Considering the regions of application of strategy 1, one can observe that the purity of the component *A* for the studied combinations (p_A; p_I; p_B) varies if the mixture comprises a low value of α_{BI} (hard separation between the *B* and *I*) and $\alpha_{IA} = 1.5$. For the cases where p_I parameter is kept constant, the purity of species *A* increases when the value of p_B decreases. This is related to the need of larger flow rates of both phases in JO sections for an operation in which the concentration wave of the species *B* must be far from the concentration wave of the species *I*. Since concentration waves become more dispersed at higher flow rates, the concentration wave of the species *I* enters into section 4. Therefore, the purity of the species *B* decreases when p_B increases. The tail of the concentration wave of *I* reaches the extract outlet when higher flow rates are required.

For larger values of p_I (keeping constant p_B), the concentration wave of the species *I* moves away from the collection point of species *A* and the probability of contamination of the raffinate by the species *I* is reduced. On the other hand, the concentration wave of the species *I* approaches to the

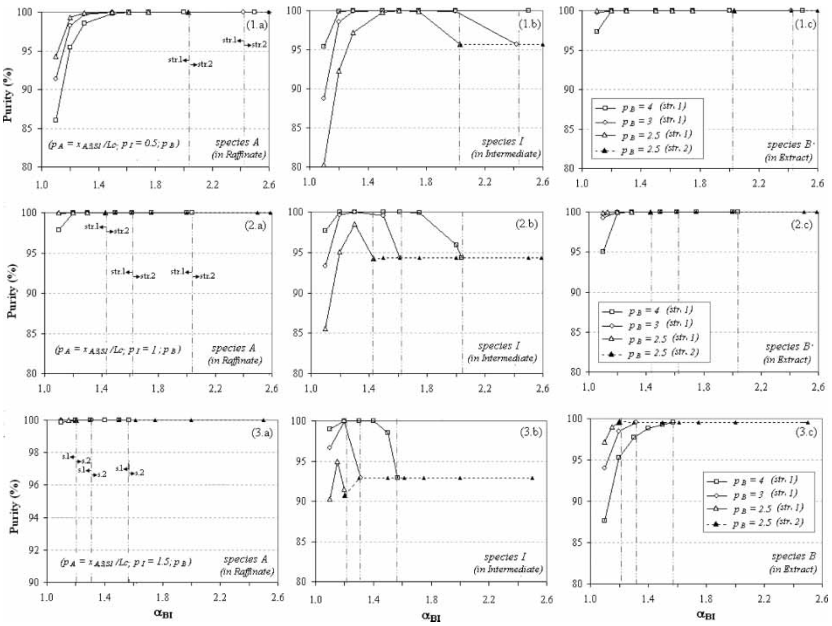


Figure 6. Purity of (a) *A* in raffinate, (b) *I* in intermediate and (c) *B* in extract stream of the 4-section JO as a function of the separation factor α_{BI} ($\alpha_{IA} = 1.5$). Operational conditions: Step 1 from Table 2 and Step 2 from strategy 1 and 2 for the combinations: $p_A = x_{A,3,S1}/L_C//$(1a–c) $p_I = 0.5$; (2a–c) $p_I = 1.0$; (3a–c) $p_I = 1.5//p_B = $ 2.5, 3, 4.

extract outlet and it increases the possibility of contamination of this stream. Therefore, the purity of *B* is lower for higher p_I.

The analysis of the purity of the species *I* for a set of p_i parameters shows that it presents a maximum purity in the region of application of the strategy 1. Such behavior is due to the fact that the intermediate stream can be contaminated either by the tail of the concentration wave of the species *A* until the end of the step 2 or by the elution of the species *B* together with the peak of *I* during the step 1. The first situation occurs when the value of p_A parameter leads to operational conditions that provide a stationary concentration wave of *A* (or with a low displacement in the direction of the liquid phase) such that it enters section 2 due to mass transfer effects. The situation in which mixtures (α_{IA}; α_{BI}) are on the line of delimitation of strategy represents this critical condition, i.e., no displacement of the wave of A occurs. The second situation can occur mainly when the separation process involves a hard separation between the *B* and *I* and higher $Q_{j,S2/}$ Q_S ratios in sections 2 and 3 in the step 2 must be used. Considering only the variation of the p_B parameter, it is observed that increasing p_B the purity of the intermediate compound increases. The wave of *B* travels a distance far from the wave of *I*, therefore reducing the contamination.

The influence of p_I on the purity of the component I is shown by comparing Fig. 6.1b–6.3b for the same values of the parameter p_B. For larger p_I, the purity of the intermediate species is higher. However, the region of application of the strategy 1 becomes smaller for larger p_I. This could mean a situation in which the mixture (α_{IA}; α_{BI}) would be closer to the line of delimitation of strategy, and thus the purity of the species I would be lower because of the contamination by the species A. The case of the mixture (1.5; 1.2) illustrates this statement.

With regard to those regions where strategy 2 should be used, Fig. 6 shows that there is a maximum purity that can be reached in the collection ports for any combinations ($p_A = x_{A,3,S1}/L_C$; $p_I =$ constant; $p_B =$ variable). As the value of the p_B parameter does not modify the operational conditions calculated by the strategy 2, such behavior is already expected. Analyzing combinations ($p_A = x_{A,3,S1}/L_C$; $p_I =$ variable; $p_B =$ constant), lower values of p_I lead to higher purities of the components I and B.

Some conclusions can be made for the studied cases of mixture (1.5; α_{BI}) using $p_A = x_{A,3,S1}/L_C$ ($=$0.516, according to data from the Table 2). The value of p_I to achieve a high-purity product in raffinate is in conflict with that needed to obtain a pure product in extract. This statement indicates that an optimum value of p_I should exist to obtain high-purity products in both outlets for one given configuration of the unit. The use of a lower p_B value can allow more concentrated products at the outlet streams as well as higher purity for components A and B, but it can also decrease the purity of the intermediate compound. For a separation of a ternary mixture in JO, those combinations ($p_A = x_{A,3,S1}/L_C$; p_I; p_B) used to define operating conditions that lead to more concentrated products in the raffinate and the intermediate stream are the same combinations that provide a decrease of the purity at collection intermediate outlet.

Since it is not easy to achieve high-performance from a 4-section JO in both requirements of low product dilution and high-purity of outlet streams, there is a need to specify the objective of the separation and which performance parameters must be optimized.

Eluent Consumption

Figure 7 shows the variation of the average eluent consumption for the separation of mixtures (1.5; α_{BI}) using combinations ($p_A = x_{A,3,S1}/L_C$; $p_I =$0.5, 1, 1.5; $p_B =$2.5, 3, 4). One can observe that to separate a given ternary mixture, the operational conditions defined by the strategy 1, using the lower value of p_B and keeping p_I constant, lead to a recovery of the species with lower average eluent consumption. A similar situation occurs when the value of p_B is kept constant and the value of p_I is increased. However, if the mixture (1.5; 1.5) is taken as an example, one could notice that for the use of the strategy 1 applying $p_I = 1.5$ a value of $p_B \geq 4$ is required. These combinations lead to a larger eluent consumption than that from the combination

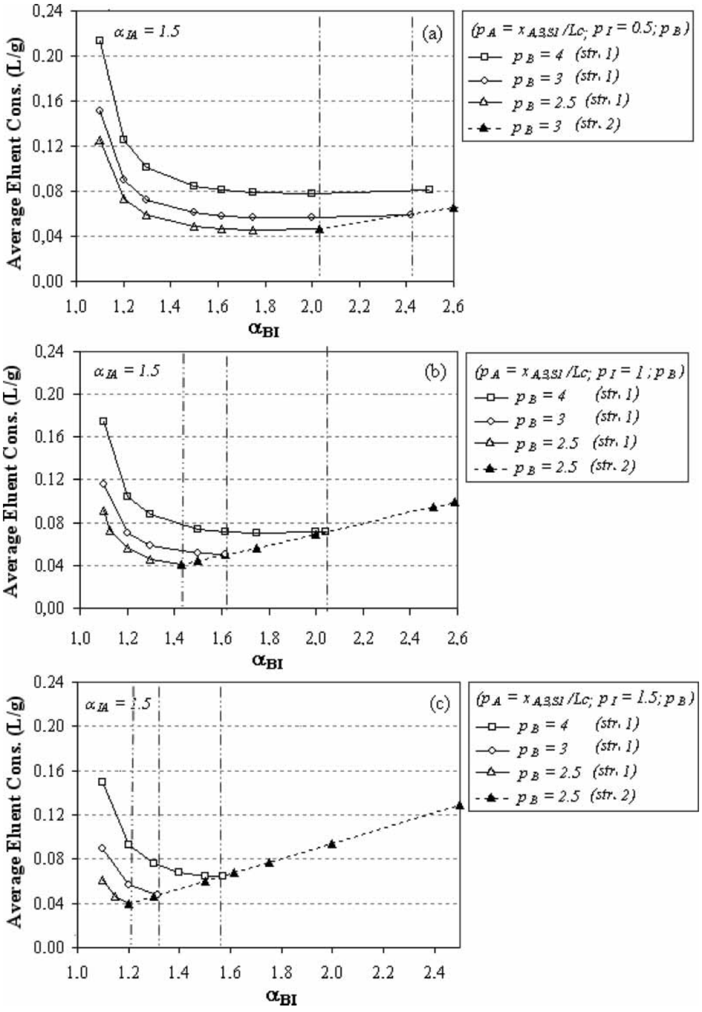


Figure 7. Average eluent consumption in the 4-section JO as a function of the separation factor α_{BI} (α_{IA} =1.5). Operational conditions: Step 1 from Table 2 and Step 2 from strategy 1 and 2 for the combinations $p_A = x_{A,3,S1}/L_C$; (a) $p_I = 0.5$; (b) $p_I = 1$; (c) $p_I = 1.5$; $p_B = 2.5, 3, 4$.

($p_A = x_{A,3,S1}/L_C$; p_I =1; p_B =3). For this mixture, the application of $p_I = 0.5$ and $p_B = 2.5$ is also valid and, although the value of p_I is lower among these mentioned combinations, this last has the lowest average eluent consumption for the separation of the mixture (1.5; 1.5).

Figure 7 also shows the eluent consumption for operating conditions calculated by strategy 2 when $p_I = 0.5$, 1 and 1.5 and $p_B = 2.5$. Since the value of p_B does not change the operational conditions calculated by the strategy 2, the eluent consumption shown in Fig. 7 for combinations ($p_A = x_{A,3,S1}/L_C$; $p_I = 0.5$, 1 and 1.5; $p_B = 2.5$) with strategy 2 are also valid for other values of p_B (3, 4 or higher). From the regions delimited by the vertical lines in Fig. 7, one can see that the operational conditions determined by strategy 2 lead to a separation with lower eluent consumption (remembering that here $p_A = x_{A,3,S1}/L_C$). Therefore, the best conditions for a lower eluent consumption will be those calculated for a combination in which the p_B parameter has the lowest value possible and the value of p_I is chosen in a way that the mixture (α_{IA}; α_{BI}) to be separated lies on the line of delimitation of strategy.

Analysis of the p_A Parameter

To complement this analysis on the effect of the p_i parameters in the operation of the JO system, Fig. 8 shows the performance when the system is working with operational conditions calculated with the combinations ($p_A = (3.6 + x_{A,3,S1})/L_C$, $(0.4 + x_{A,3,S1})/L_C$ and $x_{A,3,S1}/L_C$, $p_I = 1$; $p_B = 2.5$). As mentioned before, the value of the parameter p_A does not interfere with the calculations of the operational conditions by strategy 1. This means that the plot built with the combination ($p_A = x_{A,3,S1}/L_C$; $p_I = 1$; $p_B = 2.5$) is also valid for the cases of p_A equal to $(3.6 + x_{A,3,S1})/L_C$ and $(0.4 + x_{A,3,S1})/L_C$ where strategy 1 can be applied.

One can observe that in separating any ternary mixture (1.5; $\alpha_{BI} > 1.43$), when strategy 2 is necessary, the lower dilution of species A and B are obtained when the minimum value of p_A is used. The dilution of species I is not affected too much in this analysis. Also increasing the value of p_A, the

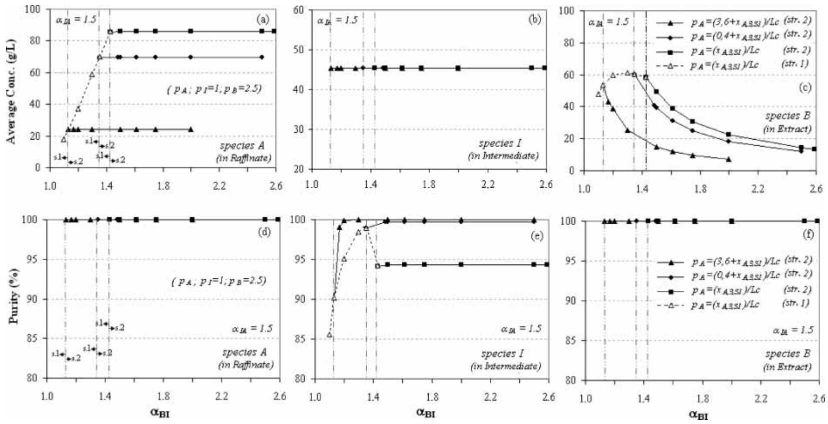


Figure 8. Average concentration and purity of the species in enrichment streams of the 4-section JO as a function of the separation factor α_{BI} ($\alpha_{IA} = 1.5$) Operational conditions: Step 1 from Table 2 and Step 2 from strategy 1 and 2 for the combinations ($p_A = (3.6 + x_{A,3,S1})/L_C$, $(0.4 + x_{A,3,S1})/L_C$ and $x_{A,3,S1}/L_C$; $p_I = 1$; $p_B = 2.5$).

purity of the intermediate species is increased. Of course, due to the displacement of the species A along with the liquid phase, it is prevented that such species spread over section 2. Thus, when larger values of p_A are used, the contamination of the intermediate stream in the separation of the mixtures with small α_{BI} is mainly due to species B.

Considering the operational conditions defined by strategy 2, Figs. 8d–f show that the purity of the components A and B for mixtures (1.5; α_{BI}) is not influenced by the changing the p_A parameter.

Figure 9 shows the average eluent consumption of the JO system when operational conditions of the step 2 are calculated with different values of p_A. One notices that strategy 1 leads to lower eluent consumption than strategy 2 for the separation of mixtures (1.5; $1.12 < \alpha_{BI} < 1.42$). In Figs. 8a and 8c, one can verify that strategy 1 for $1.12 < \alpha_{BI} < 1.42$ would also allow more concentrated species A and B in their collection streams. However, if strategy 1 is applied, a larger contamination at the intermediate outlet is observed.

This analysis indicates that when the purity of component I is an important requirement, an increment in the value of p_A parameter could avoid the contamination of I by the species A.

Design of a JO System

A methodology for the design of a 4-section JO is proposed for the separation of ternary mixtures under conditions of linear adsorption isotherms. The design consists in determining the columns dimension, duration of steps in a JO cycle, flow rates in sections in both steps that allow required purities

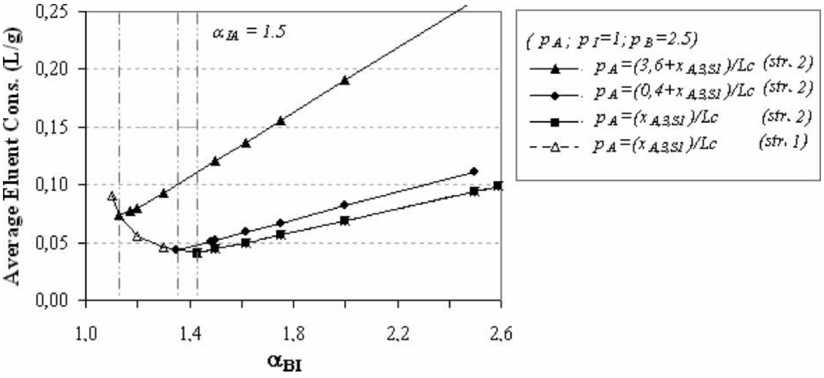


Figure 9. Average eluent consumption in the 4-section JO as a function of the separation factor α_{BI} ($\alpha_{IA} = 1.5$). Operational conditions: Step 1 from Table 2 and Step 2 from strategy 1 and 2 for the combinations ($p_A = (3.6 + x_{A,3,S1})/L_C$, $(0.4 + x_{A,3,S1})/L_C$ and $x_{A,3,S1}/L_C$; $p_I = 1$; $p_B = 2.5$).

at the outlet streams with a given productivity and taking into account the pressure drop limit imposed by the packing material in the system. The algorithm uses the mathematical model mentioned for the prediction of the behavior and performance of the unit.

If the behavior shown in Fig. 2 was achieved by the proper selection of the section flow rates in both steps and the solid flow rate in step 2, product dilution and eluent consumption would be minimized. Of course, this idealized behavior of the concentration waves of the species into JO sections is not feasible to be obtained. As known during the step 1, there is a grouping between the breakthrough curves of the species A and I from feed operation and the pre-existing concentration waves in sections 3 and 4 of these species from a previous cycle. There is also a grouping between the concentration waves of the species B during the step 2. These associations of concentration waves will lead to the peculiar behaviors of the profiles. In design procedure, we must find operational conditions in a way that the system operates close to the ideal behavior or a desired operation.

In this design algorithm, the input data are the composition of the ternary mixture to be separated, the adsorption kinetics and equilibrium parameters for all species and the time averaged feed flow rate (Q^c_{Fe}). The term of "time averaged feed flow rate" is used to differentiate the Q^c_{Fe} flow rate from the feed flow rate (Q_f) applied in discontinuous way in the JO system. The maximum pressure drop in a column, the column length to diameter ratio, and the number total of columns are also input parameters. The length-to-diameter ratio plays a significant role in bed dynamics; pressure drop, flow distribution, and wall effects are related to this ratio. Based on productivity requirements, the dimensions of columns may be calculated:

$$\mathrm{Pr}_i = \frac{Q^c_{Fe} C_{i,Fe}}{N_{TC}(1-\varepsilon)V_C}(i = A, I, B) \tag{8}$$

where N_{TC} is the total number of column in unit.

In each step of the system, the highest flow rate can be found in section 1. Thus, the velocity in section 1 cannot exceed the allowed maximum velocity defined by the upper boundary for pressure drop in a column either in step 1 or in step 2. When the pressure drop is the highest possible in a system, a highest production is expected. However, there is a trade off between the throughput and product purity. In general, a lower throughput results in higher product purity and vice versa. Starting with the step 1, a correlation relating the pressure drop with the liquid dynamics properties of the columns, such as the Karman Kozeny equation – Eq. (9) –, allows the calculation of the flow rate in section 1. The values of t_{S1} and Q_f can be defined with an initial guess for the parameters p_{ts1} and p_{Qs1} (range for these parameters was discussed previously). In fact, there is only feed flow rate Q_f during step 1 in the JO system; however, the cycle has two steps ($t_{S1} + t_{S2}$). Therefore, the time average feed flow rate and the feed flow rate in the step 1 are related as in Eq. (10).

$$\frac{\Delta P_{k,Sn}}{L_C} = 150 \frac{(1-\varepsilon)^2}{\varepsilon^2 d_p^2} \mu \, v_{k,Sn} \tag{9}$$

$$Q_{Fe}^c = Q_f \frac{t_{S1}}{t_{S1} + t_{S2}} \tag{10}$$

Equation (10) is used for the calculation of t_{S2} such that, at least, the required productivity is achieved. In order to define the solid and liquid flow rates in each section of step 2, parameters p_i (p_A; p_B; p_C) must be chosen and one of the discussed strategies will be used. The designed operation conditions for the 4-section JO are validated by simulation using the model and must satisfy purity constraints. The objective function can be the productivity and the goal will be to find a maximum throughput for a given purity requirement for all three species.

The performance variables calculated by simulation are compared with those required ones. If any constraint is not satisfied, some decisions must be taken to obtain the desired performance. These decisions to find new operational conditions in order to satisfy the performance constraints should be made in such a way that the desired initial productivity is maintained. Figure 10 shows a flow sheet of an algorithm to be a help tool in the design of operational conditions for 4-section JO. The decision-making process of the algorithm is dependent on different contamination situations taking place in a particular process. The algorithm takes as constraint the required purity of the three species to be recovered from the unit. Based on the results, the following applicable rules to satisfy the constraints of purity of the different components are:

(1a) If species A in the raffinate is being contaminated by species I: in order to prevent contamination of the raffinate, section 3 can be increased (only changing the configuration) or the wave concentration of species I can be placed far away from the raffinate (increasing the value of p_I). Another action can be the reduction of the load parameter p_{tS1}. However, it will cause a decrease in JO feed flow rate and consequently a reduction of the value of t_{S2}, which leads to a broadening of the concentration waves. The minimum possible value of t_{S2} must also take into account that the maximum possible flow rate in section 1 during the step 2 is not exceeded (according to the allowed maximum pressure drop). The higher loading on the unit, the more concentrated solutions in outlet streams (19);

(1b) If species A in the raffinate is being contaminated by species B: consider the increasing on the β_I parameter. It is worth noting that the condition of $\beta_I > 1$ in Eq. (T9) does not completely guarantee that species B remains in section 1 when mass transfer resistance is there.

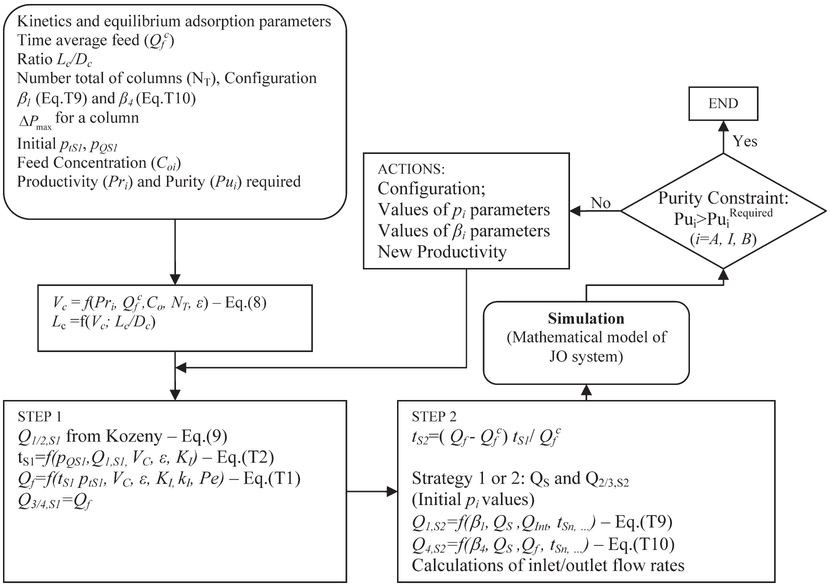


Figure 10. Flow chart of the algorithm used to design 4-section JO dimensions and operating conditions for both operation steps.

(2a) If species *B* in the extract is being contaminated by species *I*: it occurs when the tail of the concentration wave of this compound reaches the collection port of *B* compound in that time calculated for step 2. This can be avoided by changing the position of the wave of *I* for a location away from the extract, i.e., diminishing the parameter p_I. Alternatively, section 2 can be increased (altering the configuration). The reduction of p_{tS1} is also another option but with those consequences discussed before;

(2b) If species *B* in the extract is being contaminated by species *A*: when the flow rate in section 4 is so high in order to allow species *A* to go from the section 4 to section 1, one can decrease the value of β_4 parameter.

(3a) If species *I* in the intermediate stream is being contaminated by species *A*: consider the increase of p_A to move the wave concentration of *A* to far from the collect port of species *I*;

(3b) If species *I* in the intermediate stream is being contaminated by species *B*: consider the increasing parameter p_B, which moves species *B* away from the collection port of species *I*. However, this action leads to larger eluent consumption. Another alternative is to set smaller values of p_{QS1} in Eq. (T2), which leads to a decreasing in the time of elution of the intermediate *I* and consequently a reduction in the possibility of contamination of *I* by species *B*. Nevertheless, this choice can mean an accumulation of a larger amount of species *I* in the system and it is necessary to check if this will affect the purity of the extract.

Moreover, it also leads to a larger feed flow rate in the step 1, which can lead to a contamination of the raffinate by species *I*.

One notices that some decisions to satisfy a certain constraint can also affect the behavior and the performance of the system for the other species of the mixture. Hence, if the required productivity does not allow the desired purity at the collection outlet, it can be necessary to revise the performance constraints. For example, if there is an excessively high throughput, a required purity can be impracticable on a given JO system. A new value of productivity must be assigned if the constraint of purity is not satisfied.

Application of the Design Methodology

The design procedure of the Fig. 10 is applied to a 4-section JO to separate ternary mixture of sugars. Equilibrium and mass transfer parameters are listed in Table 4 (26). Those adsorption parameters were obtained from columns packed with silica gel (particle size 22 μm; $\varepsilon = 0.45$; at 25°C). For a feed concentration of 100 g/L each sugar, two situations are considered: (1) a mixture of fructose, raffinose and dextran T6 and (2) a mixture of dextran T6, dextran T9 and raffinose. The performance of the JO system is compared with two SMB in series for both the situations and considering a productivity equal to 2.5 g/L h (according to Eq. (8)). The input parameters used to JO design are also described in Table 4. These parameters are used for both the analyzed mixtures (except JO system configuration for the case of mixture 2).

Mixture 1

The difficulty of separation of this first ternary mixture—fructose (*B*), raffinose (*I*), and dextran T6 (*A*)—can be considered hard to separate the fructose from the raffinose ($\alpha_{FrRa} = 1.23$) and easy to separate the raffinose from the dextran T6 ($\alpha_{RaT6} = 2.43$). For the required productivity and 65 mL/min time average feed flow rate, the column dimensions calculated by the Eq. (8) for the 4-section JO (12 columns) are 1.63 m and 0.136 m I.D. We have assumed a maximum pressure limit at 55 bar per

Table 4. Adsorption parameters for separating sugars in silica gel at 25°C (26) and input parameters used in JO design algorithm illustrated in Fig. 10

Species	K	k, s^{-1}	Input parameters in design flow sheet			
Fructose	0.69	0.010	$\Delta P^{\max}$	55 bar	C_{oi}	100 g/L each
Raffinose	0.56	0.047	Productivity	2.5 g/L h	p_{tS1}; p_{QS1}	1; 2
Dextran T6	0.23	0.057	L_c/D_c	12	β_1; β_4	1.1; 1.1
Dextran T9	0.13	0.091	Q_F^c	65 mL/min	JO Config.	2/4/4/2

column in JO configuration (including columns packing itself and connections and valves). This high limit value for column pressure drop is due to the particle size used in the experiments from the literature. Energy cost associated with pumping or the packing mechanical strength limitations is not discussed; however, a profitable column pressure drop would allow us to perform the same analysis shown. The performance is represented by the purity, the recovery, the average concentration in enriched stream and the eluent consumption.

Since the most difficult separation is between the fructose and raffinose when both must be propagated in the solid phase direction, strategy 1 has been used to find the operational variables $Q_{2/3,S2}$ and Q_S in the system. According to the analysis performed on p_{i} parameters, a more concentrated product in the extract would be obtained if the value of parameter p_B was low. The value of p_I also affects the average concentration of collection of the species B (fructose), and larger values lead to an increment in this performance variable. Although, it has been verified that lower values of p_I lead to an increase in extract purity. Such statements can be evidenced by the analysis of the Table 5 showing the cases of ($p_A = 1$; $p_I = 0.6$; $p_B = 2.6$) and ($p_A = 1$; $p_I = 1.6$; $p_B = 2.6$). This last combination ensures more concentrated fructose in the extract but with lower purity.

As discussed, the lower dilution condition for the weakly adsorbed species is obtained when the pair (α_{IA}; α_{BI}) lies on the line of limitation of strategy for a certain combination (p_A; p_I; p_B). Due to the low mass transfer coefficients, this condition does not provide pure products in collection outlets for the required productivity, amongst the listed combinations of p_i in Table 5. For lower mass transfer coefficient for the species, concentration waves are quite broader which increases the possibility of contamination in collection outlets. The set of ($p_A = 1$; $p_I = 1.6$; $p_B = 2.6$) is that one where ($\alpha_{IA} = 2.43$; $\alpha_{B\mathrm{I}} = 1.23$) is located closer to the line of limitation of strategy and, therefore, dextran T6 is more concentrated in raffinate and lower average eluent consumption is obtained.

With regard to the intermediate component (raffinose), the trend shown in Table 5 is that the purity of raffinose becomes higher when the difference between p_I and p_B is higher. Although, larger flow rates in section 2 and 3 in step 2 and the larger solid flow rate are required in these situations leading to broader concentration waves and to larger dilution of the species in the outlets streams.

The design results obtained from the set ($p_A = 1$; $p_I = 1.4$; $p_B = 3$) show a situation where higher purity and recovery are achieved with more concentrated products for the three components of mixture. The result for this combination ($p_A = 1$; $p_I = 1.4$; $p_B = 3$) can be compared with three other situations shown in Table 5:

a. the same configuration is kept but with the half of the project parameter L_c/D_c (=6);

Table 5. Comparison of design Results for values of p_i parameters (configuration 2/4/4/2). Mixture 1: dextran T6 (A); raffinose(I); fructose (B)

(p_A; p_I; p_B)	Species	Purity, %	Recovery, %	Av. Conc., g/L	El. Cons., L/g
(1; 0.6; 2.6)	D.T6 (Ra)	97.2	100	13.5	0.13
	Raf (Int St.)	84.2	94.9	37.6	
	Fr (Ex)	99.9	82.1	26.7	
(1; 0.6; 3.0)	D.T6 (Ra)	94.7	100	11.3	0.15
	Raf (Int St.)	89.8	92.6	36.7	
	Fr (Ex)	99.5	89.2	22.8	
(1; 1.6; 2.6)	D.T6 (Ra)	100	99.9	36.7	0.07
	Raf (Int St.)	93.4	92.0	36.5	
	Fr (Ex)	96.1	93.5	39.0	
(1; 1.6; 3.8)	D.T6 (Ra)	99.7	100	13.9	0.14
	Raf (Int St.)	98.7	85.3	33.8	
	Fr (Ex)	87.5	98.7	20.0	
(1; 1.4; 3.0)	D.T6 (Ra)	99.9	99.7	19.4	0.10
	Raf (Int St.)	95.7	96.2	38.1	
	Fr (Ex)	97.0	95.8	28.4	
(1; 1.4; 2.8)[a]	D.T6 (Ra)	100	100	22.7	0.09
	Raf (Int St.)	95.0	95.2	37.7	
	Fr (Ex)	95.2	95.0	32.2	
(1; 1.4; 3.0)[b]	D.T6 (Ra)	99.9	99.7	17.8	0.11
	Raf (Int St.)	95.2	96.3	34.8	
	Fr (Ex)	96.8	95.2	26.0	
SMB1 + SMB2[c]	D.T6 (Ra)	98.1 (99.9)	98.9 (99.5)	87.6 (93.4)	0.18 (0.07)
(SMB1 + SMB2)[d]	Raf (Int St.)	81.0 (99.1)	89.2 (98.4)	25.7 (34.7)	
	Fr (Ex)	88.3 (98.5)	79.1 (99.0)	7.5 (35.4)	

[a] Configuration – 3/3/3/3;

[b] $L_C/D_C = 6$;

[c] SMBs in cascade with 12 columns; configuration: SMB1-1/2/2/1 and SMB2- 1/2/2/1. SMB model is used.

[d] SMBs in cascade with 24 columns; configuration: SMB1-2/3/3/2 and SMB2- 3/4/4/3. TMB model is used.

b. for a new configuration 3/3/3/3 and
c. two SMB in series.

The SMB operational conditions are described in Table 6 (obtained from the equilibrium theory) and they must have:

i. the same time average feed flow rate required in JO operation;
ii. the same adsorbent volume and number of columns used in the 4-section JO;
iii. the same condition of maximum pressure in the system.

Table 6. Operational conditions for separation of (a) mixture 1 – fructose, raffinose, dextran T6 – and (b) mixture 2 – raffinose, dextran T6 and dextran T9 – by two four-section SMBs in row

	Mixture 1		Mixture 2	
	First SMB[a]	Second SMB[b]	First SMB[a]	Second SMB[b]
Feed (mL/min)	65.16	117.71	65.00	106.79
Raffinate (mL/min)	73.57	224.72	106.79	175.44
Recycle (mL/min)	214.02	1367.77	206.19	1385.50
Extract (mL/min)	117.71	684.86	90.54	228.84
Swit. Time (min)	61.68	12.11	55.85	8.5
Feed Conc. (g/L)	100 g/L each (*Fr, Raf, T6*)	55 g/L each (*Fr, Raf*)	100 g/L each (*Raf, T6, T9*)	55 g/L each (*T6, T9*)
Config.	1/2/2/1	1/2/2/1	1/2/2/1	1/2/2/1

[a] $L_C = 1.63$ m; $D_C = 0.136$ m.
[b] $L_C = 1.03$ m; $D_C = 0.171$ m.

The reduction of the L_c/D_c ratio leads to an increase of the intermittent feed flow rate in JO system and consequently to a lower loading time (since the productivity must be the same). The obtained performance is not so different from that for $L_c/D_c = 12$. For the configuration 3/3/3/3, the design algorithm shows that the better performance achieved by the JO system, considering the analysed set of p_i parameters, is for the combination ($p_A = 1$; $p_I = 1.4$; $p_B = 2.8$). As expected, there is a slight reduction in the purity of the strongly adsorbed component and also a more concentrated product in raffinate.

The performance variables of two SMBs in cascade and of the 4-section JO can be compared in Table 5. The purity of the fructose and raffinose obtained from the SMBs in row is lower than that reached using the 4-section JO. The connection between the SMBs is carried out by the extract outlet of the first SMB containing fructose and raffinose. The mixture (fructose + raffinose; T6) to be separated in the first SMB is classified as an easy separation and a high performance is expected. However, the second SMB must perform the harder separation. It is well known that the complete separation conditions (i.e., constraints of sections 1 to 4) for SMB units are considerably different from those calculated from the equilibrium theory when mass transfer effects are present. Hence, considering the required feed flow rate to be processed by the SMB2 and the low mass transfer coefficients of the involved species, the complete separation is unfeasible in this second unit. In this case, the JO system provides the best performance variables. However, it is worth mentioning that the cascade of SMBs can perform better than JO system if number of columns is higher (e.g., 24) and properly distributed in the two SMBs for adequate operational conditions (as an example, 10 columns in first SMB and 14 columns in second SMB).

Mixture 2

The separation of the mixture 2 – dextran T9 (A), dextran T6 (I) and raffinose (B) – is performed using the column set as before for mixture 1, since the input parameters of the design algorithm are the same: $Pr = 2.5\ \mathrm{g/L \cdot h}$; $L_c/D_c = 12$ and a maximum pressure of 55 bar. This separation is different from the previous one because the hard separation is between the weakly adsorbed species and the compound with intermediate affinity to the adsorbent. The degree of difficulty to separate the intermediate compound and strongly adsorbed species is considered easy.

This kind of mixture – ($\alpha_{IA} = 1.77$; $\alpha_{BI} = 2.43$) – favors the use of strategy 2 since the separation of B is not critical. The operational conditions for step 1 are determined from the application of the design flow chart using $p_{tS1} = 1$ and $p_{Qs1} = 2$, while strategy 2 is applied for step 2. Some results from the design algorithm for the separation of the mixture 2 are showed in Table 7.

Lower eluent consumption is achieved when smaller values of p_A and p_I are used (p_B does not interfere with the definition of the operational conditions in strategy 2). However, the purity of the dextran T6 (species I) is lower when p_A is small due to the low mass transfer coefficient of the dextran T9 (species A) mainly. The conditions allowing the species A to travel towards the raffinate lead to the increase of the eluent consumption and to the dilution of the species in outlets.

The increase of p_I leads to a higher purity of the dextran T9 (A) and a higher recovery of the dextran T6 (I) but it also leads to the decrease of the purity of the raffinose (B) and the decrease of the recovery of the dextran T9 (A) mainly. The higher the difference between the p_I and p_A is, the higher the flow rates in the system are; therefore, for larger mass transfer resistance, the concentration waves of the species becomes more dispersed allowing species to enter into unwanted sections. A favorable condition for the separation of these three species is the combination ($p_A = 2.17$; $p_I = 0.6$; $p_B = 2.5$), where purities above 90% can be reached. Although, when comparing this performance with the performance from the system of SMBs in cascade, one can verify that this last is quite superior in almost all performance variables (operational conditions for the two SMBs in series are described in Table 6).

It is worth reporting that two SMB units involve a larger number of valves and connections and then a detailed economic study should be done to confirm this choice instead of the JO technology. Of course, the SMB in cascade has larger degree of freedom (i.e. flexibility) for operation and there is a well-established theory for such technology.

Table 7. Comparison of design results for values of p_i parameters (configuration 3/3/3/3). Mixture 2: dextran T9 (A); dextran T6 (I); raffinose (B)

(p_A; p_I; p_B)	Species	Purity, %	Recovery, %	Av. conc., g/L	El. cons., L/g
(0.45; 0.4; 2.5)	D.T9 (Ra)	99.8	76.5	68.44	0.05
	D.T6 (Int St.)	80.6	94.6	38.4	
	Raf (Ex)	100	97.8	41.5	
(2.17; 0.4; 2.5)	D.T9 (Ra)	89.1	87.4	26.8	0.15
	D.T6 (Int St.)	90.7	87.1	35.3	
	Raf (Ex)	96.2	100	10.3	
(0.45; 1.4; 2.5)	D.T9 (Ra)	100	56.6	44.8	0.14
	D.T6 (Int St.)	71.3	95.2	38.6	
	Raf (Ex)	92.9	100	12.0	
(1.18; 1.4; 2.5)	D.T9 (Ra)	99.9	70.7	32.4	0.18
	D.T6 (Int St.)	79.5	89.5	36.3	
	Raf (Ex)	85.8	100	8.7	
(2.17; 0.6; 2.5)	D.T9 (Ra)	94.4	85.2	25.9	0.17
	D.T6 (Int St.)	90.1	93.1	37.8	
	Raf (Ex)	94.8	100	9.1	
SMB1 + SMB2[a]	D.T9 (Ra)	98.5	96.3	35.8	0.08
	D.T6 (Int St.)	98.4	98.0	28.0	
	Raf (Ex)	99.9	99.5	71.5	

[a] SMBs in cascade with 12 columns; configuration: SMB1-1/2/2/1 and SMB2-1/2/2/1. SMB model is used.

CONCLUSIONS

A design methodology used to determine the flow rates and the operation time of both operation modes in a 4-section JO has been proposed based on the equilibrium theory for compounds characterized by linear adsorption isotherms. The design algorithm used a dispersive plug flow model for obtaining the JO system performance for the separation of ternary mixtures.

When the system operates in SMB mode, two strategies for the definition of the two critical flow rates in the JO system (in sections 2 and 3) and solid flow rate are suggested. The application of these strategies depends on the degree of separation difficulty of the components in the mixture and the positioning of the concentration waves of these species in the four sections of the system. The p_i parameters are linked to the positioning of the concentration waves of the species in JO sections and constraints on these p_i parameters for the use of one or another strategy in a given mixture is shown.

It was found that the JO system performance is strongly sensitive to the chosen values of the positioning parameters. There is also a complex connection among the performance parameters for the three species of the mixture.

For this reason, the choice of the best set of p_i parameter depends on the performance parameter one want to maximize or on the more valuable compound.

The proposed design methodology was applied for two cases of sugar ternary mixtures: mixture ($\alpha_{RaT6} = 2.43$; $\alpha_{FrRa} = 1.23$) and mixture ($\alpha_{T6T9} = 1.77$; $\alpha_{RaT6} = 2.43$). The trend on the 4-section JO performance and behavior in the separation of the ternary mixtures in relation to the chosen p_i parameters has been tested. For example, one can observe that a decrease in value of p_A keeping with the values of p_B and p_I leads to a higher purity of the intermediate species and a more concentrated product in raffinate (with lower eluent consumption); or decreasing the value of p_I, a more diluted product will be in extract and raffinate with larger eluent consumption but also with higher purity of the extract product. In order to complete the performance map formulated from this work, an optimization algorithm should be addressed to establish the best operational conditions to be applied.

Finally, the comparison between two SMBs in cascade and a 4-section JO for the two ternary mixtures shows that this last can lead to better performance when mass transfer effects are present. A final decision on which alternative could be more advantageous needs a cost analysis, since two SMBs in cascade would involve a large set of valves and other additional accessories.

NOTATION

A_C	cross-section area of a JO column, m^2
C	liquid phase concentration, g/L
$\bar{C}$	average concentration, g/L
d_p	particle diameter, m
D_c	column diameter, m
D	axial dispersion coefficient, m^2/s
E_C	eluent consumption, L/g
k_i	mass transfer coefficient, s^{-1}
K	linear adsorption constant, dimensionless
L_c	column length, m
n_{Se2}; n_{Se3}	number of columns in section 2; in section 3, dimensionless
p	parameter for the positioning of conc. peak – step 2 (4-JO), dimensionless
p_{tS1}; p_{QS1}	operational parameters in Eqs. (T1)–(T2) – step 1, dimensionless
Pe	Peclet number, dimensionless
$\bar{q}$	average adsorbed phase concentration, g/L
q^*	adsorbed concentration in equilibrium with liquid concentration, g/L
Pu	purity, dimensionless

Pr	productivity, g/L · h
Q^c_{Fe}	averaged time feed flow rate, m^3/s
Q, Q_S	liquid and solid flow rate, respectively, m^3/s
Re	recovery, dimensionless
t^*	switching time, s
$\bar{t}$	retention time, s
$t_{S1}; t_{S2}$	operation time of step 1; of step 2, s
u_S	interstitial solid velocity, m/s
v	interstitial liquid velocity, m/s
V_C	column volume, m^3
x	position of concentration propagation, m
z	axial coordinate, m

Greek Letters

α	separation factor, dimensionless
β	operational parameter in Eqs. (T9)–(T10) – step 2, dimensionless
ε	bed porosity, dimensionless
θ	related to the cycle in JO process

Subscripts and Superscripts

A, B, I	less, more and intermediate retained species, respectively
$El; Ex$	eluent; extract
f	feed stream
i	chemical species
Int	intermediate stream
$j; k$	JO sections; JO columns
m	external streams in JO system
n	step index
Ra	raffinate stream
$S1; S2$	related to the step 1; to the step 2

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