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Influence of the Transfer Line Dead Volume on the Performance of an Industrial Scale Simulated Moving Bed for p-Xylene Separation

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ABSTRACT

The modeling and simulation of simulated moving bed (SMB) unit is needed for the choice of its operating conditions; however, it usually does not consider the surrounding equipment (pipe transfer lines, valves, and pumps). The effect of the dead volume on SMB performance is normally associated with laboratory scale units, where the volume of the surrounding equipment could represent significant part of SMB unit volume. The presence of the dead volume is also significant in the industrial-scale SMB units applied for production of high purity component; for example, p-xylene. Different techniques are applied in industry to overcome the negative impact of the dead volume on the SMB performance. In this work,

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the UOP technique for flushing of the transfer lines before withdrawing the extract, applied in Parex process/(industrial scale SMB unit for p-xylene separation) was analyzed. First, the need of the flushing lines was assessed by simulation of SMB unit in presence of the transfer lines' dead volume. The simulated moving bed strategy of modeling was used; the transfer lines' dead volume was introduced into the model through the node mass balances and was assumed as plug flow and continuous stirred tank in different stages of the transfer line use. The transfer lines' dead volume has negative effect on the extract purity. The extract purity falls to 85.54% and 75.22% when the total transfer line dead volume is 0.6% and 1% of the total SMB unit volume, respectively. The advantage of the flushing lines in presence of transfer line dead volume was demonstrated by simulation of Parex unit allowing extract purity above 99.9% and recovery above 98.5%.

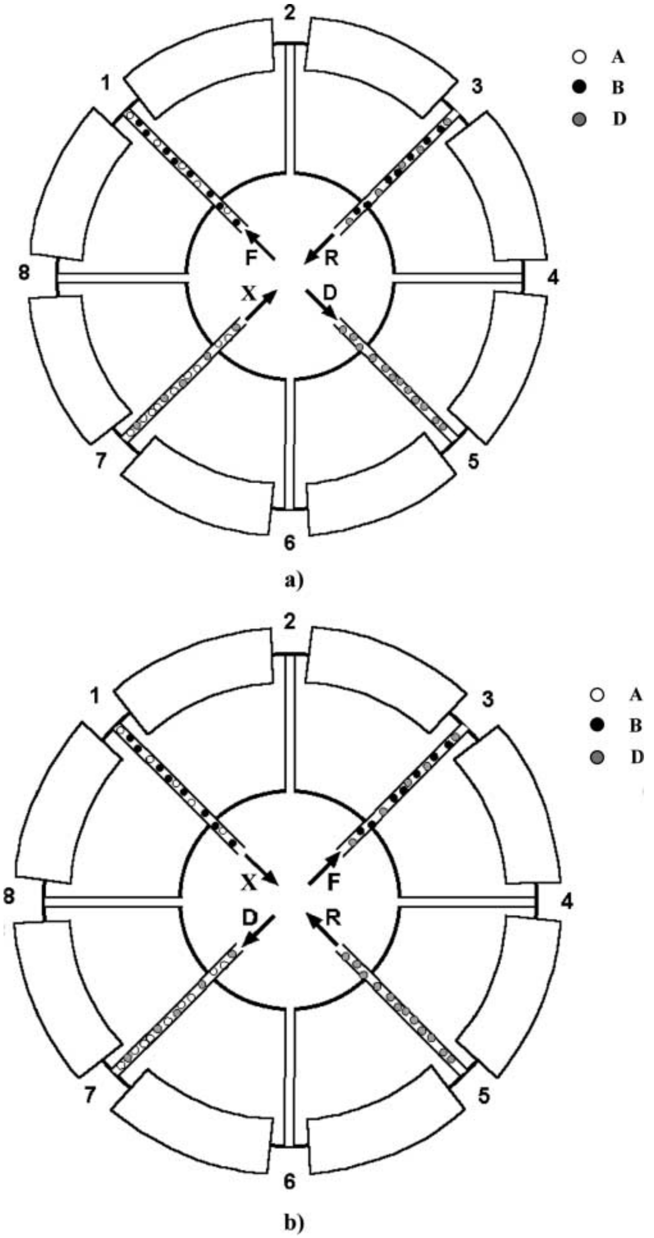
Key Words: Simulated moving bed; p-Xylene separation; Parex process; Dead volume; Flushing technique.

INTRODUCTION

Xylene isomers are used on large scale as industrial solvents or intermediates for many derivatives. The most important isomer in the modern polyester industry is p-xylene, which is almost exclusively used for polyester and polyethylene terephtalate production. The p-xylene demand is determined by the polyester demand, which is directly linked to its use in packaging of food products, and in particular, in containers for beverages.[1] The average annual growth rate for p-xylene is expected to be 6% for the next decade.[2]

A classical problem in the petrochemical industry is the separation of the xylene isomers, because of their close boiling points. The first separation processes were based on solvent extraction or crystallization. Since 1971, when UOP commercialized the first Parex unit,[3] simulated moving bed (SMB) chromatography has emerged as a superior technology for continuous counter current separation of a p-xylene from C_8 aromatics mixture. Typical p-xylene recovery per pass is more than 95% for simulated moving bed technology, compared with only 60% to 65% for crystallization.[4]

Today there are three main industrial processes for p-xylene separation operating on the principle of SMB technology (Fig. 1a): UOP's Parex,[3] Toray's Aromax,[5] and IFP's Eluxyl.[6] The year of commercialization, the number of the units in operation, their capacity, and the total p-xylene capacity of Parex,[7] Eluxyl,[8] and Aromax are presented in Table 1. Adsorbents such as molecular sieves, mainly zeolite X and Y exchanged with K and/or Ba, are used to produce high-purity p-xylene by preferentially removing p-xylene (A)



a)

b)

Figure 1. Schematic diagram of four-stream SMB unit with a rotary valve: a) position of the streams at t = 0 and b) position of the streams at t = 2t*.

Table 1. UOP Parex, IFP Eluxyl and Toray Aromax, year of commercialization, number of units, unit capacity, and total production capacity.

	Year of commercialization	Number of units	Unit capacity in MTA p-xylene	Total capacity in millions MTA p-xylene
UOP Parex[a]	1971	71	24,000-1,200,000	8.2 + 5.5 (in construction)
IFP Eluxyl[b]	1995	7	180,000-500,000	2.5
Toray Aromax	1973	2	200,000	~0.4

[a] Parex™ Process-http://www.uop.com/framesets/petrochemicals.html

[b] Eluxyl simulated countercurrent adsorption of paraxylene IFP Industrial division brochure —http://www.cpchem.com/commoditychemicals/products/DataSheets/eluxylprocess.pdf

from mixed xylene (B) streams.[4] Separation is accomplished by exploiting the differences in affinity of adsorbent for p-xylene relative to the other C_8-isomers. The adsorbed p-xylene is removed from the adsorbent by displacement with a desorbent (D). The SMB process is realized by connecting several single chromatographic columns in series. The counter current movement is approximately realized by a cyclic switching of the inlet (feed [F] and desorbent [D]) and outlet (raffinate [R] and extract [X]) ports one column forward in fluid phase the direction (see Fig. 1a).

The position of introduction and withdrawal of the process streams divide the SMB unit into four zones, each of which performs a different function. Zone 1 is located between desorbent (D) and extract (X) nodes, and its purpose is to regenerate the adsorbent; zone 2 is between extract (X) and feed (F) nodes, and its function is to adsorb component B; zone 3 is placed between feed (F) and raffinate (R) nodes, and its function is to adsorb component A; and zone 4 is located between raffinate (R) and desorbent (D) nodes, and its purpose is to regenerate the desorbent.

The typical industrial scale SMB unit for p-xylene separation consists of 24 interconnected fixed beds between which it is possible to inject or remove the process streams.[7,9] The fixed beds are placed in two individual columns. Pumps provide the liquid circulation between two columns, allowing the two adsorbent columns to function as a single continuous loop of fixed beds. The main difference between commercial SMB units for p-xylene separation is on how the movement of the adsorbent-solid phase is simulated.

In the Parex unit the shifting of the injection and withdrawal points is realized by a complex rotary valve.[10] Each distribution plate situated between two consecutive beds is connected to one of the 24 peripheral ports of the rotary valve by a single transfer line.[7] Each transfer line is used for introducing and withdrawing the process streams (feed, extract, raffinate, and desorbent). This means that the same transfer line is used for introducing the feed into the unit and later for withdrawing the extract from the unit. This could result in reduced product purity because of contamination of the withdrawn extract by the unwanted components of the feed stream. This problem in the Parex unit is overcome by removing the residue from the transfer lines by flushing them with a medium which would not affect the extract purity.[11]

In the Eluxyl and Aromax process, individual on-off valves under computer control instead of the rotary valve are used to move inlet and withdrawal ports around the bed. In the Eluxyl units the problem of transfer lines dead volume is solved by an alternative technique that consists of connecting each distribution plate located between two consecutive beds to the exterior by at least two distinct distribution lines. One of them is used to transport the “clean” fluids (desorbent and extract), and the other for the “dirty” fluids (feed and raffinate).[12]

The adsorption of xylenes on ion-exchanged faujasite-type zeolites has been studied in the liquid phase[13–17] and also in the vapor phase.[18,19] The liquid phase xylene adsorption studies are mainly done at temperatures lower than the temperature applied in industry.[13–16]

A detailed analysis of the design and optimization of four-section laboratory SMB unit for separation of a mixture of o-, m-, and p-xylene and ethylbenzene, operating in liquid phase and vapor phase has been presented by Storti et al.[20]

There are two main approaches for modeling of the SMB process: the true moving bed (TMB) approach and the SMB approach. The first one treats the simulated moving bed process as the equivalent true moving system. The second approach represents the actual simulated moving bed configuration. Each of these two modeling strategies leads to models with different degrees of complexity depending of the detail of the description of SMB unit operation. The final purpose of these models is to be used for simulation of the operation of real industrial SMB separation process, namely for tuning the industrial operating conditions in order to get best unit performance. Only few models[9,21,22] take into account the effect of the surrounding equipment (valves, pumps, and transfer pipe lines).

Azevedo et al.[23] used the TMB modeling strategy to simulate the p-xylene separation (PAREX) unit operation. They used the “lumped pore diffusion model," in which mass transfer in the particle is described by linear driving force (LDF) model using an overall mass transfer coefficient, function of the local mass transfer coefficients in the external, and internal (or pore) liquid phase. Later the model was extended including the dead volume because of piping and recirculating pumps.[21] The flow pattern inside the dead zone was treated either as a plug flow or as an ideal mixed tank. They show that even the presence of very small dead volume (1% of total volume) affects the unit performance, yielding considerably worse performance for the plug flow approach.

Migliorini et al.[22] analyzed the effect of the extracolumn dead volume present on the small-scale SMB unit performance. For this purpose, they used a detailed mathematical model that accounts for the dead volumes, assumed to be located at the beginning and end of the column. The model accounts for the mixing effects in the dead volume, which can be tuned between plug flow and perfectly stirred tank.

Pavone and Hotier[10] simulated the real cases that can happen during the Eluxyl operation, such as slow opening and closing of the valves, a missing valve under maintenance, and leaking of a valve. They also show that the systems approach modeling can be used for selecting the best design of the mixing chambers required for the Eluxyl process.

The aim of this work is:

1. To study the effect of the transfer line dead volume on the SMB performance and
2. To illustrate the UOP flushing line technique for overcoming the negative effect of transfer line dead volume on the SMB performances.

Both aims relate to the industrial-scale SMB unit for separation of p-xylene from C_8 aromatics fraction-Parex unit. For this purpose, the simulated moving bed strategy of modeling was used; the transfer lines' dead volume was introduced in the model through the node mass balances and was assumed as plug flow and continuous stirred tank in different stages of their use.

PAREX UNIT—WHY FLUSHING OF THE TRANSFER LINES?

The Parex unit, besides the four main SMB streams (feed, desorbent, extract, and raffinate), includes also the flushing streams. In this section the need, the purpose, and way of acting of the flushing streams will be explained in detail.

A representative SMB unit for p-xylene separation without flushing streams is presented in Fig. 1a. The unit here is constituted of eight columns for convenience; the four process streams (feed, raffinate, desorbent, and extract) divide the unit in four zones (two columns per zone). Between each two columns there is one distribution plate that is connected to the rotary valve by one transfer line. Feed is entering in the SMB unit through transfer line 1, the raffinate is leaving the unit through line 3, the desorbent is entering through line 5, and the extract is leaving the unit through line 7. After one switching period, all the streams will be shifted one column ahead. Because of the shifting of the process streams, a certain volume (equal to the volume of the transfer lines) of the feed will be kept in line 1; similarly, a certain volume of raffinate will be kept in line 3 and desorbent and extract in lines 5 and 7, respectively. It is interesting to see what will happen after two switching periods starting from the initial position of the process stream (Fig. 1b). Now, transfer line 1 is used for withdrawing the extract, line 3 for introducing the feed, line 5 for withdrawing the raffinate, and line 7 for introducing the desorbent. The residue of the feed trapped in the line 1 would contaminate the extract. The desorbent would be contaminated by the residue of the extract in line 7. This could result in reduced extract purity because of contamination of the withdrawn extract by the unwanted components of the feed stream.

In the Parex unit, this is overcome by applying the UOP technique[11] of flushing the transfer lines between withdrawing the extract and introducing the feed; and introducing the desorbent and withdrawing the extract. Figure 2a presents the same SMB unit as in Fig. 1a with two additional streams called the flushing-in and flushing-out streams. The starting position of the process streams is: line 1, feed; line 3, raffinate; line 5, desorbent; line 6, flushing-out; line 7, extract; and line 8, flushing-in. The flushing-out stream is connected to the flushing-in stream with a pump forming an internal recirculation loop; therefore, the flow rates of both streams are equal. The flushing-out stream is withdrawn between desorbent and extract stream; it is mainly the desorbent component, with the extract component (p-xylene). The flushing-out stream is recirculated and introduced in the unit between the extract and feed node as a flushing-in stream.

After one switching period (Fig. 2b) the feed would be introduced through line 2, and the raffinate would be withdrawn from line 4. Desorbent would be introduced through line 6, in which the residue of the flushing-out stream is trapped. Desorbent would not be contaminated because it is the major component of the flushing-out stream. The flushing-out stream would be taken out through line 7, which was previously used for withdrawing of the extract. The extract trapped in this transfer line would increase the concentration of the p-xylene in the flushing-out stream. This stream would be introduced in the unit as with the flushing-in stream through line 1 pushing the feed stream trapped in the line 1 into the unit. The extract

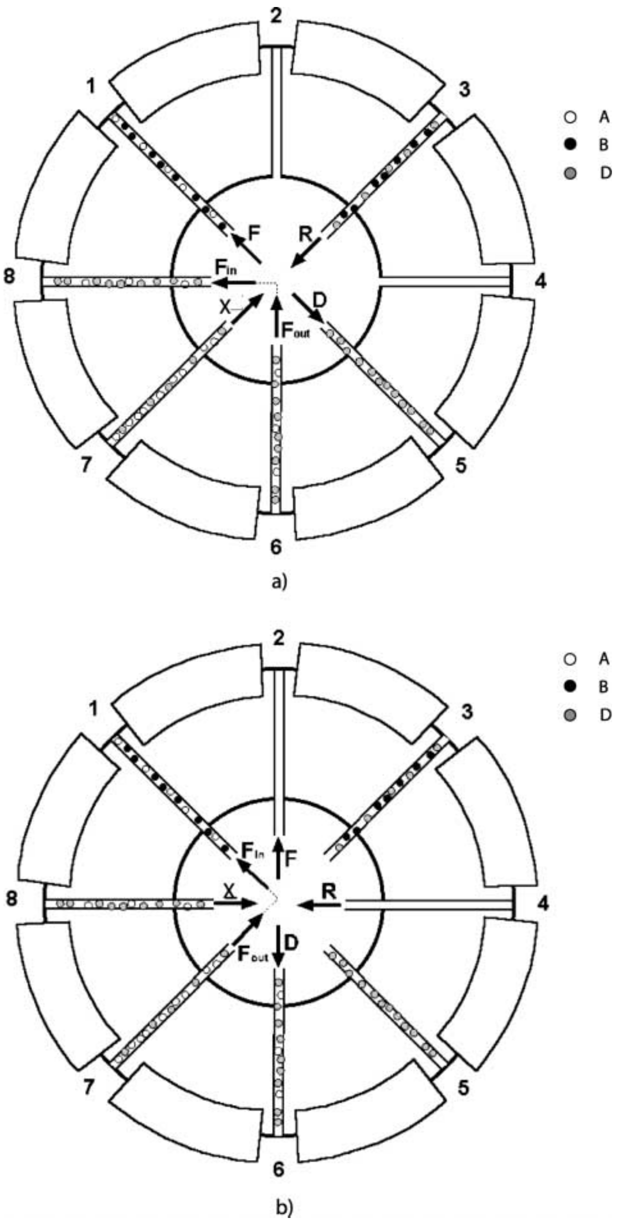


Figure 2. Schematic diagram of SMB unit with the flushing streams and a rotary valve: a) position of the streams at t = 0 and b) position of the streams at t = t*.

would be taken out from the line 8, which was previously used for introducing the flushing-in stream. In this way, the extract would not be contaminated with the unwanted component present in the feed stream, because the flushing-in stream contains the desorbent and extract component (p-xylene). In any case, the extract is going to be diluted because the desorbent is the major species in the flushing-in stream.

To overcome this problem, the secondary flushing-in stream of p-xylene is introduced between extract and flushing-in stream, which guarantees that the extract stream is always withdrawn from the line which was previously used to introduce the secondary flushing-in stream (i.e., p-xylene stream).

MODELING AND SIMULATION OF FOUR-STREAM SMB UNIT FOR p-XYLENE SEPARATION IN PRESENCE OF TRANSFER LINE DEAD VOLUME

To better understand the purpose of flushing-in and flushing-out streams, the four-stream industrial scale simulated moving bed unit for p-xylene separation, in presence of the transfer lines' dead volume was studied by simulation. The SMB unit consists of 24 adsorption columns and includes the four common SMB streams (feed, desorbent, extract, and raffinate).

The simulated moving bed strategy of modeling was used. In the formulation of the model, the following assumptions have been considered:

1. Bed void fraction, radius, and porosity of the particles are constant along the columns;
2. Mass transfer coefficients and physico-chemical parameters are independent of mixture composition;
3. Negligible thermal effects; and
4. Negligible pressure drop.

Simulated moving bed model includes axial dispersion flow for the liquid phase, LDF for the intraparticle mass transfer rate and multicomponent adsorption equilibria described by nonstoichiometric Langmuir isotherm. The model equations are:

Mass balance in a volume element of the column k:

$$\varepsilon \frac{\partial c_{ik}}{\partial t} + (1-\varepsilon)\rho_p \frac{\partial q_{ik}}{\partial t} = \varepsilon D_{L_k} \frac{\partial^2 c_{ik}}{\partial z^2} - \varepsilon v_k \frac{\partial c_{ik}}{\partial z} \tag{1}$$

Particle mass balance:

$$\frac{\partial q_{ik}}{\partial t} = k_{mi}(q_{ik}^{*} - q_{ik}) \tag{2}$$

Multicomponent adsorption equilibrium isotherm:

$$q_{ik}^{*} = \frac{q_{mi}K_i c_{ik}}{1 + \sum_{l=1}^{NC} K_j c_{lk}} \tag{3}$$

Initial conditions:

$$t = 0; \quad c_{ik} = c_{Dk}^{0} \quad q_{ik} = q_{ik}^{*}(c_{Dk}^{0}) \tag{4}$$

Boundary conditions:

$$z = 0; \quad c_{ik}^{in} = c_{ik} - \frac{D_{L_k}}{v_k}\frac{\partial c_{ik}}{\partial z} \tag{5}$$

$$z = L_k \quad \frac{dc_{ik}}{dz} = 0 \tag{6}$$

c_{ik}, q_{ik} and q_{ik}^{*} are the fluid phase, average adsorbed phase, and equilibrium adsorbed phase concentration of the component i ($i = 1, 2\ldots 5$) in k ($k = 1, 2\ldots 24$) column, respectively; K_i and q_{mi} are the adsorption equilibrium constant and adsorbed phase saturation concentration of component *i;* k_{mi} is the intraparticle mass-transfer coefficient of the component *i;* D_{Lk} is the axial dispersion coefficient in column k; v_k is the interstitial fluid velocity in k column; ρ_p is the apparent particle density; ε is the bed porosity; t is the time variable; and z is axial coordinate.

The mathematical model also accounts for the transfer lines' dead volume. Some assumptions have been made before introducing the transfer lines' dead volume in the model. As mentioned previously, each distribution plate between two columns is connected by the transfer line to the rotary valve. The length of the transfer lines is different and depends of their distance from the rotary valve. To simplify the mathematical model, it was assumed that all the lines have the same length (i.e., same volume).

During one switching period, just 4 of the 24 transfer lines were used. The number of the switching periods during one cycle (1 to 24) determines the position of the four transfer lines used for introduction and withdrawing of the process streams.

From the modeling point of view, it is necessary to distinguish three different stages during one switching period:

1. The first stage of the switching time when the liquid volume trapped in the transfer line is pushed in or out of the transfer line with the stream, which is introduced or withdrawn from the SMB unit during that switching period (which corresponds to given position of process streams). The concentration profile of the liquid volume trapped in the line is defined by the concentration profile of the stream, which was previously transported through the same line.
2. The second stage of the switching time period when the concentration of the stream entering or leaving the transfer line corresponds to the concentration of the stream entering or living the SMB unit during that particular switching time.
3. The third stage is when certain volume (equal to the volume of the transfer line) of the stream passing through the transfer line will be trapped in the line as a result of the switching of the position of the process stream. The concentration profile of the trapped liquid volume corresponds to the concentration of the stream actually passing through the transfer line and would determine the concentration profile of the liquid phase in the first stage next time when the transfer line will be used for introducing or withdrawing of some process stream.

The flow rate during all three stages is constant and corresponds to the flow rate of the stream passing through the transfer line. The flow in the transfer line is assumed as plug flow. The duration of the three stages is calculated on the basis of the stream flow rate and the line volume. The first and third stages have equal duration calculated as the ratio between the transfer line volume and stream flow rate, which corresponds to the time needed to push or fill the transfer line volume under certain stream flow rate. The duration of the second stage is calculated as the difference between the switching period and the sum of first and third stage. It should be noticed that these three stages have different duration for each of the four process streams, because they are calculated on the basis on the stream flow rates.

The time between two consecutive uses of the same transfer line is determined by the unit configuration (i.e., number of columns per zone). Therefore, the minimum time between two consecutive uses of one line could be one switching period, which corresponds to one column per zone and the maximum time would correspond to the maximum number of columns per zone. This means that the liquid volume trapped in a certain transfer line could remain in the line a different period, which will determine the concentration profile in the transfer line in the moment of its reuse.

For modeling purposes, the transfer lines were assumed to be continuous stirred tanks during the period between their two consecutive uses.

The concentration of the volume trapped in the transfer line was calculated as average value of the plug flow concentration profile in the transfer line during the third stage of its previous use.

The transfer line dead volume was modeled on the basis of above assumption. The transfer lines' dead volume was introduced in the mathematical model by the node mass balances. The node mass balances depend of the unit configuration and the steam flow rates, which set the duration of the three stages during one switching time and therefore the concentration profiles in the transfer lines. The node mass balances do not have universal form and should be written for each particular unit (configuration).

To illustrate the transfer line dead volume modeling strategy, the four-stream SMB unit for p-xylene separation was selected. The SMB unit configuration, operation conditions, and equilibrium data are presented in Table 2. The equilibrium data for the p-, m-, o-xylene; ethylbenzene; and p-diethylbenzene at 180 °C, were provided by Azevedo et al.[21] Feed was considered to be a typical C_8 aromatics mixture containing 23.6% p-xylene, 49.7% m-xylene, 12.7% o-xylene, and 14% ethylbenzene.

The node balances were written taking into consideration that: the desorbent will be always introduced in the SMB unit through the line that was used for withdrawing the extract six switching time periods ago (extract trapped in the line); the extract will be always withdrawn from the line that was used for the introduction of the feed nine switching time periods ago (feed trapped in the line); the feed will be always introduced through the line that was used for withdrawing the raffinate six switching

Table 2. Four-stream SMB unit configuration, operating conditions, and model parameters.

SMB unit geometry	Operating conditions	Model parameters
$L_c = 1.1\,\mathrm{m}$	T = 180°C, liquid phase	$Pe = v_k L_k / D_{L_k} = 2000$
$d_c = 4.1\,\mathrm{m}$	$t^* = 1.15\,\mathrm{min}$	$k = 2\,\mathrm{min}^{-1}$
		$\varepsilon = 0.39\; d_p = 9.2 \times 10^{-4}\,\mathrm{m}$
No. of columns: 24	$Q_D = 173.4\,\mathrm{m}^3/\mathrm{hr}$	
No. of zones: 4	$Q_X = 99.0\,\mathrm{m}^3/\mathrm{hr}$	$q_{mPX(MX;OX;EB)} = 0.1303\,\mathrm{kg/kg}$
	$Q_F = 87\,\mathrm{m}^3/\mathrm{hr}$	$K_{PX} = 1.0658\,\mathrm{m}^3/\mathrm{kg}$
	$Q_R = 161.4\,\mathrm{m}^3/\mathrm{hr}$	$K_{MX} = 0.2299\,\mathrm{m}^3/\mathrm{kg}$
Configuration: 6-9-6-3	$Q_1 = 496.8\,\mathrm{m}^3/\mathrm{hr}$	$K_{OX} = 0.1884\,\mathrm{m}^3/\mathrm{kg}$
		$K_{EB} = 0.3067\,\mathrm{m}^3/\mathrm{kg}$
		$q_{mPDEB} = 0.1077\,\mathrm{kg/kg}$
		$K_{PDEB} = 1.2935\,\mathrm{m}^3/\mathrm{kg}$

time periods ago (raffinate trapped in the line); and raffinate will be always withdrawn from the line that was used for the introduction of the desorbent three switching time periods ago (desorbent trapped in the line).

The total transfer line volume, $V_{l,t}$, was considered as 0.6% and 1% of the volume of the SMB unit ($V_{l,t} = 0.006^* V_{SMB}$ and $V_{l,t} = 0.01^* V_{SMB}$). Because it was assumed that all transfer lines have the same volume, the single line dead volume, V_l, was calculated as $V_l = \frac{V_{l,t}}{N_c}$; N_c is the total number of columns in the SMB unit.

The stream flow rates (Q_D, Q_X,Q_F, Q_R) and transfer line volume (V_l) were used to calculate the time in which each stream will push the liquid trapped in the transfer line or fill the transfer line with the liquid (i.e., $t_D = \frac{V_l}{Q_D}$, $t_X = \frac{V_l}{Q_X}$, $t_F = \frac{V_l}{Q_F}$, $t_R = \frac{V_l}{Q_R}$).

These times correspond to the duration of the first and third stages during one switching period for the transfer lines used for transporting of desorbent, extract, feed, and raffinate, respectively. Having all the data needed, the node mass balances are written as follows:

Desorbent node:

$$Q_4 + Q_D = Q_1 \tag{7}$$

$$c_{i,k}^{out} Q_4 + c_{i,D} Q_D = c_{i,k+1}^{in} Q_1 \tag{8}$$

Q_Z is the flow rate in zone Z (Z $= 1, 2, 3, 4$);
$c_{i,k}^{out}$ is the outlet concentration of the component i in column k; and
$c_{i,k+1}^{in}$ is the inlet concentration of the component i in column $k+1$.

Extract node:

$$Q_1 - Q_X = Q_2 \tag{9}$$

$$c_{i,k}^{out} = c_{i,k+1}^{in} \tag{10}$$

Feed node:

$$Q_2 + Q_F = Q_3 \tag{11}$$

$$c_{i,k}^{out} Q_2 + c_{i,F} Q_F = c_{i,k+1}^{in} Q_3 \tag{12}$$

Raffinate node:

$$Q_3 - Q_R = Q_4 \tag{13}$$

$$c_{i,k}^{out} = c_{i,k+1}^{in} \tag{14}$$

where in the:
First stage: $t = (Nt^*, Nt^* + t_S)$

t^* is the switching time period;

N is number of the switching time periods $N = 0, 1, 2, 3.\ldots.;$

$$c_{i,S} = \frac{\int_{(N-M_Z)t^*+(t^*-t_{S+1})}^{(N-M_Z)t^*+t^*} c_{i,S+1}\,dt}{\int_{(N-M_Z)t^*+(t^*-t_{S+1})}^{(N-M_Z)t^*+t^*} dt} \quad \text{for } S = Z = 1, 3 \quad \text{and} \quad \mathrm{N} \geq 6;$$

$$S = \mathrm{Z} = 2 \quad \text{and} \quad \mathrm{N} \geq 9;$$

$$c_{i,S} = \frac{\int_{(N-M_Z)t^*+(t^*-t_1)}^{(N-M_Z)t^*+t^*} c_{i,1}\,dt}{\int_{(N-M_Z)t^*+(t^*-t_1)}^{(N-M_Z)t^*+t^*} dt} \quad \text{for } S = Z = 4 \quad \text{and} \quad \mathrm{N} \geq 3. \tag{15}$$

otherwise, $c_{i,S} = c_{i,D}$, because, at the begining, all the columns and transfer lines are filled with desorbent.

S is the number of the stream ($S = 1, 2, 3, 4$). The streams are numbered starting from the desorbent stream and finishing with the raffinate stream (i.e., 1-desorbent [D]; 2-extract [X]; 3-feed [F]; 4-raffinate [R].

M_Z is the number of the columns in the zone Z.

Second and third stages: $t = (Nt^* + t_S, Nt^* + (t^* - t_S))$ and $t = (Nt^* + (t^* - t_S), Nt^* + t^*)$ in the inlet nodes (desorbent, feed):

$$c_{i,S} = c_{i,S} \quad \text{for} \quad \mathrm{S} = 1, 3 \tag{16a}$$

in the outlet nodes (extract, raffinate):

$$c_{i,S} = c_{i,k}^{out} = c_{i,k+1}^{in} \quad \text{for} \quad \mathrm{S} = 2, 4 \tag{16b}$$

It can be seen that the stream concentration in the second and third stages are calculated in an identical way. It was necessary to distinguish these two stages because the stream concentration histories from the third stage will be stored during the solution of the mathematical model and will be used later for calculation of the stream concentration in the first stage in the next switching periods.

The mathematical model (Eq. 1–6 and 7–16) was solved using gPROMS (general PROcess Modelling System).[24] Both space and temporal domains were discretized simultaneously. A third-order orthogonal collocation method in finite elements was used in the discretisation of spatial domain and a second-order backward difference method was used for discretization of temporal domain. It can be seen that, in the mathematical model, besides the switching of the column boundary conditions, the concentration of the process stream also changes during each switching time period as a result of the liquid trapped into the transfer line dead volume. The discretization of the time domain allows the description of the change of the process stream concentration in each moment during the switching time period. The PDAE systems (Eq. 1–6 and Eq. 7–16) are reduced directly into a set of nonlinear algebraic equations and solved using a Newton-type iterative method implement in gPROMS. All simulations were performed on Pentium III 1000 MHz processor with 725 Mb RAM memory.

The cyclic steady state concentration profiles at the end of the cycle for the total transfer line dead volume 0.6% of SMB volume ($V_{l,t} = 0.006^* V_{SMB}$) and 1% of SMB volume ($V_{l,t} = 0.01^* V_{SMB}$) are presented in Fig. 3. The concentration profiles around the feed node for $V_{l,t} = 0.006^* V_{SMB}$ are slightly above those for $V_{l,t} = 0.01^* V_{SMB}$. The main reason for this is the feed stream composition. Namely, the feed stream is introduced in the SMB through the line, which was previously used for withdraw of raffinate; therefore, the feed stream would be contaminated (diluted) by the raffinate trapped in the line. This contamination (dilution) will be more significant as the transfer line dead volume increases.

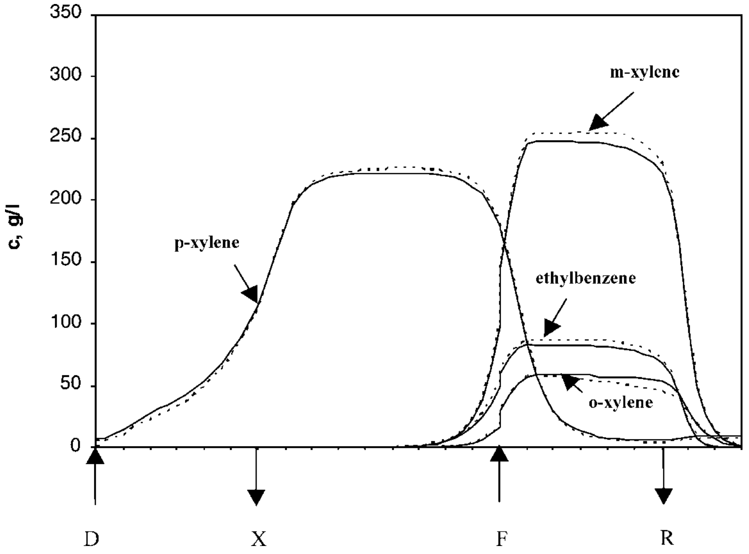


Figure 3. Cyclic steady state concentration profile (at the end of the cycle) of the four-stream SMB unit in a presence of transfer line dead volume ((- - - -$V_{l,t} = 0.006^* V_{SMB}$ and ——$V_{l,t} = 0.01^* V_{SMB}$).

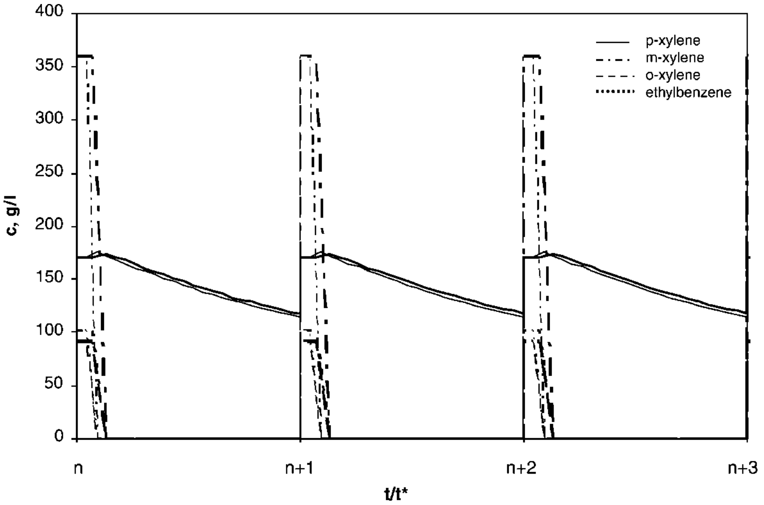
The cyclic steady state extract concentration history during few switching time periods and cyclic steady state extract performances are presented in Fig. 4a and Table 3. The equations used for calculation of extract performances are also given in Table 3. The extract purity for $V_{l,t} = 0.006{*}\,V_{SMB}$ is 85.54% and for $V_{l,t} = 0.01{*}\,V_{SMB}$ is 75.22%, as a result of the contamination of the extract by the feed trapped in the line used for withdrawing of the extract. This could be observed at the beginning of the switching period of the cyclic steady state extract concentration history presented in Fig. 4b. Higher transfer line dead volume led to a bigger quantity of the feed trapped in the line and therefore lower purity of the extract.

The purity of the extract (i.e., p-xylene) should be at least 99.9%; as mentioned previously, this was the major reason for introduction of the flushing streams technique in the Parex unit.

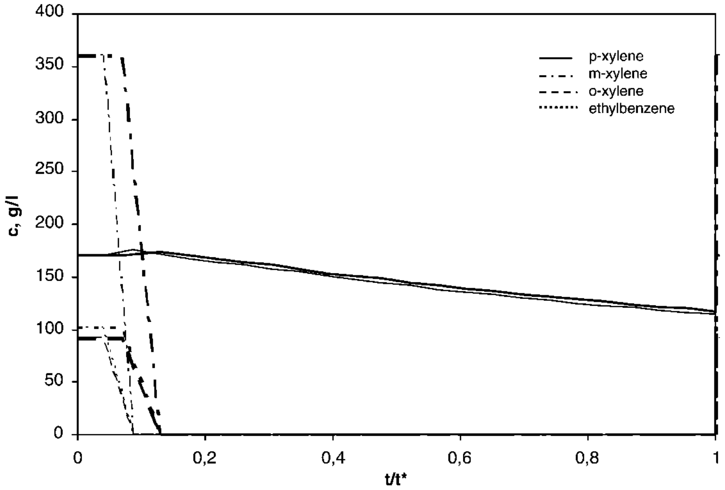
MODELING AND SIMULATION OF THE REAL PAREX UNIT INCLUDING FLUSHING-IN AND FLUSHING-OUT LINES

To illustrate the benefits of the flushing streams the real industrial scale SMB unit for PAREX including the three additional flushing streams was simulated. The unit configuration, stream flow rates, and equilibrium data used in the simulation are presented in Table 4. The total number of columns is the same in the four-stream SMB simulation. The configuration chosen for the Parex unit is 1-5-1-6-2-6-3, seven zones ($Z = 1, 2 \ldots 7$): zone 1 between desorbent and flushing-out streams, zone 2 between flushing-out and extract streams, zone 3 between extract and secondary flushing-in (p-xylene) streams, zone 4 between secondary flushing-in and flushing-in streams, zone 5 between flushing-in and feed streams, zone 6 between feed and raffinate streams, and zone 7 between raffinate and desorbent streams. The feed, desorbent, and raffinate flow rates of the real Parex unit are equal to those in the four-stream SMB unit. The extract flow rate of the real Parex unit (Q_X^{PAREX}) was calculated as a sum of the four-stream extract flowrate (Q_X^{SMB}) and the secondary flushing-in flowrate (Q_{SF}^{PAREX}) to keep the total Parex mass balance ($Q_X^{PAREX} + Q_R^{PAREX} + Q_{SF}^{PAREX} = Q_F^{PAREX} + Q_D^{PAREX}$) identical to that of the four-stream SMB unit ($Q_X^{SMB} + Q_R^{SMB} = Q_F^{SMB} + Q_D^{SMB}$).

The mathematical model used for simulation of four-stream SMB for p-xylene separation was applied. The node mass balances were written taking into consideration that during one switching time period (1) the desorbent stream will be introduced through the line used for withdrawing of the flushing-out stream one switching period ago; (2) the flushing-out stream will be withdrawn through the line that was used for withdrawing of



a)



b)

Figure 4. Cyclic steady state extract history of the four-stream SMB unit in a presence of transfer line dead volume a) during few switching periods and b) zoomed during one switching period (thin lines correspond to $V_{l,t} = 0.006^* V_{SMB}$ and bold lines correspond to $V_{l,t} = 0.01^* V_{SMB}$).

Table 3. The four-stream SMB unit extract performance in the presence of the transfer line dead volume.

		Value	
Performance	Formulation	$V_{l,t} = 0.006V_{SMB}$	$V_{l,t} = 0.01V_{SMB}$
Purity (%)	$\frac{c_X^{PX}}{(c_X^{PX}+c_X^{MX}+c_X^{OX}+c_X^{EB})} \times 100$	85.54	75.22
Recovery (%)	$\frac{c_X^{PX} Q_X}{c_F^{PX} Q_F} \times 100$	95.59	97.66
Desorbent consumption (m^3/kg)	$\frac{Q_D}{c_X^{PX} Q_X}$	0.0122	0.0199
Productivity (kg/h/m^3)	$\frac{c_X^{PX} Q_X}{Vads}$	63.95	65.34

the extract five switching periods ago; (3) the extract stream will be withdrawn from the line that was used for introduction of the secondary flushing-in one switching period ago; (4) the secondary flushing-in stream will be introduced through the line that was used for introduction of flushing-in stream six switching periods ago; (5) the flushing-in stream will be introduced through the line used for introduction of the feed two switching periods ago; (6) the feed stream will be introduced through the line used for withdrawing of the raffinate six switching time periods ago; and (7) raffinate

Table 4. Real Parex unit configuration, operating conditions, and model parameters.

SMB unit geometry	Operating conditions	Model parameters
$L_c = 1.1\,\text{m}$	T = 180°C, liquid phase	$Pe = v_k L_k / D_{L_k} = 2000$
$d_c = 4.1\,\text{m}$	$t^* = 1.15\,\text{min}$	$k = 2\,min^{-1}$
		$\varepsilon = 0.39\; d_p = 9.2 \times 10^{-4}\,\text{m}$
No. of columns: 24	$Q_D = 173.4\,\text{m}^3/\text{hr}$	
No. of zones: 7	$Q_{Fout} = Q_{Fin} = 18.91\,\text{m}^3/\text{hr}$	$q_{mPX(MX;OX;EB)} = 0.1303\,\text{kg}/\text{kg}$
	$Q_X = 114.0\,\text{m}^3/\text{hr}$	$K_{PX} = 1.0658\,\text{m}^3/\text{kg}$
	$Q_{SF} = 15\,\text{m}^3/\text{hr}$	$K_{MX} = 0.2299\,\text{m}^3/\text{kg}$
Configuration: 1-5-1-6-2-6-3	$Q_F = 87\,\text{m}^3/\text{hr}$	$K_{OX} = 0.1884\,\text{m}^3/\text{kg}$
	$Q_R = 161.4\,\text{m}^3/\text{hr}$	$K_{EB} = 0.3067\,\text{m}^3/\text{kg}$
	$Q_1 = 496.8\,\text{m}^3/\text{hr}$	$q_{mPDEB} = 0.1077\,\text{kg}/\text{kg}$
		$K_{PDEB} = 1.2935\,\text{m}^3/\text{kg}$

stream will be withdrawn from the line used for introduction of the desorbent stream three switching time ago.

The node mass balances are:

Desorbent node:

$$Q_7 + Q_D = Q_1 \tag{17}$$

$$c_{i,k}^{out} Q_7 + c_{i,D} Q_D = c_{i,k+1}^{in} Q_1 \tag{18}$$

Flushing-out node:

$$Q_1 - Q_{Fout} = Q_2 \tag{19}$$

$$c_{i,k}^{out} = c_{i,k+1}^{in} \tag{20}$$

Extract node:

$$Q_2 - Q_X = Q_3 \tag{21}$$

$$c_{i,k}^{out} = c_{i,k+1}^{in} \tag{22}$$

Secondary flushing-in (p-xylene) node:

$$Q_3 + Q_{SF} = Q_4 \tag{23}$$

$$c_{i,k}^{out} Q_3 + c_{i,SF} Q_{SF} = c_{i,k+1}^{in} Q_4 \tag{24}$$

Flushing-in node:

$$Q_4 + Q_{Fin} = Q_5 \tag{25}$$

$$c_{i,k}^{out} Q_4 + c_{i,Fin} Q_{Fin} = c_{i,k+1}^{in} Q_5 \tag{26}$$

Feed node:

$$Q_5 + Q_F = Q_6 \tag{27}$$

$$c_{i,k}^{out} Q_5 + c_{i,F} Q_F = c_{i,k+1}^{in} Q_6 \tag{28}$$

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Raffinate node:

$$Q_6 - Q_R = Q_7 \tag{29}$$

$$c_{i,k}^{out} = c_{i,k+1}^{in} \tag{30}$$

where in the:
First stage: $t = (Nt^*, Nt^* + t_S)$

$$c_{i,S} = \frac{\int_{(N-M_Z)t^*+(t^*-t_{S+1})}^{(N-M_Z)t^*+t^*} c_{i,S+1}dt}{\int_{(N-M_Z)t^*+(t^*-t_{S+1})}^{(N-M_Z)t^*+t^*} dt} \quad \text{for} \quad S = Z = 1,3 \quad \text{and} \quad \mathrm{N} \geq 1;$$

$$S = Z = 2 \quad \text{and} \quad \mathrm{N} \geq 5; \quad S = Z = 4,6 \quad \text{and} \quad \mathrm{N} \geq 6;$$

$$S = Z = 5 \quad \text{and} \quad \mathrm{N} \geq 2.$$

$$c_{i,S} = \frac{\int_{(N-M_Z)t^*+(t^*-t_1)}^{(N-M_Z)t^*+t^*} c_{i,1}dt}{\int_{(N-M_Z)t^*+(t^*-t_1)}^{(N-M_Z)t^*+t^*} dt} \quad \text{for} \quad S = Z = 7 \quad \text{and} \quad \mathrm{N} \geq 3 \tag{31}$$

otherwise $c_{i,S} = c_{i,D}$, because at the begining all the columns and transfer lines are filled with desorbent.

The streams are numbered ($S = 1, 2\ldots7$) starting from the desorbent stream and finishing with the raffinate stream (i.e., 1-desorbent [D]; 2-flushing-out [F_{out}]; 3-extract [X]; 4-secondary flushing-in (p-xylene) [SF]; 5-flushing-in [F_{in}]; 6-feed [F]; 7-raffinate [R].

Second and third stage: $t = (Nt^* + t_S, Nt^* + (t^* - t_S))$ and $t = (Nt^* + (t^* - t_S), Nt^* + t^*)$
in the inlet nodes (desorbent, feed, p-xylene):

$$c_{i,S} = c_{i,S} \quad \text{for} \quad S = 1,4,6 \tag{32a}$$

in the outlet nodes (flushing-out, extract, raffinate):

$$c_{i,S} = c_{i,k}^{out} = c_{i,k+1}^{in} \quad \text{for} \quad S = 2,3,7 \tag{32b}$$

in the flushing-in node:

$$c_{i,S} = c_{i,2} \quad \text{for} \quad S = 5 \tag{32c}$$

The cyclic steady state concentration profiles at the end of the cycle for the total transfer line dead volume 0.6% of Parex unit volume ($V_{l,t} = 0.006^* V_{PAREX}$) and 1% of Parex unit volume ($V_{l,t} = 0.01^* V_{PAREX}$) are presented in Fig. 5. The position of the concentration profiles is related to the composition of the process input streams. Namely, higher transfer line dead volume leads to bigger contamination of the: feed stream by raffinate trapped; flushing-in stream by feed trapped; secondary flushing stream by flushing-in trapped; and desorbent stream by flushing-out trapped. These contaminations lead to lower feed concentration but higher flushing-in, secondary flushing-in and desorbent concentration when transfer line dead volume is increased.

The cyclic steady state extract concentration history during few switching periods and zoomed during one switching period are presented in Figs. 6a and 6b, respectively. The cyclic steady state extract performances and the equations used for their calculation are given in Table 5. The Parex unit performance in terms of extract purity and recovery does not change significantly when the transfer line dead volume increase from 0.6% up to 1% of the Parex unit volume. The productivity is slightly higher for 1% transfer line dead volume, because the extract concentration is higher at the beginning of the switching period as a result of the bigger quantity of secondary flushing-in (p-xylene) stream trapped in the transfer line (see Fig. 6b).

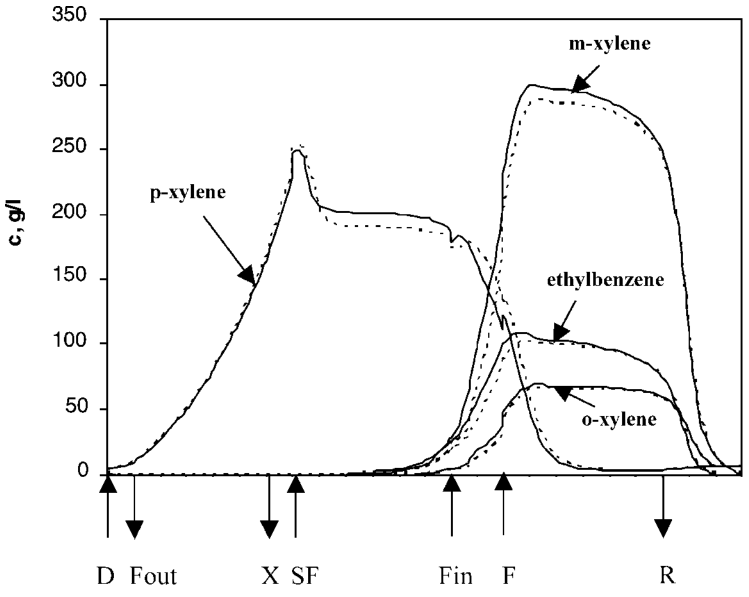
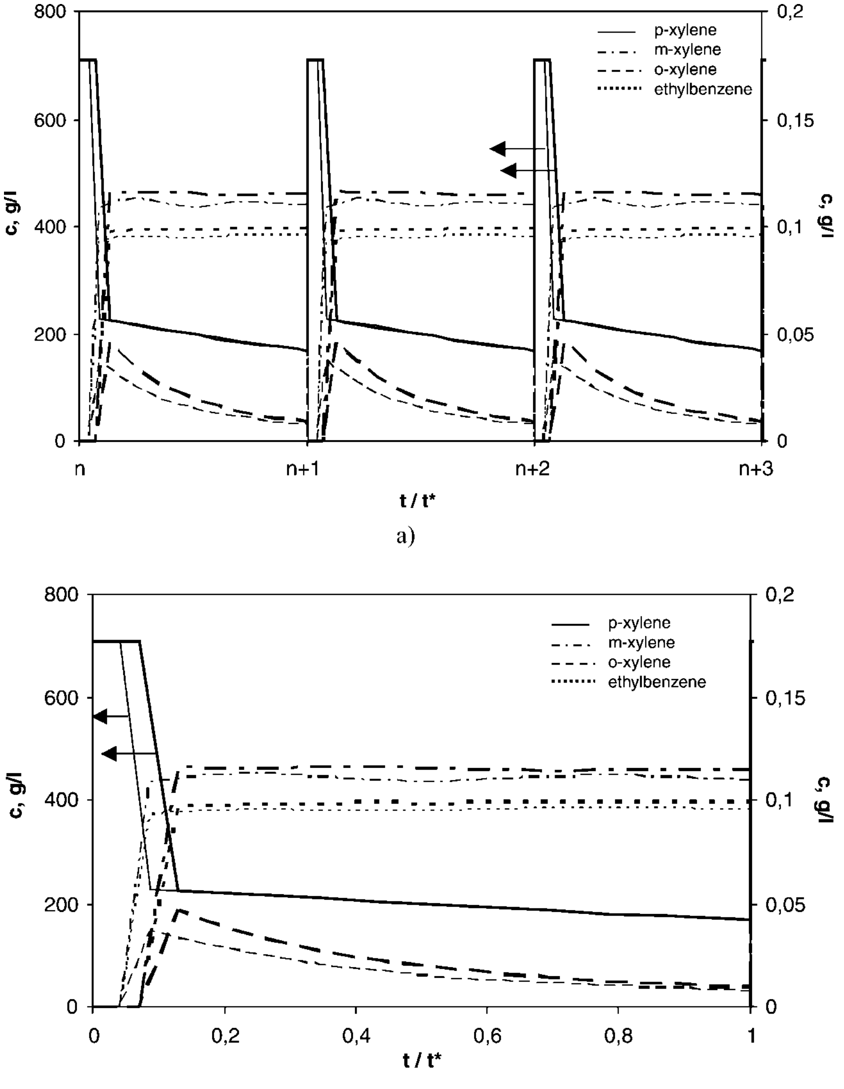


Figure 5. Cyclic steady state concentration profile (at the end of the cycle) of the real Parex unit in a presence of transfer line dead volume (----$V_{l,t} = 0.006 * V_{PAREX}$ and ——$V_{l,t} = 0.01 * V_{PAREX}$).



a)

b)

Figure 6. Cyclic steady state extract history of the real Parex unit in a presence of transfer line dead volume a) during few switching period; and b) zoomed during one switching period (thin lines correspond to $V_{l,t} = 0.006{*}V_{PAREX}$ and bold lines correspond to $V_{l,t} = 0.01{*}V_{PAREX}$).

Table 5. The real Parex unit extract performance.

		Value	
Performance	Formulation	$V_{l,t} = 0.006\,V_{PAREX}$	$V_{l,t} = 0.01V_{PAREX}$
Purity (%)	$\frac{c_X^{PX}}{(c_X^{PX}+c_X^{MX}+c_X^{OX}+c_X^{EB})} \times 100$	99.91	99.92
Recovery (%)	$\frac{c_X^{PX} Q_X}{c_F^{PX} Q_F + c_{SF}^{PX} Q_{SF}} \times 100$	98.56	98.72
Desorbent consumption (m^3/kg)	$\frac{Q_D}{c_X^{PX} Q_X}$	0.0069	0.0067
Productivity (kg/h/m^3)	$\frac{c_X^{PX} Q_X}{Vads}$	113.135	116.689

The comparison of the extract performances of the real Parex unit (see Table 5) with those of four-stream SMB unit for p-xylene separation (see Table 3) shows that the all extract performances have been improved as a result of flushing of the transfer lines.

INFLUENCE OF THE FLUSHING STREAMS ON THE PAREX UNIT PERFORMANCE

The simulation of the Parex unit taking into consideration the transfer line dead volume and flushing stream is time consuming, because the SMB strategy must be used to simulate the shifting of the process stream positions, and also the presence of the five components (p-, o-, m-xylene; ethylbenzene; and p-diethylbenzene). To find faster way for prediction of the influence of the three additional Parex streams (flushing-in, flushing-out, and secondary flushing-in (i.e., p-xylene stream)) onto Parex unit performances the use of the TMB strategy was explored. It is clear that the TMB strategy could not describe the phenomena of the trapped liquid volume in the transfer lines, because it does not account for the shifting of the process streams. However, it could help getting a close picture about the influence of the flushing stream flow rates and secondary flushing-in stream composition on the Parex performance.

The Parex unit (see Table 4) was simulated using steady state TMB strategy of modeling.[26] It was assumed that in each moment the concentration of flushing-in stream is equal to the concentration of the flush-out stream, which is not true, because the liquid withdrawn from the flushing-out node travels some time through the recirculation loop before entering in the unit through the flushing-in node.

The Parex steady state concentration profiles calculated using TMB strategy of modeling and the cyclic steady state concentration profiles at the middle of the switching time period calculated by SMB strategy of modeling considering the line dead volume ($V_{l,t} = 0.006 * V_{PAREX}$) are presented in Fig. 7. The TMB concentration profile follows the shape of the SMB concentration profile. The SMB concentration profiles of raffinate component are above the TMB concentration profiles. This behavior is a result of the presence the transfer line dead volume considered in the SMB model (i.e., the feed stream is always introduced through the transfer line that was previously used for withdrawing of the raffinate as a result of what in the first period of the switching time the raffinate [trapped in the transfer line] is practically introduced in the Parex unit as a feed). The difference in the extract TMB and SMB concentration profiles is also the result of the presence of the transfer line dead volume considered in the SMB strategy of modeling.

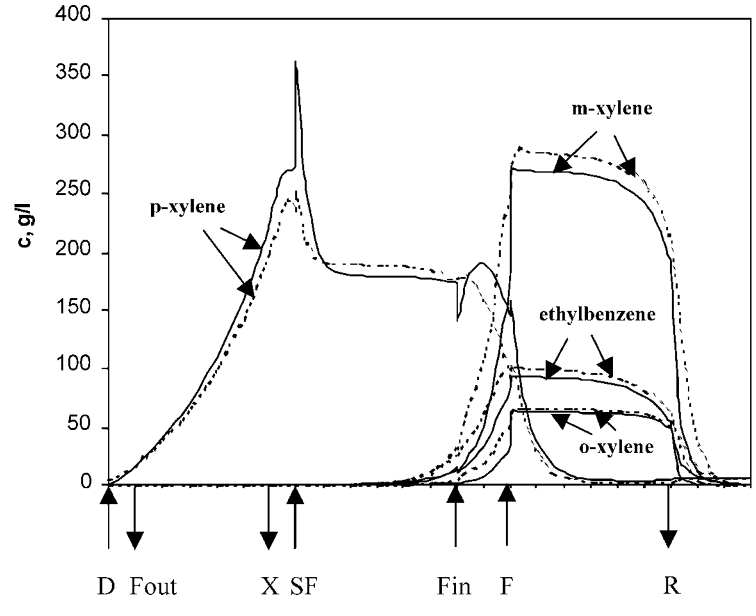


Figure 7. Comparison of steady state concentration profiles of the Parex unit predicted by: ——TMB strategy and - - - -SMB strategy (at the middle of the switching time period, taking in account lines dead volume).

The Parex performance calculated by the TMB strategy of modeling are: extract purity, 99.97%; extract recovery, 97.42%; desorbent consumption, 0.007 m^3/kg; and productivity, 111.83 kg/h $m^3_{adsorbent}$.

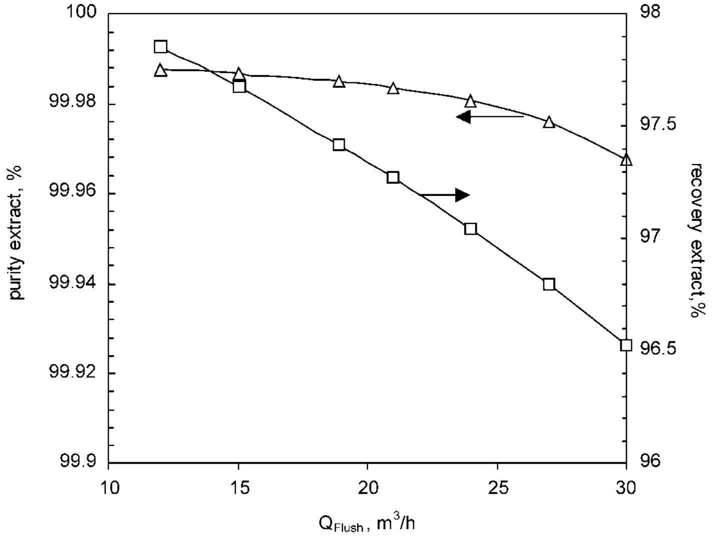
The values of the Parex extract performance calculated by TMB strategy of modeling are relatively close to those calculated by SMB strategy of modeling taking into account the transfer line dead volume. Therefore the TMB modeling strategy was used for fast visualization of the effect of:

1. The flushing-out/flushing-in and the secondary flushing-in (p-xylene) flow rates and
2. The secondary flushing-in stream composition.

EFFECT OF THE FLUSHING STREAMS FLOWRATE ON THE PAREX PERFORMANCE

The effect of the flushing-out/flushing-in flow rate was studied by changing its flow rate in the range of 12 to 30 m^3/hr and keeping constant all the other flow rates (see Table 4). The influence of the flushing-out/flushing-in stream on the Parex extract purity and recovery is presented on Fig. 8a; and on the desorbent consumption and the p-xylene productivity on Fig. 8b. The increase of the flushing-out/flushing-in stream flow rate decreases the Parex performance. This behavior could be explained by the composition of the flushing-out/flushing-in stream. Namely, the flushing-out stream is withdrawn immediately after the desorbent stream it is constituted by the desorbent component in majority. The withdrawn flushing-out stream is introduced as flushing-in stream before the feed stream as a result of what the concentration of the p-xylene would decrease. The decrease of the p-xylene concentration depends of the flushing-out/flushing-in stream flow rate: higher flow rate lowers the p-xylene concentration.

The influence of the secondary flushing-in (p-xylene) stream on the Parex performance was studied by changing its flow rate in the range of 6 to 24 m^3/hr; the extract flow rate was also changed to keep the total mass balance unchanged, and the other streams were those given in Table 4. The effect of the secondary flushing-in stream flow rate on extract purity and recovery (Fig. 9a) and desorbent consumption and p-xylene productivity (Fig. 9b) is presented. Higher secondary flushing-in flow rates lead to slightly higher



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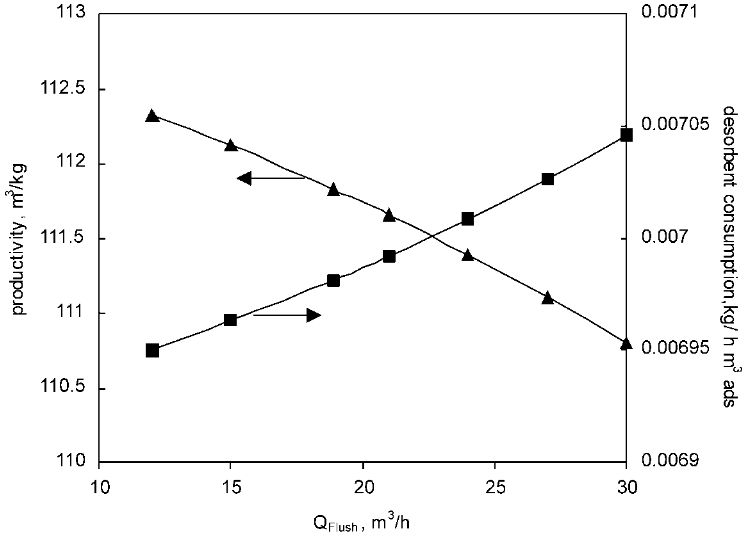

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Figure 8. Effect of the flushing stream flow rate on the Parex: a) extract purity and recovery; and b) p-xylene productivity and desorbent consumption. (Predicted by TMB strategy of modeling.)

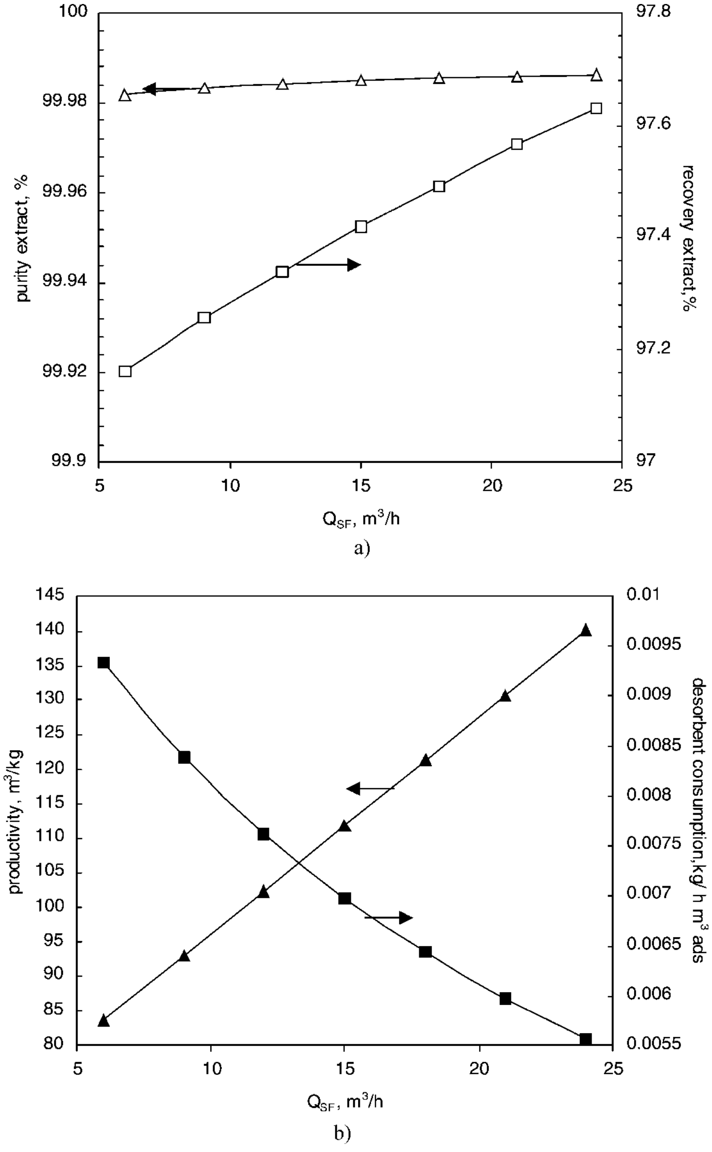


Figure 9. Effect of the secondary flushing-in (p-xylene) stream flow rate on the Parex: a) extract purity and recovery and b) p-xylene productivity and desorbent consumption. (Predicted by TMB strategy of modeling.)

extract purity and recovery, and also to higher p-xylene productivity and lower desorbent consumption.

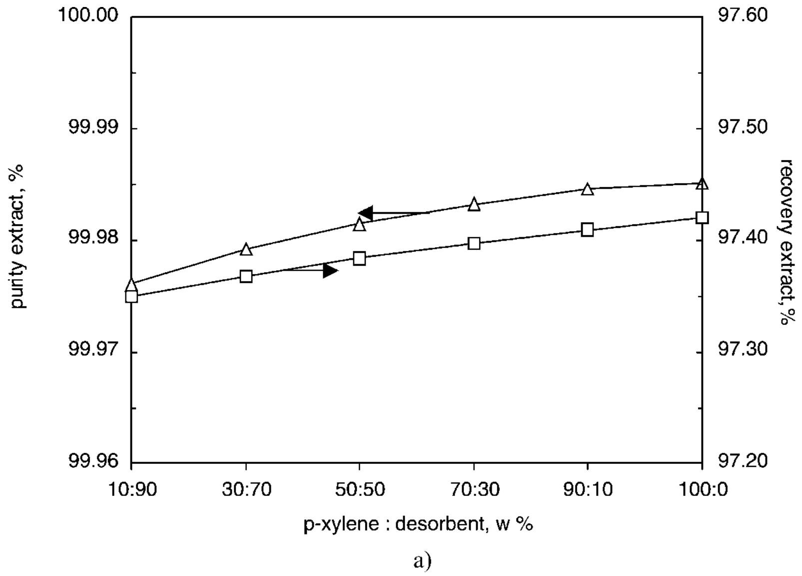
EFFECT OF THE COMPOSITION OF SECONDARY FLUSHING-IN STREAM ON THE PAREX PERFORMANCE

In all simulations, the secondary flushing-in stream was assumed as pure p-xylene stream that could be recycled from the distillation column used for separation of the extract stream into p-xylene and desorbent. To explore the possibility of using a mixture of p-xylene and desorbent instead the pure p-xylene as secondary flushing-in stream, the influence of the secondary flushing-in stream composition on the Parex performance was studied. The compositions of secondary flushing-in stream used in the study were: 10:90; 30:70; 50:50; 70:30; 90:10; and 100:0 of p-xylene: desorbent in weight percent. The operating conditions were identical to those presented in Table 4. Figure 10a shows that the extract purity and recovery increase as the weight fraction of p-xylene in the p-xylene/desorbent mixture increases, and are maximal when pure p-xylene is used as secondary flushing stream. Also, the productivity increases and desorbent consumption decreases as the weight fraction of p-xylene in the secondary flushing-in stream increases (Fig. 10b). The use of the pure p-xylene as a secondary flushing-in stream would be more favorable in the Parex units with strong desorbent, to increase the p-xylene concentration in the zone between extract and feed ports so that the liquid inside the adsorbent pores passing to the zone between desorbent and extract port is exclusively p-xylene.

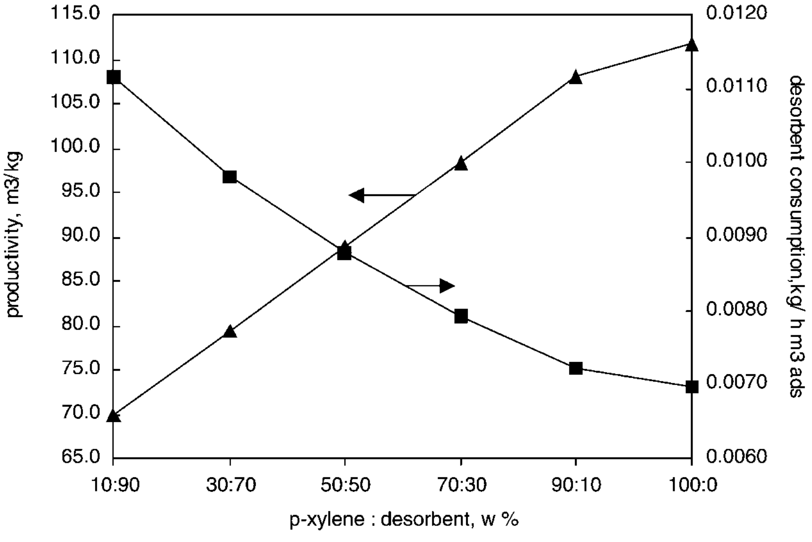
EQUIVALENCE BETWEEN THE IDEALIZED FOUR-STREAM SMB UNIT FOR p-XYLENE SEPARATION AND THE REAL PAREX UNIT

Most of the models used for simulation of SMB units for p-xylene do not account for the transfer line dead volume and presence of the flushing streams.[20,23,25] These models are applied in the prediction of SMB unit performance and in the tuning of the SMB operating conditions.

To calculate the error in the calculation of SMB performances resulting from the assumption previously stated (i.e., no transfer lines dead volume and no flushing streams), the idealized four-streams industrial scale SMB unit for p-xylene separation was simulated. The transfer lines' dead volume and the flushing streams were not taken into consideration. The idealized SMB unit



a)



b)

Figure 10. Effect of the secondary flushing-in (p-xylene) stream composition on the Parex: a) extract purity and recovery and b) p-xylene productivity and desorbent consumption. (Predicted by TMB strategy of modeling.)

configuration, operation conditions and equilibrium data are identical as those in Table 2.

The equivalence between the idealized four-stream SMB unit for p-xylene separation and the real Parex unit is established by keeping in the real Parex unit the total mass balance unchanged. Therefore the extract flow rate of the idealized four-stream SMB, Q_X^{SMB}, was calculated as a difference between the real Parex extract flowrate, Q_X^{PAREX}, and real Parex secondary flushing-in flowrate, Q_{SF}^{PAREX}, ($Q_X^{SMB} = Q_X^{PAREX} - Q_{SF}^{PAREX}$).

The idealized four-stream SMB unit cyclic steady state concentration profiles at the end of the cycle are presented in Fig. 11. The extract concentration history during few switching periods and its zoom during one switching period are shown in Figs. 12a and 12b, respectively. The extract performances calculated by the equations given in Table 3 are: extract purity, 99.88%; extract recovery, 98.56%; desorbent consumption, 0.012 m^3/kg; and productivity, 65.94 kg/h $m^3_{adsorbent}$.

The idealized four-stream SMB unit extract purity and recovery are very close to those of the equivalent real Parex unit. This is not a case for

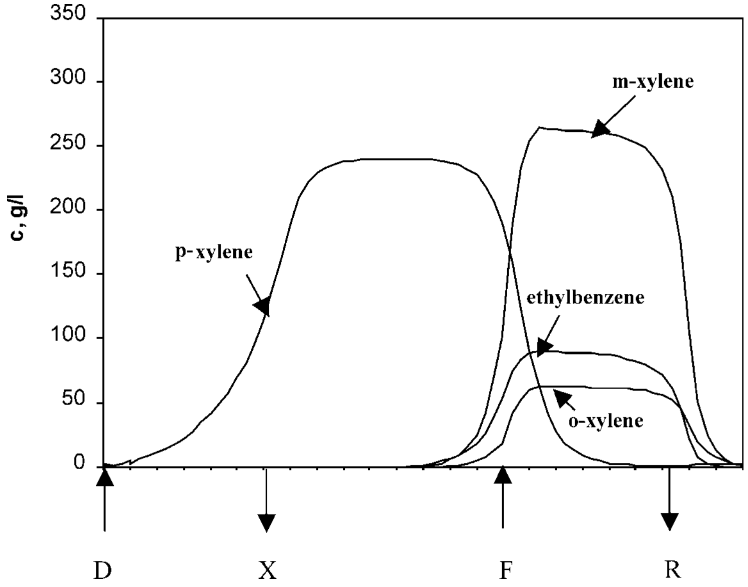


Figure 11. Cyclic steady-state concentration profile (at the end of the cycle) of the idealized four-stream SMB (neglected transfer line dead volume).

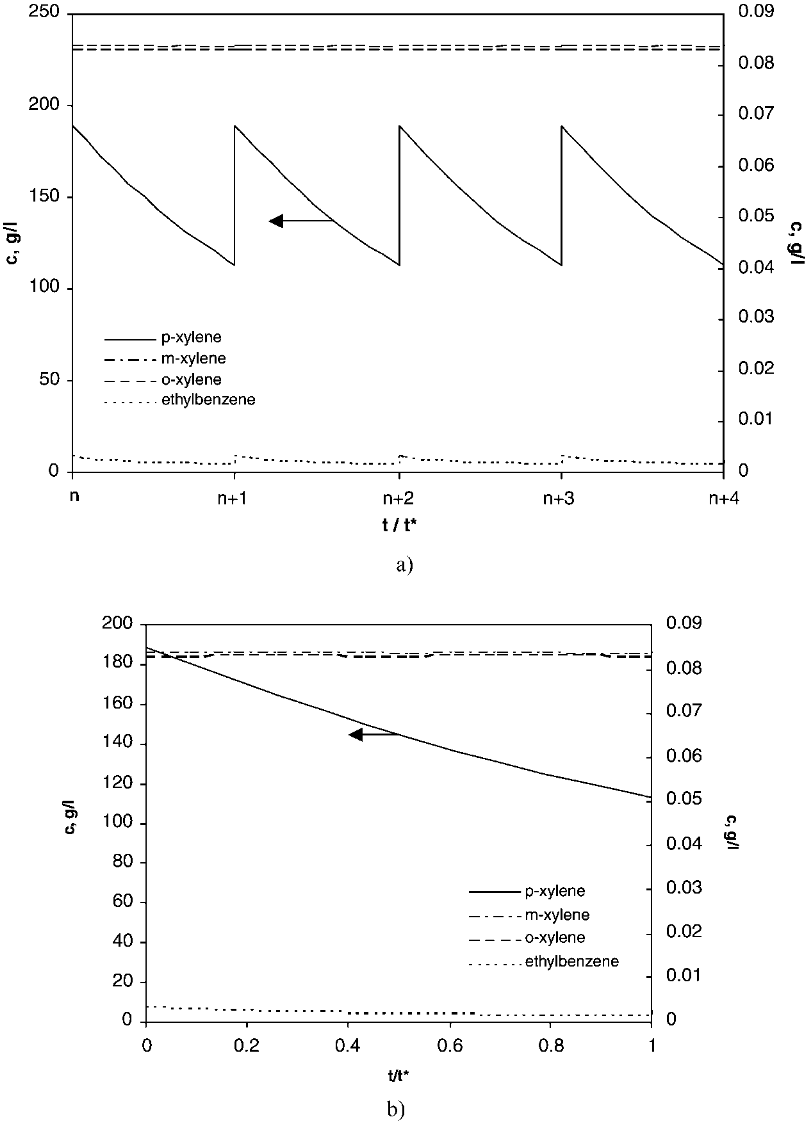


Figure 12. Cyclic steady-state extract history of the idealized four-stream SMB (neglected transfer line dead volume) a) during few switching periods and b) zoomed during one switching period.

the idealized four-stream SMB unit desorbent consumption and productivity, which are quite different from those of the real Parex unit.

The modeling of the real Parex unit in a presence of the transfer line volume and flushing stream as an equivalent four-stream SMB unit could yield high error in the prediction of the real Parex unit performance therefore should be applied with caution.

CONCLUSIONS

In this work the influence of the transfer line dead volume on the performance of an industrial scale SMB for p-xylene separation was studied through simulation. The SMB strategy of modeling was used; the model includes axial dispersion flow for the liquid phase, LDF for the intraparticle mass transfer rate and multicomponent adsorption equilibria described by nonstoichiometric Langmuir isotherm. The transfer line dead volume was assumed as plug flow or continuous stirred tank in different stages of transfer line use and was introduced into the mathematical model through the node mass balances.

The conclusions of this work can be summarized as follows:

1. The presence of the dead volume is also significant in the industrial-scale SMB units applied for production of high purity component as p-xylene. The p-xylene purity falls to 85.54% and 75.22% when the total transfer line dead volume is 0.6% and 1% of the total SMB unit volume.
2. The UOP technique of flushing the transfer lines between the desorbent and extract port and between the extract and feed port is efficient in overcoming the negative influence of the transfer line dead volume on SMB unit performances.
3. The steady-state TMB strategy of modeling was used to study the influence of the flushing streams flow rate and secondary flushing-in stream composition on the Parex performance. It was shown that the flushing stream flow rates should be also tuned as the four classical SMB unit streams (feed, extract, desorbent and raffinate) to get the best unit performances.
4. The modeling of the real Parex unit in a presence of the transfer line volume and flushing stream as an equivalent four-stream SMB unit could yield high error in the prediction of the real Parex unit performance.

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