

An optimal three fractions yielding simulated moving bed chromatographic separation: Triple switch SMBC

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Abstract: Among the various degrees of freedom Simulated moving bed chromatography possesses, the current work deals with manipulation of operating conditions comprising internal flow rates and switching period. The conventional mode of operation yields a single fraction of the extract and raffinate with a single set of operating conditions whereas the current work proposes a novel triple switch mode of operation which is characterised by three sets of internal flow rates and switching period and yields three fractions. Under optimal conditions, the higher degrees of freedom have the potential of yielding higher extract purities than conventional as well as dual switch modes of operation with two sets of operating conditions. A multi-objective optimisation problem has been solved which maximizes the purity of one of the three extract fractions, for a certain minimum extract recovery and minimum feed flow rate. It is through a lower purity in two of the three fractions that a superior extract purity is achieved. This finding has been corroborated by a modeling based study on the linear adsorption isotherm based separation of fructose-glucose in deionised water on a cation exchange resin.

Keywords: Simulated moving bed, novel operation, multi-objective optimisation

1. INTRODUCTION

As shown in Fig. 1, the separation of two components (m : more adsorbed, l : less adsorbed) in feed using Simulated Moving Bed Chromatography (SMBC) into extract and raffinate with a solvent doubling as desorbent, in a continuous manner, is achieved through a synchronous periodic switching or shifting of the inlet and outlet ports, by a column, in the direction of fluid flow (Rajendran et al., 2009). The internal flow rate (Q) in the four sections (I-IV) along with the period of port switching known as (t^*), constitute the set of operating conditions (O). After sufficient number of port switches, a single period cyclic steady state (CSS) is attained wherein the temporal behaviour of the concentration profile repeats after every cycle.

With the operating conditions O (internal flow rates and switching period) repeating after every port switch, the conventional mode of operation has been referred to in the current work and by Vignesh et al. (2016), as single switch mode of operation, shown in Fig. 1. At CSS, each cycle of the single switch SMBC results in a fraction with the same cycle averaged purity and recovery, at the extract and raffinate ports. If the internal flow rates and switching period are varied over the course of separation, additional degrees of freedom are obtained, which can be optimised as studied in the works of Kearney and Hieb (1992), Zhang et al. (2003) and Vignesh et al. (2016). More recently, Maruyama et al. (2019) proposed bypass-SMB whereas works of Yao et al. (2018), Chung et al. (2017) are extensions of previously proposed advanced modes, all

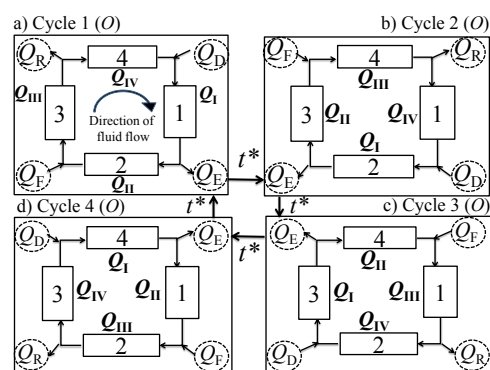


Fig. 1. Single switch mode of operation shown on a one-column per section SMB, for four consecutive cycles (Feed enters column 3 at the start of separation)
 F - Feed ($m+l$ +solvent), D - Desorbent, E - Extract (m predominantly), R - Raffinate (l predominantly)

dealing with innovations not involving dynamic operating conditions.

In the current work, we propose a strategy, involving three sets of operating conditions, as opposed to two sets in dual switch (Vignesh et al., 2016), applied on consecutive cycles and termed as triple switch. With each set repeating after every three port switches, this mode of operation enables a further enrichment of the extract purity than possible in dual switch, due to the availability of higher degrees of freedom. The contribution of dual switch and triple switch modes is the production of more than one fraction in addition to acquiring higher extract

purity. As opposed to Fractionation and feedback SMB (Li et al., 2010) wherein one of the fraction gets recycled as feed, the proposed strategy yields all the fractions as product, albeit during different cycles. The proposed mode of operation has been demonstrated using simulation, unaided by experimental validation, on the separation of fructose-glucose in deionized water on a cation exchange resin, using a linear adsorption isotherm. Modeling studies show that, under optimal operating conditions, for same process constraints, the triple switch is advantageous over single as well as dual switch modes of operation with triple switch yielding a maximum extract purity of 90.54%, as opposed to 86.53%, 88.32% for single switch and dual switch, respectively. This has, however, been obtained at the cost of the purity of the other extract fractions and productivity of the said enriched fraction.

Section 2 explains the working of triple switch SMBC and gives the model in brief. Section 3 discusses the possible merits of triple switch and the problem formulation adopted to implement the same. This is followed by the results and discussion in Section 4 ending with the conclusion in the last section.

2. MODEL OF TRIPLE SWITCH SMBC

Considering a single column as a fixed bed, mass balance is applied along the axial direction. A linear driving force along with axial dispersion has been assumed and the following PDEs were obtained with $c_{i,j}$, $n_{i,j}$ being concentration for i^{th} component in j^{th} column in liquid and solid phases, respectively (Rajendran et al. (2009)).

$$\frac{\partial c_{i,j}}{\partial \theta} = \gamma_j \left(\frac{1}{Pe_j} \frac{\partial^2 c_{i,j}}{\partial x^2} - \frac{\partial c_{i,j}}{\partial x} \right) - \frac{(1-\epsilon)}{\epsilon} \frac{\partial n_{i,j}}{\partial \theta} \quad (1)$$

$$\frac{\partial n_{i,j}}{\partial \theta} = k_i t^* (n_{i,j}^* - n_{i,j}), n_{i,j}^* = f_i(c_{m,j}, c_{l,j}) \quad (2)$$

i = component m, 1

j = 1, 2, ..., N_j (the total number of columns)

where $\theta = t/t^*$ and t is time, t^* is the switching period, $x = z/L_j$ and z is length in axial direction, L_j is the length of j^{th} column, $\gamma_j = v_j t^*/L_j$ and $v_j = Q_{sec}/A_j \epsilon$ is the interstitial fluid velocity with Q_{sec} referring to volumetric flow rate of section (I-IV), $A_j = \pi d_j^2/4$ is the cross sectional area of the column with d_j being the column diameter, ϵ is the bed porosity, $Pe_j = v_j L_j/D_i$ is the Peclet number and D_i is the axial dispersion coefficient which may depend on fluid velocity, k_i is the mass transfer coefficient, $n_{i,j}^*$ is the solid phase concentration in equilibrium with the liquid phase concentration given by an adsorption isotherm f as in (2).

Eqs. (1)-(2) are solved along with the equations for balance of flow rate and mass at the four nodes, omitted for brevity, corresponding to two inlet and two outlet ports, to account for the external flow rates in the system which do not feature in PDEs (1), (2). The above equations along with one initial condition for each of $c_{i,j}$, $n_{i,j}$ in time and two boundary conditions for $c_{i,j}$ in space, constitute the SMBC model for a single cycle. We cite Kawajiri and Biegler (2006), Rajendran et al. (2009) for further details. The following section gives the working of the proposed triple

switch along with brief details about its model for which a one-column per section SMB ($N_j = 4$) has been assumed.

2.1 Working of Triple Switch SMBC

The triple switch mode of operation is characterised by three sets of operating conditions denoted by O_s ($s = 1, 2, 3$) comprising of $Q_{I,s}$, $Q_{II,s}$, $Q_{III,s}$, $Q_{IV,s}$, t_s^* . The three sets are applied on consecutive cycles with each set being repeated after three port switches or three cycles, as seen in Fig. 2 for six consecutive cycles

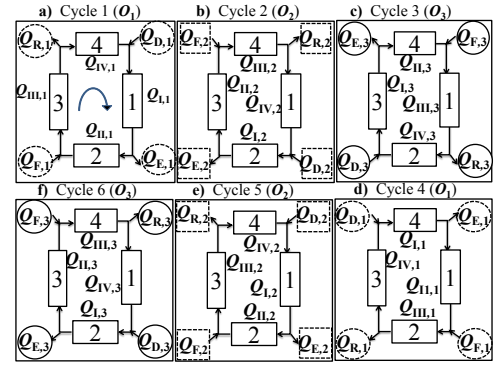


Fig. 2. Triple switch strategy for a one-column per section SMB (Feed enters column 3 at start of separation)

Table 1. Duration of six consecutive cycles in Triple switch mode of operation

Cycle	Duration
1	t_1^*
2	$t_1^* - (t_1^* + t_2^*)$
3	$(t_1^* + t_2^*) - (t_1^* + t_2^* + t_3^*)$
4	$(t_1^* + t_2^* + t_3^*) - (2t_1^* + t_2^* + t_3^*)$
5	$(2t_1^* + t_2^* + t_3^*) - (2t_1^* + 2t_2^* + t_3^*)$
6	$(2t_1^* + 2t_2^* + t_3^*) - (2t_1^* + 2t_2^* + 2t_3^*)$

Table 1 gives the duration for each of six consecutive cycles, when the separation starts with feed entering column 3 and operated using O_1 .

After sufficient port switches, the concentration profiles repeat in time after the same duration as operating conditions repeat i.e. three cycles and hence the name. This results in the requirement of model equations corresponding to any three consecutive port switches denoted as *Cycle* (k) ($k = 1, 2, 3$). Here, k indicates the sequence of three consecutive cycles at triple period CSS. *Cycle* (k) ($k = 1, 2, 3$) considered in model pertain to feed entering columns 3, 4, 1 respectively which are operated using O_1, O_2, O_3 , respectively.

Each *Cycle* (k) of triple switch SMBC model comprises of 16 PDEs giving mass balance as described in (1), (2) for the two components in four columns, 8 algebraic equations giving adsorption isotherms f as given by (2), 16 algebraic equations describing nodal balance, 16 algebraic equations giving initial condition and 16 PDEs giving boundary conditions. The model enforces the said steady state by equating concentration profiles across different columns at the beginning of *Cycle* (1) with that at the end of *Cycle* (3) and shifted by 3 columns and thus enabling one to solve model equations for only 3 cycles to obtain CSS profiles directly.

The current work assumes a perfect plant model without any plant-model mismatch. The use of feedback to overcome plant model mismatch has been discussed in Wang et al. (2003), and Song et al. (2006) but is beyond scope of current work.

The following section briefly gives the contribution of triple switch SMBC and details out the problem formulation used to evaluate the advantage, if any, of the said strategy.

3. OPTIMAL OPERATION OF TRIPLE SWITCH SMBC

At CSS, triple switch mode of operation yields three distinct fractions, during three consecutive cycles, at the extract and raffinate ports. In the current work, extract is assumed to be the desired or key product with the extract fractions E_1, E_2, E_3 having been obtained by implementing operating conditions O_1, O_2, O_3 , respectively. The purity of one of the three fractions needs to be maximized in presence of constraints on the quantities of the various feed flow rates and extract recoveries as well as purity of one of the other two fractions.

$$[Pur]_{E_s,m} = \frac{\int_0^{t_s^*} c_m^{E_s}(t) dt}{\int_0^{t_s^*} c_1^{E_s}(t) dt + \int_0^{t_s^*} c_m^{E_s}(t) dt} \quad (3)$$

$$Q_{F,s} = Q_{III,s} - Q_{II,s} \quad (4)$$

$$[Rec]_{E_s,m} = \frac{Q_{E,s} \int_0^{t_s^*} c_m^{E_s}(t) dt}{Q_{F,s} c_m^F} \quad (5)$$

$s = 1, 2, 3$ indicates operating conditions O_1, O_2, O_3 , respectively, $[Pur]$ is purity and $[Rec]$ is recovery, both quantities time-averaged over the cycle of duration t^* .

In addition to the above metrics, the following two metrics, which although not a part of the formulation, have also been used to measure the performance of separation.

$$\frac{Q_D^{avg}}{Q_F^{avg}} = \frac{D}{F}, [Prod]_{m,E_s} = \frac{Q_{E,s} \int_0^{t_s^*} c_m^{E_s}(t) dt}{N_j A_j L_j (1 - \epsilon)} \quad (6)$$

where avg indicates the quantity being averaged over a given duration, $[Prod]$ is productivity giving the rate of production of given component in an outlet for the total volume of adsorbent in the system

It has been shown by Vignesh et al. (2016) that optimal operation of SMB by two sets of operating conditions applied on alternate cycles yielded higher extract purity than optimal single switch, at CSS. This is obtained for one of the two extract fractions of the former at the expense of extract purity of the other fraction. In the current work, the optimal operation of SMB by three different sets of operating conditions, applied on three consecutive cycles at CSS, is evaluated. We investigate if the proposed triple switch operation would result in a maximum extract purity that is higher than the maximum extract purity obtainable for dual switch operation.

The model equations are discretized in both space (x) and time (θ) using orthogonal collocation on finite elements (OCFE). $[FE]$ number of finite elements and $[OC]$ number of interior orthogonal collocation points (roots of shifted Legendre polynomial) in each finite element, were considered per column. They are chosen to be same in both space

and time. The optimisation studies have been carried out using interior point optimiser IPOPT in Matlab2013a[®].

3.1 Problem formulation: Maximization of purity of E_3

A multi-objective optimisation problem is solved using ϵ -constraint method wherein purity of fraction E_3 is maximized by placing a lower bound ϵ_{Rec} on the extract recovery of each of the three fractions E_1, E_2, E_3 and a lower bound ϵ_F on the feed flow rate of each of the three consecutive cycles. The bounds take care of the trade-off in these quantities while maximizing purity of E_3 .

$$\max_{c_{i,j}, n_{i,j}, Q_{sec,s}, t_s^*} [Pur]_{E_3,m} \quad (7)$$

$$\text{s.t. } [Pur]_{E_1,m} \geq \epsilon_{Pur} \quad (8)$$

$$[Rec]_{E_s,m} \geq \epsilon_{Rec}, Q_{F,s} \geq \epsilon_F \quad (9)$$

Completely discretized model equations for *Cycle* (k) (10)

$$Q_{I,s} = Q_{max} \quad (11)$$

$$0 \leq Q_{sec,s} \leq Q_{I,s}, 1 \text{ ml/min} \leq Q_{D,s}, Q_{E,s}, Q_{R,s} \leq Q_{I,s} \quad (12)$$

$$0 \leq c_{i,j} \leq c_i^F, 0 \leq n_{i,j} \leq n_i^* = f_i(c_m^F, c_1^F) \quad (13)$$

$$t_{min}^* \leq t_s^* \leq t_{max}^* \quad (14)$$

$sec = I - IV, j = 1 - 4, i = m \text{ and } l, s = 1 - 3, k = 1 - 3$

The discretized model equations for three consecutive cycles have been given as equality constraints. All the aforementioned constraints are similar to single and dual switch modes of operation differing only in the number of distinct sets of operating conditions characterising a given mode of operation. Also, the extract purity of any one of the fractions whose purity is not being maximized, is constrained by placing a lower bound ϵ_{Pur} , which is irrelevant for single switch. It is at the cost of this purity that the objective function improves (Vignesh et al., 2016), with bound being placed on the only other fraction available in dual switch whereas for triple switch it is placed on the purity of either of the fractions E_1 or E_2 (E_1 in our case, as shown in (8)). At higher values of the bound, it is active for the optimal value of objective function $[Pur]_{E_3,m}$. In order to obtain the maximum possible extract purity, the bound is decreased till the value below which it ceases to become active. Among the decision variables, nodal balance indicates that the flow rate in section I is maximum among all the internal as well as external flow rates. For the sake of simplicity, this value is fixed at some value and all the internal and external flow rates cannot exceed this value. Also, the external flow rates are constrained to ensure certain minimum flow. The solid and liquid phase concentrations cannot exceed the corresponding feed concentrations. Bounds have been placed on the switching period based on heuristics.

4. FRUCTOSE-GLUCOSE SEPARATION

The separation under consideration is that of fructose-glucose mixture in deionized water on a cation exchange resin. Fructose (Fru) is the more adsorbed component and glucose (Glu) is the less adsorbed component, being predominantly obtained in extract and raffinate, respectively. This linear isotherm ($n_{i,j}^* = H_i c_{i,j}$) based separation with H being adsorption coefficient or Henry's coefficient determining distribution of component i in between liquid and

solid phases, has parameter H_i for *Fru* and *Glu* as 0.5634, 0.3401 respectively. $k_i=0.1 \text{ s}^{-1}$, $c_i^F=30 \text{ g/L}$ for both the components and $Pe_j=2000$. The columns parameters are $L_j=10 \text{ cm}$, $d_j=2 \text{ cm}$, $\epsilon=0.4$, $N_j=4$.

A comparison is done between the optimal operation of proposed triple switch mode of operation and single switch as well as dual switch from which the triple switch has been derived, with results in Table 2. The optimisation parameters/bounds ϵ_F , ϵ_{Rec} , ϵ_{Pur} Q_{max} considered are 1 ml/min, 70%, 60%, 15 ml/min respectively and discretization parameter $[FE]_{x,\theta}$ for single, dual and triple switch modes is 7, 9, 14 respectively with $[OC]_{x,\theta} = 2$ in common.

4.1 Single switch

The optimal single switch yields a maximum extract purity of 86.53% at CSS. It can be seen that the bounds on feed flow rate and extract recovery become active ($Q_F=\epsilon_F=1 \text{ ml/min}$, $[Rec]_{E,Fru}=\epsilon_{Rec}=70\%$). This ensues in order to decrease the amount of feed processed and thus achieve the maximum possible extract purity. Also, maximization of extract purity results in removal of high amount of glucose (1) in the raffinate resulting in a high recovery ($\sim 90\%$). The low purity of 74.79% could be attributed to the low value of minimum extract recovery (70%) resulting in considerable amount of fructose (m) being obtained in raffinate.

4.2 Dual switch

The dual switch with two sets of operating conditions applied on alternate cycles is optimised to yield maximum purity for one of the two extract fractions, at CSS. This is done using optimisation parameters and bounds same as above but applied on two consecutive cycles at a dual period CSS, denoted as *Cycle* (1, dual), *Cycle* (2, dual) and yielding extract fractions E_1^{dual} and E_2^{dual} , respectively. The optimal dual switch yields a higher extract purity (88.32%) compared to optimal single switch (86.53%), for the fraction E_2^{dual} obtained during *Cycle* (2, dual). The superior purity is due to a lower average concentration of glucose (1.42 g/L) relative to fructose (10.73 g/L), in the extract, compared to single switch (1.32, 8.49 g/L respectively). This is the consequence of a higher switching period (124.71 s) and higher internal flow rates in sections II and III (13.03, 14.03 ml/min), compared to the single switch, during the previous cycle *Cycle* (1, dual). This results in sufficient time and speed for the less adsorbed glucose, which is faster than the more adsorbed fructose, to exit the columns of sections II, III during *Cycle* (1, dual). Consequently, a lower amount of glucose relative to fructose is available for elution as extract, when the column acting as section II during *Cycle* (1, dual) becomes part of section I, after port switching, during the current cycle i.e. *Cycle* (2, dual). However, the higher flow rates and switching period if applied during every cycle, would eventually lead to contamination of all the columns, due to the low flow rates of extract (1.97 ml/min) and raffinate (1 ml/min). This necessitates a second set of operating conditions to contain the contamination. Similar to optimal single switch, the lower bounds on feed flow rate and extract recovery during *Cycle*(1, dual) become active ($Q_{F,1}=\epsilon_F=1 \text{ ml/min}$, $[Rec]_{E_1,Fru}=\epsilon_{Rec}=70\%$). This ensues in order to reduce the amount being processed

and prevent the eventual contamination of section II via propagation in the direction of fluid flow.

With lower internal flow rates in sections II, III (10.78, 12.94 ml/min) and switching period (71.73 s) than single switch, the second set applied during *Cycle* (2, dual) serves the purpose of contamination prevention, with glucose having lower speed and lesser time to exit the said section. However, this also results in an increase in the amount of glucose relative to fructose in section II during *Cycle* (2, dual). This yields an extract fraction (E_1^{dual}) with purity (81.72%) inferior to optimal single switch (86.53%), when the column acting as section II during *Cycle* (2, dual) becomes part of section I during the next cycle i.e. when *Cycle* (1, dual) is repeated.

It is to be noted that, during *Cycle* (2, dual), the lower bound on only the extract recovery becomes active ($[Rec]_{E_2,Fru}=\epsilon_{Rec}=70\%$), in order to reduce the amount being processed for higher purity. Unlike single switch and *Cycle* (1, dual) of dual switch, the lower bound on feed flow rate is no longer active ($Q_{F,2}=2.15 \text{ ml/min} \neq \epsilon_F$). This happens in order to facilitate the extract recovery of 70%, same as optimal single switch i.e. at the minimum possible, when section III becomes section I after two cycles, but in a reduced duration (71.73 s). The flow rates in sections II, III decrease to the extent that they yield a feed flow rate that satisfies all the process constraints without contaminating E_2^{dual} (section I) during *Cycle* (2, dual). Therefore, the purity of the non-objective extract fraction (E_1^{dual}) is allowed to drop as low as possible by providing such a value for the lower bound on its purity that the bound does not become active ($[Pur]_{E_1,Fru}=81.72\% \neq \epsilon_{Pur}$).

In summary, at CSS, the optimal dual switch yielding two extract fractions, namely E_1^{dual} and E_2^{dual} , is characterised by a sequential enrichment of section II during *Cycle* (1, dual) and elution of resultant enriched E_2^{dual} from section I during the next cycle *Cycle* (2, dual). However, in order to maintain the superior purity of the eluted product E_2^{dual} , a containment of contamination also happens during *Cycle* (2, dual). This results in the inferior quality of E_1^{dual} which is eluted during the cycle when E_2^{dual} (section II) is getting enriched. Hence, an enriched and a more contaminated extract are obtained over every two consecutive cycles.

The trend of the average purity of raffinate fractions obtained during any two consecutive cycles is same as that of the corresponding extract fractions. In spite of a high switching period of 124.71 s during *Cycle* (1, dual), compared to 97.56 s of single switch, the low raffinate flow rate (1 ml/min) during *Cycle* (1, dual) results in a low raffinate recovery of 32.04%. This is compensated by the high raffinate flow rate of 7.32 ml/min during the shorter cycle *Cycle* (2, dual) yielding an extremely high recovery of 132.97%, thus preventing the accumulation in the system.

4.3 Triple switch

The extent to which the enrichment of sections and the contamination containment can happen, during optimal dual switch, to result in a better extract purity than single switch, is limited by the process constraints. If a third set of operating conditions were introduced with each of the three sets repeating after every three port

Table 2. Comparison: Optimal results of Single, Dual and Triple switch modes of operation for Fructose-Glucose ($\epsilon_F=1$ ml/min, $\epsilon_{Rec}=70\%$, $\epsilon_{Pur}=60\%$)

Parameter	Units	Mode of operation							
		Single switch	Dual switch			Triple switch			
			Cycle (1, dual)	Cycle (2, dual)	Avg. (hr ⁻¹)	Cycle (1)	Cycle (2)	Cycle (3)	Avg. (hr ⁻¹)
t^*	(s)	97.56	124.71	71.73		171.56	44.62	82.64	
Q_I	(ml/min)	15.00	15.00	15.00	4.62	15.00	15.00	15.00	4.99
Q_{II}		12.53	13.03	10.78		13.47	13.00	8.55	
Q_{III}		13.53	14.03	12.94		14.47	14.00	10.95	
Q_{IV}		10.53	13.03	5.62		13.47	13.00	1.16	
Q_D		4.47	1.97	9.38		1.53	2.00	13.84	
Q_E		2.47	1.97	4.22		1.53	2.00	6.45	
Q_R		2.99	1.00	7.32		1.00	1.00	9.79	
Q_F		1.00	1.00	2.15		1.41	1.00	1.00	
Extract	Fru	g/L	8.49	10.67	10.73	13.69	10.52	7.82	
	Glu	g/L	1.32	2.39	1.42	4.20	4.22	0.82	
	$[Pur]$	(%)	86.53	81.72	88.32	76.53	71.38	90.54	
	$[Rec]$	(%)	70.00	70.00	70.00	70.00	70.00	70.00	
D/F		4.47			3.28				3.59
$[Prod]_{Fru,E}$	g/(L hr)	16.71	10.72	12.91		9.62	2.49	11.07	
Raffinate	Fru	g/L	3.01	4.54	3.71	1.76	3.87	4.38	
	Glu	g/L	8.93	9.61	11.74	1.84	7.10	11.40	
	$[Pur]$	(%)	74.79	67.91	75.99	51.14	64.75	72.24	
	$[Rec]$	(%)	89.10	32.04	132.97	6.14	23.66	154.81	

The portions highlighted other than extract purity indicate the lower bound on that quantity becoming active. The highlighted purity indicates the maximum obtainable extract purity for a given mode of operation.

switches, two cycles will be available for the same as opposed to only one cycle in dual switch. The triple switch

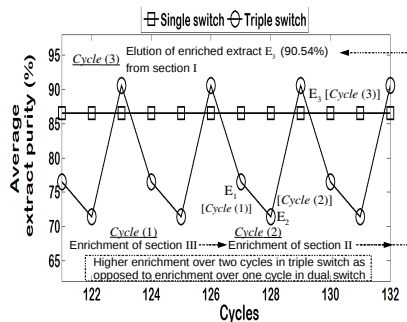


Fig. 3. Average extract purity at cyclic steady state (CSS) has been attained well ahead of 120 cycles, found after carrying out transient simulations)

is optimised (7), to obtain maximum extract purity for one out of the three distinct extract fractions obtained at the triple period CSS. The constraints, optimisation parameters and bounds are same as single and dual switch but are applied on three consecutive cycles as opposed to one or two consecutive cycles, respectively. The optimal triple switch yields a maximum extract purity of 90.54% for extract fraction E_3 , during *Cycle (3)*, which is higher than the corresponding value in dual switch (88.32% for E_2^{dual}). This becomes possible with the internal flow rates in sections II, III (13.47, 14.47 ml/min) and switching period (171.56 s) during *Cycle (1)* being higher than the corresponding values of dual switch (13.03, 14.03 ml/min, 124.71 s) for *Cycle (1, dual)*, resulting in enrichment of section III. Next, with the internal flow rates in sections II, III (13.0, 14.0 ml/min) during the consecutive cycle (*Cycle (2)*) being similar to the corresponding values of enriching *Cycle (1, dual)* of dual switch, there is further enrichment of erstwhile section III behaving as section II during *Cycle*

(2). This happens in spite of lesser time (44.62 s < 71.73 s) being available for enrichment. An extract (E_3) more enriched than the enriched extract (E_2^{dual}) of dual switch is eluted during next cycle *Cycle (3)*, when the column acting as section II during the current cycle behaves as section I.

With the extent of enrichment being higher than that of dual switch, the extent of containment of contamination required to maintain the enrichment, is also higher. This results in the flow rate in sections II, III (8.55, 10.95 ml/min), during *Cycle (3)*, being significantly lower than the corresponding values (10.78, 12.94 ml/min) of the cycle (*Cycle (2, dual)*) containing the contamination in dual switch. As a result, the extracts E_1, E_2 subsequently eluted after one and two cycles respectively, after *Cycle (3)*, as seen in Fig. 3, are inferior to the inferior fraction E_1^{dual} of dual switch. The switching period of *Cycle (3)* being only slightly higher than of (*Cycle (2, dual)*) of dual switch does not contribute much in terms of giving more time to the components to exit the said sections. The nature of the extract purities wherein the purity of fraction E_2 (71.38%) is lower than that of fraction E_1 (76.53%), can be attributed to section III having a feed flow rate of 2.4 ml/min and 1 ml/min during *Cycle (3)* and *Cycle (2)*, respectively. This is in contrast to the containment of contamination in section II during *Cycle (2, dual)*, which not involving any feed into the said section results in an extract fraction E_1^{dual} during *Cycle (1, dual)* which is superior to both the fractions E_1, E_2 of triple switch.

The lower bounds on extract recovery and feed flow rate are active during *Cycle (1)* as well as *Cycle (2)*, in order to reduce the amount processed, for high purity of the resultant extract E_3 being eluted subsequently during *Cycle (3)*. Similar to *Cycle (2, dual)*, the bound on extract recovery of *Cycle (3)* becomes active to prevent contamination of sections and bound on the feed flow rate

does not become active. The latter happens in order to attain sufficient amount in section III for the minimum extract recovery of 70% after two cycles, during *Cycle* (1), when section III of current cycle behaves as section I. This is due to the factors like reduced duration (82.64 s < 171.56 s) available for adsorption as well as higher rate of removal from the system due to the high raffinate flow rate during *Cycle* (3). Also, the raffinate purities and recoveries follow an increasing trend, unlike that of the extract purities.

4.4 Comparison of D/F and Productivity

Due to higher degrees of freedom, the dual switch is better than single switch and triple switch is better than dual switch, in terms of maximum possible extract purity. The enriched product, however, is being obtained during only part of the operation and thus results in a reduced productivity. The relative amounts of desorbent (Q_D) and feed (Q_F) being consumed during the whole operation also need to be considered.

Table 3. D/F and Productivity

Parameter	Units	Mode of operation		
		Single switch	Dual switch	Triple switch
$[Pur]_{E,Fructose}$	(%)	86.53	88.32	90.54
D/F	Avg. (hr^{-1})	4.47	3.28	3.59
$[Prod]_{Fructose,E}$	g/(L hr)	16.71	12.91	11.07

Table 3 summarizes productivity of fructose in the extract with maximum purity and average D/F, from Table 2, for an hourly operation, through the three modes of operation. For a litre of total adsorbent, optimal single switch yields 16.71 g of fructose in a 86.53% pure extract for an average hourly D/F value of 4.47. The optimal dual switch yields a slightly better extract with a purity of 88.32%, at a reduced average D/F value of 3.28 but yields only 12.91 g of fructose. In the case of optimal triple switch, with a slightly higher value of average D/F (~3.6) than dual switch (3.28) but considerably lower than single switch (4.47), an extract more enriched (90.54% pure) than dual switch (88.32%) is obtained with, however, a lower amount (11.07 g) of fructose. The higher extract purities are not only characterised by the desirable low value of average D/F but also undesirable low productivities. A detailed economic analysis comparing the gain due to the higher extract purity obtained through a low value of average D/F with the loss due to low productivity and production of inferior extract fractions, will help evaluate the feasibility of experimental implementation of the proposed triple switch mode of operation.

5. CONCLUSION

Manipulation of the sets of operating conditions over different cycles results in different fractions, which when optimised yields a higher extract purity than the conventional mode of operation. In a general manner, for q number of consecutive cycles operated by q different sets of operating conditions, this is attained by section enrichment happening over $q-1$ consecutive cycles followed by elution of the resultant enriched extract and containment of contamination during the last (q^{th}) cycle, yielding $q-1$ number of fractions inferior to said enriched fraction, over the next

cycles. This has been evaluated for three ($q=3$) sets of operating conditions in the current work and two ($q=2$) sets previously. As the sets of operating conditions increase, the extent of enrichment and contamination containment also increases, as much as permitted by the process constraints. Thus, the maximum extract purity possible also improves.

By extension of the above mechanism to a switching of higher order like quadruple switch (say), with four sets of operating conditions, one could expect enrichment of sections IV, III, II over three consecutive cycles, as much as permitted by the process constraints, and elution of an extract more enriched than triple switch, during the fourth cycle from section I. However, since section IV is on the downstream side of the section (section III) into which feed enters and involves removal of feed entering from another section as opposed to residual feed from a previous cycle, it might not be that straightforward.

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