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Arithmetic approach for complex PSA cycle scheduling

Amal Mehrotra · Armin D. Ebner · James A. Ritter

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Abstract An algebraic model was derived for obtaining complex pressure swing adsorption (PSA) cycle schedules. This new approach involves *a priori* specifying the cycle steps, their sequence and any constraints, and then solving a set of analytical equations. The solution identifies all the cycle schedules for a given number of beds, the minimum number of beds required to operate the specified cycle step sequence, the minimum number and location of idle steps to ensure alignment of coupled cycle steps, and a simple screening technique to aid in identifying the best performing cycles that deserve further examination. The methodology was tested successfully against 10, 12 and 16 bed PSA systems in the literature that all utilized the same 13 step cycle sequence that has four pressure equalization steps. It completely resolved all the corresponding cycle schedules for these 13 step multi-bed PSA systems with ease, and showed that the number of cycle schedules was hundreds to thousands of times greater than the few ever reported in the literature for each one. Overall, this new methodology for complex PSA cycle scheduling can be applied to any number of cycle steps, any corresponding cycle step sequence, and any number of constraints, with the outcome being the complete set of cycle schedules for any number of beds greater than or equal to the minimum number it determines.

Keywords Pressure swing adsorption · PSA · Cycle scheduling · Cycle sequencing · PSA cycle schedules

A. Mehrotra · A.D. Ebner · J.A. Ritter (✉)
Department of Chemical Engineering, Swearingen Engineering Center, University of South Carolina, Columbia, SC 29208, USA
e-mail: ritter@cec.sc.edu

Nomenclature

D duration of a unit block
I_i duration of idle step i
J_i duration between two coupled cycle steps i
N number of beds
S_i duration of a cycle step i
T total cycle time
U duration of a unit cell
x maximum number of unit cells occupied by any cycle step except the feed step
y number of unit cells in a unit block
z number of beds fed simultaneously

Abbreviations

CnD countercurrent depressurization step
EeD depressurization equalization step ($1 \leq e \leq$ number of such steps)
EeR repressurization equalization step ($1 \leq e \leq$ number of such steps)
F feed step
FP feed pressurization step
LR light reflux step
PP cocurrent depressurization step
PSA pressure swing adsorption

1 Introduction

Pressure swing adsorption (PSA) is a widely used commercial process for gas separation and purification (Ruthven et al. 1994). Generally, two or more beds are interconnected and operate in a cyclic fashion according to a specified sequence of cycle steps. There are just six basic cycle steps comprising any cycle step sequence in a PSA process (Ruthven et al. 1994). These are feed, rinse (heavy reflux), co-current or countercurrent depressurization, purge (light reflux), pressure equalization, and repressurization steps. A minimum of two of these steps must be used, including one production step (e.g., feed) and one regeneration step (e.g., purge), to achieve the characteristic periodic behavior associated with all PSA processes.

For typical PSA systems, especially the ones designed to process large feed throughputs, these six basic steps are arranged in a variety of ways, with multiple beds and steps interacting with one another. Such an interaction is clearly evident during the operation of the pressure equalization step (Ruthven et al. 1994). Here, two beds are interconnected till their pressures equalize. Another example includes the heavy reflux step (also called the rinse step), which uses the gas produced from the purge or countercurrent depressurization step as the source of rinse gas (Reynolds et al. 2008).

During a PSA cycle many such interactions take place between different beds, which, in turn, gives rise to many constraints that must be met while constructing a PSA cycle schedule. For example, during the equalization step, the beds involved must initialize and terminate the step at the same instant in time. Similarly, if the entire product from the countercurrent depressurization step is used as the source of the heavy reflux gas, both of these cycle steps must start and end at the same instant in time. Therefore, the steps in these two examples must be coupled in time throughout the cycle schedule.

Cycle scheduling is relatively simple when dealing with a small number of beds. However, the complexity of the problem increases tremendously when multiple beds and numerous constraints are involved. Only a paucity of information is available in the literature for such complex PSA cycle scheduling (Chiang 1988; Smith and Westerberg 1990; Ebner et al. 2009).

Chiang (1988) presented an arithmetic model for scheduling PSA cycles. However, this first of its kind analysis does not consider the possibility of idle steps being incorporated into the final schedule. During an idle step, the bed is isolated and all valves leading to it are closed. Sometimes this step has to be included in a cycle schedule to align all the interacting steps in different beds.

Smith and Westerberg (1990) suggested a method based on mixed integer nonlinear programming. Under certain conditions, the nonlinearities in the model are linearized and the program is restructured as a mixed integer linear program (MILP). This method requires the use of complex programming techniques and numerical methods to solve the MILP. Although powerful, the implementation of this approach can be a daunting task, especially for multi-bed PSA systems.

Ritter and coworkers (Ebner et al. 2009) developed the first of its kind graphical approach to obtain PSA cycle schedules. This analysis is simple, quick to adapt, and follows a systematic procedure to fill up a 2-D grid based on a few rules and some heuristics. Virtually any PSA cycle schedule can be devised using this graphical approach, no matter the complexity. However, this approach lacks the ability to positively identify all the possible cycle schedules for a given cycle step sequence and number of beds.

Therefore, the objective of this article is to present a methodology for obtaining algebraic expressions that can used to devise all the possible complex PSA cycle schedules for a given cycle step sequence, any associated constraints, and any number of beds equal to or greater than the minimum number it determines. Complex PSA systems found in the literature are used to demonstrate this new arithmetic approach. Examples include 10, 12 and 16 bed systems that all utilize the same 13 step cycle sequence and that all have many coupled steps (i.e., constraints), including four pressure equalization steps. The effectiveness of this new approach for complex PSA cycle scheduling is discussed.

2 Graphical representation of the cycle schedule

The terminology used in the analysis is based on the arithmetic approach outlined by Chiang (1988) and the graphical approach developed by Ebner et al. (2009) for a 13 step cycle sequence (Xu et al. 2004). This cycle sequence (excluding the idle steps) goes as follows:

1. feed (F) at high pressure, where a bed receives feed gas in its heavy end and produces light product from its light end;
2. four consecutive depressurization pressure equalization steps where E1D, E2D, E3D and E4D are in succession and coupled with E1R, E2R, E3R and E4R, respectively;
3. cocurrent depressurization (PP), where the light gas exiting a bed is used to purge another bed undergoing light reflux (LR);
4. countercurrent depressurization (CnD), where a bed is depressurized from the heavy end and the gas exiting it is taken as heavy product;
5. light reflux (LR), where a bed receives purge gas in its light end from the light end of a bed undergoing cocurrent depressurization (PP);
6. four consecutive repressurization pressure equalization steps where E4R, E3R, E2R and E1R are in succession and coupled with E4D, E3D, E2D and E1D, respectively; and
7. feed pressurization (FP), where a bed receives gas in its heavy end from the feed source.

PSA systems operating this cycle schedule are being run on a commercial scale for the production of high purity hydrogen, with many 10 and 12 bed cycle schedules discussed by

Xu et al. (2004). For brevity, the methodology, and its applications and examples are based exclusively on this 13 step cycle sequence.

Figure 1 shows a typical PSA cycle schedule in graphical form for a 10 bed system that uses the 13 step cycle sequence (Xu et al. 2004). The 10 beds are placed along the vertical direction, and time is placed along the horizontal direction. The 20 columns in the grid, i.e., A through T along the horizontal direction represent unit cells or time steps of equal length. A row of the grid represents all the cycle steps a bed undergoes over the entire cycle, whereas a column of the grid shows which cycle step is being run by which bed at a particular instant in time. The intersection of a row and a column is a unit cell (shaded) and is the smallest repeating element of the grid. This analysis assumes that a unit cell cannot be further divided, i.e., a unit cell can be occupied by only one cycle step.

It is clear from this 2D grid that each bed follows the same sequence of steps but out of phase with each other by two unit steps. The thick rectangle that encapsulates these two unit cells (or the phase) for all columns is defined as the unit block. A unit block thus comprises the time it takes for a specific step (operating in a particular bed) to be repeated by the next bed in a different phase. Consequently, the number of unit blocks equals the number of beds, e.g., 10 in this case. Also, within the time frame of a unit block, all the cycle steps in the sequence are being run somewhere in the beds.

3 Development of the methodology

In this section, the methodology behind obtaining a powerful analytical tool for complex PSA cycle scheduling is explained qualitatively. All that is needed to get started is a sequence of cycle steps and a list of associated constraints. With both of them in hand, the methodology involves carrying out three stages.

Stage I involves determining the relationships for the time durations between coupled cycle steps in a column. This stage necessarily establishes all the time relationships between the cycle steps and idle steps of a given cycle sequence. To start, all the idle steps must be defined. Since the locations of the idle steps are unknown at this point, it is necessary to place an idle step in between every cycle step, unless a constraint prevents it from being there. An idle step must also be placed in between the last and first step of the cycle sequence.

Next, a relationship must be determined for the time duration of each pair of coupled cycle steps in the cycle sequence. For example, two relationships are needed in a cycle sequence with two equalization steps. Recall that because a coupled step requires the interconnection of two beds, the

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	Feed		Feed		E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FP
2	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R
3	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R
4	I	E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP		CnD		LR	
5	LR		I	E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP		CnD	
6	CnD		LR		I	E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP	
7	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D
8	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D
9	E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FP	Feed			
10	Feed		E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FP	Feed	

Fig. 1 Cycle schedule for a 10 bed 13 step system with one idle step and four pressure equalization steps (Xu et al. 2004)

steps in these beds must run for the same duration and start and stop at the same instant in time. Since D, the duration of a unit block, is also the time taken for a specific step (operating in a particular bed) to be repeated by any of the remaining beds, the time between two coupled steps in the cycle sequence undergone by a single bed must be a multiple of D. This multiple of D is expressed in terms of a positive integer J, where J is unique to each coupling. Consequently, in each relationship, the time between each pair of coupled steps is expressed on the right side of it as the sum of the durations of all the cycle and idle steps from the start of the first step in the coupling to the start of the second step in the coupling, and on the left side of it simply as the product of J and D. An additional relationship is needed to express the total cycle time T as the sum of the durations of all the cycle and idle steps. Because T is equal to the product of the number of beds N and the duration of the unit time block D, the duration of all the cycle and idle steps can be expressed in terms of N and D. Thus, for M pairs of coupled steps, $M+1$ equations must be established, i.e., M equations for M pairs of coupled steps and one equation involving the total cycle time T. The resulting system of equations contains all the J parameters, the number of beds N, and the durations of all the cycle and idle steps.

Stage II involves determining the number of beds N and all the J parameters, because they are used in the relationships established in stage I to solve for the durations of all the cycle and idle steps, which is done in stage III. To obtain values of J and N, a set of relationships in the form of inequalities is derived based on restrictions imposed on both the cycle and idle steps. For example, by default, the duration of an idle step can be zero, while the duration of a cycle step cannot be less than the duration of a unit cell U. Also, the duration of a certain step may be limited to a specific value based on experience. For example, an equalization step is normally assumed to occupy only one unit cell. For steps that are not *a priori* restricted by an equality and are already expressed in multiples of unit cells, it is necessary to restrict the durations of the remaining cycle and idle steps to a certain number of unit cells. This is done to avoid an infinite number of solutions, which are possible because the inequality relationships inherently lead to multiple solutions for each J and N, as shown later.

With these imposed conditions and the set of equations constructed in stage I, a set of inequalities that involve N and all Js in terms of unit cells is built. An assumption must be made at this point for expressing the unit block in terms of a chosen number of unit cells y, i.e., $D = yU$; thus, the integer y establishes the length of or equivalently the number of unit cells in a unit block. The resulting solution set consists of one of the many combinations of the different values of J (i.e., M values of J for M pairs of coupled steps) and N that satisfy the inequalities containing them. This means that many such solution sets exist that lead to the total number of solutions in stage III. From these solution sets it becomes apparent that N is never less than a given number, with this number corresponding to the minimum number of beds allowed for the given cycle sequence and conditions imposed in stage II.

Stage III involves determining all the durations of the cycle and idle steps, i.e., the total number of solutions, once all the solution sets are determined in stage II. This is done by replacing the values of J and N in the equations established in stage I, while keeping in mind the conditions imposed on them in stage II. Because the number of variables (i.e., the durations for the cycle and idle steps) is normally larger than the number of relationships, many solutions are possible for each solution set, i.e., for each set of Js and N. Once all the solutions are determined, the construction of the corresponding cycle schedules in graphical form is straightforward, as described later.

4 Results and discussion

4.1 Application of the methodology

In this section, the methodology explained qualitatively above is developed into a quantitative set of relationships based on applying the three stages to the specific cycle schedule in Fig. 1 and its associated constraints. Table 1 shows the notation used to represent the durations of the individual cycle and idle steps for the 13 step cycle sequence

Table 1 Notation for the duration of each cycle step and all idle times for– the 13 step cycle sequence: F → E1D → E2D → E3D → E4D → PP → CnD → LR → E4R → E3R → E2R → E1R →FP

Notation	Cycle step
S_1	Step time for the feed step
S_2	Step time for each of the equalization steps (E1D, E2D, E3D, E4D, E1R, E2R, E3R, E4R)
S_3	Step time for PP and LR
S_4	Step time for CnD
S_5	Step time for FP
I_1	Idle time between E4D and PP
I_2	Idle time between PP and CnD
I_3	Idle time between CnD and LR
I_4	Idle time between LR and E4R
I_5	Idle time between E4R and E3R
I_6	Idle time between E3R and E2R
I_7	Idle time between E2R and E1R
I_8	Idle time between E1R and FP
I_9	Idle time between FP and Feed
I_{10}	Idle time between F and E1D

shown in Fig. 1. Each of the 13 steps (excluding the idle steps) in this cycle sequence is given a duration denoted by S_i, with i normally taking on values $1 \le i \le 13$. However, in this case, i takes on values $1 \le i \le 5$ because it is known *a priori* that certain cycle steps have identical durations. For example, the four equalization steps are assumed to operate for the same duration S_2, and to minimize the time associated with equalization, the duration of these steps is assumed to be that of a unit cell, i.e., $S_2 = U$. As the PP and LR steps are coupled, they also operate for the same duration S_3. This leaves the F, CnD and FP steps with corresponding durations of S_1, S_4 and S_5.

To ensure that the system is fed continuously, the duration of the feed step is set equal to a multiple number of unit blocks, i.e., $S_1 = zD$, where z is a positive integer and physically indicates the number of beds being fed simultaneously. Also, to maximize the feed time per cycle, cycle steps other than the feed and equalization steps are restricted to being no longer than x number of unit cells, i.e., $S_i \le xU$ (with $3 \le i \le 5$).

Recall that it is necessary to account for idle time between each cycle step, unless otherwise stated. For example, in this case it is assumed that there are no idle steps between the four consecutive pressure equalization steps, i.e., E1D, E2D, E3D and E4D. The idle time between each remaining cycle step, which amounts to 10 possible idle steps, is represented by I_i with $1 \le i \le 10$. To minimize the total idle time in a cycle schedule, the idle steps are also limited to a maximum duration equal to D, i.e., $I_i \le D = yU$.

In summary, the conditions imposed on this particular 13 step cycle are:

$$S_1 = zD = zyU \tag{1}$$

$$S_2 = U \tag{2}$$

$$U \le S_i \le xU; \quad 3 \le i \le 5 \tag{3}$$

$$0 \le I_i \le D = yU; \quad 1 \le i \le 10 \tag{4}$$

It must be emphasized that these relationships are unique to the cycle schedule shown in Fig. 1 that utilizes the 13 step cycle sequence and has its own set of constraints. A different set of relationships may result if the sequence or any of the constraints are changed. This is also the point in the analysis where a new constraint can be added, e.g., like restricting the LR step to be no longer than the F step.

Stage I involves identifying the relationships between the time variables defined in Table 1. Because there are four pairs of equalization steps and a coupling between the PP and LR steps ($M = 5$), a total of six ($M + 1$) equations are required. Recall that the time between two coupled steps is the time from the start of the first step in the coupling till the start of the second step in the coupling. For example, for the coupled equalization steps E1D and E1R in Fig. 1, when moving in time from left to right, the duration from the start of E1D till the start of E1R is 7D (i.e., $J = 7$). Obviously, the integer J has to be less than N, otherwise the product of J and D becomes greater than T, which is impossible. Also, as stated before, the total cycle time T, which is the sum of all the individual cycle and idle steps, satisfies the relationship $T = ND$ (or $T = NyU$).

The six corresponding relationships are obtained by analyzing the cycle step sequence in one bed as follows:

a) For coupled steps E1R and E1D, the duration from the start of E1R till the start of E1D is:

$$DJ_1 = S_1 + S_2 + S_5 + I_8 + I_9 + I_{10} \tag{5}$$

b) For coupled steps E2R and E2D, the duration from the start of E2R till the start of E2D is:

$$DJ_2 = S_1 + 3S_2 + S_5 + I_7 + I_8 + I_9 + I_{10} \tag{6}$$

c) For coupled steps E3R and E3D, the duration from the start of E3R till the start of E3D is:

$$DJ_3 = S_1 + 5S_2 + S_5 + I_6 + I_7 + I_8 + I_9 + I_{10} \tag{7}$$

d) For coupled steps E4R and E4D, the duration from the start of E4R till the start of E4D is:

$$DJ_4 = S_1 + 7S_2 + S_5 + I_5 + I_6 + I_7 + I_8 + I_9 + I_{10} \tag{8}$$

e) For coupled steps PP and LR, the duration from the start of LR till the start of PP is:

$$DJ_5 = S_1 + 8S_2 + S_3 + S_5 + I_1 + I_4 + I_5 + I_6 + I_7 + I_8 + I_9 + I_{10} \tag{9}$$

f) Finally, for the total cycle time:

$$T = DN = S_1 + 8S_2 + 2S_3 + S_4 + S_5 + I_1 + I_2 + I_3 + I_4 + I_5 + I_6 + I_7 + I_8 + I_9 + I_{10} \tag{10}$$

For the sake of clarity, (5) to (10) are listed in order of increasing time duration, i.e., $J_1 < J_2 < J_3 < J_4 < J_5 < N$. Note that these equations are derived by evaluating time from left to right in the given cycle sequence; a different set of equations that leads to identical results can also be obtained by evaluating time from right to left.

Stage II involves the determination of all the Js (i.e., J_1 to J_5) and N, now that the stage I relationships are defined. This is done by establishing relationships between the conditions imposed on the steps, as indicated by (1) to (4), and the equations derived in stage I. The first of these relationships is obtained by subtracting (5) from (6), substituting

$D = yU$ and $S_2 = U$, and then using the restriction imposed on the idle steps. This leads to

$$2U \le yU(J_2 - J_1) = 2U + I_7 \le (2 + y)U \tag{11a}$$

which, after eliminating U and simplifying, becomes

$$\frac{2}{y} \le (J_2 - J_1) \le \frac{2 + y}{y} \tag{11b}$$

Similarly, when repeating the same procedure for (6) and (7), (7) and (8), (8) and (9), and (9) and (10), while remembering that $T = NyU$, and using restrictions given in (2) to (4) when appropriate, the remaining relationships are obtained as

$$\frac{2}{y} \le (J_3 - J_2) \le \frac{2 + y}{y} \tag{12}$$

$$\frac{2}{y} \le (J_4 - J_3) \le \frac{2 + y}{y} \tag{13}$$

$$\frac{2}{y} \le (J_5 - J_4) \le \frac{1 + x + 2y}{y} \tag{14}$$

$$\frac{2}{y} \le (N - J_5) \le \frac{2(x + y)}{y} \tag{15}$$

Equations (11) to (15) constitute 10 inequalities that contain six unknowns (J_1, J_2, J_3, J_4, J_5 and N). However, because they are all difference relationships in the unknowns, a value of one of them is needed to begin generating solutions. Notice also that in establishing the relationships from (5) to (10) S_1 cancels out in every case. To bring S_1 back into the analysis, (1) and (5) are used. Equation (5) is useful as it contains both S_1 and J_1, and (1) is useful as it imposes the restriction on S_1 and thus supplies the value of one of the unknowns that is needed to start generating solutions. By following a procedure identical to that which leads to (11) to (15) and making the assumption that z in (1) cannot be less than unity, the following inequality is obtained that contains J_1:

$$\frac{2 + y}{y} \le J_1 \le \frac{1 + x + (3 + N)y}{y} \tag{16}$$

Note that in (16) the upper limit for J_1 is always satisfied (as $N > J_1$, and x and y are positive integers) and is therefore inconsequential.

The above equations are now used to obtain all the possible cycle schedules for the 13 step cycle sequence in Table 1 for 7, 8 and 9 bed systems. Recall that the length of a unit block D is expressed as a multiple of unit cells using the parameter y (a positive integer), i.e., $D = yU$. In this example, the length of the unit block is assumed to be 2 unit cells, i.e., $y = 2$, which is the same as the case shown in Fig. 1. Also, in this example, x is assumed to be 4, which means that any of the cycle steps other than the feed step are restricted to occupying no more than 4 unit cells. Notice that $x = 2$ in Fig. 1. This is not a problem because using $x = 4$ guarantees all solutions are obtained for $x = 1$ to 4.

Table 2 Solution sets for $N = 7$, 8 and 9 when $x = 4$ and $y = 2$[a]

N	J_1	J_2	J_3	J_4	J_5	Total solution sets
7	2	3	4	5	6	1
8	2	3	4	5	6	6
	2	3	4	5	7	
	2	3	4	6	7	
	2	3	5	6	7	
	2	4	5	6	7	
	3	4	5	6	7	
9	2	3	4	5	6	18
	2	3	4	5	7	
	2	3	4	6	7	
	2	3	5	6	7	
	2	4	5	6	7	
	3	4	5	6	7	
	2	3	4	5	8	
	2	3	4	6	8	
	2	3	5	6	8	
	2	3	5	7	8	
	2	4	5	6	8	
	2	4	5	7	8	
	2	4	6	7	8	
	3	4	5	6	8	
	3	4	5	7	8	
	3	4	6	7	8	
	3	5	6	7	8	
	4	5	6	7	8	

[a]The solution set shaded in grey is used to obtain all the possible solutions shown in Table 3

Table 2 shows all the possible solution sets for J_i ($i = 1$ to 5) obtained by solving the above system of inequalities for N equal to 7, 8 and 9. Every row in the table is a separate solution set, as it contains distinct values of J_1, J_2, J_3, J_4, J_5 and N. The algorithm used to determine these solutions starts with the least possible value of J_1 that satisfies (16). Then, for every value of J_1, multiple values of J_2 are possible. Similarly, for every value of J_2, multiple values of J_3 are possible, and so on. This procedure is repeated by incrementing the values of J_1 and continued till no more solutions are possible that simultaneously satisfy (11) to (16). It should be clear at this point how important the restrictions are in (1) to (4) for limiting the number of solution sets to a discrete number; otherwise, the number of solutions becomes infinite. Also, it is noteworthy that no solution set can be obtained for $N = 6$, because J_1 for this particular problem cannot be less than 2 and all the differences between either consecutive Js or between N and J_5 in (11) to (16) are not less than unity. This implies that a minimum of 7 beds are needed for operating this 13 step cycle sequence.

Stage III involves determining the total number of solutions for each solution set resolved in stage II and thus the durations of the cycle and idle steps for each of these solutions. To proceed, (5) to (10) must express all the unknowns in terms of J_i ($i = 1$ to 5), N and U, while using all the imposed restrictions in terms of equalities. By following a procedure analogous to that of stage II, (17) to (21) are obtained by respectively subtracting (5) from (6), (6) from (7), (7) from (8), (8) from (9), and (9) from (10). This leads to:

$$(y(J_2 - J_1) - 2)U = I_7 \quad (17)$$

$$(y(J_3 - J_2) - 2)U = I_6 \quad (18)$$

$$(y(J_4 - J_3) - 2)U = I_5 \quad (19)$$

$$(y(J_5 - J_4) - 1)U = S_3 + I_1 + I_4 \quad (20)$$

$$y(N - J_5)U = S_3 + S_4 + I_2 + I_3 \quad (21)$$

Equation (22) is obtained from (5), which contains J_1.

$$(y(J_1 - z) - 1)U = S_5 + I_8 + I_9 + I_{10} \quad (22)$$

For this 13 step cycle sequence, the final set of relationships that must be solved are (1), (2) and (17) to (22), as they contain all the unknowns, namely S_1 to S_5 and I_1 to I_{10}. S_i ($i = 3$ to 5) and I_i ($i = 1$ to 10) are subject to the limits imposed by (3) and (4), while the integer z, representing the number of beds being fed simultaneously, is restricted by the condition that $y(J_1 - z) - 1$ from (22) cannot be negative, i.e., $z < J_1$ for this specific 13 step cycle sequence. It is noteworthy that the system of equations given by (1), (2) and (17) to (22) is over specified, as it contains 16 variables, namely S_1 to S_5, I_1 to I_{10}, and z in 8 equations. This is the reason why there are multiple solutions for each solution set.

For the solution set shaded in grey for $N = 9$ in Table 2, Table 3 shows the 33 solutions that result from solving (1), (2) and (17) to (22). Figure 2 shows the cycle schedule for just one of these solutions, denoted as solution 24 in Table 3. To convert this solution into the symmetrical 2D grid shown in Fig. 2, start with an empty grid of nine rows ($N = 9$) and 18 (i.e., yN) columns representing the unit cells. Then, in the first row start filling in the unit cells from the first step to the last step of the cycle sequence, including the surviving idle steps, starting from unit cell A1. For solution 24, idle step I_8 is the only one needed. To continue with the next row or bed 2, start with the feed step two unit cells to the right relative to bed 1 (i.e., unit cell C2) and then proceed as

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
											$J^*_1=1$	$J^*_2=2$	$J^*_3=3$	$J^*_4=4$	$J^*_5=5$			
1	Feed				E1D	E2D	E3D	E4D	PP	CnD	LR	E4R	E3R	E2R	E1R	I_8	FP	
2	FP		Feed				E1D	E2D	E3D	E4D	PP	CnD	LR	E4R	E3R	E2R	E1R	I_8
3	E1R	I_8	FP		Feed				E1D	E2D	E3D	E4D	PP	CnD	LR	E4R	E3R	E2R
4	E3R	E2R	E1R	I_8	FP		Feed				E1D	E2D	E3D	E4D	PP	CnD	LR	E4R
5	LR	E4R	E3R	E2R	E1R	I_8	FP		Feed				E1D	E2D	E3D	E4D	PP	CnD
6	PP	CnD	LR	E4R	E3R	E2R	E1R	I_8	FP		Feed				E1D	E2D	E3D	E4D
7	E3D	E4D	PP	CnD	LR	E4R	E3R	E2R	E1R	I_8	FP		Feed				E1D	E2D
8	E1D	E2D	E3D	E4D	PP	CnD	LR	E4R	E3R	E2R	E1R	I_8	FP		Feed			
9	Feed		E1D	E2D	E3D	E4D	PP	CnD	LR	E4R	E3R	E2R	E1R	I_8	FP		Feed	
									$J_5=8$	$J_4=7$	$J_3=6$	$J_2=5$	$J_1=4$					

Fig. 2 Cycle schedule for a 9 bed 13 step system corresponding to solution 24 highlighted in grey in Table 3. The shaded cells identify the coupled steps, as described in the text

Table 3 Solutions for the solution set shaded in grey in Table 2: $J_1 = 4$, $J_2 = 5$, $J_3 = 6$, $J_4 = 7$, $J_5 = 8$, and $N = 9$; with $x = 4$ and $y = 2$.[a] Results for S_i and I_i are given as multiples of unit cells U. $I_1 = I_2 = I_3 = I_4 = I_5 = I_6 = I_7 = 0$, $S_1 = zyU$, and $S_2 = S_3 = S_4 = U$ in all cases

Solution	z	S_5	I_8	I_9	I_{10}	Total solutions
1	1	1	2	1	1	33
2	1	1	1	2	1	
3	1	1	1	1	2	
4	1	1	2	2	0	
5	1	1	2	0	2	
6	1	1	0	2	2	
7	1	2	1	1	1	
8	1	2	2	1	0	
9	1	2	1	2	0	
10	1	2	2	0	1	
11	1	2	1	0	2	
12	1	2	0	1	2	
13	1	2	0	2	1	
14	1	3	2	0	0	
15	1	3	0	2	0	
16	1	3	0	0	2	
17	1	3	1	1	0	
18	1	3	1	0	1	
19	1	3	0	1	1	
20	1	4	1	0	0	
21	1	4	0	1	0	
22	1	4	0	0	1	
23	2	3	0	0	0	
24	2	2	1	0	0	
25	2	2	0	1	0	
26	2	2	0	0	1	
27	2	1	2	0	0	
28	2	1	0	2	0	
29	2	1	0	0	2	
30	2	1	1	1	0	
31	2	1	1	0	1	
32	2	1	0	1	1	
33	3	1	0	0	0	

[a]The solution shown in grey is used to obtain the cycle schedule in Fig. 2

before to the right by filling in the rest of the unit cells with steps. Once the last unit cell (i.e., unit cell R2) is reached, continue the process from the beginning of the row (i.e., unit cell A2) until reaching unit cell B2. The process is repeated likewise for the rest of the rows until the grid is completely filled in, thereby systematically forming the complete cycle schedule.

5 Implications of the methodology

In this section, unique features that emerge from the methodology are illuminated. First, an alternative meaning of J is illustrated, along with a way of finding all the solutions for a particular cycle schedule, i.e., solution set, in the literature. Then, the total number of solutions is differentiated from the total number of distinct solutions, which differ simply by the placement of one or more idle steps. The implications of x (which limits the duration of all the steps but the feed step), y (which limits the number of unit cells in a row, i.e., the width of a unit block), and z (which is the number of beds being fed simultaneously) are also revealed. In particular, the effect of z on the resulting cycle schedule is demonstrated; and the effects of x and y on the number of solutions and number of distinct solutions are shown.

In Fig. 2, notice that the cycle schedule has unit cells highlighted in two different shades of grey. The cells highlighted in lighter grey identify the steps that are coupled to those taking place in bed nine, while the cells highlighted in darker grey identify the steps that are coupled to those taking place in bed one. The coupled cells are located at the top and bottom ends of the highlighted cells in a given column. For example, step E3D in framed unit cell K3 and its coupled step E3R in framed unit cell K9 are at the top and bottom, respectively, of the highlighted unit cells K3 to K9. An alternate definition of the value of J is given using these shaded regions.

In Fig. 2, take the row at the bottom of the cycle schedule (i.e., row 9) and place the value of each J just under the starting step of a set of coupled steps for which the equation containing this J is derived. For example, locate $J_1 = 4$ under unit cell M9 that corresponds to step E1R for which (5) is derived; locate $J_2 = 5$ under unit cell L9 that corresponds to E2R for which (6) is derived; and so on, as depicted in the figure. Notice that each J corresponds exactly to the number of rows or beds above the identified step where the corresponding coupled step is located (bottom to top). As stated earlier, in a given row J is also equal to the number of unit blocks traversing the start of the first step in the coupling to the start of the second step in the coupling (from left to right). These are in fact two equivalent definitions of J, as the number of unit blocks must equal the number of beds in a cycle schedule.

Also, recall that the methodology which leads to a solution set, i.e., the Js, can be obtained by one of two approaches, i.e., either from left to right or from right to left in time. The Js in this example are obtained by the former approach (bottom to top). The J^*'s in Fig. 2 located above the coupled cells in bed 1 correspond to a solution set that is obtained by the latter approach (top to bottom). The region shaded in darker grey corresponds to this solution set. It is easy to prove that $J + J^* = N$, an interesting outcome.

Clearly, for any cycle schedule in the literature, which must have a corresponding cycle step sequence, all the Js can be readily identified using either of these definitions. These Js and N correspond to one of its solution sets. If another cycle schedule has the same Js and N, it also belongs to this same solution set. Moreover, values of x, y and z can also be extracted from its 2D grid, as well as all the coupled steps. This means that the methodology can be readily applied to find the rest of the solutions for this solution set, barring any additional constraints that may be unknown or hidden. Of course, to find all the solution sets and their solutions corresponding to the cycle step sequence in the cycle schedule a full analysis must be carried out and a larger value of x may be chosen just to capture more solutions, as shown below.

For a 13 step 10 bed system ($N = 10$), with $D = 2U$ and $U \le S_i \le 4U$ ($i \ne 1$), 38 solution sets exist, one of which is $J_1 = 3$, $J_2 = 4$, $J_3 = 5$, $J_4 = 6$ and $J_5 = 8$. The total number of solutions for this solution set depends on the value of z, because z can be either 1 or 2 ($z < J_1$ with $J_1 = 3$ for this 13 step cycle sequence). In this case, the total number of solutions is 50 for this solution set, with 25 solutions belonging to each value of z. Moreover, when $z = 1$, only one bed is being fed at any given time, the F step occupies two unit cells (from (1)) and the FP step occupies three unit cells (22) (perhaps, not an optimum situation); however, when $z = 2$, two beds are being fed simultaneously, the F step occupies four unit cells and the FP step occupies only one unit cell (perhaps, a more optimum situation). The total number of solutions for all 38 solution sets is shown later for this 10 bed 13 step system.

For the above solution set, three cycle schedules are shown in Fig. 3. The cycle schedules in Figs. 3a and 3c are exactly the ones shown by Xu et al. (2004). For this case, $x = 4$, $y = 2$ and $z = 2$. Notice that $x = 3$ in Fig. 3a, and $x = 2$ in Figs. 3b and 3c. Recall that with $x = 4$, the analysis provides all the solutions corresponding to $x = 1$ to 4. It is also interesting that the solutions shown in Figs. 3b and 3c have identical step times for all the individual cycle steps. The only difference between them is the position of the idle step. Instead of the idle step being between E4D and PP as in Fig. 3b, it is between LR and E4R as in Fig. 3c. Thus, these are two separate solutions that the methodology correctly differentiates. So, a solution or cycle schedule is defined as being distinct if each of its cycle steps has the same duration and differs from other solutions or cycle schedules only in the placement of idle steps. A distinct solution may thus have many solutions, as shown later. Unfortunately, the affect of the position of an idle step in an otherwise identical cycle schedule has not been discussed in the literature.

A similar exercise can be carried out for 12 and 16 bed systems. A 12 bed system ($N = 12$), with $D = 2U$ and $U \le S_i \le 4U$ ($i \ne 1$), has 100 solution sets, one of which is $J_1 = 5$, $J_2 = 6$, $J_3 = 7$, $J_4 = 8$ and $J_5 = 10$. In this case, $z < 5$, since $J_1 = 5$. When $z = 4$, one of them is shown in Fig. 4a, which is the same as one published by Xu et al. (2004). This particular solution set has 80 total solutions. A 16 bed system ($N = 16$), with $D = 2U$, $U \le S_i \le 6U$ ($i \ne 1$), has 268 solution sets, one of them being $J_1 = 5$, $J_2 = 6$, $J_3 = 7$, $J_4 = 8$ and $J_5 = 12$. Again, $z < 5$ in this case. When $z = 4$, one of them is shown in Fig. 4b, which is the same as another one published by Xu et al. (2003). Notice that 4 beds are being fed simultaneously in both cases ($z = 4$). This is the largest value of z found in the literature. Also, notice that $x = 2$ for the 12 bed system (Fig. 4a) and $x = 6$ for the 16 bed system (Fig. 4b). This latter value of x is the largest value of x found in the literature.

The values of x and y change the total number of solutions and the number of distinct solutions considerably. All the examples considered so far deal with $y = 2$ and $x = 4$ or 6. Interestingly, all the cycle schedules developed by Xu et al. (2003, 2004) have $y = 2$; however, the x in their cycle schedules varies from 2 to 6, depending on the number of beds. Figure 5a shows the change in the total number of solutions and the number of distinct solutions as x is varied with $N = 10$ and $y = 2$. The solutions represented by $U \le S_i \le xU$ ($i \ne 1$) keep adding to the solutions of $S_i = D$, $S_i = 2D$, $S_i = 3D \ldots$, $S_i = xD$ in a cumulative manner, but leading to a value of x after which the total number of solutions become constant. The reason the total number of solutions and the number of distinct solutions hit upper limits is simple. For a given y, the number of unit cells in a row is fixed. So, if a cycle step occupies too many unit cells in a row, not enough unit cells remain for the other cycle steps to occupy or the coupled steps to be aligned.

Figure 5b shows the change in the total number of solutions and the number of distinct solutions as y is varied with $N = 10$ and $x = 4$. Recall that the value of y sets the length of a unit block or equivalently is the number of unit cells in a unit block. A larger value of y expands the cycle schedule in the horizontal direction, which means more unit cells are available in a row to accommodate all the cycle steps. As a consequence, the 13 cycle steps can be arranged in increasingly more ways with increasing y, thereby increasing the number of total and distinct solutions without bound. Clearly, having $y > 4$ makes the total number of solutions in this case unwieldy. Notice that y starts from 2 in this figure. For a 13 step 10 bed system, the $y = 1$ case is not possible, as it results in a grid where all the cycle steps are the same duration, i.e. an equal step time cycle, which requires 13 beds to run 13 steps.

Also, observe that Figs. 5a and 5b represent two slices of a 3-D surface in which x and y are independent variables.

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	Feed				E1D	E2D	E3D	E4D	PP			CnD	LR			E4R	E3R	E2R	E1R	FP
2	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP			CnD	LR			E4R	E3R	E2R
3	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP			CnD	LR			E4R
4	LR	E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP			CnD	LR	
5	LR			E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP			CnD
6	PP	CnD	LR			E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D	PP	
7	PP			CnD	LR			E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D	E3D	E4D
8	E3D	E4D	PP			CnD	LR			E4R	E3R	E2R	E1R	FP	Feed				E1D	E2D
9	E1D	E2D	E3D	E4D	PP			CnD	LR			E4R	E3R	E2R	E1R	FP	Feed			
10	Feed		E1D	E2D	E3D	E4D	PP			CnD	LR			E4R	E3R	E2R	E1R	FP	Feed	

(a)

1	Feed	E1D	E2D	E3D	E4D	I	PP	CnD	LR	E4R	E3R	E2R	E1R	FP	
2	E1R	FP	Feed	E1D	E2D	E3D	E4D	I	PP	CnD	LR	E4R	E3R	E2R	
3	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	I	PP	CnD	LR	E4R	
4	LR	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	I	PP	CnD	LR
5	CnD	LR	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	I	PP	CnD
6	PP	CnD	LR	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	I	PP
7	I	PP	CnD	LR	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	
8	E3D	E4D	I	PP	CnD	LR	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	
9	E1D	E2D	E3D	E4D	I	PP	CnD	LR	E4R	E3R	E2R	E1R	FP	Feed	
10	Feed	E1D	E2D	E3D	E4D	I	PP	CnD	LR	E4R	E3R	E2R	E1R	FP	Feed

(b)

1	Feed	E1D	E2D	E3D	E4D	PP	CnD	LR	I	E4R	E3R	E2R	E1R	FP	
2	E1R	FP	Feed	E1D	E2D	E3D	E4D	PP	CnD	LR	I	E4R	E3R	E2R	
3	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	PP	CnD	LR	I	E4R	
4	I	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	PP	CnD	LR	
5	LR	I	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	PP	CnD	
6	CnD	LR	I	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	PP	
7	PP	CnD	LR	I	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	E3D	E4D	
8	E3D	E4D	PP	CnD	LR	I	E4R	E3R	E2R	E1R	FP	Feed	E1D	E2D	
9	E1D	E2D	E3D	E4D	PP	CnD	LR	I	E4R	E3R	E2R	E1R	FP	Feed	
10	Feed	E1D	E2D	E3D	E4D	PP	CnD	LR	I	E4R	E3R	E2R	E1R	FP	Feed

(c)

Fig. 3 Cycle schedules for a 10 bed 13 step system with (**a**) no idle step, (**b**) one idle step, (**c**) and one idle step. The cycle schedules in (**b**) and (**c**) differ only by the placement of the idle step

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X
1	Feed								E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR
2	E1R	FR	Feed								E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R
3	E3R	E2R	E1R	FR	Feed								E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R
4	I	E4R	E3R	E2R	E1R	FR	Feed								E1D	E2D	E3D	E4D	PP		CnD		LR	
5	LR		I	E4R	E3R	E2R	E1R	FR	Feed								E1D	E2D	E3D	E4D	PP		CnD	
6	CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed								E1D	E2D	E3D	E4D	PP	
7	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed								E1D	E2D	E3D	E4D
8	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed								E1D	E2D
9	E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed							
10	Feed		E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed					
11	Feed				E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed			
12	Feed						E1D	E2D	E3D	E4D	PP		CnD		LR		I	E4R	E3R	E2R	E1R	FR	Feed	

(a)

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Z	AA	AB	AC	AD	AE	AF	AG
1	Feed								E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP
2	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R
3	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R
4	I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP						CnD		LR					
5	LR		I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP						CnD		LR			
6	LR				I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP						CnD		LR	
7	LR						I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP						CnD	
8	CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP					
9	PP		CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP			
10	PP				CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D	PP	
11	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D	E3D	E4D
12	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed								E1D	E2D
13	E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed							
14	Feed		E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed					
15	Feed				E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed			
16	Feed						E1D	E2D	E3D	E4D	PP						CnD		LR						I	E4R	E3R	E2R	E1R	FP	Feed	

(b)

Fig. 4 Cycle schedules for (**a**) 12 bed 13 step and (**b**) 16 bed 13 step systems

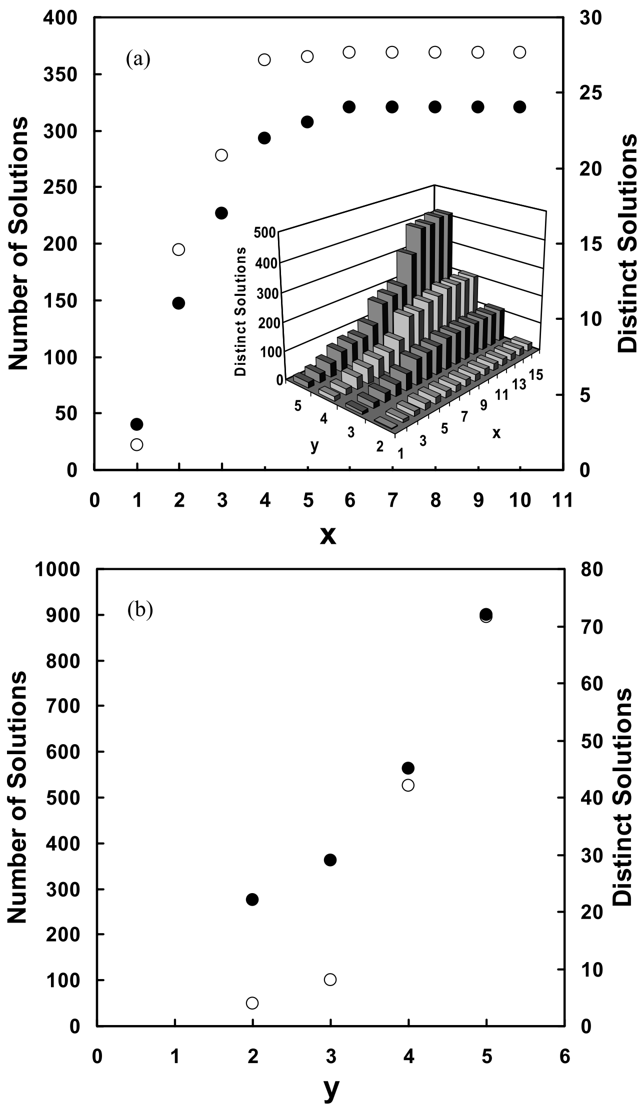

Fig. 5 Effect of changing (**a**) x with $N = 10$ and $y = 2$, and (**b**) y with $N = 10$ and $x = 4$ on the total number of solutions (*empty symbols*) and number of distinct solutions (*filled symbols*). *Insert* in (**a**) shows the resulting 3-D surface for the distinct solutions when changing both x and y with $N = 10$

This 3-D surface is shown in the insert in Fig. 5a for the distinct solutions (not shown is a similar 3-D surface for the total number of solutions). Based on the above discussion, for a fixed y, the total number of solutions and the number of distinct solutions reaches an upper limit with increasing values of x; but, for larger values of y this upper limit occurs at larger and larger values of x. Conversely, for a fixed x, increasing y dramatically increases the total number of solutions and the number of distinct solutions, both without bound; so, for larger values of x more and more solutions are obtained. These trends are seen very clearly in the insert in Fig. 5a.

It is instructive to compare the number of distinct solutions for this 10 bed system in terms of the duration of each cycle step plotted as a fraction of the total cycle time. In this case, there are 22 distinct solutions, as shown in Fig. 6a. Each one of them can be arranged in a variety of ways depending on the positions of the idle steps. This makes the total number of solutions equal to 361. Figure 6b shows the number of solutions for each distinct solution in Fig. 6a. Since solutions 11, 18, 21 and 22 have no idle time, they can be arranged in only one way. Other solutions have considerable idle time, which gives rise to many solutions for each distinct solution, in one case even exceeding 100.

It should be clear at this point that when all the solutions of each solution set are resolved, literally thousands of cycle schedules exist for each of these 10, 12 and 16 bed systems, with few of them ever appearing in the literature. A plot like that shown in Fig. 6a can be used to narrow down the number of cycle schedules for further study. By plotting the relative duration of each cycle step, the ones that have an obvious shortcoming, like too short of a feed time or too much idle time, can easily be eliminated. It then becomes a straightforward and much less daunting exercise to study the remaining cycle schedules in more detail using a suitable PSA process simulator or experimental system to determine the ones that maximize performance. Although it is not obvious that the cycle schedules in the literature are the best ones, it is probably not a coincidence that solutions 17 and 18 in Fig. 6a, which are the same as the ones reported by Xu et al. (2004), are the ones that have the longest relative feed and purge times, which improve production and regeneration, respectively.

6 Conclusions

An arithmetic methodology was developed for obtaining complex pressure swing adsorption (PSA) cycle schedules. This approach involved *a priori* specifying the cycle steps, their sequence, any constraints and then solving a set of algebraic equations. This information was used to obtain the total number of cycle schedules, the minimum number of beds required to operate the given cycle sequence, the minimum number and location of the idle steps needed to align the various coupled cycle steps, and a simple graphical approach for identifying the cycle schedules worthy of further examination via simulation or experiment.

This technique was tested successfully against cycle schedules comprising 13 steps with numerous constraints, including four pressure equalization steps, for 10, 12 and 16 bed PSA systems in the literature. This methodology resolved thousands of cycle schedules for each one of these systems, with the number increasing with the number of beds. The cycle schedules in the literature represented just a few of them.

Although this approach cannot pinpoint which cycle schedule among the many thousands it can resolve is the

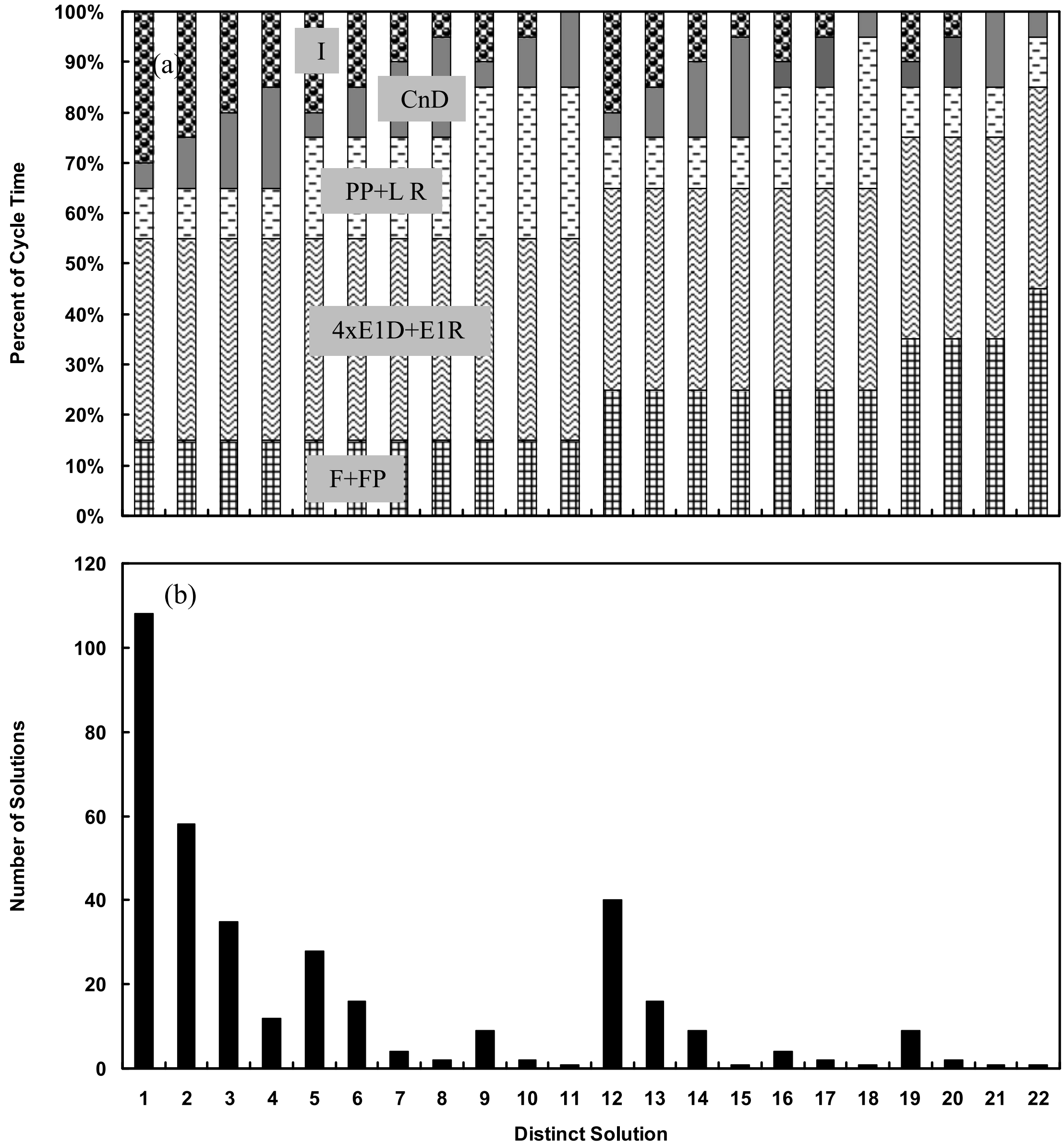

Fig. 6 (**a**) Bar graph showing the 22 distinct solutions for $N = 10$, $x = 4$ and $y = 2$ in terms of the duration of each cycle step as a fraction of the total cycle time: from bar *bottom to top*, *checks* represent time for F and FP steps combined (FP occupies one unit cell), *waves* represent total equalization time (Eq), *dashes* represent time for PP and LR steps combined, *solids* represent time for CnD step, and *dots* represent total idle time. (**b**) Bar graph showing the total number of solutions for every distinct solution in (**a**)

best, it does provide a very accurate and complete way to determine all the cycle schedules for a given cycle sequence and set of constraints. By plotting the relative duration of each cycle step for every cycle schedule resolved, the cycle schedules that have an obvious shortcoming, like too short of a feed time or too much idle time, can be easily eliminated. It then becomes a straightforward and much less daunting task to study the remaining cycle schedules in more detail using a suitable PSA process simulator or experimental system to determine the ones that maximize performance.

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