

Simplified graphical approach for complex PSA cycle scheduling

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Abstract A simple, graphical, unit block approach for rapid complex pressure swing adsorption (PSA) cycle scheduling has been developed. This new methodology involves *a priori* specifying the cycle steps, their sequence, and the number of beds, and then following a systematic procedure that requires filling in a 2-D grid. The outcome or solution is a unit block which can easily be extended to form the complete cycle schedule. This new approach has been tested successfully against several multi-bed and multi-step cycle schedules taken from the literature. It should thus be very useful for quickly scrutinizing different PSA cycle schedules for further PSA process development.

Keywords Pressure swing adsorption · PSA · Cycle schedule · Cycle sequence

1 Introduction

Typical PSA processes operate multiple beds and numerous cycle steps. However, the various cycle steps can be arranged and configured in a variety of ways, which can give rise to numerous cycle configurations. In addition, most of the PSA cycles have beds that interact with each other. As a consequence, scheduling of complex PSA cycles becomes a daunting task.

Chiang (1988) presented an arithmetic approach for scheduling rather simple PSA cycles. This analysis did not consider the possibility of idle steps being included in the

cycle schedule. An idle step is one where the bed is isolated from the rest of the PSA process by closing all of the valves leading to it and has to be incorporated only to satisfy various alignment constraints in a PSA cycle. This method did give the total idle time required, but not their positions and durations.

Smith and Westerberg (1990) introduced a mathematical approach to schedule PSA cycles. The model encompassed a set of equations and constraints while considering it as an optimization problem. However, solving these systems of equations for a large number of beds and constraints becomes an overwhelming task.

Ebner et al. (2009) developed the first of its kind graphical approach for obtaining various PSA cycle schedules. This novel methodology followed a systematic procedure to fill the entire cycle schedule grid simultaneously and could easily be used for complex, multi-bed, multi-step, PSA systems. Mehrotra et al. (2010) also introduced an arithmetic approach for complex PSA cycle scheduling. This new approach involved *a priori* specifying the cycle steps, their sequence and any constraints, and then required solving a set of algebraic equations. The solution identified 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 deserved further examination. However, this arithmetic approach is specific for the pre-defined cycle step sequence and the analysis needs to be redone if the cycle step sequence is changed.

Therefore, the objective of this work is to introduce a comparatively rapid and simple, graphical, unit block approach for complex PSA cycle scheduling, based on similar but simpler reasoning as that outlined by Ebner et al. (2009)

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Cycle Sequence: F→E1D→E2D→CoD→E3D→CnD→LR→E3R→E2R→E1R→FP

Time →

Bed ↓	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	E3R	E2R	E1R	FP			F		E1D	I	E2D	CoD	E3D	CnD	LR
2	FP			F		E1D	I	E2D	CoD	E3D	CnD	LR	E3R	E2R	E1R
3	F		E1D	I	E2D	CoD	E3D	CnD	LR	E3R	E2R	E1R	FP		F
4	I	E2D	CoD	E3D	CnD	LR	E3R	E2R	E1R	FP		F			E1D
5	E3D	CnD	LR	E3R	E2R	E1R	FP			F		E1D	I	E2D	CoD

Fig. 1 PSA cycle schedule (Chiang 1988) of a five-bed eleven-step process, depicting the unit block (cells contained within the *thick black rectangle*)

in their more rigorous, graphical approach. Instead of filling in the entire cycle schedule grid simultaneously as shown in the previous work by Ebner et al. (2009), this work involves filling in only a portion of the grid called the unit block, which makes this approach much easier and quicker to implement. This simple yet robust methodology is first described using a generic example of a PSA cycle schedule. Then, the graphical unit block approach is used to obtain the cycle schedules of several PSA cycles taken from the patent literature, including those with multi-beds, multi-steps, multi-couplings and multi-idle steps.

2 Cycle schedule grid

A typical PSA cycle schedule or grid of a PSA system is shown in Fig. 1 (Chiang 1988). It consists of five beds and eleven steps, including three equalization steps and two idle (I) steps. Each of the five beds operates the following sequence of steps:

1. high pressure feed (F), provides light product;
2. first pressure equalization (E1D), coupled with E1R;
3. second pressure equalization (E2D), coupled with E2R;
4. co-current depressurization (CoD), coupled with light reflux (LR) purge;
5. third pressure equalization (E3D), coupled with E3R;
6. counter-current depressurization (CnD), provides heavy product;
7. light reflux (LR) purge, coupled with CoD;
8. third pressure equalization (E3R), coupled with E3D;
9. second pressure equalization (E2R), coupled with E2D;
10. first pressure equalization (E1R), coupled with E1D; and
11. feed pressurization (FP).

In the grid shown in Fig. 1, time is placed along the horizontal direction, whereas all five beds are placed along the vertical direction. The fifteen columns in the grid, i.e., A through O along the horizontal direction, represent unit

time steps or time steps of identical length. A row of the grid represents all the different cycle steps a given bed undergoes over the entire cycle, whereas a column of the grid represents which cycle step is being run by which bed at a particular unit time step. The total cycle time is the sum of all the individual unit time steps of a particular row. The intersection of a row and a column of the grid is a unit cell and is the smallest repeating element of the grid.

A unit cell is denoted by its row and column position in the grid. For example, unit cell B-4 contains the step which runs in bed 4 during unit time step B (i.e., E2D). For a particular bed, one unit cell corresponds to the minimum time of operation of any cycle step. In other words, a unit cell can be occupied by only one cycle step. In addition, the total length of an individual cycle step is always a multiple of the unit time step. For instance, in Fig. 1, the CnD step occupies one unit time step, and the F step occupies three unit time steps.

Since every bed operates identically in a PSA process, the same cycle steps are run by successive beds after a fixed interval of time. This means that the same operation in one bed is repeated in another bed after this interval, the duration of which constitutes a unit block. A thick solid line enclosing unit time steps A through C represents one unit block for the cycle shown in Fig. 1. Notice that within the unit block, all the steps in the schedule are being run by one of the five beds. The unit block occurs again during unit time steps D through F. In the same way, the total cycle time is made up of five consecutive unit blocks, and this number must match the total number of beds.

3 Methodology

This graphical unit block scheduling methodology is divided into three parts. In the first part, the goal is to build the primary skeleton of a unit block. The primary skeleton of a unit block is formed when the array of a given number of rows (i.e., beds) and a given number of columns (i.e., width of a

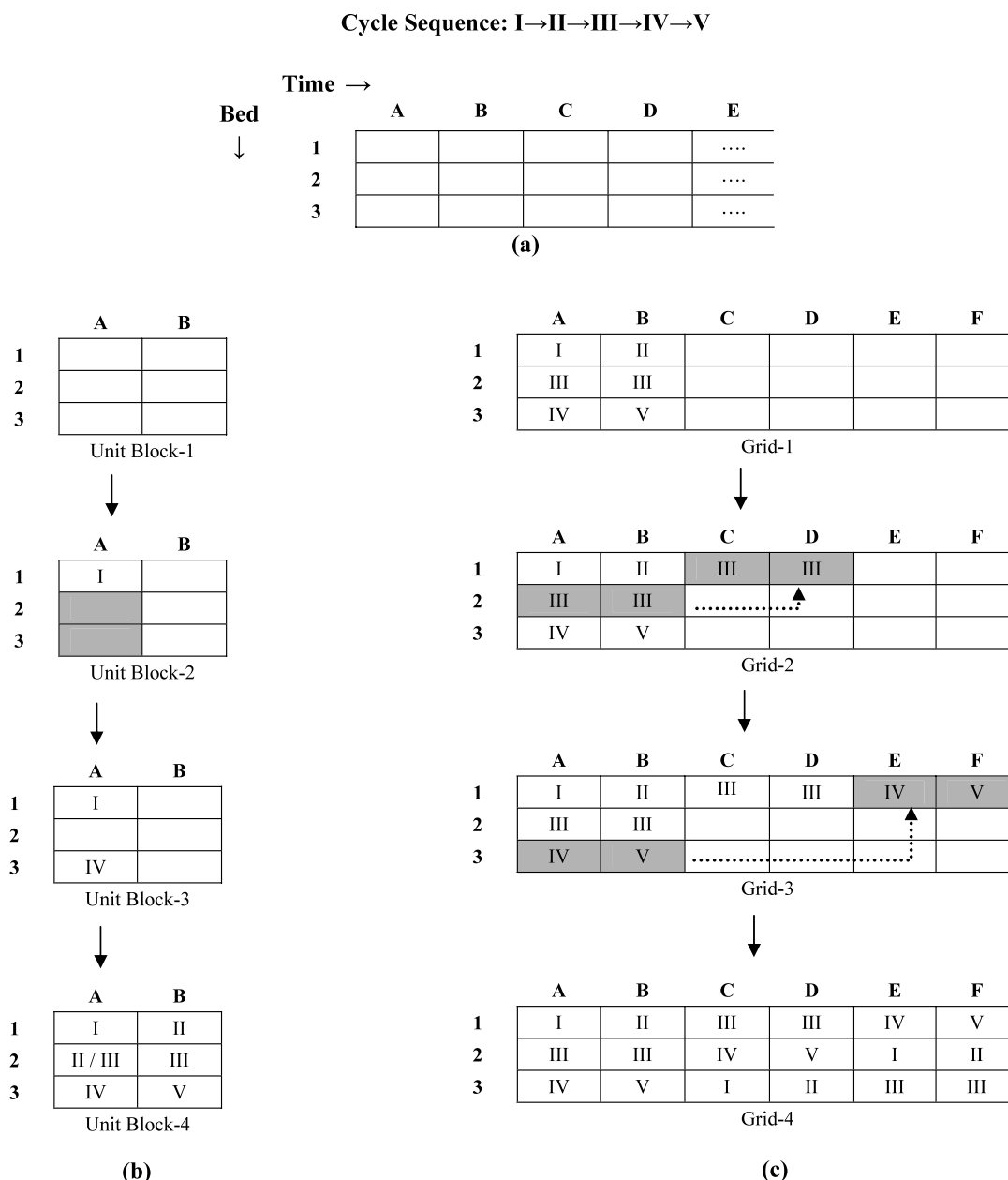


Fig. 2 Construction of a unit block for a three-bed five-step process: **a** initial empty unit block; **b** sequential filling of one possible unit block; **c** construction of the final cycle schedule from the unit block shown in (b)

unit block) is determined. In the second part, the unit block is built by filling in the empty unit cells. During this second part, the number of idle steps (if any), and their duration and relative location within the grid is determined. Finally, in the third part, the final cycle schedule is derived by extending the unit block N consecutive times, where N is the number of beds.

First, two pieces of information about the PSA cycle must be decided *a priori* to start construction of the cycle schedule. (1) The individual cycle steps of the cycle must

be chosen, along with their sequence of operation. (2) The number of beds must be chosen.

Consider the hypothetical PSA cycle shown in Fig. 2, where the number of beds is chosen to be three and the sequence of cycle steps is defined generically by I through V. Typically, for any PSA cycle schedule a few constraints must be satisfied. For instance, in the sequence shown in Fig. 1, the gas exiting the light end of the bed undergoing the E1D step enters the light end of the bed undergoing the E1R step till the pressure in both beds equalizes. Thus, these two steps are coupled, so they must initiate and terminate at the same

time. In the schedule shown in Fig. 2, the same is assumed for steps I and IV. In other words, at a given unit time step, at least two different beds must have these steps operating simultaneously.

Figure 2a shows an empty grid of a unit block with three rows (equivalent to the total number of beds) and multiple vertical columns (representing different unit time steps). At this point, the total number of unit time steps in a unit block has not been determined. In other words, the unit block is free to expand or contract horizontally.

Next, the width of the unit block must be decided. Although, a wider unit block allows for more flexibility, it also increases the probability of needing idle steps in the final cycle schedule, which is undesirable. Therefore, as a starting point, a minimum width for the unit block must be chosen. Recall, that within a unit block, all the cycle steps in the sequence are operated by one or the other beds. As a consequence, in this three-bed five-step example, the unit block cannot be one unit cell wide, as only three unit cells would be available to accommodate five cycle steps. Thus, the minimum width of the unit block has to be two unit cells, as shown in Fig. 2b Unit Block-1 in order to accommodate the different cycle steps. At this point, part one of the methodology, i.e., formation of the primary skeleton of the unit block, is complete.

Part two of the methodology involves building the unit block by strictly filling in the empty unit cells from left to right and from top to bottom. Notice the unit block shown in Fig. 1 at unit time steps G, H and I (thick encapsulated line). Sequentially following the cycle steps occupying various unit cells from one bed to the other gives the same sequence of steps that is followed by every bed. For instance, sequentially moving from G-1 to I-1, G-2 to I-2, G-3 to I-3, G-4 to I-4 and G-5 to I-5 gives the same sequence of steps that is followed by any one of the five beds. In this methodology, after the formation of the primary skeleton of the unit block, the empty unit cells must be filled in a way that a similar continuity is maintained.

Typically, there are multiple constraints that must be satisfied in a PSA cycle, like the one shown in Fig. 1. At this point in the methodology, at least one coupled step (if any) should be selected and placed in the unit block. The duration of this coupled step should be assumed *a priori* before proceeding to the next step in the methodology. For example, in this three-bed five-step case, where steps I and IV are coupled, step I is assumed to occupy one unit cell and is placed in unit cell A-1, as shown in Fig. 2b Unit Block 2. The coupled step IV corresponding to step I in unit cell A-1 can be placed in either of the darker shaded unit cells A-2 or A-3, as both these steps should initiate and terminate at the same time. Cycle step IV cannot be placed in unit cell A-2, as doing so would leave only one unit cell (B-1) for steps II and III. As a result, cycle step IV is placed in unit cell A-3,

as shown in Fig. 2b Unit Block-3. At this point, the coupled steps in the cycle sequence are aligned. As each of the cycle steps have to occupy at least one unit cell, B-1, B-2 and B-3 are occupied by cycle steps II, III and V, respectively. However, unit cell A-2 can be filled in with either cycle step II or cycle step III. Therefore, two different unit blocks can be formed in this specific example depending on which cycle step occupies unit cell A-2.

Part three of the methodology involves building the final cycle schedule from the completed unit block formed in part two. Recall, that when a unit block is repeated N times, with N being the number of beds, the complete cycle schedule is formed. In this example, the unit block, when repeated three times, will result in the formation of the complete cycle schedule. Figure 2c Grid-1 shows one of the unit blocks derived in part two of the methodology occupying the first two unit time steps A and B of the grid which has a total of six unit time steps (A to F). Next, the two unit cells (C-1 and D-1) next to the first row of the unit block (A-1 and B-1) are filled in with cycle steps occupying the second row of the unit block, i.e., A-2 and B-2. Therefore, cycle step III, which occupies unit cells A-2 and B-2, now also occupies unit cells C-1 and D-1, as shown in Fig. 2c Grid-2. Finally, the last two unit cells of bed 1 (E-1 and F-1) are filled in with cycle steps occupying the last row of the unit block, i.e., in unit cells A-3 and B-3, as shown in Fig. 2c Grid-3. The entire sequence for bed 1 is now ready and the same is followed by beds 2 and 3, resulting in the complete cycle schedule shown in Fig. 2c Grid-4.

A similar procedure can be followed for the cases where there is more than one coupled step. Also, further possibilities can be explored when the width of the unit block is increased. More illustrations of the versatility of this methodology are provided in the *Applications* section, where it is used to obtain actual PSA cycle schedules from the literature.

4 Applications

First, a simple two-bed four-step Skarstrom PSA cycle (Skarstrom 1960) is analyzed to exemplify the application of this new unit block graphical approach to construct PSA cycle schedules. In this example, every bed undergoes the following steps: feed (F) at high pressure, countercurrent depressurization (CnD) from high pressure to a low pressure, light reflux purge (LR) at low pressure, and light product pressurization (LPP) from low to high pressure. In this particular sequence, the light gas exiting the F step is used to purge the bed during the LR step and also pressurize the bed during the LPP step. Therefore, the two constraints that must be met while constructing the cycle schedule are: the F and LR steps must be coupled, and the F and LPP steps must be coupled.

Cycle Sequence: $F \rightarrow CnD \rightarrow LR \rightarrow LPP$

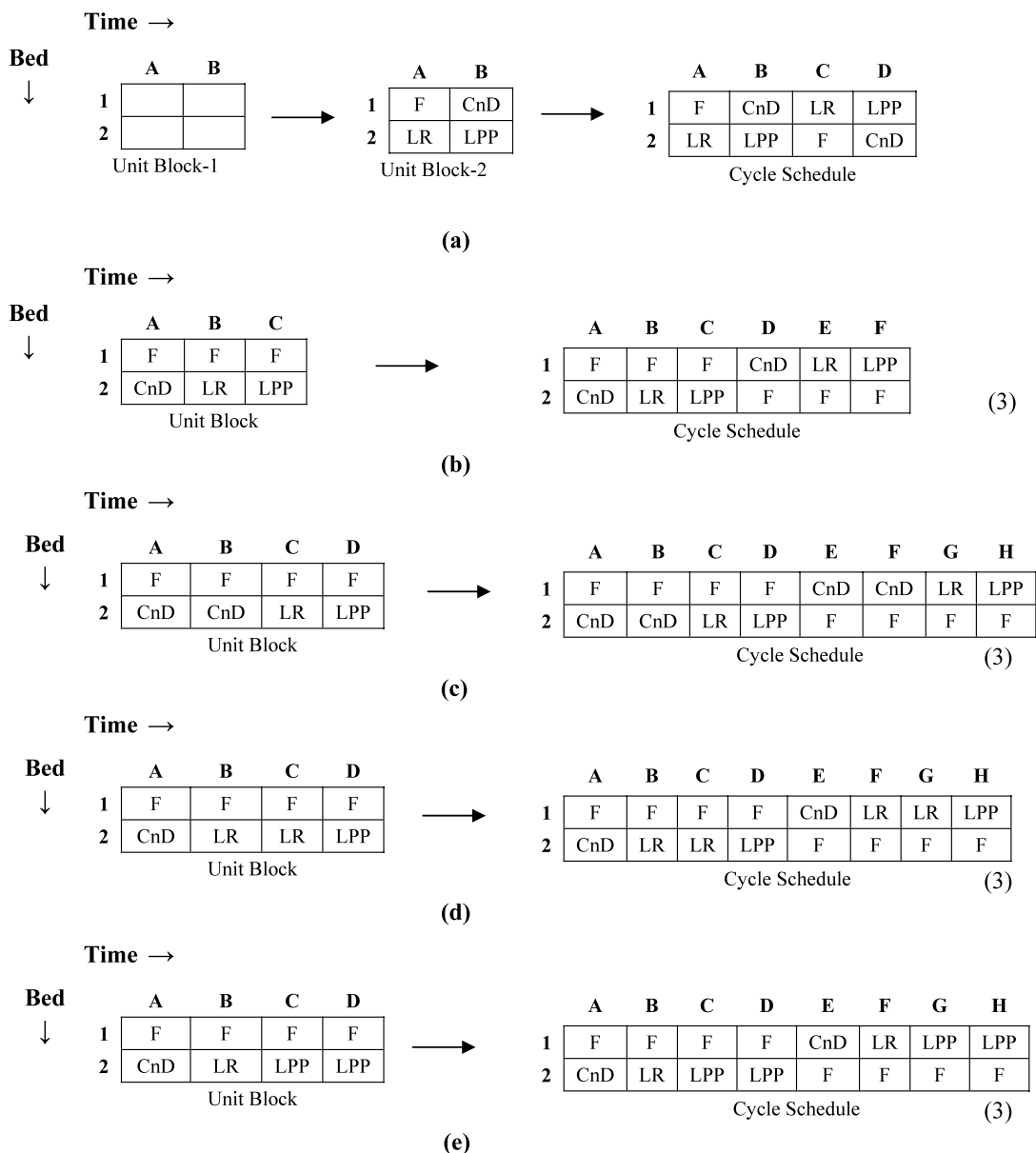


Fig. 3 Construction of a PSA cycle schedule for a two-bed four-step process: **a** sequential filling of a unit block which is two unit cells wide and construction of the final cycle schedule; **b** possible unit block

which is three unit cells wide and construction of the final cycle schedule; and **c** to **e** possible unit blocks which are four unit cells wide and construction of the final cycle schedule

Numerous PSA cycle schedules can be constructed depending upon the width of the unit block. For a two-bed PSA system, following the above described four cycle steps, the width of a unit block has to be greater than one unit cell to accommodate all the cycle steps. For a unit block which is one unit cell wide, a minimum of four beds are required to accommodate these four cycle steps. When the unit block is two unit cells wide, as seen in Fig. 3a Unit Block-1, there are four unit cells available to fill the four

cycle steps. This results in only one possibility as shown in Fig. 3a Unit Block-2. The complete cycle schedule shown in Fig. 3a can be created from this unit block by following the same principles discussed in the previous section. In addition, the constraint of coupling the F and LPP steps is not met in this particular cycle schedule.

In most PSA processes, to maintain feed and product continuity, it is important that the PSA process is fed continuously at all times. The cycle schedule derived in Fig. 3a is

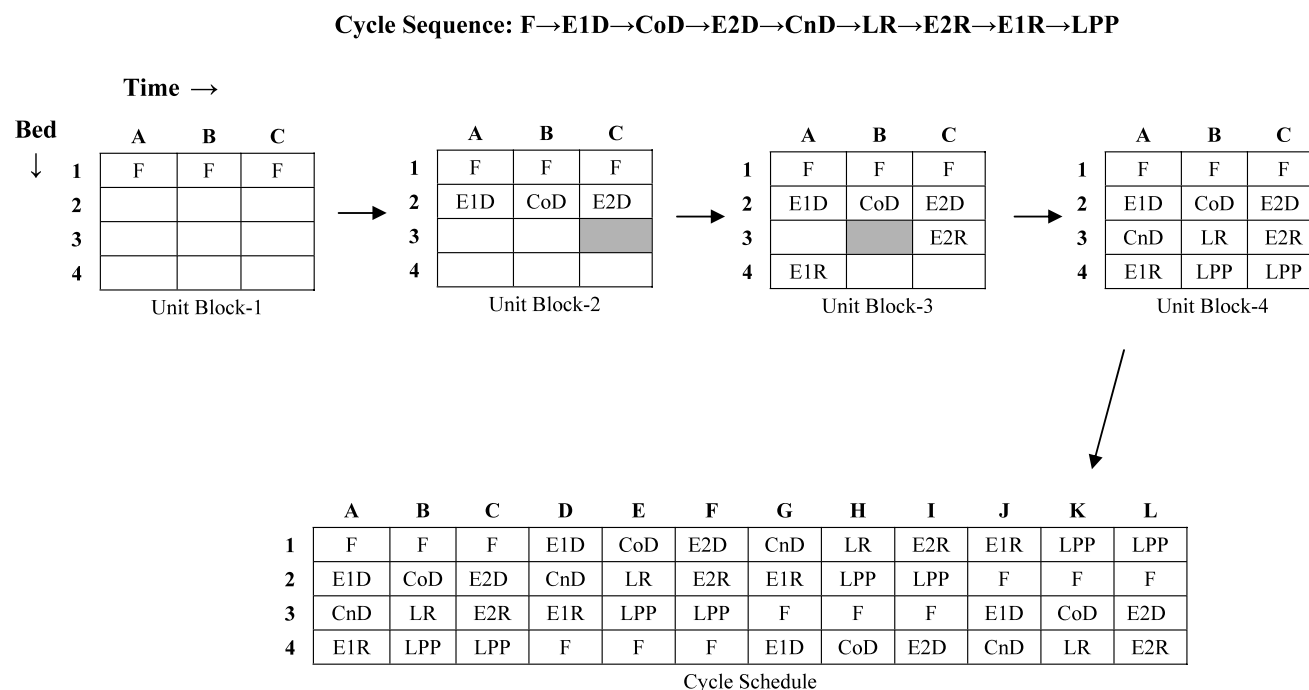


Fig. 4 Construction of a PSA cycle schedule for a four-bed nine-step process: Figure shows the sequential filling of a unit block which is three unit cells wide and construction of the final cycle schedule

unable to meet this criterion. A continuous feed step can be incorporated in a cycle schedule while creating the unit block by ensuring that each column in the unit block has at least one F step. For example, continuous feed in the cycle schedule in Fig. 3a is only possible when both unit cells A-1 and B-1 in Fig. 3a Unit Block-1 incorporate the F step. However, that would leave only two unit cells (A-2 and B-2) for three cycle steps (CnD, LR and LPP), which is clearly infeasible. In this example of a two-bed system, a continuous F step in the final cycle schedule can only be achieved when the width of the unit block is increased beyond two unit cells.

Figure 3b shows a unit block which is three unit cells wide. For a continuous feed, the F step is incorporated in each column of the unit block (i.e., unit cells A-1, B-1 and C-1). Now, three unit cells (A-2, B-2 and C-2) are available for incorporating the CnD, LR and LPP steps. The resulting cycle schedule formed from this unit block is shown in Fig. 3b. The unit block can be further widened to four unit cells as shown in Fig. 3c with the F step occupying the first row (unit cells A-1, B-1, C-1 and D-1). As a consequence, there are four unit cells (A-2, B-2, C-2 and D-2) where the remaining three cycle steps (CnD, LR and LPP) can be placed. This results in three possibilities as shown in Figs. 3c, d and e, which have different relative cycle step times. Notice, that in all cycle schedules shown in Figs. 3b to e, since the F step is continuous, the criterion of F and LR steps and F and LPP steps being coupled is always satisfied.

Pressure equalization steps are quite common in the PSA literature and are typically used to save on operating costs. The next example encompasses two pressure equalization steps in a nine-step cycle designed for a four-bed PSA system. The nine cycle steps are:

1. high pressure feed (F), provides light product;
2. first pressure equalization (E1D), coupled with E1R;
3. co-current depressurization (CoD), coupled with light reflux (LR) purge;
4. second pressure equalization (E2D), coupled with E2R;
5. counter-current depressurization (CnD), provides heavy product;
6. light reflux (LR) purge, coupled with CoD;
7. second pressure equalization (E2R), coupled with E2D;
8. first pressure equalization (E1R), coupled with E1D; and
9. light product pressurization (LPP), coupled with F.

In this example of a four-bed PSA system, the unit block has to be at least three unit cells wide to accommodate all nine cycle steps. When the unit block is only two unit cells wide, a total of only eight unit cells are available for the nine different cycle steps in all four beds, making it infeasible to construct the cycle schedule. Figure 4 Unit Block-1 shows a unit block three unit cells wide with the F step occupying the first row, i.e., unit cells A-1, B-1 and C-1, which forces the F step to be continuous. Next, as shown in Fig. 4 Unit Block-2, cycle steps E1D, E2D and the CoD are placed in unit cells A-2, B-2 and C-2, based on the assumption that

Cycle Sequence: F→E1D→CoD→E2D→CnD→LR→E2R→E1R→LPP

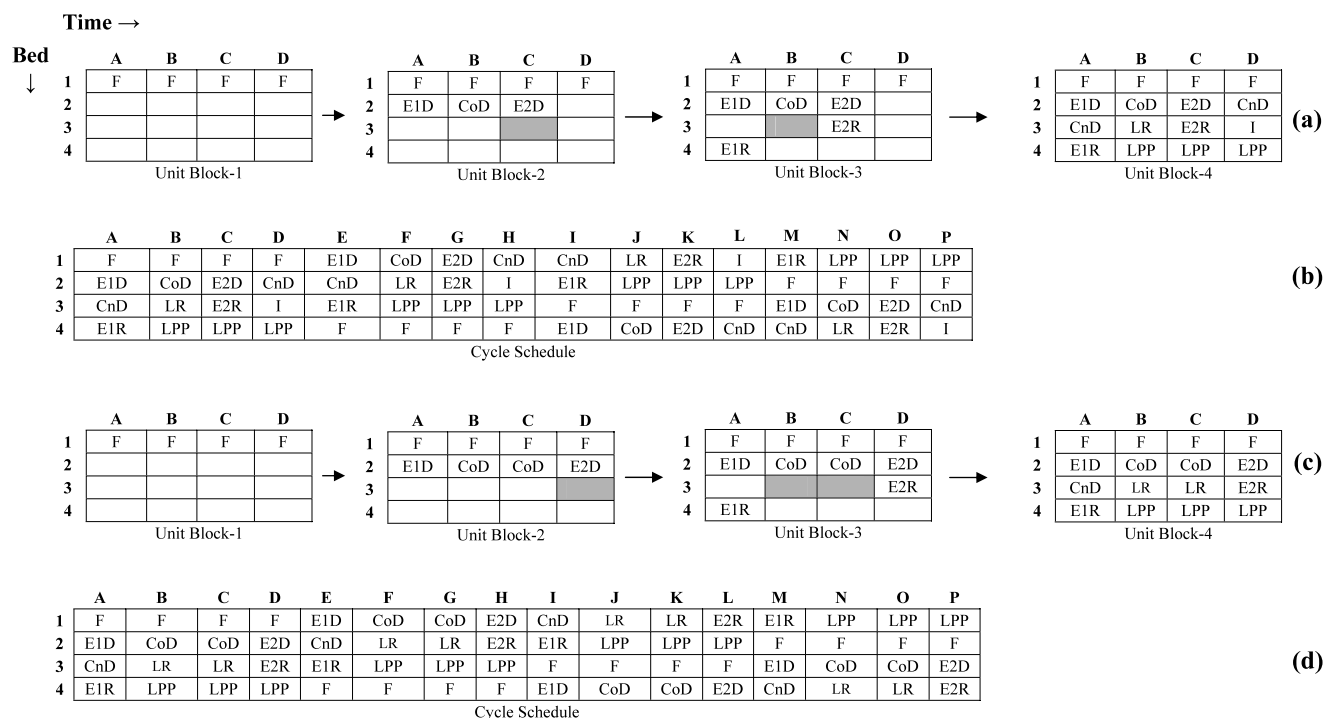


Fig. 5 Construction of a PSA cycle schedule for a four-bed nine-step process: **a** sequential filling of a possible unit block that is four unit cells wide; **b** resulting cycle schedule formed from unit block

shown in (a); **c** another possible way of sequentially filling the unit block that is four unit cells wide compared to (a); and **d** resulting cycle schedule formed from the unit block shown in (c)

each of these cycle steps occupies only one unit cell. As the pressure equalization steps are coupled, the darker shaded cell shows the only possible place where E2R can be placed (corresponding to E2D in C-2). E2R cannot be placed in C-4, as doing so would not leave any space for cycle steps E1R and LPP. Figure 4 Unit Block-3 shows both pressure equalization steps coupled. Also, the darker shaded unit cell B-3 is the only place where the LR step can be placed as the CoD and LR steps are coupled. LR cannot occupy unit cell B-4 as doing so will force E1R to operate before LR thereby violating the specified operating order of the steps. Unit cells A-3 and B-3 can now accommodate the CnD and LR steps, respectively, whereas, LPP can occupy both B-4 and C-4. Figure 4 Unit Block-4 shows the completed unit block from which the complete cycle schedule is derived.

Numerous possibilities in terms of deriving other PSA cycle schedules can be explored when the unit block is further widened. Figure 5a Unit Block-1 shows a unit block that is four unit cells wide with the F step occupying the first row (unit cells A1 to D-1). Next, based on the assumption that E1D, E2D and CoD occupy one unit cell each, Fig. 5a Unit Block-2 is obtained. The darker shaded unit cell C-3 is the only place where E2R (corresponding to E2D) can be placed. Figure 5a Unit Block-3 shows the placement and coupling of each of the pressure equalization steps. As a re-

sult of the positioning of E2R and E1R in unit cells C-3 and A-4, respectively, an I step is required in unit cell D-3. Also, the darker shaded unit cell B-3 is the only place where the LR step can be placed to satisfy the alignment constraint that the LR and CoD steps are coupled. The remaining cycle steps can be placed in the empty unit cells, as shown in Fig. 5a Unit Block-4. The resulting unit block can be extended to derive the complete cycle schedule, as shown in Fig. 5b.

The cycle schedule shown in Fig. 5b was based on the assumption that the CoD step occupies only one unit cell. When the CoD step is lengthened and forced to occupy two unit cells, with E1D and E2D occupying one unit cell each, the unit block shown in Fig. 5c Unit Block-2 is obtained. The darker shaded unit cell D-3 shows the only position where E2R (corresponding to E2D) in D-2 can be placed. Figure 5c Unit Block-3 shows the positioning and placement of both the pressure equalization steps. Also, as CoD occupies unit cells B-2 and C-2, the darker shaded unit cells B-3 and C-3 are the only two places where the LR step can be placed, as both the CoD and LR steps are coupled. Notice that by extending the duration of the CoD step, relative to that in Fig. 5a, the I step is no longer required. The completed unit block is shown in Fig. 5c Unit Block-4. This resulting unit block, when extended, results in the cycle schedule shown

Cycle Sequence: F→E1D→E2D→CoD→E3D→CnD→LR→E3R→E2R→E1R→FP

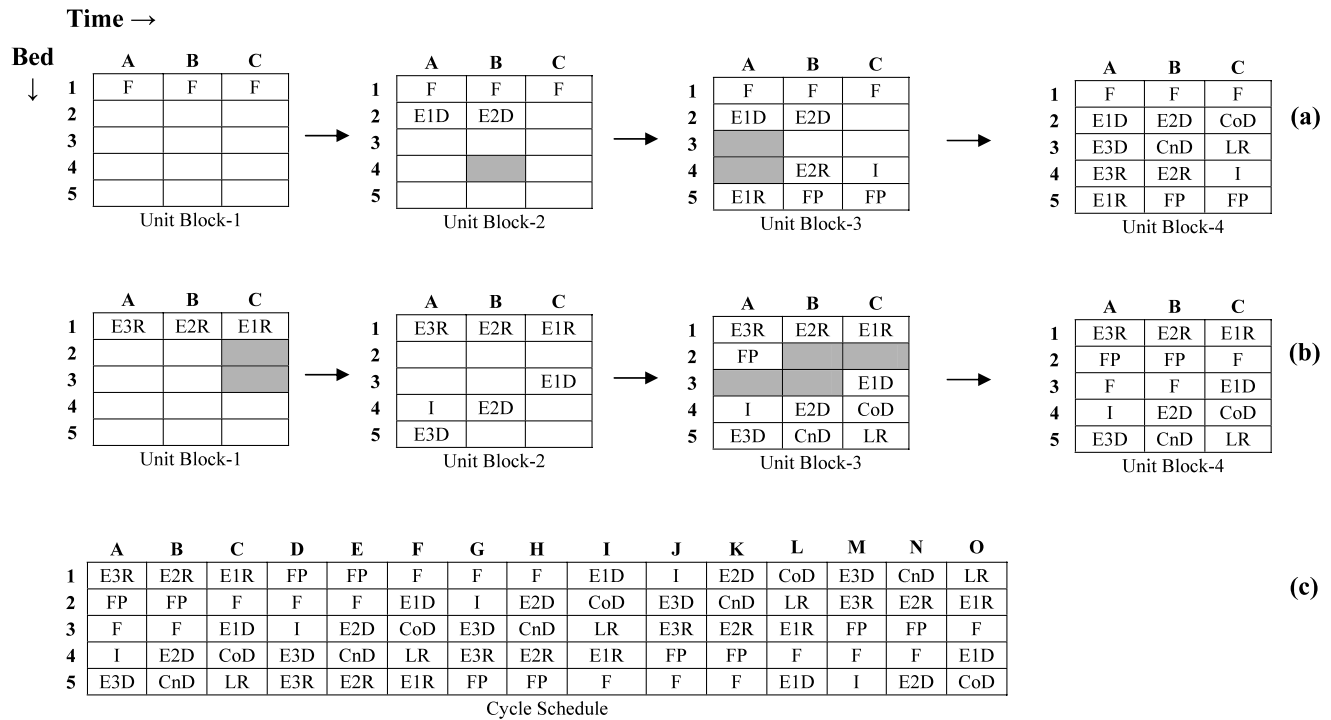


Fig. 6 Construction of a PSA cycle schedule for a five-bed eleven-step process: **a** sequential filling of a possible unit block that is three unit cells wide; **b** starting from different coupled steps, another possible

way of sequential filling the unit block that is three unit cells wide compared to **(a)**; **c** resulting cycle schedule formed from the unit block shown in **(b)**

in Fig. 5d. This grid is the same as that proposed by Cassidy and Holmes (1984).

This novel methodology can also be extended to derive PSA cycles with numerous pressure equalization steps and other coupled steps. Next, consider the five-bed eleven-step cycle shown and described in Fig. 1. The sequence of steps is described in detail in the *Cycle Schedule Grid* section.

In this specific five-bed example, the unit block has to be at least three unit cells wide in order to accommodate the eleven cycle steps. Figure 6a Unit Block-1 shows a unit block three unit cells wide with the F step occupying the first row (unit cells A-1 to C-1), forcing the F step to be continuous. Next, E1D and E2D are assumed to occupy one unit cell each, resulting in the unit block shown in Fig. 6a Unit Block-2. The darker shaded cell represents the only possible place where E2R (corresponding to E2D in B-2) can be placed. E2R cannot occupy B-3 as that would leave only two unit cells (C-2 and A-3) for the five cycle steps, CoD, E3D, CnD, LR and E3R. Similarly, E2R cannot occupy B-5 as that would leave only one unit cell (C-5) for the two cycle steps, E1R and FP. Therefore, E2R occupies unit cell B-4 and E1R occupies unit cell A-5 with an I step in unit cell C-4 to satisfy the alignment constraints. The resulting unit block is shown in Fig. 6a Unit Block-3 with the darker shaded cells representing the only possible places to accommodate the third

pressure equalization steps, E3D and E3R. The completed unit block is shown in Fig. 6a Unit block-4, which can be extended to derive the entire cycle schedule (not shown).

In this five-bed eleven-step example, the unit block can also be constructed by starting from the assumption that the pressure equalization steps, E3R, E2R and E1R, occupy one unit cell each, as shown in Fig. 6b Unit Block-1. The darker shaded unit cells (C-2 and C-3) represent the possible places where E1D (corresponding to E1R in C-1) can be placed. E1D in C-2 would result in the F step occupying just one unit cell, which is not desirable. Therefore, placing E1D in C-3 is the obvious choice. Similarly, E2D (corresponding to E2R in B-1) and E3D (corresponding to E3R in A-1) can be placed in unit cells B-4 and A-5, respectively. As a consequence, one I step (in unit cell A-4) is necessary to align the various coupled steps, resulting in the unit block shown in Fig. 6b Unit Block-2. Placement of the CoD, CnD, LR and FP steps in unit cells C-4, B-5, C-5 and A-2, respectively, results in the unit block shown in Fig. 6b Unit Block-3. The darker shaded cells represent the possible places that can be occupied by the F step. However, placing the F step in these four unit cells would make the feed step discontinuous, as there would be instances during the cycle where two beds would be fed simultaneously, while during the rest of the cycle only one bed would be fed. This situation can be avoided

by extending the FP step. The FP step, when placed in unit cell B-2, with the remaining unit cells occupied by the F step, results in the completed unit block shown in Fig. 6b Unit Block-4. The final cycle schedule can easily be derived from the resulting unit block, as shown in Fig. 6c, which is the same grid as that proposed by Chiang (1988).

5 Conclusions

A simple and rapid graphical unit block approach for complex pressure swing adsorption (PSA) cycle scheduling was developed. This new methodology involved *a priori* specifying the cycle steps, their sequence, and the number of beds, and then following a systematic procedure that required filling in a 2-D grid. The outcome or solution was a unit block, which was easily extended to form the complete cycle schedule. This unique methodology can be applied to any number of beds, any number of cycle steps, and any number of coupled steps or constraints.

This new approach was tested successfully against cycle schedules taken from the literature, including a two-bed four-step Skarstrom cycle, a four-bed nine-step process with two equalization steps, and a five-bed eleven-step process with three pressure equalization steps. The methodology

easily revealed that multiple PSA cycle schedules could be derived for any number of beds involving multiple constraints with numerous bed interactions. This new methodology should prove to be very useful for rapidly deriving all kinds of PSA cycle schedules in minutes that can then be compared to each other to scrutinize each of them for possible incorporation into a PSA process.

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