

Graphical approach for complex PSA cycle scheduling

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Abstract A simple graphical approach for 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 based on a few simple rules, some heuristics and some experience. The outcome or solution is a grid comprised of columns that represent the total cycle time, rows that represent the total number of beds, and cells that represent the duration of each cycle step, i.e., the complete cycle schedule. This new approach has been tested successfully against several cycle schedules taken from the literature, including a two-bed four-step Skarstrom cycle, a four-bed nine-step process with two equalization steps, a nine-bed eleven-step process with three pressure equalization steps, and a six-bed thirteen-step process with four pressure equalization steps and four idle steps. This approach also revealed the existence of numerous cycle schedules for each bed and cycle step combination examined. Although it cannot identify the total number of permutations or which one is better, it does provide a very straightforward way to determine some of the possible cycle schedules of virtually any PSA process that can be conceived.

Keywords Pressure swing adsorption · Cycle scheduling · Cycle sequencing

1 Introduction

There are just six basic cycle steps associated with any PSA process (Ruthven et al. 1994). These are the feed, rinse (or heavy reflux), co-current or counter-current depressurization, purge (or light reflux), pressure equalization, and repressurization steps. However, since a typical PSA process has multiple beds operating simultaneously and every bed following the same set of cycle steps in order, these six different cycle steps can be scheduled in many different ways. This gives rise to a multitude of different cycle configurations, including cycles that have beds interacting with each other.

In fact, each one of the six basic cycle steps can be coupled to another cycle step, which necessarily results in pairs of beds being periodically linked during operation of a PSA process. The most obvious step is the pressure equalization step. In this case, two beds are interconnected to allow their pressures to equalize. The gas used for purge can also come from a bed under going either the feed step or the co-current depressurization step (Ruthven et al. 1994). Similarly, the gas used for rinse can come from a bed undergoing either the counter-current depressurization step or purge step (Reynolds et al. 2008). Finally, the gas used for repressurization can come from a bed undergoing the feed step (Ruthven et al. 1994).

In addition, each one of the six basic cycle steps does not always operate for the same length of time, unless it is coupled to another step. These two features, i.e., unequal step time cycles and coupled steps, naturally give rise to numerous constraints that must be met when developing a cycle step schedule for a PSA process. For instance, the operation of two beds undergoing equalization steps must have these steps initiate and terminate at the same time. Likewise,

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Cycle Sequence: F→E1D→E2D→E3D→CoD→DeD→CnD→LR→E4R→E3R→E2R→E1R→FR

Bed ↓	Time →																			
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1	CoD	DeD	CnD		LR	E4R	E3R	I	E2R	I	I	E1R			FR			F		
2	E1D	E2D	I	E3D	CoD	DeD	CnD	LR	E4R	E3R	I	E2R	I	I	E1R			FR		
3			F		E1D	E2D	I	E3D	CoD	DeD	CnD	LR			E4R	E3R	I	E2R	I	I
4	E1R		FR				F		E1D	E2D	I	E3D			CoD	DeD	CnD	LR	E4R	E3R
5	I	E2R	I	I	E1R		FR				F			E1D	E2D	I	E3D	CoD	DeD	CnD
6	LR	E4R	E3R		I	E2R	I	I	E1R		FR				F		E1D	E2D	I	E3D

Fig. 1 PSA cycle schedule of a six-bed thirteen-step process, depicting the primary set (each *lighter shaded row* of cells), the beginning unit step and ending unit step in the primary set (darker shaded cells),

the primary diagonal (all *lighter shaded cells*), and the unit block (cells contained within the thick black rectangle)

if light product from the feed step is used for repressurization, the length of the pressurization step must be less than or equal to that of the feed step. Clearly, the scheduling of complex PSA cycles is a daunting task, with a paucity of information available in the literature.

Chiang (1988) presented an arithmetic approach for scheduling rather simple PSA cycles. However, his 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 for a certain amount of time by closing all of the valves leading to it. It sometimes has to be incorporated to make a set of interacting steps line up properly in the schedule. From Chiang's work, the total idle time for a particular bed can be obtained, but not the positions where the idle steps are to be placed and their respective durations.

Smith and Westerberg (1990) approached this problem from a different perspective. Their idea was to model and solve a set of equations and constraints, considering it as an optimization problem. However, the models became very complicated as the number of beds or constraints increased, due to a corresponding increase in the number of interactions. Understanding and solving such a system of equations and constraints can become an overwhelming and time consuming task, especially for complex, multi-bed, multi-step, PSA systems.

The objective of this work is to introduce a comparatively simple, graphical approach for complex PSA cycle scheduling. The mechanics of this new methodology are described using a generic example of a PSA cycle schedule. Then, the graphical 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. Strengths and weaknesses of this new graphical approach for complex PSA cycle scheduling are discussed.

Before introducing the graphical approach, it is worth pointing out the pedagogy behind the arrangement of the PSA cycle schedules presented below. This analysis begins with a 3-bed PSA cycle, not a 2-bed one. It is difficult, if not

impossible, to start with a 2-bed system because it is so simple that all the features of a typical PSA cycle schedule can not be included in it. In fact, it is so simple that it does not allow all the definitions and heuristics of the methodology to be defined and discussed concisely in one section. However, a 3-bed system has just enough complexity to explain all the features and heuristics of the graphical approach in a logical fashion without being overly complex. Only after the graphical approach is explained with a hypothetical 3-bed system are examples provided with actual PSA cycle schedules. These examples begin with the analysis of 2-bed systems to show that the graphical approach does indeed apply to this simple case. Then, 3-bed, 4-bed, 5-bed, 6-bed and 9-bed systems are analyzed and discussed to provide increasingly more complex examples, with each one teaching a new feature of the graphical approach.

2 Cycle schedule grid

Figure 1 shows a typical PSA cycle schedule or grid of a PSA system (Xu and Weist 2002). It consists of six beds and thirteen steps, including four equalization steps and four idle (I) steps. The sequence of the thirteen cycle steps (excluding the I steps) goes as follows:

1. feed (F) at high pressure, where a bed receives gas in its heavy end from the feed source while producing light product from its light end;
2. first pressure equalization step (E1D), where a bed provides gas from its light end to the light end of a bed undergoing pressure equalization (E1R);
3. second pressure equalization step (E2D), where a bed provides gas from its light end to the light end of a bed undergoing pressure equalization (E2R);
4. third pressure equalization step (E3D), where a bed provides gas from its light end to the light end of a bed undergoing pressure equalization (E3R);
5. co-current depressurization (CoD), where a bed provides purge gas from its light end to the light end of a bed undergoing light reflux (LR);

6. dual ended depressurization (DeD), where a bed is depressurized from both the light and heavy ends, with the gas exiting its light end being provided to the light end of a bed receiving pressure equalization (E4R) and the gas exiting its heavy end being taken as heavy product;
7. counter-current depressurization (CnD), where a bed is depressurized through its heavy end to provide most of the heavy product;
8. light reflux (LR), where a bed receives purge gas in its light end from the light end of a bed undergoing co-current depressurization (CoD);
9. fourth pressure equalization step (E4R), where a bed receives gas in its light end from the light end of a bed undergoing dual ended depressurization (DeD);
10. third pressure equalization step (E3R), where a bed receives gas in its light end from the light end of a bed undergoing pressure equalization (E3D);
11. second pressure equalization step (E2R), where a bed receives gas in its light end from the light end of a bed undergoing pressure equalization (E2D);
12. first pressure equalization step (E1R), where a bed receives gas in its light end from the light end of a bed undergoing pressure equalization (E1D); and
13. feed repressurization (FR), where a bed receives gas in its heavy end from the feed source.

In the corresponding grid, all six beds are placed along the vertical direction, whereas time is placed along the horizontal direction. The twenty-four columns in the grid, i.e., A through X 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 D-4 contains the step which runs in bed 4 during unit time step D (i.e., FR). 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 four unit time steps.

The lighter shaded cells in Fig. 1 represent one of many primary diagonals that can be identified in this grid. As shown later, the primary diagonal is the fundamental element that is required for the formation of any grid. Notice that the primary diagonal consists of the same repeating blocks (for every bed) placed diagonally along the grid.

Each repeating block is denoted as a primary set. In this case, a primary set is six unit cells long and consists of cycle steps CoD, DeD, CnD, and LR. As there are six beds, six primary sets are arranged diagonally along the grid. The primary sets can be arranged diagonally in different ways, which gives rise to many other solutions or schedules other than the one shown in Fig. 1. Such possibilities are discussed in detail in the next section.

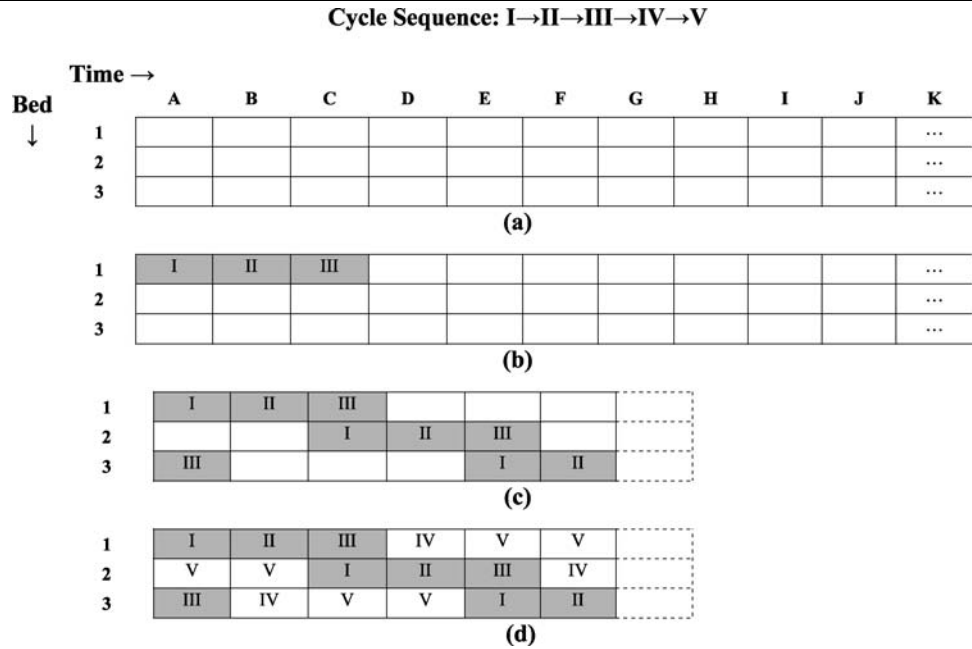
Every primary set has two key elements, i.e., the beginning unit step, which is the first unit time step in the set, and the ending unit step, which is the last unit time step in the set. For example, the beginning unit and ending unit steps for the primary sets in rows three and four are indicated in Fig. 1 by the darker shaded cells. The ending unit step of the first row must also be aligned properly with the beginning unit step of the second row and so on in subsequent rows to initiate and complete the formation of the primary diagonal and thus the primary grid. There are three possibilities. First, these two steps can be aligned vertically with one unit time step overlapping. Second, the beginning unit step can be shifted to the left from this vertical position with multiple unit time steps overlapping. For example, the schedule in Fig. 1 has its primary sets shifted to the left from the vertical position by one unit cell. Third, the beginning unit step can be shifted to the right by multiple unit time steps with no unit time steps overlapping. This choice may or may not be arbitrary, depending on the imposed constraints, as illustrated later by example.

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 step times A through D 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 six beds. The unit block occurs again during unit step times E through H. In the same way, the total cycle time is made up of six consecutive unit blocks, and this number must match the total number of beds.

3 Methodology

This graphical scheduling methodology is divided into two parts. In the first part, the goal is to build the primary grid. A primary grid is formed when the array of a given number of rows (i.e., beds) and a given number of columns (i.e., unit time steps) is determined. In the second part, the final cycle schedule is built around the primary grid by filling in the rest of the remaining empty unit cells. During this second part, the number of idle steps (if any), their duration, and relative location within the grid is determined.

Fig. 2 Construction of a PSA cycle schedule for a three-bed five-step process: (a) initial empty grid; (b) grid from (a) showing primary set (shaded cells); (c) grid from (b) showing primary set added to every row, forming the primary diagonal and primary grid (shaded cells); and (d) grid from (c) showing all cycle steps added, forming a cycle schedule



In part one, two pieces of information about the PSA cycle must be decided *a priori* to start building a grid. First, the individual cycle steps of the cycle must be chosen from the six basic steps, along with their sequence of operation. Second, 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. Figure 2a shows an empty grid 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 or the total cycle time has not been determined. In other words, the grid is free to expand or contract horizontally.

Typically, for any PSA cycle schedule a few constraints must be satisfied. For instance, in the sequence shown in Fig. 1, the gas from the CoD step is used to purge the bed undergoing the LR step. 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 III. In other words, at a given unit time step, at least two different beds must have these steps operating simultaneously. Although there is usually more than one constraint that must be satisfied in a PSA cycle, like that shown in Fig. 1, only one constraint (if any) should be selected for the formation of the primary grid, because it allows for more flexibility in part two, i.e., during grid filling. **Heuristic:** choose the constraint associated with a coupled set of steps that has the least number of cycle steps in between them.

The next stage of part one involves the formation of the primary set. The length of the primary set is chosen arbitrarily, while keeping the above heuristic in mind. At this point,

it must be decided whether all the cycle steps in the primary set are the same duration, with each one being only one unit time step long, or whether one or more of the cycle steps occupies more than one unit time step. The beginning unit and ending unit steps of the primary grid are then identified, with the caveat that these steps can be only one unit time step long, even if the cycle step they belong to is more than one unit time step.

In this example, to build the primary set, one of the two coupled cycle steps, i.e., I or III, must be chosen to begin the set, while the other must be chosen to end it. Since, the cycle steps always run in order, step I can be chosen as either the beginning unit step or the ending unit step, and the same holds true for step III. Hence, a primary set can be formed in two ways. For the cycle sequence shown in Fig. 2, the two possible primary sets are [I, II, and III] and [III, IV, V, I], with the shorter one preferred because it also allows for more flexibility with placement of the remaining steps during grid filling, especially if any one of the remaining steps is expected to be longer than one unit cell, like a feed step. Constructing a primary set with more cycle steps requires the lengths of the intermediate steps to be decided *a priori*, which for certain cases thwarts the possibility of considering other options that a smaller primary set may allow. **Heuristic:** choose the primary set with the least number of cycle steps.

Based on the above heuristic, the first primary set is placed in the first row of the grid in Fig. 2b in unit cells A-1, B-1, and C-1. This makes step I the beginning unit step and step III the ending unit step. For the particular case shown in Fig. 2, the total length of the primary set is based on the stipulation that the lengths of steps I, II and III are equal

and that they each occupy only one unit time step. Thus, the primary set shown in Fig. 2 is three unit time steps long.

The next stage of part one is to take the primary set that has been established for bed 1 in row one and place it in consecutive rows by aligning it in such a way that it forms the primary diagonal along the grid. Recall that this diagonal arrangement with the primary set to form the primary diagonal can be done in three ways. The ending unit step in row one can align vertically with the beginning unit step in row two, or the beginning unit step can be shifted to the left or to the right of this position. For the schedule in Fig. 1, the shift in the alignment from the vertical position is to the left by one unit time step, logically resulting in overlap of the LR and CoD steps, which are each two unit time steps long and coupled. In contrast, for the example in Fig. 2, the simplest case is considered, where the ending unit step in row one (step III) and the beginning unit step in row two (step I) overlap and each cycle step happens to be only one unit time step long (Fig. 2c). In other words, these two steps are vertically aligned. The primary diagonal is thus formed by placing the primary set in each consecutive row with the proper alignment of the ending unit step and beginning unit step until the last row is reached. **Heuristic:** consider the simplest alignment first; shifts to the left second, especially if they make a coupled set of steps that each occupy more than one unit cell to be completely aligned; and shifts to the right last, if grid expansion is deemed necessary.

Observe that while proceeding down the primary diagonal, unit cell F-3 is occupied by step II. If step III is aligned along its side in unit cell G-3 like in the rest of the rows, then there is no corresponding step III for step I of bed 1 in A-1. Hence, step III must be placed in A-3 to complete the primary grid. This primary grid is unique to the specified cycle sequence, number of beds, and primary set.

The importance of forming the primary grid, i.e., the primary diagonal from the primary set cannot be overstated. It fixes the length of the grid horizontally, which, in turn, fixes the number of unit time steps in the grid and thus the total cycle time. In the example in Fig. 2, the diagonal arrangement makes sure that steps I and III are always coupled, as seen in Fig. 2c at unit times A, C and E. Moreover, as mentioned above, the primary grid can be formed in different ways. For example, if steps I and III are coupled for only part of the time, then they do not need to be the same duration. In other words, an equally valid primary set is [I, I, II, II, II, II, and III], which occupies seven unit time steps. This primary set stipulates that steps I and III are coupled during only one of the unit time steps, the duration of step I is two times this unit time step, and the duration of step II is four times this unit time step. Another equally valid primary set is [I, I, II, III and III], which occupies five unit time steps. Steps I and III are still coupled for the entire time, but their duration is twice that of step II. **Heuristic:** to make a cycle

step longer in a primary set choose to have it occupy more than one unit cell.

With respect to primary set alignment, there is no limit to the number of unit time step shifts that can be taken to the right, as the total number of unit time steps in the grid has not been determined. However, there is a limit to the number of unit time step shifts that can be taken to the left. This limit is reached when the two primary sets become completely aligned in two consecutive rows. The PSA cycle schedule that forms for such a situation corresponds to one where all the beds operate independent of each other with no coupled steps possible. A PSA cycle can surely operate without overlap, but generally there are benefits of incorporating one or more overlapping steps (e.g., to reduce the need for large receivers or surge tanks). However, one shift to the left less may result in a more viable, overlapping PSA cycle schedule.

In addition, the total unit time steps in the primary grid increases with an increase in the number of right shifts and it decreases with an increase in the number of left shifts. These may be positive or negative attributes and may even lead to nonsensical solutions or schedules, depending on the number of beds, particular cycle sequence, and relative time of the shortest cycle step to that of the longest cycle step. Clearly, some trial and error is involved with the choice of the primary set and its alignment to form the corresponding primary grid, where experience with PSA cycles is paramount to minimizing the number of options to consider.

In part two, the final PSA cycle schedule is built around the primary grid by filling in the rest of the remaining empty unit cells using intuition, experience, and also some trial and error. Notice that for the primary grid in Fig. 2c, there are three empty unit cells (for each row) in which the two remaining cycle steps must be placed. Clearly, there are two possible ways to do this ([IV, IV, V] and [IV, V, V]), with each resulting in a unique solution or cycle schedule. **Heuristic:** if there are coupled cycle steps to deal with during part two, choose to add each set of coupled steps one at a time in such a way that it minimizes the number of idle steps. This heuristic becomes clear later in an example.

By assuming that no additional constraints need to be satisfied in this example, one possible cycle schedule of many is shown in Fig. 2d. In this case, step V takes up two unit step times and step IV takes up only one unit step time. More illustrations of the versatility afforded in part two are provided in the *Applications* section, where this methodology is used to obtain actual PSA cycle schedules from the literature.

In closing this section, it is noteworthy that the methodology presented so far is very restrictive due to the constraints imposed by the coupled cycle steps. However, a completely general methodology is also possible that relaxes all constraints during the formation of the primary grid in part one. This relaxation allows for the most flexibility in deriving

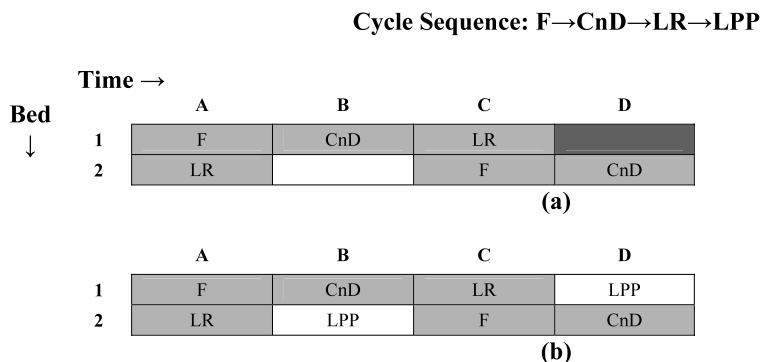


Fig. 3 Construction of a PSA cycle schedule for a two-bed four-step process: (a) grid showing primary set, primary diagonal and primary grid (lighter shaded cells), and empty cells for filling with remaining

cycle steps (darker shaded cells); and (b) grid from (a) showing all cycle steps added, forming an equal step time cycle schedule

uniquely different PSA cycle schedules. Any constraints are then handled one at a time in a logical fashion during the filling of the grid in part two. One of the applications addressed later illustrates this more general approach to primary grid formation and solution or schedule refinement.

4 Applications

To illustrate how to apply this new graphical approach to an actual PSA cycle schedule, a relatively simple two-bed four-step Skarstrom PSA cycle is analyzed first (Skarstrom 1960). In this example, every bed undergoes the same 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. For this configuration, gas leaving the light end of the bed undergoing the F step is provided as purge to the light end of the bed undergoing the LR step and is also used to pressurize the bed during LPP. Hence, two constraints must be considered while forming such a cycle schedule. These are coupling of F with LR, and F with LPP. Also, if a buffer tank is not to be used, the length of the LPP and LR steps must be less than or equal to the F step.

One possible grid is depicted in Fig. 3a. The F, CnD and LR steps are arbitrarily chosen to constitute the primary set. F is the beginning unit step while LR is the ending unit step, with their durations the same and each equal to one unit time step. The simplest alignment is also selected in this case to satisfy one of the constraints mentioned above on coupled steps. So, the ending unit step of the primary set in the first row is vertically aligned with the beginning unit step of the primary set in the second row, which is shown in Fig. 3a. This particular primary grid leaves one unit cell (darker shaded cell) for LPP to be placed in. There is only one solution for this situation, i.e., the equal step time cycle

schedule shown in Fig. 3b. However, notice that the F step is not continuous, which may not be acceptable depending on the application.

One of the primary goals in designing a PSA process is to maximize the feed throughput, which can be accomplished by feeding longer or by feeding multiple beds at the same time. To increase the feed time of this two-bed four-step PSA process, the grid needs to be expanded horizontally. Clearly, this is not possible with the primary set used in Fig. 3. Figure 4a shows a primary set where the F step occupies two unit cells and the CnD and LR steps take one unit cell each. The formation of the primary grid is again based on vertical alignment, which also satisfies one of the constraints on the coupled steps. But now the grid size is six unit time steps (Fig. 4a) instead of five (Fig. 3), which makes two unit cells (darker shaded cells in Fig. 4a) available for the placement of LPP and/or the F step. The only solution which can accommodate continuous feed for a two-bed four-step cycle arranged in six unit cells is shown in Fig. 4b. In other words, for the feed to be continuous, it must occupy three of the six unit cells. This leaves only three unit cells for the remaining three steps; hence, there is only one solution for this case.

All the two-bed four-step cycles discussed so far were based on coupling the F and LR steps. The primary set and consecutively the primary diagonal can also be formed by considering the other constraint instead, i.e., by coupling the F and LPP steps together. For this particular case, choosing LPP to be the beginning unit step and F to be the ending unit step results in a primary grid where no space is left for the rest of the cycle steps. However, this might not be true when the number of beds is more than two. Alternatively, the primary set can be constructed with F being the beginning unit step and LPP being the ending unit step, as shown in Fig. 5a. This is an interesting case where all the cycle steps in the sequence are used to form the primary grid. For this case, the

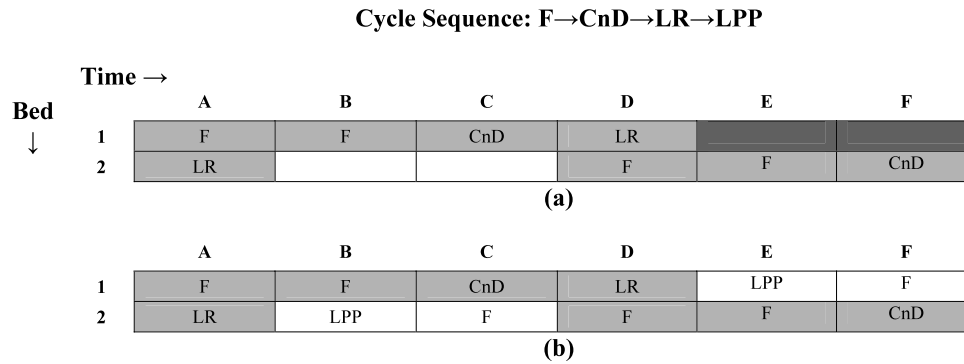


Fig. 4 Construction of a PSA cycle schedule for a two-bed four-step process: (a) grid showing primary set, primary diagonal and primary grid (lighter shaded cells) with more intermediate steps between the beginning unit step (F) and ending unit step (LPP) and with empty

cells for filling with remaining cycle steps (darker shaded cells); and (b) grid from (a) showing all cycle steps added, forming the final cycle schedule

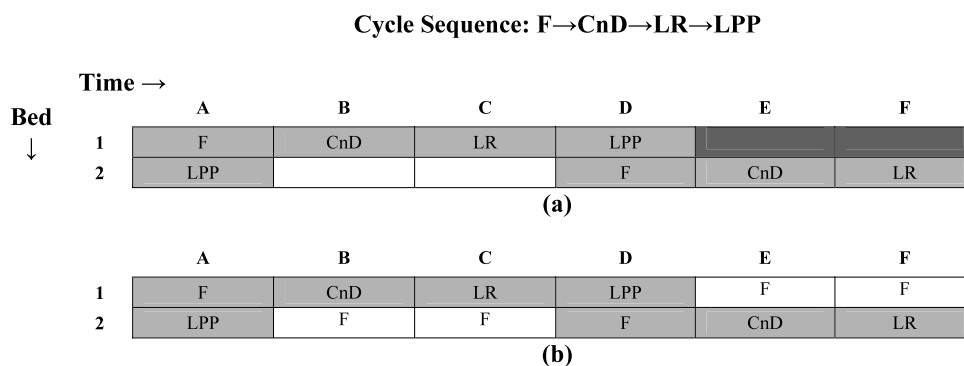


Fig. 5 Construction of a PSA cycle schedule for a two-bed four-step process: (a) grid showing primary set, primary diagonal and primary grid (lighter shaded cells) formed with F and LPP being coupled and

empty cells for filling with remaining cycle steps (darker shaded cells); and (b) grid from (a) showing all cycle steps added, forming the final cycle schedule

only solution with continuous feed is shown in Fig. 5b. Notice that this solution is the same as that shown in Fig. 4b. This implies that the same solution might be obtained even when starting from a different primary set.

Figures 6a, 6b and 6c show an example where the primary grid can be expanded even further. The expansion results from using different relative lengths of any of the steps including the beginning unit step, ending unit step and any intermediate steps. For example, intermediate steps occupy three unit cells in Fig. 6a (B-1 to D-1 in bed 1), four unit cells in Fig. 6b (B-1 to E-1 in bed 1), and five unit cells in Fig. 6c (B-1 to F-1 in bed 1). Notice that the length of the feed step is the same in all three cases (50% relative to the total cycle time); but, the relative lengths of the other steps constituting the sequence are different. Such a procedure can prove to be very useful while exploring different PSA cycles for a specific application. Also, the grid shown in Fig. 6c is exactly the same as that in Fig. 4b i.e., if the duration of every unit cell of Fig. 4b is doubled, Fig. 6c is obtained. This demonstrates that if every unit cell in a par-

ticular grid is expanded by a constant factor, like 2, 3 or 4, then it results in the same grid (provided they both represent the same total cycle time).

It is noteworthy that a variation of the two-bed four-step PSA cycle schedules depicted in Figs. 4 to 6 are used commercially in gasoline vapor recovery units (Dinsmore and Young 1984). All of these cycle schedules have one bed being fed while the other bed is undergoing CnD, LR and LPP. In this way the feed is continuous to the PSA unit, as required when recovering gasoline vapor from large tank filling operations.

These concepts can be implemented and extended easily for a larger number of beds. Figures 7a and 7b show two primary grids for a three-bed four-step PSA cycle with F and LR coupled in one case, and F and LPP coupled in the other case. Based on the heuristics and procedure discussed above, the rest of the unit cells can be filled in easily, resulting in the cycle schedules shown in Figs. 7c, 7d and 7e. In Fig. 7c, two LPP steps and one F step are chosen to fill in the grid, with the only other option being LR, LPP and F. The

Cycle Sequence: F→CnD→LR→LPP

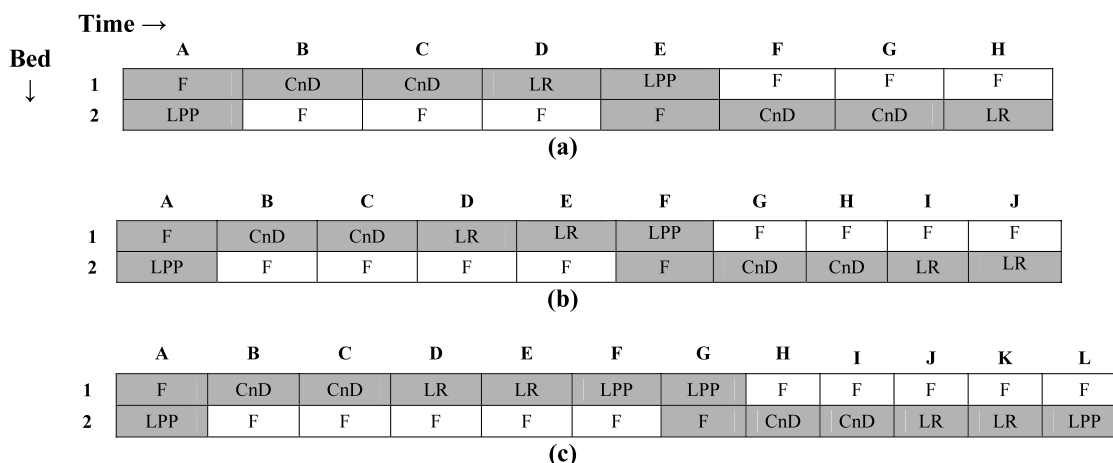


Fig. 6 Construction of PSA cycle schedules for a two-bed four-step process showing the importance of grid expansion: (a) grid showing primary set, primary diagonal and primary grid (shaded cells) formed with F and LPP being coupled, intermediate steps occupying three unit

cells, and the entire grid formed with eight unit time steps; (b) intermediate steps occupying four unit cells and entire grid formed with ten unit time steps; (c) intermediate steps occupying five unit cells and entire grid formed with twelve unit time steps

schedule in Fig. 7d is unique because two beds are being fed simultaneously at all times. With the F steps occupying 33.3% and 66.7% of the total cycle time in Figs. 7c and 7d, respectively, it is interesting that the feed throughput can be doubled simply by choosing a different coupled step to form the primary step and the primary diagonal. Other options are possible, like that shown in Fig. 7e.

This cycle schedule has an idle (I) step after the LPP step and before the F step. Sometimes it may be necessary to accommodate an I step in the final cycle schedule for two reasons. First, an I step can be used to align the various coupled steps in different beds (as shown in later examples), and second, for a particular bed, an I step can be used to shorten an individual cycle step (if needed). In the grid shown in Fig. 7e, placing the I step in between the F and LPP steps causes the length of both these steps to be equal. Placing F in G-1 results in a variable feed cycle (where one bed is being fed sometimes and two beds are being fed other times), whereas placing LPP there makes the LPP step longer than the F step, which is impossible without a buffer tank.

As discussed earlier, it is not always necessary for the ending unit step to align vertically with the beginning unit step of consecutive beds to form the primary grid. Consider the primary set shown in Fig. 7b, where F, CnD, LR and LPP occupy one unit cell each and the ending unit step (LPP) of any one bed is aligned vertically with the beginning unit step (F) of another bed. If this alignment is broken, the ending unit step of a particular bed can be displaced one (or more) position(s) either to the left or to the right relative to the ending unit step of another bed. These cases are depicted in

Fig. 8. Compared to Fig. 7b, Fig. 8a shows the primary grid with the alignment shifted one position to the left. Following the same logic from previous examples, the primary grid can be completed, resulting in Fig. 8b. This is the only possible solution. Figure 8c shows the grid with the alignment shifted one position to the right. Notice in this case, none of the coupled steps are aligned along the primary diagonal, which means care must be taken to ensure alignment of coupled steps when filling in the grid. One possible solution is shown in Fig. 8d. In this case two columns are again being fed simultaneously at all times. Other solutions are possible, but they allow only one bed to be fed at a time and involve one or two LPP steps and numerous I steps.

As realized from the PSA cycle schedule shown in Fig. 1, pressure equalization steps are quite common in the PSA patent literature and used commercially not only to save on operating costs (intuitive) but also to improve the performance (not intuitive) (Ruthven et al. 1994). The next example is more complicated in that it adds two pressure equalization steps to a four-bed PSA cycle. One such way is presented below, based on the following nine-step cycle sequence:

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;

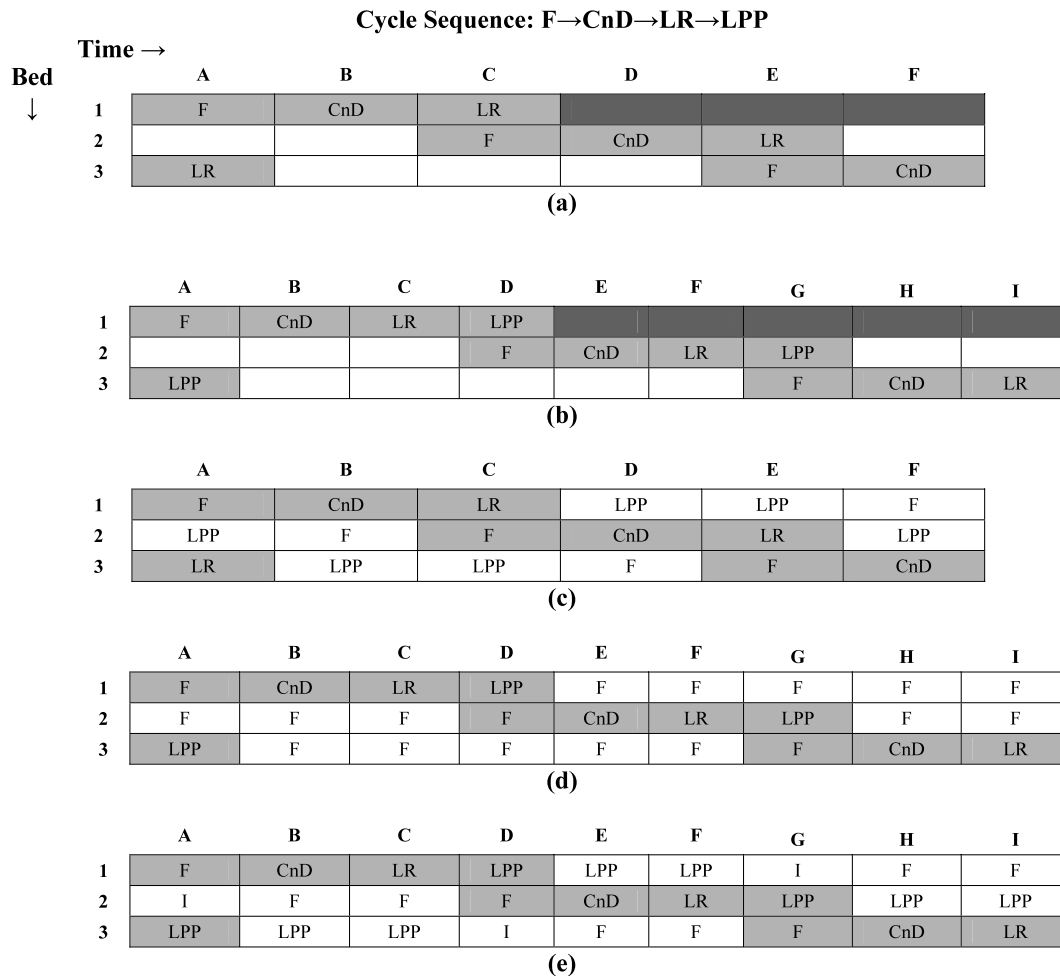


Fig. 7 Construction of a PSA cycle schedule for a three-bed four-step process: **(a)** and **(b)** grid showing primary set, primary diagonal and primary grid (lighter shaded cells), and empty cells for filling with remaining cycle steps (darker shaded cells) with F and LR and F and LPP forming the coupled steps; **(c)** grid from **(a)** showing all cycle

steps added, forming a cycle schedule; **(d)** grid from **(b)** showing all cycle steps added, forming a cycle schedule where two beds are being fed simultaneously at any instant; **(e)** grid from **(b)** showing all cycle steps added, forming a cycle schedule with one idle step

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.

Figure 9a shows the resulting primary grid. Clearly, CoD, E2D, CnD and LR form the primary set (shaded cells in every row) with the alignment being vertical. CoD and LR steps are two unit time steps long, whereas E2D and CnD are each a unit time step long. In addition, CoD and LR are the beginning unit step and ending unit step, respectively. These are logical choices, especially since they satisfy one constraint on step coupling, i.e., CoD and LR are coupled. The darker shaded cells C-3 and C-4 depict the possible places that E2R (corresponding to E2D in C-1) can occupy. C-2 is eliminated because placing E2R in it leaves no space for

other steps between E2R and CoD, and placing E2R in C-3 results in four I steps between LR and E2R (occupying O-3 to B-3). Figure 9b shows E2R placed in C-4. As every bed follows the same sequence of steps, E2R is further placed in G-1, K-2 and O-3. Notice that for the steps shown in Fig. 9b, the grid is completely balanced. In other words, the coupled steps are properly aligned. Figure 9c shows E1R being placed next to E2R in all the beds. The darker shaded cells show two possible places where E1D can be placed (corresponding to E1R in D-4). D-2 is the logical choice as placing E1D in D-3 results in four I steps (in cells F-3 to H-3) between E1D and CoD. The result is the grid depicted in Fig. 9d. Observe that for every bed, seven unit cells are occupied by the LPP and F steps (combined). To have continuous feed, LPP must occupy three unit cells, whereas F must occupy four unit cells. This results in the grid shown

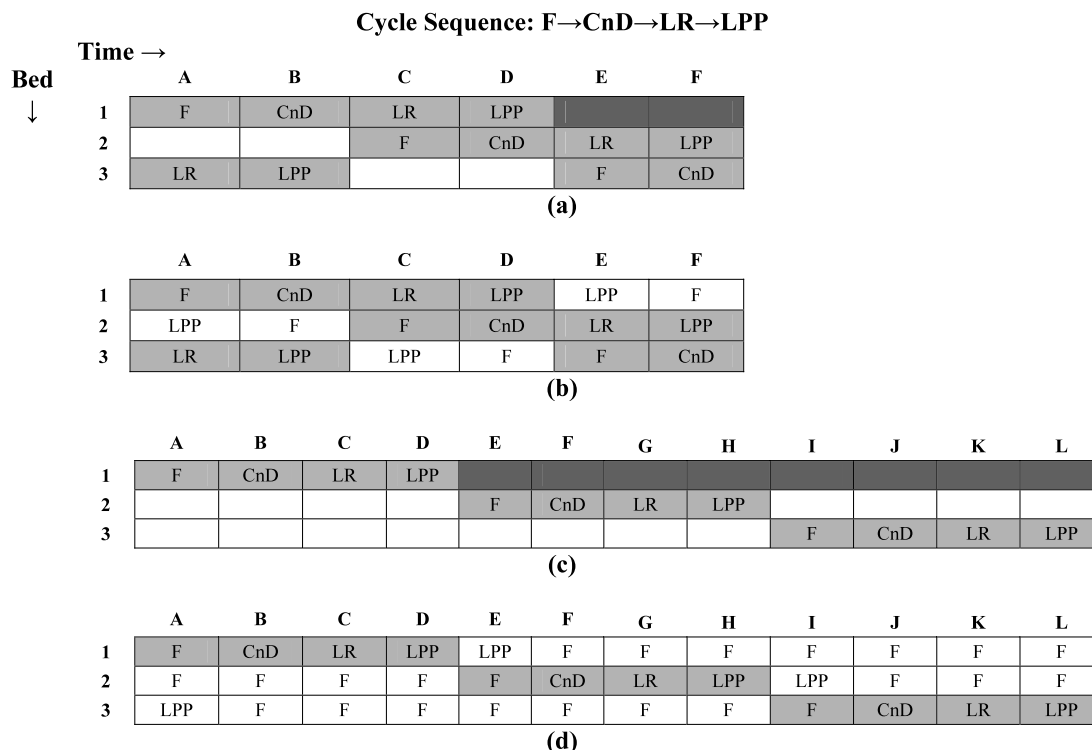


Fig. 8 Construction of PSA cycle schedules for a three-bed four-step process showing the relative importance of aligning primary sets in different beds: **(a)** grid showing primary set, primary diagonal and primary grid (lighter shaded cells), and empty cells for filling with remaining cycle steps (darker shaded cells) with the beginning unit step (F) aligned one unit time step to the right relative to the end step (LPP) in consecutive beds; **(b)** grid from **(a)** showing all cycle steps

added, forming a cycle schedule; **(c)** grid showing primary set, primary diagonal and primary grid (lighter shaded cells), and empty cells for filling with remaining cycle steps (darker shaded cells) with the beginning unit step (F) aligned one unit time step to the right relative to the end step (LPP) in consecutive beds; **(d)** grid from **(c)** showing all cycle steps added, forming a cycle schedule

in Fig. 9e, which is the same as proposed by Cassidy and Holmes (1984).

At this point it is probably becoming obvious that there are many ways to configure PSA cycles. Next consider a five-bed eleven-step cycle based on the following sequence:

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 repressurization (FR).

Figure 10a shows the resulting primary grid. Clearly, CoD, E3D, CnD and LR form the primary set, the duration

of each step is equal to the unit time step, CoD and LR are the beginning unit step and ending unit step, and the alignment is vertical. These are logical choices, especially since they satisfy one constraint on step coupling, i.e., CoD and LR are coupled. The darker shaded cells B-4 and B-5 depict the possible places that E3R (corresponding to E3D in B-1) can occupy. B-2 and B-3 are eliminated because placing E3R in them leaves no space for other steps between E3R and CoD. Also, E3R in B-4 requires I steps in three unit cells (N-4, O-4 and A-4), resulting in a shorter F step. Hence, E3R occupying B-5 is the logical choice. This result is shown in Fig. 10b.

The darker shaded cells in Fig. 10b represent two choices where E1D can be placed corresponding to E1R in A-4. When E1D occupies A-3, only one unit cell (O-3) becomes available for the F step, thereby lowering the feed throughput considerably. Contrarily, Fig. 10c shows E1D in A-2, and depending on the length of E1D, two solutions are possible. These are shown in Figs. 10d and 10e. The grid in Fig. 10d is the same as that shown by Chiang (1988). Note that these grids can be configured in many ways, resulting in

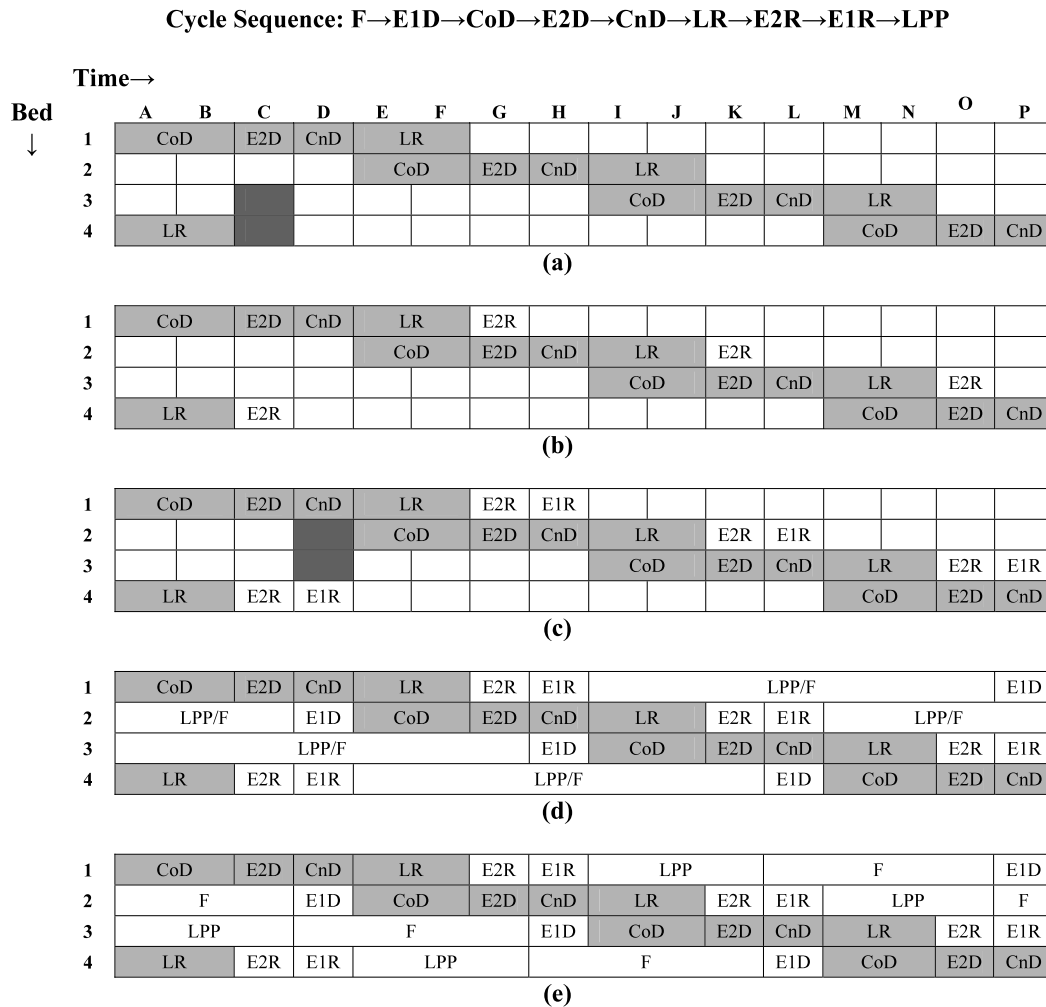


Fig. 9 Construction of a PSA cycle schedule for a four-bed nine-step process with two equalization steps: (a) grid showing primary set, primary diagonal and primary grid (lighter shaded cells); (b) and (c) showing placement of two equalization steps; (d) and (e) grids from (b) and (c) showing all cycle steps added, forming two cycle schedules

many solutions, depending upon the relative lengths of FR and F.

The next example illustrates how to form the primary grid with overlap of the unit cells during left shifting alignment of the primary sets. Consider the same sequence of steps for the six-bed system shown in Fig. 1. The not so obvious choice for the primary set is CoD, DeD, CnD, and LR. The durations of the CoD and LR steps are each twice the unit time step, with the other two steps having durations equal to the unit time step. The beginning unit step and ending unit step are associated with the first unit time step occupied by CoD and the second unit time step occupied by LR. The alignment is such that the beginning unit step in row two is shifted one unit time step to the left from the vertical alignment position. This alignment choice puts the coupled CoD and LR steps in complete alignment with each other. The resulting primary grid is given in Fig. 11a. Observe that because the CoD and LR steps occupy two unit cells each,

the primary grid expands to twenty-four columns (A through X). It is worth insisting that the decision to start with longer CoD and LR steps to expand the grid horizontally depends on the relative gain in the feed time without compromising the process performance. However, this can be judged only after solutions are obtained.

Since E4R follows LR and E3D precedes CoD, they each occupy only one unit time step, resulting in the grid in Fig. 11b. This makes steps DeD and E4R overlap in consecutive beds, as required since they are coupled (see Fig. 1 and the *Cycle Schedule Grid* section). The darker shaded cells show the possible places where E3R can be placed corresponding to E3D in D-2. E3R cannot occupy D-3 as this leaves no space for the six steps in between E3R and E3D. Also, E3R in D-4 gives a solution where the equalization steps do not align. So, the only two places that E3R can occupy are D-5 or D-6. By observation, D-5 is not the preferred choice, as it forces four I steps in between E4R and

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

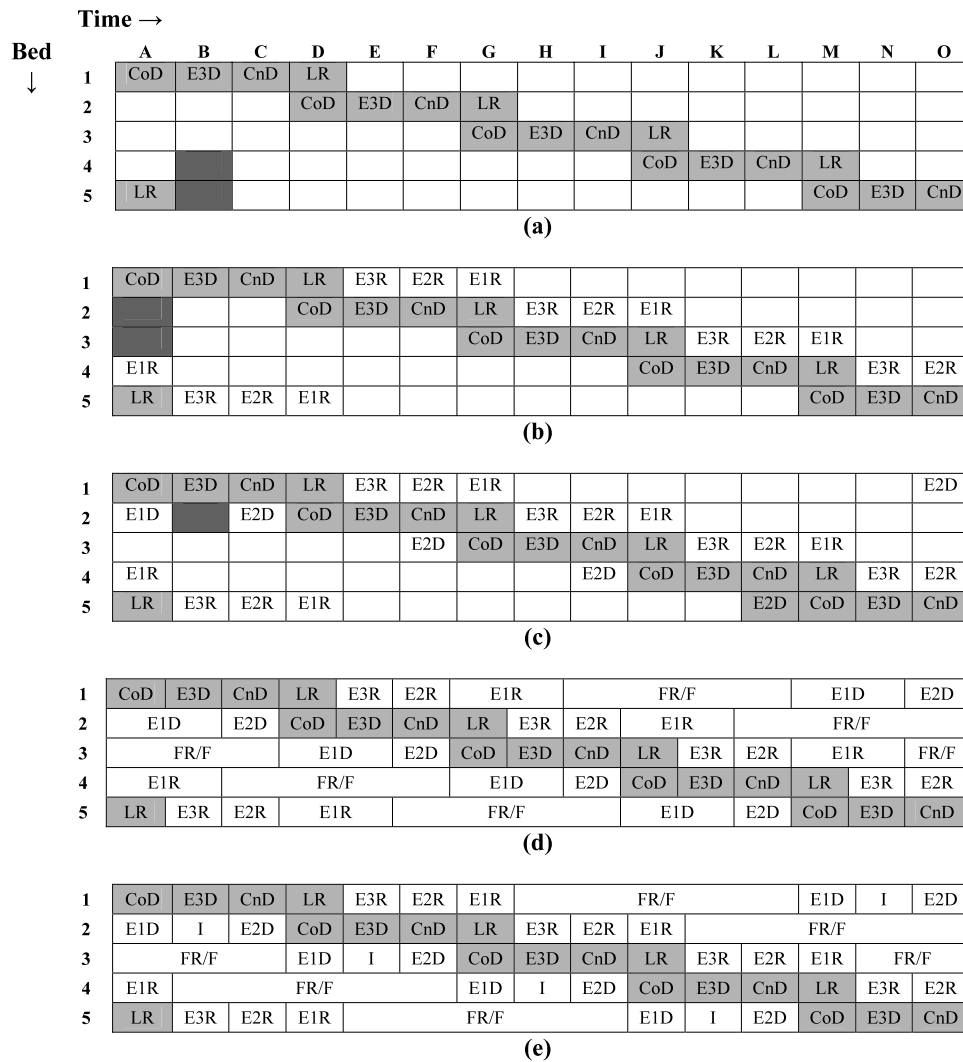


Fig. 10 Construction of a PSA cycle schedule for a five-bed eleven-step process with three equalization steps: (a) grid showing primary set, primary diagonal and primary grid (lighter shaded cells), and two empty cells for filling with remaining cycle steps (darker shaded cells); (b) grid from (a) showing new cycle steps added and two new empty cells for filling with remaining cycle steps (darker shaded

cells); (c) grid from (b) showing more cycle steps added and two new empty cells for filling with remaining cycle steps (darker shaded cells); (d) grid from (c) showing all cycle steps added, forming a cycle schedule; and (e) grid from (a) showing all cycle steps added, but forming an alternative cycle schedule than that in (d), because the cycle steps are added differently than in (b) and (c)

E3R, leaving little room for the feed step. This leaves D-6 as the place to put E3R. This arrangement is shown in Fig. 11c, with equalization steps E1D, E2D and E3D also added and placed together. The darker shaded cells represent the two places that E2R can occupy in unit time step W. To minimize the idle steps, E2R is placed in W-4. The resulting cycle schedule is shown in Fig. 11d. Seven unit cells are now available for any combination of the FR and F steps, with longer feed times usually preferred.

A different schedule is obtained if equalization steps E4R, E3R and E2R instead of equalization steps E1D, E2D and E3D are placed together in the primary grid shown in

Fig. 11c. This grid is shown in Fig. 12a. Again, to minimize the number of I steps in the solution, E1R (corresponding to E1D in H-4) is placed in H-6. The resulting cycle schedule is shown in Fig. 12b. However, if an I step is placed *a priori* between E3R and E2R after the formation of the primary grid (Fig. 11a) and the same procedure discussed above is followed, then the cycle schedule depicted in Fig. 12c results. This cycle schedule has been reported by Xu and Weist (2002). Note that the lengths of the different cycle steps in Fig. 12c are exactly the same as those in Fig. 11d. The only difference between the two solutions is the position of the four I steps; thus, in essence, they are the same cycle

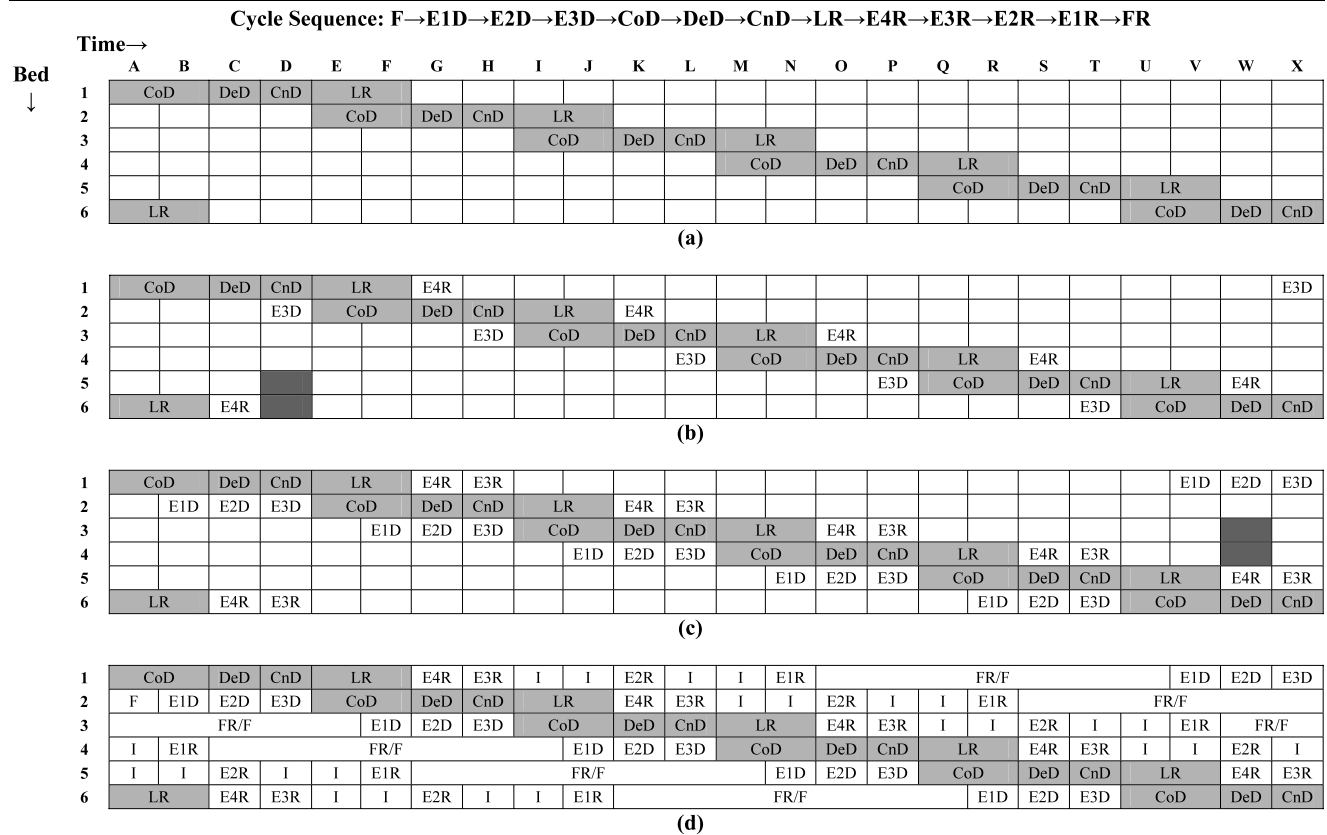


Fig. 11 Construction of a PSA cycle schedule for a six-bed thirteen-step process with four equalization steps: **(a)** grid showing primary set, primary diagonal and primary grid (shaded cells); **(b)** grid from **(a)** showing new cycle steps added and two empty cells for filling with

remaining cycle steps (darker shaded cells); **(c)** grid from **(b)** showing more cycle steps added and two new empty cells for filling with remaining cycle steps (darker shaded cells); and **(d)** grid from **(c)** showing all cycle steps added, forming a cycle schedule

schedule, if the position of the idle step has no effect on the process performance. Clearly, this comparison shows the utility of the graphical scheduling methodology, as it can be used in a logical fashion to obtain cycle schedules that have been obtained perhaps by less rational approaches.

The last example takes the nine-bed eleven-step PSA cycle sequence shown in Fig. 13 and illustrates the situation when the primary grid is comprised of uncoupled cycle steps. The nomenclature for the various steps is the same as that for the configurations in Fig. 11. Unlike all the previous cycle sequences, the primary set E1D, E2D and E3D has no coupled steps, with the beginning unit step as E1D, the ending unit step as E3D, and the alignment being vertical. It is worth pointing out that aligning E1D and E2D makes the grid too small, and other combinations may result in the grid being too wide, thereby reducing the equalization times compared to the total cycle time. This grid is also based on the initial stipulation that the E3D and E1D equalization steps operate for the same duration. This is a reasonable assumption for equalization steps.

The darker shaded cells in Fig. 13a show the possible places where E1R can be placed in a unit step time A. E1R

and E1D are separated by two steps, FR and F. So, to increase the feed throughput, it is desirable to put E1R in A-6, which, in turn, leaves nine unit cells (B-6 to J-6) in which the FR and F steps can be distributed. As a consequence, the depressurization and LR steps are comparatively shortened, which may be undesirable. To avoid such a scenario, E1R is placed in A-5, which produces the grid shown in Fig. 13b. This grid is now balanced for the first equalization steps.

To couple the third equalization steps, E3R (corresponding to E3D in A-9) can occupy either A-6 or A-7. When E3R is placed in A-6, the grid shown in Fig. 13c is reached. This grid provides multiple solutions depending on the lengths of the CoD, CnD, LR, FR, and F steps. As the CoD and LR steps are coupled, the two combinations possible for CoD, CnD, and LR are (2, 1, 2) and (1, 3, 1). Similarly, for FR and F, the possibilities include (1, 6), (2, 5), (3, 4), (4, 3), (5, 2) and (6, 1). When the CoD, CnD, and LR steps are distributed as (2, 1, 2), and the FR and F steps are distributed as (1, 6), the solution shown in Fig. 13d is realized. This cycle schedule has been reported by Fuderer and Rudelstorfer (1976). On the other hand, when E3R occupies A-7 in Fig. 13b,

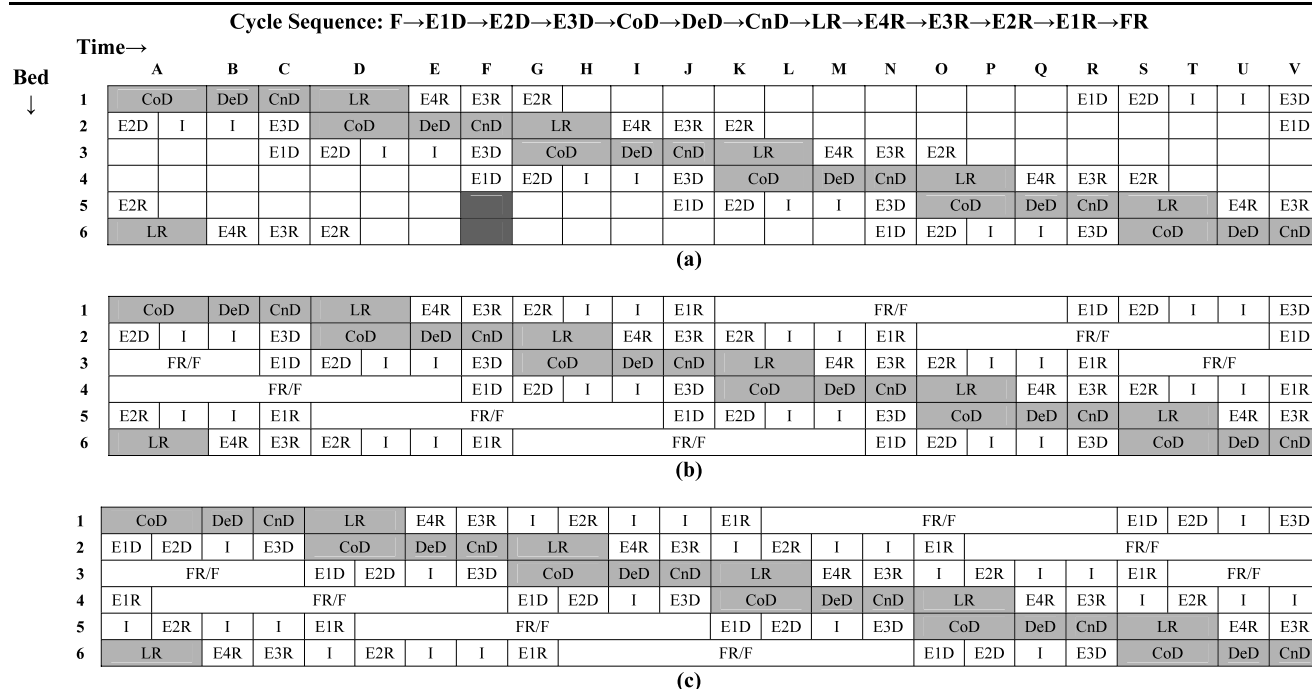


Fig. 12 Construction of a PSA cycle schedule for a six-bed thirteen-step process with four equalization steps: **(a)** grid from Fig. 11a showing a different placement of cycle steps than in Fig. 11b or 11c; **(b)** grid from (a) showing all cycle steps added, but forming an alternative cycle

schedule than that in Fig. 11d; and **(c)** grid from Fig. 11a showing all cycle steps added, but forming another alternative cycle schedule than those in Fig. 11d and (b)

the cycle schedule depicted in Fig. 13e is reached. Here, the lengths of the FR and F steps remain the same as the previous schedules, but the depressurization and LR steps are shortened. It is clear that there are many possible cycle schedules for this nine-bed eleven step PSA cycle, some desirable and some not.

5 Conclusions

A simple graphical approach to scheduling complex pressure swing adsorption (PSA) cycles was introduced. 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 based on a few simple rules, some heuristics, some experience, and possibly a trial and error approach. The outcome from a single graphical analysis is a grid comprised of columns that represent the total cycle time, rows that represent the total number of beds, and cells that represent the duration of each cycle step, i.e., a complete cycle schedule. This cycle schedule is usually one of many possible cycle schedules that can be obtained for the chosen set of cycle steps, their sequence, and number of beds.

This new graphical approach was tested successfully against several PSA cycle schedules taken from the literature, including a two-bed four-step Skarstrom cycle, a four-

bed nine-step process with two equalization steps, a nine-bed eleven-step process with three pressure equalization steps, and a six-bed thirteen-step process with four pressure equalization steps and four idle steps. The results revealed the existence of numerous cycle schedules for each of those bed and cycle step combinations. Hence, many possible cycle schedules were easily derived for any number of beds involving multiple constraints with numerous bed interactions through the application of this graphical approach.

It must be emphasized that the intent behind the development of this approach was to provide a simple set of rules from which a PSA cycle schedule can be built. It was never the intent to provide an optimum schedule for a given PSA cycle. Thus, although this graphical approach cannot be used to indicate the total number of permutations from a given set of cycle steps, their sequence and number of beds, and although it cannot be used to indicate which one is better, it can be employed in a very straightforward fashion to determine cycle schedules for virtually any PSA process that can be conceived. To determine the best cycle schedule from the multitude of possibilities that typically result, significant experience, sound intuition, and a good PSA process simulator are needed.

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

Time→

Bed ↓

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R
1	E1D	E2D	E3D															
2			E1D	E2D	E3D													
3				E1D	E2D	E3D												
4					E1D	E2D	E3D											
5						E1D	E2D	E3D										
6							E1D	E2D	E3D									
7								E1D	E2D	E3D								
8									E1D	E2D	E3D							
9	E3D																E1D	E2D

(a)

1	E1D	E2D	E3D								E1R						FR/F	
2		FR/F		E1D	E2D	E3D							E1R				FR/F	
3			FR/F		E1D	E2D	E3D							E1R			FR/F	
4				FR/F		E1D	E2D	E3D									E1R	
5	E1R				FR/F		E1D	E2D	E3D									
6				E1R			FR/F		E1D	E2D	E3D							
7					E1R			FR/F		E1D	E2D	E3D						
8						E1R			FR/F		E1D	E2D	E3D					
9	E3D							E1R			FR/F						E1D	E2D

(b)

1	E1D	E2D	E3D				CoD/CnD/LR		E3R	E2R	E1R					FR/F		
2		FR/F		E1D	E2D	E3D		CoD/CnD/LR		E3R	E2R	E1R				FR/F		
3			FR/F		E1D	E2D	E3D		CoD/CnD/LR		E3R	E2R	E1R			FR/F		
4				FR/F		E1D	E2D	E3D		CoD/CnD/LR		E3R	E2R	E1R		FR/F		
5	E1R				FR/F		E1D	E2D	E3D		CoD/CnD/LR		E3R	E2R				
6	E3R	E2R	E1R			FR/F		E1D	E2D	E3D		CoD/CnD/LR		E3R	E2R			
7	CoD/CnD/LR	E3R	E2R	E1R			FR/F		E1D	E2D	E3D		CoD/CnD/LR		E3R	E2R		
8		CoD/CnD/LR		E3R	E2R	E1R			FR/F		E1D	E2D	E3D		CoD/CnD/LR			
9	E3D			CoD/CnD/LR		E3R	E2R	E1R			FR/F						E1D	E2D

(c)

1	E1D	E2D	E3D		CoD	CnD	LR		E3R	E2R	E1R	FR				F		
2		F		E1D	E2D	E3D		CoD	CnD	LR	E3R	E2R	E1R	FR			F	
3			F		E1D	E2D	E3D		CoD	CnD	LR	E3R	E2R	E1R	FR			F
4				F		E1D	E2D	E3D		CoD	CnD	LR	E3R	E2R	E1R	FR		
5	E1R	FR							E1D	E2D	E3D		CoD	CnD	LR		E3R	E2R
6	E3R	E2R	E1R	FR						E1D	E2D	E3D		CoD	CnD	LR		
7		LR		E3R	E2R	E1R	FR						E1D	E2D	E3D		CoD	CnD
8	CoD	CnD	LR		E3R	E2R	E1R	FR						E1D	E2D	E3D	CoD	
9	E3D		CoD	CnD		LR	E3R	E2R	E1R	FR						E1D	E2D	

(d)

1	E1D	E2D	E3D	CoD	CnD	LR	E3R	E2R	I	I	E1R	FR/F								
2	FR/F		E1D	E2D	E3D	CoD	CnD	LR	E3R	E2R	I	I	E1R	FR/F						
3	FR/F			E1D	E2D	E3D	CoD	CnD	LR	E3R	E2R	I	I	E1R	FR/F					
4	FR/F					E1D	E2D	E3D	CoD	CnD	LR	E3R	E2R	I	I	E1R				
5	E1R	FR/F					E1D	E2D	E3D	CoD	CnD	LR	E3R	E2R	I	I	E1R			
6	I	I	E1R	FR/F							E1D	E2D	E3D	CoD	CnD	LR	E3R	E2R		
7	E3R	E2R	I	I	E1R	FR/F						E1D	E2D	E3D	CoD	CnD	LR			
8	CnD	LR	E3R	E2R	I	I	E1R	FR/F					E1D	E2D	E3D	CoD	CnD	LR		
9	E3D	CoD	CnD	LR	E3R	E2R	I	I	E1R	FR/F				FR/F			E1D	E2D	E3D	CoD

(e)

Fig. 13 Construction of a PSA cycle schedule for a nine-bed eleven-step process with three equalization steps: (a) grid showing primary set, primary diagonal and primary grid (lighter shaded cells), and three empty cells for filling with remaining cycle steps (darker shaded cells); (b) grid from (a) showing new cycle steps added and two new empty cells for filling with remaining cycle steps (darker shaded cells);

(c) grid from (b) showing all cycle steps added, forming a cycle schedule; (d) grid from (a) showing all cycle steps added, but forming an alternative cycle schedule than that in (c); and (e) grid from (b) showing all cycle steps added, but forming another alternative cycle schedule than those in (c) and (d)

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