Adsorption (2015) 21:229–241
DOI 10.1007/s10450-015-9665-9

Graphical unit block approach for complex PSA cycle scheduling of parallel interacting trains of columns and tanks

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

Received: 24 July 2014 / Revised: 25 February 2015 / Accepted: 27 February 2015 / Published online: 7 March 2015

Abstract A simple, graphical, unit block approach for complex pressure swing adsorption (PSA) cycle scheduling has been developed for parallel interacting trains of PSA columns, possibly assisted by trains of tanks. For parallel interacting trains of PSA columns, this new methodology involves a priori specifying for each train the cycle steps, their sequence, and the number of beds, and then following a systematic procedure that requires filling in a 2-D grid for each of these coupled trains. For parallel interacting trains of PSA columns assisted by trains of tanks, a similar methodology has been developed; however, the number of tanks to include and their steps is an output from the methodology rather than an input to it. The reason for this is that tanks are inherently required when the coupling between steps is otherwise impossible or leads to the generation of undesirable idle steps. The overall outcome is a unit block for each train that can easily be extended to form its complete cycle schedule, thereby forming the grand cycle schedule of the coupled train–train or train-tank system. Three heuristics were also discovered about the minimum number of beds required to satisfy the number and types of steps in the cycle step sequence. These new methodologies and heuristics should be very useful for quickly scrutinizing different PSA cycle schedules for complex PSA processes comprising any number of parallel interacting trains of PSA columns, including the possibility of being assisted by one or more trains of tanks.

Keywords Pressure swing adsorption · Cycle step scheduling · Cycle step sequencing · Multi-train PSA processes · PSA trains with tanks · Cycle schedule heuristics

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

1 Introduction

Three approaches have been offered to design cycle schedules for pressure swing adsorption (PSA) processes. These include the arithmetic approaches of Chiang (1988) and Ritter and coworkers (Mehrotra et al. 2010), the numerical optimization approach of Smith and Westerberg (1990), and the graphical approaches of Ritter and coworkers (Ebner et al. 2009; Mehrotra et al. 2011). However, no attention has been given to the scheduling of parallel interacting trains of PSA columns that may also be assisted by or interacting with trains of tanks.

Most PSA processes have been designed as a single train of columns to recover, remove, concentrate or purify a single component from a multicomponent, often binary, gas stream (Ruthven et al. 1994). However, several patents and a few articles describe the use of multiple trains of PSA columns interacting in parallel mostly for separating multicomponent gas mixtures (Sircar 1979a, b, 1988, 1989; Wang et al. 1988; Kumar et al. 1990, 1992; Kumar and Kratz 1992), but also for separating binary gas mixtures (Grande and Blom 2012), purifying a gas where a single train of columns may not be viable (D'Amico et al. 1966; Jee et al. 2005), and improving the process performance beyond that possible with a single train of columns (Fuderer 1983). These patents and articles all considered 2-train PSA systems except for one which considered a 3-train PSA system (Sircar 1988). It is clear from these works that parallel interacting trains of PSA columns allow for considerable flexibility in designing a gas separation process because each train, although coupled to each other, can operate with different numbers of columns, sizes of columns, cycle schedules and/or adsorbents.

There are also two very interesting patents that nebulously disclose the use of 2-tanks with a 4-bed (single train) PSA system (Reinhold et al. 1996) in one case and n-tanks with an n-bed (single train) PSA system (Reinhold 2010) in the other case. These are not feed or product tanks; these tanks are judiciously positioned in lines between certain columns. Both patents indicate they are used for gas storage and recycle within the process. These works do not offer nor were any other works found in the literature that offer any information on the useful role of tanks in PSA cycle scheduling. Nevertheless, it is easy to envision that it may be prudent to have one or more tanks interacting with single or even multiple trains of PSA columns. They can be used not only for gas storage and recycle, but also for equalization between PSA beds and to assist in aligning coupled cycle steps between columns within a train or between trains, potentially reducing the number of beds and/or decreasing the number of undesirable idle steps in the cycle schedule.

Therefore, the objective of this work is to extend the graphical unit block approach developed by Mehrotra et al. (2011) for deriving complex PSA cycle schedules for any number of parallel interacting trains of PSA columns that may also be assisted by or interacting with one or more trains of tanks. This graphical approach is developed first for any number of parallel interacting trains of PSA columns. It is then extended for handling the inclusion of one or more tanks between columns in a train or between trains of columns. Finally, two examples are provided along with three heuristics on the use of this new graphical unit block approach for deriving complex PSA cycle schedules of parallel interacting trains of PSA columns and tanks.

2 Theory

2.1 Terminology for multi-train PSA systems

The methodology behind the scheduling of a multi-train PSA system, possibly interacting with trains of tanks, is similar to that recently developed for single train PSA systems (Mehrotra et al. 2011). The only difference is that at a given moment in the cycle, the beds may interact not only with other beds belonging to the same train, but also with beds belonging to another train or with trains of tanks. Each train within a multi-train system is identified with the letters α, β, γ, δ, etc., and the corresponding cycle steps are each labeled with a subscript using these letters to identify their respective train. Likewise, each tank, as an individual train, is numbered T1, T2, etc., and the corresponding cycle steps are each labeled with a subscript using these identifiers to indicate their interaction with a specific tank. Figure 1 shows a multi-train PSA cycle schedule labeled in this way that is associated with the 2-train PSA process developed by Sircar (1979a). One of the trains contains 6 beds (α Train) while the other one contains 3 beds (β Train). Because each train of beds has its own unique cycle schedule, the overall cycle schedule is termed the grand cycle schedule. The sequence of cycle steps associated with each train in this 2-train 6-bed 3-bed PSA process is given below.

2.1.1 *α Train*

(a) High pressure feed (F_α) step. A bed receives high pressure feed and it produces light product that is sent to a bed undergoing the feed step (F_β) in the β train.
(b) Heavy reflux (HR_α) or rinse step. A bed receives heavy product from a bed undergoing the first counter-current depressurization ($CnD1_\alpha$) step and it produces light product that is mixed with fresh feed and sent to a bed undergoing the F_α step.
(c) First counter-current depressurization ($CnD1_\alpha$) step. A bed produces heavy product that is sent to a bed undergoing the HR_α step.
(d) Second counter-current depressurization ($CnD2_\alpha$) step. A bed produces heavy product that is taken as heavy product.
(e) Counter-current evacuation ($Evac_\alpha$) step. A bed produces heavy product that is taken as heavy product.
(f) First pressure equalization up ($E1{\uparrow}_\alpha$) step. A bed receives gas in its light product end that is produced from the heavy product end of a bed undergoing the first pressure equalization down ($E1{\downarrow}_\beta$) step in the β train.
(g) Idle step (I_α). A bed rests idle with both ends closed.
(h) Light product pressurization (LPP_α) step. A bed receives light product from the heavy product end of a bed undergoing the second light product pressurization step in the β train ($LPP2_\beta$).

2.1.2 *β Train*

(a) High pressure feed (F_β) step. A bed receives as feed light product from a bed undergoing the F_α step in the α train and it produces light product: some of it is sent to a bed undergoing the light reflux (LR_β) or purge step, some of it is sent to a bed undergoing the light product pressurization (LPP_β) step, and the rest is taken as light product.
(b) First pressure equalization down ($E1{\downarrow}_\beta$) step. A bed produces gas from its heavy product end that is sent

Cycle Step Sequences

α Train: $F_\alpha \rightarrow HR_\alpha \rightarrow CnD1_\alpha \rightarrow CnD2_\alpha \rightarrow Evac_\alpha \rightarrow E1{\uparrow}_\alpha \rightarrow LPP_\alpha$

β Train: $F_\beta \rightarrow E1{\downarrow}_\beta \rightarrow E2{\downarrow}_\beta \rightarrow CnD_\beta \rightarrow LR_\beta \rightarrow E2{\uparrow}_\beta \rightarrow LPP1_\beta \rightarrow LPP2_\beta$

	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_α	F_α				HR_α				$CnD1_\alpha$				$CnD2_\alpha$				Evac				$E1{\uparrow}_\alpha$	I_α		LPP_α
2_α	HR_α				$CnD1_\alpha$				$CnD2_\alpha$				$Evac_\alpha$				$E1{\uparrow}_\alpha$	I_α		LPP_α	F_α			
3_α	$CnD1_\alpha$				$CnD2_\alpha$				$Evac_\alpha$				$E1{\uparrow}_\alpha$	I_α		LPP_α	F_α				HR_α			
4_α	$CnD2_\alpha$				$Evac_\alpha$				$E1{\uparrow}_\alpha$	I_α		LPP_α	F_α				HR_α				$CnD1_\alpha$			
5_α	$Evac_\alpha$				$E1{\uparrow}_\alpha$	I_α		LPP_α	F_α				HR_α				$CnD1_\alpha$				$CnD2_\alpha$			
6_α	$E1{\uparrow}_\alpha$	I_α		LPP_α	F_α				HR_α				$CnD1_\alpha$				$CnD2_\alpha$				$Evac_\alpha$			
1_β	F_β				$E1{\downarrow}_\beta$	$E2{\downarrow}_\beta$	CnD_β		LR_β	$E2{\uparrow}_\beta$	$LPP1_\beta$	$LPP2_\beta$	F_β				$E1{\downarrow}_\beta$	$E2{\downarrow}_\beta$	CnD_β		LR_β	$E2{\uparrow}_\beta$	$LPP1_\beta$	$LPP2_\beta$
2_β	$E1{\downarrow}_\beta$	$E2{\downarrow}_\beta$	CnD_β		LR_β	$E2{\uparrow}_\beta$	$LPP1_\beta$	$LPP2_\beta$	F_β				$E1{\downarrow}_\beta$	$E2{\downarrow}_\beta$	CnD_β		LR_β	$E2{\uparrow}_\beta$	$LPP1_\beta$	$LPP2_\beta$	F_β			
3_β	LR_β	$E2{\uparrow}_\beta$	$LPP1_\beta$	$LPP2_\beta$	F_β				$E1{\downarrow}_\beta$	$E2{\downarrow}_\beta$	CnD_β		LR_β	$E2{\uparrow}_\beta$	$LPP1_\beta$	$LPP2_\beta$	F_β				$E1{\downarrow}_\beta$	$E2{\downarrow}_\beta$	CnD_β	

Fig. 1 Grand cycle schedule of a parallel interacting 2-train 6-bed 3-bed PSA system (Sircar 1979a): the α train is a 6-bed 7-step PSA process and the β train is 3-bed 7-step PSA process. The *cells within the thick black rectangle* depict the unit block

to the light product end of a bed undergoing the $E1{\uparrow}_\alpha$ step in the α train.

(c) Second pressure equalization down ($E2{\downarrow}_\beta$) step. A bed produces gas from its light product end that is sent to the light product end of a bed undergoing the second pressure equalization up ($E2{\uparrow}_\beta$) step.

(d) Counter-current depressurization (CnD_β) step. A bed produces heavy product that is taken as waste product.

(e) Light reflux (LR_β) or purge step. A bed receives gas produced from a bed undergoing the F_β step.

(f) Second pressure equalization up ($E2{\uparrow}_\beta$) step. A bed receives gas in its light product end that is produced from the light product end of a bed undergoing the second pressure equalization down $E2{\downarrow}_\beta$ step.

(g) Light product pressurization (LPP_β) step. A bed receives gas produced from a bed undergoing the F_β step.

(h) Second light product pressurization ($LPP2_\beta$) step. A bed receives light product from the heavy product end of a bed undergoing the F_β step and it produces gas from its light product end that is sent to the light product end of a bed undergoing the LPP_α step.

In the 2-D grid shown in Fig. 1, time is placed horizontally, whereas the beds in each train are placed vertically. The 24 columns in the grid, i.e., A through X along the horizontal direction, represent unit time steps or time steps of identical length. This unit time step is the smallest unit of time used in a grand cycle schedule and is the same in each train. The grand cycle time of the grand cycle schedule is the sum of all the unit time steps in a row. All the different cycle steps a bed undergoes in sequence during the grand cycle time are given along a row of the grid. One grand cycle corresponds to each bed undergoing all of its cycle steps in sequence beginning with that in column A, proceeding to that in column X, and then returning back to column A and continuing along the row as before so that the process is repeated indefinitely.

The six rows in the top cycle schedule and the three rows in the bottom cycle schedule represent the number of beds in the α and β trains, respectively. An intersection between a column and a row in the grid, defined as the unit cell, represents the cycle step being run by a particular bed in a particular train during a particular unit time step. For example, unit cell B-6_α contains the cycle step being run by bed 6 in the α train during unit time step B (i.e., the I_α step). 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 time taken by an individual cycle step must always be a multiple of the unit time step. For instance, in Fig. 1 the LR_β step occupies one unit time step, whereas the F_α step occupies four unit time steps. There are 24 unit cells in this grid that are occupied by eight different cycle steps.

Notice that the same cycle steps are run by successive beds in each train 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–D represents one unit block for the grand cycle schedule shown. Within the unit block, every cycle step in the cycle schedule of the α train is being run by one of its beds and the same is true for the β train, i.e., every cycle step in the cycle schedule of the β train is being run by one of its beds. This is an important and key feature in multi-train PSA cycle scheduling. The unit block occurs again during unit time steps E–H, and then four more consecutive times with the last one occurring during unit time steps U–X. Thus, there are six unit blocks in this grand cycle schedule. It is not a coincidence that the number of unit blocks is exactly equal to the number of beds in the α train and two times the number of beds in the β train. In the same way, the grand cycle time for the grand cycle schedule is equal to that of the α train and twice that of the β train. In other words, the number of unit blocks and length of the grand cycle time are both multiples of the number of beds and cycle time of each individual train. Generalizing this statement for any number of trains, the total number of unit blocks in a grand cycle schedule, N_{GCS}, is given by:

$$N_{GCS} = \text{ Least common multiple of } \left\{N_{\alpha}, N_{\beta}\ldots N_{\zeta}\right\} \quad (1)$$

where N_{α}, $N_{\beta} \ldots N_{\zeta}$ respectively correspond to the number of beds in the α, β, … ζ trains. The grand cycle time relative to the cycle time of the ith train is always an integer and given by

$$N_{C,i} = N_{GCS}/N_i \quad \text{with } i = \alpha, \beta, \ldots \zeta \quad (2)$$

where $N_{C,i}$ corresponds exactly to the number of cycles the ith train undergoes during the grand cycle time. In Fig. 1, the α train carries out one complete cycle while the β train carries out two complete cycles during the grand cycle time.

Notice there also are steps in alternative beds that must coincide in time, such as HR_{α} with $CnD1_{\alpha}$, or $E1{\downarrow}_{\beta}$ with $E1{\uparrow}_{\alpha}$. This temporal coincidence is defined as coupling and is an imposed restriction. Clearly, coupled beds may belong to the same train or be coupled between different trains, as shown in Fig. 1.

2.2 Terminology for PSA systems interacting with tanks

Figure 2 shows a 1-train 4-bed PSA system interacting with 1-tank. The sequences of cycle steps associated with the train and the tank in this 1-train 4-bed 1-tank PSA process are given below.

2.2.1 α Train

(a) High pressure feed (F_{α}) step. A bed receives high pressure feed and it produces light product: some of it is sent to a bed undergoing the light reflux (LR_{α}) or purge step, some of it is sent to a bed undergoing the light product pressurization (LPP_{α}) step, and the rest of it is taken as light product.

(b) First pressure equalization down ($E1{\downarrow}_{\alpha}$) step. A bed produces gas from its light product end that is sent to a tank undergoing the first pressure equalization up ($E1{\uparrow}_{T1}$) step.

(c) Second pressure equalization down ($E2{\downarrow}_{\alpha}$) step. A bed produces gas from its light product end that is sent to the light product end of a bed undergoing the second pressure equalization up ($E2{\uparrow}_{\alpha}$) step.

(d) Counter-current depressurization (CnD_{α}) step. A bed produces heavy product that is taken as waste product.

(e) Light reflux (LR_{α}) purge step. A bed receives gas produced from a bed undergoing the F_{α} step.

(f) Second pressure equalization up ($E2{\uparrow}_{\alpha}$) step. A bed receives gas in its light product end that is produced from a bed undergoing the $E2{\downarrow}_{\alpha}$ step.

(g) First pressure equalization up ($E1{\uparrow}_{\alpha}$) step. A bed receives gas in its light product end that is produced from a tank undergoing the first pressure equalization down ($E1{\downarrow}_{T1}$) step.

(h) Light product pressurization (LPP_{α}) step. A bed receives gas produced from a bed undergoing the F_{α} step.

2.2.2 Tank 1

(a) First pressure equalization up ($E1{\uparrow}_{T1}$) step. A tank receives gas produced from a bed undergoing the $E1{\downarrow}_{\alpha}$ step.

(b) Idle (I_{T1}) step. The tank rests idle with its end closed.

(c) First pressure equalization down ($E1{\downarrow}_{T1}$) step. A tank produces gas that is sent to a bed undergoing the $E1{\uparrow}_{\alpha}$ step.

The grand cycle time is identified by the 12 unit steps of the grid, i.e., A–L along the horizontal direction. The corresponding unit block is identified by the thick solid line enclosing unit time steps A–C. Notice there are four unit blocks associated with this grand cycle schedule and while the α train undergoes one cycle during the grand cycle time, the tank undergoes four cycles.

At this point it should be obvious that there are many similarities between the train-tank schedule in Fig. 2 and the multi-train schedule in Fig. 1. In fact, from a mathematical perspective, a tank is no different than a train consisting of just one bed. Thus, applying Eqs. 1 and 2 to the train-tank grand cycle in Fig. 2 leads to $N_{GCS} = 4$, $N_{C\alpha} = N_{GS}/N_{\alpha} = 1$ and $N_{CT1} = N_{GS}/N_{\alpha} = 4$, as expected.

If additional tanks are needed, each one is treated simply as another train containing just one bed. Two possibilities

Cycle Step Sequences

α Train: $F_\alpha \rightarrow E1\downarrow_\alpha \rightarrow E2\downarrow_\alpha \rightarrow CnD_\alpha \rightarrow LR_\alpha \rightarrow E2\uparrow_\alpha \rightarrow E3\uparrow_\alpha \rightarrow LPP_\alpha$

Tank 1: $E1\uparrow_{T1} \rightarrow E3\downarrow_{T1}$

	A	B	C	D	E	F	G	H	I	J	K	L
1_α	F_α			$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	CnD_α	LR_α	$E2\uparrow_\alpha$	$E3\uparrow_\alpha$	LPP_α		
2_α	$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	CnD_α	LR_α	$E2\uparrow_\alpha$	$E3\uparrow_\alpha$	LPP_α			F_α		
3_α	LR_α	$E2\uparrow_\alpha$	$E3\uparrow_\alpha$	LPP_α			F_α			$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	CnD_α
4_α	LPP_α			F_α			$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	CnD_α	LR_α	$E2\uparrow_\alpha$	$E3\uparrow_\alpha$
T1	$E1\uparrow_{T1}$	I_{T1}	$E3\downarrow_{T1}$	$E1\uparrow_{T1}$	I_{T1}	$E3\downarrow_{T1}$	$E1\uparrow_{T1}$	I_{T1}	$E3\downarrow_{T1}$	$E1\uparrow_{T1}$	I_{T1}	$E3\downarrow_{T1}$

Fig. 2 Grand cycle schedule of a parallel interacting 1-train 4-bed 1-tank PSA system: the α train is a 4-bed 8-step PSA process interacting with one tank. The *cells within the thick black rectangle* depict the unit block

arise when including one or more tanks in a grand cycle schedule. First, a tank (or tanks) may be interacting with the beds belonging to any single train in a multi-train PSA process (intra-train-tank interaction). Second, a tank (or tanks) may be interacting with the beds belonging to multiple trains of a multi-train PSA process (inter-train-tank interaction). Of course, a multi-train PSA process may include both intra-train-tank and inter-train-tank interactions, with each tank simply treated as an additional train in the grand cycle schedule.

2.3 Methodology

The graphical unit block approach developed by Merohtra et al. (2011) is extended here for deriving PSA cycle schedules of parallel interacting trains of PSA columns and tanks. Once again, the methodology is divided into four sequential parts. In Part 1, the sequence of steps needed for each train is decided, the number of beds in each train is chosen, the coupled cycle steps within a train and between trains are identified, and the cycle steps with durations longer than one unit step and the cycle steps that are continuous are also identified. In the last case the duration of the continuous cycle step is at least (but preferably a multiple of) the length of the unit block, which ensures that a bed is always available for that step to continue without interruption (such as a feed step). These are the only a priori decisions; the use of tanks and their number is not decided yet. At this point caution must be exercised when choosing the number of trains and their corresponding number of beds to avoid a very long grand cycle schedule, which could be difficult to implement. For example, a 3-train 4-bed 5-bed 6-bed PSA system does not seem unreasonable; however, according to Eq. 1, such a system would have 30 unit blocks in the grand cycle schedule, possibly an unwieldy number.

At the outset it is important to consider the following heuristics before deciding on the number of beds for a given cycle step sequence:

1. The minimum number of beds required by a schedule is never less than the sum of the number of continuous steps and the number of equalization steps within the same train plus one. For example, a schedule that requires a continuous feed step needs at least two beds; a schedule that requires a continuous feed step and a continuous light reflux step needs at least three beds; a schedule that requires a continuous feed step and three equalization steps within the same train needs at least five beds.
2. The minimum number of beds required by a schedule that contains a number of coupled steps other than equalization steps is simply the sum of the continuous steps plus two. For example, a schedule that requires a continuous feed step and a coupled step between a heavy reflux step and countercurrent depressurization step and another coupled step between a cocurrent depressurization step and a light reflux step needs at least three beds.
3. The minimum number of beds required by a schedule, based on heuristics 1 and 2, decreases by one each time a tank is added. Or, expressed in a different way: if the number of beds is already decided, then the schedule is feasible only if the number of tanks is never less than the difference between the minimum number of beds predicted by heuristic 1 and the actual number of beds

planned. For example, a schedule that requires a continuous feed step and three equalization steps needs at least three beds with the aid of two tanks, or alternatively, if three beds were already decided, then the schedule needs at least two tanks.

In Part 2, the goal is to build a primary skeleton of the unit block. For any particular PSA train, the primary skeleton of a unit block is formed when the array of a given number of rows (i.e., beds and tanks) and a given number of columns (i.e., width of a unit block) is determined. It is at this point where the number of unit steps per unit block is decided. Recall that the unit block must contain an identical number of unit steps for each train and tank in the system. If tanks are being considered, it is prudent to add several new rows below the arrays for the trains (one for each tank), even though they may not all be needed in the final grand cycle schedule, as shown later. It is also important to consider that a judicious selection of the number of unit steps per unit block is required. A small number of unit steps per unit block may not provide enough unit steps for all the cycle steps involved in the cycle step sequence and a large number of unit steps per unit block may lead to undesirable idle steps in the cycle step sequence.

In Part 3, the unit block for each train is constructed by filling in the empty unit cells, with the caveat that a cycle step time may not be shorter than the unit step time. During Part 3 the number of idle steps (if any), their duration, and their relative location within the grid are determined. If the entire sequence of cycle steps chosen for a train of beds cannot be inserted within the unit block, then the attempted design is not feasible. At this point, it must be decided whether to increase the number of beds in the train (Part 1) or increase the number of unit steps in the unit block (Part 2) and then repeat Part 3 until a feasible solution is obtained.

As an aside, it is worth providing a few comments about the use of idle steps. Idle steps are typically inserted to facilitate aligning coupled cycle steps between two different beds. They are generally undesirable because the bed is not processing any gas during the idle period. In general, the number of potential idle steps that may be needed in a schedule increases with an increase in the number of unit steps in a unit block. The effect of increasing the width of the unit block is shown in one of the train-tank examples provided later.

In Part 4, the grand cycle schedule is obtained by creating the remaining unit blocks for each bed and tank train in the system. The number of unit blocks is determined from Eq. 1. It must be emphasized that each unit block is unique and has a specific location within the grand schedule. Any disturbance in the order of the unit blocks causes an actual multi-train PSA system to malfunction because the beds and tanks are misaligned in the grand cycle schedule. To ensure proper alignment of the unit blocks, make sure the first row in the cycle schedule of each train follows the exact same sequence of cycle steps as in the first unit block when beginning in the upper left hand corner of the unit block and proceeding to the lower right hand corner of the unit block. This simple procedure is illustrated in the examples provided below.

3 Results and discussion

Two examples are provided to show how to use the methodology and associated terminology discussed above. The first example is concerned with a 1-train PSA process that takes advantage of tanks. This case explains the subtleties associated with integrating tanks into a PSA cycle schedule that is not possible without them and discusses other possible benefits of doing so. The second example is concerned with a 2-train PSA process. This case explains the intricacies associated with integrating two PSA cycle schedules together.

3.1 1-Train PSA system with tanks

In this example, the four part methodology is applied to the 1-train 4-bed PSA system shown in Fig. 3. As required in Part 1, the 10-step cycle step sequence shown in Fig. 3 and described below is chosen for the α train.

3.1.1 α Train

(a) High pressure feed (F_α) step. A bed receives high pressure feed and it produces light product: some of it is sent to a bed undergoing the light reflux (LR_α) or purge step, some of it is sent to a bed undergoing the light product pressurization (LPP_α) step, and the rest is taken as light product.

(b) First pressure equalization down ($E1{\downarrow}_\alpha$) step. A bed produces gas from its light product end that is sent to the light product end of a bed undergoing the first pressure equalization up ($E1{\uparrow}_\alpha$) step.

(c) Second pressure equalization down ($E2{\downarrow}_\alpha$) step. A bed produces gas from its light product end that is sent to the light product end of a bed undergoing the second pressure equalization up ($E2{\uparrow}_\alpha$) step.

(d) Third pressure equalization down ($E3{\downarrow}_\alpha$) step. A bed produces gas from its light product end that is sent to the light product end of a bed undergoing the third pressure equalization up ($E3{\uparrow}_\alpha$) step.

(e) Counter-current depressurization (CnD_α) step. A bed produces heavy product that is taken as waste product.

Initial Cycle Step Sequence

α Train: $F_\alpha \rightarrow E1{\downarrow}_\alpha \rightarrow E2{\downarrow}_\alpha \rightarrow E3{\downarrow}_\alpha \rightarrow CnD_\alpha \rightarrow LR_\alpha \rightarrow E3{\uparrow}_\alpha \rightarrow E2{\uparrow}_\alpha \rightarrow E1{\uparrow}_\alpha \rightarrow LPP_\alpha$

(a) Time → ; Bed ↓

	A	B	C	D	E
1_α					…..
2_α					…..
3_α					…..
4_α					…..
T1					…..
T2					…..
T3					…..

(b)

	A	B	C
1_α	F_α	F_α	F_α
2_α	$E1{\downarrow}_\alpha$	$E2{\downarrow}_\alpha$	$E3{\downarrow}_\alpha$
3_α			$E3{\uparrow}_\alpha$
4_α			
T1			
T2			
T3			

(c)

	A	B	C
1_α	F_α	F_α	F_α
2_α	$E1{\downarrow}_\alpha$	$E2{\downarrow}_\alpha$	$E3{\downarrow}_\alpha$
3_α	CnD_α	LR_α	$E3{\uparrow}_\alpha$
4_α			LPP_α
T1			
T2			
T3			

(d)

	A	B	C
1_α	F_α	F_α	F_α
2_α	$E1{\downarrow}_\alpha$	$E2{\downarrow}_\alpha$	$E3{\downarrow}_\alpha$
3_α	CnD_α	LR_α	$E3{\uparrow}_\alpha$
4_α	$E2{\uparrow}_\alpha$	$E1{\uparrow}_\alpha$	LPP_α
T1			
T2			
T3			

(e)

	A	B	C
1_α	F_α	F_α	F_α
2_α	$E1{\downarrow}_\alpha$	$E2{\downarrow}_\alpha$	$E3{\downarrow}_\alpha$
3_α	CnD_α	LR_α	$E3{\uparrow}_\alpha$
4_α	$E2{\uparrow}_\alpha$	$E1{\uparrow}_\alpha$	LPP_α
T1	$E2{\downarrow}_{T1}$	$E2{\uparrow}_{T1}$	
T2			

(f)

	A	B	C
1_α	F_α	F_α	F_α
2_α	$E1{\downarrow}_\alpha$	$E2{\downarrow}_\alpha$	$E3{\downarrow}_\alpha$
3_α	CnD_α	LR_α	$E3{\uparrow}_\alpha$
4_α	$E2{\uparrow}_\alpha$	$E1{\uparrow}_\alpha$	LPP_α
T1	$E2{\downarrow}_{T1}$	$E2{\uparrow}_{T1}$	I_{T1}
T2	$E1{\uparrow}_{T1}$	$E1{\downarrow}_{T1}$	I_{T2}

Fig. 3 Construction of the unit block for a 4-bed 10-step PSA process assisted with tanks

(f) Light reflux (LR_α) purge. A bed receives gas produced from a bed undergoing the F_α step.
(g) Third pressure equalization up ($E3{\uparrow}_\alpha$) step. A bed receives gas in its light product end that is produced from the light product end of a bed undergoing $E3{\downarrow}_\alpha$.
(h) Second pressure equalization up ($E2{\uparrow}_\alpha$) step. A bed receives gas in its light product end that is produced from the light product end of a bed undergoing $E2{\downarrow}_\alpha$.
(i) First pressure equalization up ($E1{\uparrow}_\alpha$) step. A bed receives gas in its light product end that is produced from the light product end of a bed undergoing $E1{\downarrow}_\alpha$.
(j) Light product pressurization (LPP_α) step. A bed receives light product from a bed undergoing F_α.

Constraints on this PSA process include a continuous feed step and three equalization steps that occupy no more than one unit time step each. According to heuristic 1, this 4-bed PSA system requires a minimum of 5 beds for its cycle step sequence to be feasible; or, according to heuristic 3, at least 1 tank is required. Also note that since the number of tanks is not known at this point, the initial cycle step sequence does not include any interactions with a tank. There are no other constraints or restrictions imposed on any of the other cycle steps.

Because the number of tanks and their respective cycle step sequences are not known, three rows are arbitrarily included in the 2-D grid for the potential inclusion of up to three tanks as an initial guess, while noting that the final number may be less than three. As is always the case, initially all the unit cells are empty and the total number of unit steps in the unit blocks of both the α and tank trains is not yet determined (Fig. 3a). In other words, both sets of unit blocks are free to expand or contract horizontally. Part 1 of the methodology is complete.

Part 2 involves determining the width of the unit block in the PSA process; a minimum width should be chosen (Mehrotra et al. 2011). By definition, in a unit block every cycle step in the sequence defined for a train must be assigned to a bed. In this example, the unit block cannot be 1 or 2 unit cells wide, as this would respectively leave only 4 or 8 unit cells for the placement of 10 cycle steps. Hence, a unit block 3 unit cells wide is selected, as shown in Fig. 3b, with columns A, B and C identifying each one. Part 2 of the methodology, i.e., formation of the primary skeleton of the unit block, is complete.

Part 3 of the methodology involves building the unit block by filling in the empty unit cells. This part is accomplished (Mehrothra et al. 2011) by taking the cycle step sequence in its exact order from left to right and sequentially filling in empty unit cells with each cycle step. Begin with the unit cell in the top left hand corner and end with the unit cell in the bottom right hand corner, while noting a cycle step may occupy more than one unit block. For example, the unit cells in Fig. 3a are to be filled in with cycle steps according to the specified cycle step sequence while moving from A-1_α to C-1_α, then continuing from A-2_α to C-2_α, then from A-3_α to C-3_α, and finally from A-4_α to C-4_α. The order of the cycle steps and their final duration is the same exact order and duration that is followed by every bed in a grand cycle schedule, which immediately specifies how the other unit blocks are filled in to define the grand cycle schedule, as shown in Part 4. This is the essence of the graphical unit block approach; but, keep in mind that in every conceivable cycle schedule multiple solutions exist (Mehrotra et al. 2010).

For a continuous feed process, F_α must occupy the first row of the unit block from A-1_α to C-1_α, as shown in Fig. 3b. As stated earlier, this ensures that a bed is always available to take feed without interruption; this becomes clear when the grand cycle schedule is completed in Part 4. Notice there are nine empty unit cells for use with the remaining nine steps of the cycle step sequence. Hence, at this point in the analysis, a cycle schedule for this 4-bed PSA process appears to be still feasible. The filling process continues in row 2_α with E1$\downarrow_\alpha$, E2$\downarrow_\alpha$ and E3$\downarrow_\alpha$ each occupying unit cells A-2_α, B-2_α and C-2_α. The next 2 unit cells in the sequence are shaded in gray, i.e., A-3_α and B-3_α, to indicate 2 unit cells are available for the next two cycle steps in the sequence, i.e., CnD_α and LR_α. This is the case because the next unit cell, i.e., C-3_α must be occupied by the next cycle step in the sequence, i.e., E3$\uparrow_\alpha$ because it is coupled with E3$\downarrow_\alpha$ in unit cell C-2_α, as shown in Fig. 3b. Following the order of the cycle step sequence, CnD_α and LR_α are consequently placed in A-3_α and B-3_α, respectively, as shown in Fig. 3c. As stated above, E3$\uparrow_\alpha$ is placed in unit cell C-3_α; although C-4_α is also a potentially viable unit cell for E3$\uparrow_\alpha$, it is not chosen to minimize both the number of beds and the number of idle steps (Mehrotra et al. 2011). Moreover, since C-4_α is the last unit cell available in the unit block, LPP_α must be placed there, as shown in Fig. 3c. Unit cells A-4_α and B-4_α are shaded in gray in Fig. 3c to emphasize that these are the only unit cells remaining in this 4-bed cycle schedule where E1$\uparrow_\alpha$ and E2$\uparrow_\alpha$ can be placed for proper coupling respectively with E1$\downarrow_\alpha$ and E2$\downarrow_\alpha$ in unit cells A-2_α and B-2_α. However, it is evident that this simple placement is not feasible because the cycle step sequence dictates that E2$\uparrow_\alpha$ must take place before E1$\uparrow_\alpha$. In fact, it is easy to show that it is not possible to properly couple all three equalization steps unless 5 beds are used. Heuristic 1 is thus validated and the need for at least 1 tank arises to make the solution viable.

Before adding any tanks, it is obvious that placing cycle steps E2$\uparrow_\alpha$ and E1$\uparrow_\alpha$ respectively in unit cells A-4_α and B-4_α is the only option available that preserves the ordering of the cycle steps in this cycle step sequence. This is shown in Fig. 3d. However, this placement misaligns E2$\uparrow_\alpha$ with E2$\downarrow_\alpha$ and E1$\uparrow_\alpha$ with E1$\downarrow_\alpha$. To resolve this dilemma, two tanks are added, one for each of the equalization steps. The dark cells in Fig. 3d show how tank 1 is used to assist in the coupling of cycle steps E2$\uparrow_\alpha$ and E2$\downarrow_\alpha$ with the use of two extra equalization steps. A first equalization step E2$\uparrow_{T1}$ in cell B-T1 is used to receive gas from E2$\downarrow_\alpha$ and then a second equalization step E2$\downarrow_{T1}$ in cell A-T1 is subsequently used to provide gas to E2$\uparrow_\alpha$. This train-tank coupling is shown in Fig. 3e. Similarly, the second tank is utilized to first couple cycle steps E1$\downarrow_\alpha$ with E1$\uparrow_{T2}$ and then to couple cycle steps E1$\downarrow_{T2}$ with E1$\uparrow_\alpha$, as shown in Fig. 3f.

Part 3 is now concluded by filling in the remaining empty unit cells in both the bed and tank trains. In this case only two inconsequential idle steps (I_{T1} and I_{T1}) are placed in C-T1 and C-T2. The unused tank row is also discarded. The complete unit block is shown in Fig. 3f.

The resulting cycle schedule is a 1-train 4-bed 2-tank PSA process with a continuous feed step and three equalization steps. To achieve so many equalization steps with only 4 beds two tanks are required, with each one handling a different equalization step. The inclusion of these tanks does not change the original cycle step sequence of the 4-bed PSA process; it still contains the same 10-step cycle step sequence. However, two additional 4-step cycle step sequences are added below the original cycle step sequence to account for the addition of the two tanks. Compare the initial cycle step sequence at the top of Fig. 3 with the final cycle step sequence at the top of Fig. 4. The 4-step cycle step sequence description for each tank is as follows:

3.1.2 Tank 1

(a) Second equalization down (E2$\downarrow_{T1}$) step. A tank produces gas that is sent to a bed undergoing the E2$\uparrow_\alpha$ step.

(b) Second pressure equalization up ($E2\uparrow_{T1}$) step. A tank receives gas produced from a bed undergoing the $E2\downarrow_{\alpha}$ step.
(c) Idle (I_{T1}) step. The tank rests idle with its end closed.

3.1.3 Tank 2

(a) First pressure equalization up ($E1\uparrow_{T2}$) step. A tank receives gas produced from a bed undergoing the $E1\downarrow_{\alpha}$ step.
(b) First equalization down ($E1\downarrow_{T2}$) step. A tank produces gas that is sent to a bed undergoing the $E1\uparrow_{\alpha}$ step.
(c) Idle (I_{T2}) step. The tank rests idle with its end closed.

The methodology is concluded with Part 4, which consists of deriving the grand cycle schedule of this 1-train 4-bed 2-tank PSA system by extending the unit block in Fig. 3f three times to make a total of 4 unit blocks, as determined by Eq. 1. Recall that to ensure proper alignment of the unit blocks, the first row in the cycle schedule of each train must follow the exact same sequence of cycle steps as in the first unit block (Fig. 3f) when beginning in the upper left hand corner of the unit block and proceeding to the lower right hand corner of the unit block. As shown in Fig. 4, for the bed-train, unit cells A-2_{α} to C-2_{α} must be copied in unit cells D-1_{α} to F-1_{α}, unit cells A-3_{α} to C-3_{α} must be copied in unit cells G-1_{α} to I-1_{α}, and unit cells A-4_{α} to C-4_{α} must be copied in unit cells J-1_{α} to L-1_{α}. For the first train-tank, unit cells A-T1 to C-T1 must be copied in D-T1 to F-T1, then G-T1 to I-T1, and finally J-T1 to L-T1. For the second train-tank, unit cells A-T2 to C-T2 must be copied in D-T2 to F-T2, then G-T2 to I-T2, and finally J-T2 to L-T2. It is then straightforward to fill in the rest of the 2-D grid because each unit block has to follow the same exact cycle step sequence. This exercise constructs the grand cycle schedule of this 1-train 4-bed 2-tank PSA process.

This perfectly viable grand cycle schedule of this 1-train 4-bed 2-tank PSA process is based on a unit block containing three unit steps. Recall that a unit block containing just two unit steps is not feasible. However, a unit block containing more than three unit steps is feasible. It is instructive to see how increasing the number of unit steps in the unit block from 3 to 4 and then from 4 to 5 changes the grand cycle schedule for the same 10-step cycle step sequence shown in Fig. 3 for the α-train. The grand cycle schedules created from the four step methodology by using four and five unit steps in the unit block are respectively shown in Figs. 5 and 6.

For both situations, the grand cycle schedule is a 1-train 4-bed 1-tank PSA process with a continuous feed step and three equalization steps. The significant effect of increasing the number of unit steps in the unit block in both cases is a decrease in the number of required tanks from 2 to 1. However, as indicated earlier, the addition of unit steps to the unit block may come at a cost. Figure 5 shows that increasing the number of unit steps in the unit block from 3 to 4 improves the grand cycle schedule by eliminating the need for one of the tanks. In fact, this is the better of the two grand cycle schedules because the additional unit step in the unit block does not cause any negative

Fig. 4 Grand cycle schedule of a parallel interacting 1-train 4-bed 2-tank PSA system that corresponds to a unit block 3 unit steps wide. The 10-step cycle step sequence and construction of its unit block are shown in Fig. 3 for the α-train

<u>Final Cycle Step Sequences</u>

α Train: $F_{\alpha}\rightarrow E1\downarrow_{\alpha}\rightarrow E2\downarrow_{\alpha}\rightarrow E3\downarrow_{\alpha}\rightarrow CnD_{\alpha}\rightarrow LR_{\alpha}\rightarrow E3\uparrow_{\alpha}\rightarrow E2\uparrow_{\alpha}\rightarrow E1\uparrow_{\alpha}\rightarrow LPP_{\alpha}$

Tank 1: $E2\downarrow_{T1}\rightarrow E2\uparrow_{T1}\rightarrow I_{T1}$

Tank 2: $E1\uparrow_{T2}\rightarrow E1\downarrow_{T2}\rightarrow I_{T2}$

<table>
<tr><th></th><th>A</th><th>B</th><th>C</th><th>D</th><th>E</th><th>F</th><th>G</th><th>H</th><th>I</th><th>J</th><th>K</th><th>L</th></tr>
<tr><td>1_{α}</td><td colspan="3">F_{α}</td><td>$E1\downarrow_{\alpha}$</td><td>$E2\downarrow_{\alpha}$</td><td>$E3\downarrow_{\alpha}$</td><td>CnD_{α}</td><td>LR_{α}</td><td>$E3\uparrow_{\alpha}$</td><td>$E2\uparrow_{\alpha}$</td><td>$E1\uparrow_{\alpha}$</td><td>LPP_{α}</td></tr>
<tr><td>2_{α}</td><td>$E1\downarrow_{\alpha}$</td><td>$E2\downarrow_{\alpha}$</td><td>$E3\downarrow_{\alpha}$</td><td>CnD_{α}</td><td>LR_{α}</td><td>$E3\uparrow_{\alpha}$</td><td>$E2\uparrow_{\alpha}$</td><td>$E1\uparrow_{\alpha}$</td><td>LPP_{α}</td><td colspan="3">F_{α}</td></tr>
<tr><td>3_{α}</td><td>CnD_{α}</td><td>LR_{α}</td><td>$E3\uparrow_{\alpha}$</td><td>$E2\uparrow_{\alpha}$</td><td>$E1\uparrow_{\alpha}$</td><td>LPP_{α}</td><td colspan="3">F_{α}</td><td>$E1\downarrow_{\alpha}$</td><td>$E2\downarrow_{\alpha}$</td><td>$E3\downarrow_{\alpha}$</td></tr>
<tr><td>4_{α}</td><td>$E2\uparrow_{\alpha}$</td><td>$E1\uparrow_{\alpha}$</td><td>LPP_{α}</td><td colspan="3">F_{α}</td><td>$E1\downarrow_{\alpha}$</td><td>$E2\downarrow_{\alpha}$</td><td>$E3\downarrow_{\alpha}$</td><td>CnD_{α}</td><td>LR_{α}</td><td>$E3\uparrow_{\alpha}$</td></tr>
</table>

T1	**$E2\downarrow_{T1}$**	**$E2\uparrow_{T1}$**	**I_{T1}**	**$E2\downarrow_{T1}$**	**$E2\uparrow_{T1}$**	**I_{T1}**	**$E2\downarrow_{T1}$**	**$E2\uparrow_{T1}$**	**I_{T1}**	**$E2\downarrow_{T1}$**	**$E2\uparrow_{T1}$**	**I_{T1}**
T2	**$E1\uparrow_{T2}$**	**$E1\downarrow_{T2}$**	**I_{T2}**	**$E1\uparrow_{T2}$**	**$E1\downarrow_{T2}$**	**I_{T2}**	**$E1\uparrow_{T2}$**	**$E1\downarrow_{T2}$**	**I_{T2}**	**$E1\uparrow_{T2}$**	**$E1\downarrow_{T2}$**	**I_{T2}**

Final Cycle Sequences

α Train: $F_\alpha \rightarrow E1\downarrow_\alpha \rightarrow E2\downarrow_\alpha \rightarrow E3\downarrow_\alpha \rightarrow CnD_\alpha \rightarrow LR_\alpha \rightarrow E3\uparrow_\alpha \rightarrow E2\uparrow_\alpha \rightarrow E1\uparrow_\alpha \rightarrow LPP_\alpha$

Tank 1: $I_{T1} \rightarrow E2\uparrow_{T1} \rightarrow I_{T1} \rightarrow E2\downarrow_{T1}$

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1_α	F_α				$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	$E1\uparrow_\alpha$	LPP_α		
2_α	$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	$E1\uparrow_\alpha$	LPP_α			F_α			
3_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	$E1\uparrow_\alpha$	LPP_α			F_α				$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α
4_α	$E1\uparrow_\alpha$	LPP_α			F_α				$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$
T1	I_{T1}	$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}	$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}	$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}	$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$

Fig. 5 Grand cycle schedule of a parallel interacting 1-train 4-bed 1-tank PSA system that corresponds to a unit block 4 unit steps wide. The 10-step cycle step sequence is the same as that shown in Fig. 3 for the α-train

Final Cycle Sequences

α Train: $F_\alpha \rightarrow E1\downarrow_\alpha \rightarrow E2\downarrow_\alpha \rightarrow E3\downarrow_\alpha \rightarrow CnD_\alpha \rightarrow LR_\alpha \rightarrow E3\uparrow_\alpha \rightarrow E2\uparrow_\alpha \rightarrow E1\uparrow_\alpha \rightarrow LPP_\alpha$

Tank 1: $I_{T1} \rightarrow E2\uparrow_{T1} \rightarrow I_{T1} \rightarrow E2\downarrow_{T1}$

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T
1_α	F_α					$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	CnD_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	I_α	$E1\uparrow_\alpha$	LPP_α			
2_α	$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	CnD_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	I_α	$E1\uparrow_\alpha$	LPP_α				F_α				
3_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	I_α	$E1\uparrow_\alpha$	LPP_α				F_α					$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	CnD_α
4_α	$E1\uparrow_\alpha$	LPP_α				F_α					$E1\downarrow_\alpha$	$E2\downarrow_\alpha$	$E3\downarrow_\alpha$	CnD_α	CnD_α	LR_α	LR_α	$E3\uparrow_\alpha$	$E2\uparrow_\alpha$	I_α
T1	I_{T1}	$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}		$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}		$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}		$E2\uparrow_{T1}$	I_{T1}	$E2\downarrow_{T1}$	I_{T1}

Fig. 6 Grand cycle schedule of a parallel interacting 1-train 4-bed 1-tank PSA system that corresponds to a unit block 5 unit steps wide. The 10-step cycle step sequence is the same as that shown in Fig. 3 for the α-train

consequences. In contrast, Fig. 6 shows that increasing the number of unit steps in the unit block from 4 to 5 does indeed cause negative consequences. Although it improves the grand cycle schedule by also eliminating the need for one of the tanks, an undesirable and unavoidable idle step appears in the cycle schedule of the α-train. Of these three grand cycle schedules, the best one for this 10-step cycle step sequence is clearly the one with no idle steps in the α-train schedule and that utilizes just 1 tank instead of 2.

3.2 2-Train PSA system

In this example, the four part methodology is applied to the 2-train 6-bed 3-bed PSA system (1979a) shown in Fig. 1. The 6-bed α train operates on a 7-step cycle sequence (not including the idle step), while the 3-bed β train operates on an 8-step cycle sequence. Both of these cycle step sequences are described in detail in the *Terminology for Multi-Train PSA Systems* section. Constraints on this PSA process include a continuous feed cycle; all equalization steps, LPP_α and $LPP2_\beta$ occupying no more than one unit time step each; HR_α and F_β being coupled to F_α; and $CnD1_\alpha$ being coupled to HR_α. No time restrictions are imposed on any other cycle step. Part 1 of the methodology is complete.

Part 2 involves determining the width of the unit block in the PSA process. Figure 7a shows an empty skeleton representing the unit block for this case. The block of six rows represents the α train beds and the block of three rows represents the β train beds. Recall that in a unit block every cycle step in the sequence defined for each train must be assigned to a bed and that initially a minimum width should be considered. In this example, the unit block cannot be 1 unit cell wide because only 6 and 3 unit cells would be available for the seven and eight cycle steps of the α and β trains, respectively. The unit block cannot be 2 unit cells wide either because only 6 unit cells would be available for the eight steps of the β train. A unit block 3 unit cells wide is also not viable because for a continuous feed cycle the F_β step of the β train must occupy the entire first row of the grid, leaving only 6 unit cells for the remaining seven cycle steps of the β train. Hence, a unit block 4 unit cells wide is selected, as shown in Fig. 7b, with columns A, B, C and D identifying each one. Part 2 of the methodology, i.e., formation of the primary skeleton of the unit block, is complete.

Part 3 of the methodology involves building the unit block by filling in the empty unit cells. Recall the left–right, top-down procedure described in detail in the 1-train 1-tank example. This process should be done in parallel for both trains. Consecutive steps should be kept as close as possible, with space (i.e., unit cells) being reserved for the remaining cycle steps. Also realize it may be prudent to skip one or more cycle steps in the sequence to place one of the later cycle steps in a unit cell and then go back and place the skipped steps. Finally realize there may be more than one solution. These subtle features of the graphical unit block approach are illustrated with this example.

For the α train, the process begins by filling in row 1_α from A-1_α to D-1_α, then continuing with row 2_α from A-2_α

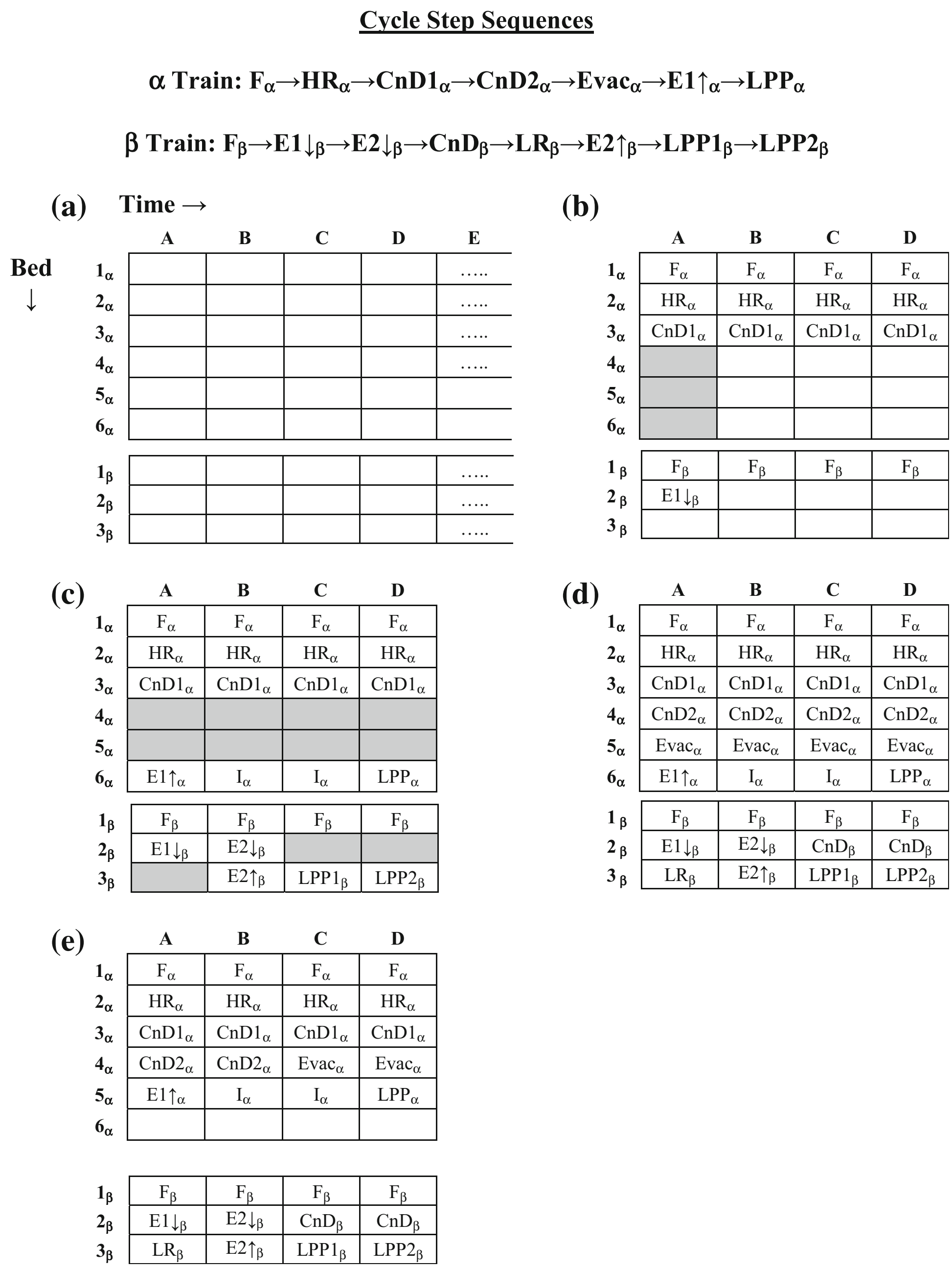

Fig. 7 Construction of the unit block for the 2-train 6-bed 3-bed PSA system shown in Fig. 1

to D-2$_\alpha$, and so on until the last row of unit cells A-6$_\alpha$ to D-6$_\alpha$ are filled in. As unit cells become occupied with the initial cycle steps of the α train, it may be necessary to skip some cells and some cycle steps to proceed in a more logical fashion. It may also be necessary to begin to place some of the cycle steps in the β train because they are coupled with a cycle step in the α train. When multiple options (solutions) arise, as many as possible should be explored, especially to minimize the number of idle steps that may be necessary to ensure coupled steps align properly. The example below illustrates some of these situations that require sometimes difficult decisions to be made during the progression of Part 3.

To satisfy the continuous feed cycle constraint of Part 1, F$_\alpha$ must occupy the first row (i.e., A-1$_\alpha$ to D-1$_\alpha$) of its unit block, as shown in Fig. 7b. Because HR$_\alpha$, CnD1$_\alpha$ and F$_\beta$ are coupled with F$_\alpha$, HR$_\alpha$ must occupy the second row (i.e., A-2$_\alpha$ to D-2$_\alpha$) of the α train, CnD1$_\alpha$ must occupy the third row (A-3$_\alpha$ to D-3$_\alpha$) of the α train and F$_\beta$ must occupy the first row (i.e., A-1$_\beta$ to D-1$_\beta$) of the β train. E1$\downarrow_\beta$ is placed in unit cell B-2$_\beta$ since it is the next step following F$_\beta$ in the β train. The unit cells shaded in gray (i.e., A-4$_\alpha$, A-5$_\alpha$ and A-6$_\alpha$) indicate three possible locations for E1$\uparrow_\alpha$, because this step is coupled with E1$\downarrow_\beta$. So, a decision must be made. It is quickly realized that E1$\uparrow_\alpha$ cannot occupy unit cell A-4$_\alpha$ since that would leave no unit cells for CnD2$_\alpha$ and Evac$_\alpha$ that must both occur before E1$\uparrow_\alpha$. This gives rise to two options, where E1$\downarrow_\beta$ can be placed in either A-5$_\alpha$ or A-6$_\alpha$. Figure 7c shows the option adopted by Sircar (1979a), which places E1$\uparrow_\alpha$ in A-6$_\alpha$. Figure 7c also shows E2$\downarrow_\beta$ and E2$\uparrow_\beta$ placed in cells B-2$_\beta$ and B-3$_\beta$. This is a logical placement for these steps, as it places E2$\downarrow_\beta$ closest to E1$\downarrow_\beta$ and it leaves two cells in the β train (i.e., C-3$_\beta$ and D-3$_\beta$) for the last two steps in the sequence, i.e., LPP1$_\beta$ and LPP2$_\beta$, as also shown in Fig. 7c. Because LPP$_\alpha$ is coupled to LPP2$_\beta$, LPP$_\alpha$ must be placed in D-6$_\alpha$. This arrangement necessarily forces the placement of idle steps in unit cells B-6$_\alpha$ and C-6$_\alpha$. The cells shaded in gray in Fig. 7c indicate there are several options to consider for placing CnD2$_\alpha$ and Evac$_\alpha$ in unit cells A-4$_\alpha$ to D-5$_\alpha$ in the α train and for placing CnD$_\beta$ and LR$_\beta$ in unit cells C-2$_\beta$, D-2$_\beta$ and A-3$_\beta$ in the β train. Figure 7d shows the solution provided by Sircar (1979a), which is just one of many solutions. Another solution, obtained by placing E1$\uparrow_\alpha$ in A-5$_\alpha$ instead of in A-6$_\alpha$ as Sircar (1979a) did, is shown Fig. 7e.

The methodology is concluded with Part 4, which consists of deriving the grand cycle schedule of this 2-train 6-bed 3-bed PSA system by extending the unit block of Fig. 7d five times to make a total of 6 unit blocks, as determined by Eq. 1. The Part 4 procedure for a multi-train PSA process is identical to that for a train-tank system and explained in detail in that example. This creates the grand cycle schedule shown in Fig. 1.

4 Conclusions

A simple, graphical, unit block approach for complex PSA cycle scheduling has been developed for parallel interacting trains of PSA columns, possibly assisted by trains of tanks. For parallel interacting trains of PSA columns (case 1), this new methodology involves a priori specifying for each train the cycle steps, their sequence, and the number of beds, and then following a systematic procedure that requires filling in a 2-D grid for each of these coupled trains. For parallel interacting trains of PSA columns assisted by trains of tanks (case 2), a similar methodology has been developed; however, the number of tanks to include and their steps is an output from the methodology rather than an input to it. The reason for this is that tanks are inherently required when the coupling between steps is otherwise impossible or leads to the generation of undesirable idle steps. The overall outcome is a unit block for each train that can easily be extended to form its complete cycle schedule, thereby forming the grand cycle schedule of the coupled train–train or train-tank system.

The new methodology was applied universally to either case 1 or 2, because the analysis of a multi-train system and a train-tank system are very similar. Each tank was simply treated as a train consisting of just one bed. Two examples were provided to show how to use the methodology for multi-train and train-tank systems.

The first example considered a 1-train PSA process with tanks. This case explained the subtleties associated with integrating one or more tanks into a PSA cycle schedule and discussed the possible benefits of doing so. It also revealed the effect of increasing the number of unit steps in a unit block. Three grand cycle schedules resulted for the same 10-step cycle step sequence. For 3, 4 and 5 unit steps in the unit block, the grand cycle schedule respectively changed from a 1-train 4-bed 2-tank PSA system to a 1-train 4-bed 1-tank PSA system to a 1-train 4-bed 1-tank PSA system with an undesirable idle step in the cycle schedule. The 1-train 4-bed 1-tank PSA system without the idle step was the best grand cycle schedule.

The second example considered a 2-train PSA process. This case explained the intricacies associated with integrating two PSA cycle schedules together. The resulting grand cycle scheduled was for a 2-train 6-bed 3-bed PSA system from the literature.

Three heuristics were also discovered about the minimum number of beds required to satisfy the number and types of steps in the cycle step sequence. Heuristic 1 states the minimum number of beds required by a schedule is never less than the sum of the number of continuous steps and the number of equalization steps within the same train plus one. Heuristic 2 states the minimum number of beds required by a schedule that contains a number of coupled steps other than equalization steps is never less than the sum of the continuous steps plus two. Heuristic 3 states the minimum number of beds required by a schedule, based on heuristics 1 and 2, decreases by one each time a tank is added.

Overall, these new methodologies and heuristics should be very useful for quickly scrutinizing different PSA cycle schedules for complex PSA processes. These PSA processes may comprise a single train of PSA columns; they may comprise a single train of PSA columns assisted by one or more trains of tanks; they may comprise any number of parallel interacting trains of PSA columns; or they may comprise any number of parallel interacting trains of PSA columns assisted by one or more trains of tanks. The possibilities are seemingly endless.

Acknowledgments The authors gratefully acknowledge financial support provided in part by the National Space Biomedical Research Institute through NASA NCC9-58, in part by the SAGE Center at the University of South Carolina, and in part by the Process Science and Technology Center, a consortium composed of the University of Texas at Austin, the University of South Carolina, and the Texas A&M University.

Conflict of interest The authors declare they have no conflict of interest.

References

Chiang, A.S.T.: Arithmetic of PSA process scheduling. AIChE J. **34**, 1910–1912 (1988)

D'Amico, J.S., Reinhold, III, H.E., Knaebel, K.S.: Helium recovery. US Patent 5,542,966, 1966

Ebner, A.D., Mehrotra, A., Ritter, J.A.: Graphical approach for complex PSA cycle scheduling. Adsorption **15**, 406–421 (2009)

Fuderer, A.: Pressure swing adsorption process and system. US Patent 4,381,189, 1983

Grande, C.A., Blom, R.: Dual pressure swing adsorption units for gas separation and purification. Ind. Eng. Chem. Res. **51**, 8695–8699 (2012)

Jee, J.G., Lee, S.J., Kim, M.B., Lee, C.H.: Three-bed PVSA process for high-purity O_2 generation from ambient air. AIChE J. **51**, 2988–2999 (2005)

Kumar, R., Kratz, W.C., Rarig, D.L., Guro, D.E., Schmidt, W.P.: Adsorptive process for separating multi-component gas mixtures. U.S Patent 4,914,218, 1990

Kumar, R., Kratz, W.C.: Separation of multicomponent gas mixtures by selective adsorption. US Patent 5,133,785, 1992

Kumar, R., Kratz, W.C., Rarig, D.L., Guro, D.E., Schmidt, W.P.: Gas mixture fractionation to produce two high purity products by pressure swing adsorption. Sep. Sci. Techol. **27**, 509–522 (1992)

Mehrotra, A., Ebner, A.D., Ritter, J.A.: Arithmetic approach for complex PSA cycle scheduling. Adsorption **16**, 113–116 (2010)

Mehrotra, A., Ebner, A.D., Ritter, J.A.: Simplified graphical approach for complex PSA cycle scheduling. Adsorption **17**, 337–345 (2011)

Reinhold, III, H.S., D'Amico, J.S., Knaebel, K.S.: Natural gas enrichment process. US Patent 5,536,300, 1996

Reinhold, III: Pressure swing adsorption method for separating gas components. US Patent 7,740,687, 2010

Ruthven, D.M., Farooq, S., Knaebel, K.S.: Pressure Swing Adsorption. VCH Publishers Inc, New York (1994)

Sircar, S: Separation of multi-component gas mixtures. US Patent 4,171,206, 1979a

Sircar, S: Separation of multi-component gas mixtures by pressure swing adsorption. US Patent 4,171,207 ,1979b

Sircar, S.: Fractionation of multicomponent gas mixtures by pressure swing adsorption. US Patent 4,790,858 ,1988

Sircar, S.: Recovery of nitrogen, hydrogen and carbon dioxide from hydrocarbon reformate. US Patent 4,813,980, 1989

Smith, O.J.I.V., Westerberg, A.W.: Mixed-integer programming for pressure swing adsorption cycle scheduling. Chem. Eng. Sci. **45**, 2833–2842 (1990)

Wang, S.-I., Patel, N.M., Sircar, S., Allam, R.J.: Ammonia synthesis. US Patent 4,792,441, 1988