Arithmetic of PSA Process Scheduling

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Pressure swing adsorption (PSA) process is a very attractive route for many industrial gas separation problems. Presently, commercial processes exist for the separation of air, the purification of hydrogen, the separation of iso- and normal paraffins as well as the separation of CO_2 from flue gas (Keller and Jones, 1980). A PSA system usually involves a series of adsorption beds, each executing the same sequence of operations but shifted in phase. The basic operations that are performed on each bed include pressurization, production, depressurization, and purge (Skarstrom, 1960). However, diverse designs have been proposed, which may include such steps as pressure equalization, product pressurization, and cocurrent depressurization (Tondeur and Wankat, 1985; Yang, 1987).

In a pressure equalization step, the high-pressure gas in an adsorption bed before depressurization is transferred to a lower-pressure bed so that the latter can be pressurized with less effort in the following steps. Low-quality product may also be used to pressurize a bed countercurrently to a medium pressure, so that its production end is enriched with ligher adsorbates, and a high-quality product can be obtained later (Yang, 1987). The equalization and product repressurization steps necessarily involve the connection of two beds at different operational stages. A schedule must thus be planned so that the two beds involved arrive at the connection stage simultaneously. For a dual-bed system which is common for small capacity applications, the schedule is rather obvious. However, for a larger-scale system with more adsorption beds, it becomes more difficult to arrange such a schedule by intuition. A rational approach must be established to accomplish this work. We report here an attempt to rationalize the planning of such a schedule.

Theory

Let N be the number of beds in a PSA system, where each bed is designed to perform the same sequence of M operations—O_1, O_2, O_3, . . . , O_m. The duration of operation O_i is represented by S_i with T representing the time required for the entire sequence. In the examples of this paper, the sequence of operations is assumed to be initiated at the lowest pressure conditions. If each bed is operated identically, there will be a shift of $D = T/N$ time interval between the sequence initiation of successive beds. Therefore, the same operation in one bed will always be performed in the next bed D time later.

Assume the sequence contains several operations that require the connection of two beds. Therefore, for each such operation O_i, there must exist a counteroperation O_i' of the same duration in the sequence. A workable schedule requires that all of the dual-bed operations pairs be initiated, and terminated, at the same time in each of the two beds. After the initiation of O_i in one bed, the same operation will be initiated by every D interval in the other beds. The synchronization of the dual-bed operations suggests that the duration between the initiation of operations O_i and O_i' on the same bed should be equal to an integer multiple of D interval, $J_i \cdot D$, where J_i is a positive integer less than N. Also, the sum of the duration of all operations (S_1, S_2, S_3, . . . , S_m) must be equal to T.

If a continuous production is expected, the duration of the production step must be larger than or equal to D: i.e., there will always be at least one bed in the production step. Furthermore, if a constant flow of product is also required, the number of beds in the production step should be the same at any instant. In other words, the duration of the production step S_p should be equal to an integer multiple of D.

Similar relations may exist for other operations based on their rate or other considerations. For example, vacuum to a subatmospheric pressure is usually slower than the pressure equalization of two beds. One may want to specify that the duration of a vacuum step be longer than the equalization step. However, without such a specific requirement, the duration S_i of an operation O_i will be assumed to be smaller than or equal to D. This assumption will minimize the number of beds needed to accomplish a matching schedule.

With the above assumptions, it is possible to schedule the following procedures.

Examples

Example 1. The operation sequence of a PSA system is to be designed as followed:

1) Pressure equalization with a higher pressure bed (O_1)
2) Pressurization with the product of another bed (O_2)
3) Pressurization with feed (O_3)

4) Adsorption and production (O_4)
5) Pressurization of the other bed with its product (O_2')
6) Equalizing its pressure with a lower pressure bed (O_1')
7) Vent or vacuum (O_5)

To synchronize the dual-bed operations, one has

$$D \cdot J_1 = S_1 + 2S_2 + S_3 + S_4$$
$$D \cdot J_2 = S_2 + S_3 + S_4.$$

Also $T = D \cdot N = 2S_1 + 2S_2 + S_3 + S_4 + S_5$.
With the requirement of continuous production, we may write $S_4 \geq D_1$, and $S_j \leq D$ for $j \neq 4$. Thus,

$$2D \geq D(N - J_1) = S_1 + S_5 > 0 \quad (1)$$

$$2D \geq D(J_1 - J_2) = (S_1 + S_2) > 0. \quad (2)$$

Subtracting Eq. 2 from Eq. 1, one gets

$$-D < D(N - 2J_1 + J_2) = S_5 - S_2 < D$$

Because N, J's are positive integers, it implies:

$$N = 2J_1 - J_2. \quad (3)$$

The above equations can also be arranged to give:

$D(2J_2 - J_1) = S_4 + S_3 - S_1 > 0$, which says

$$J_2 > (J_1 - J_2) \quad (4)$$

Based on Eqs. 1 to 4, the permissible values for $(N - J_1, J_2, J_1 - J_2)$ or $[(S_5 + S_1)/D, (S_2 + S_3 + S_4)/D, (S_2 + S_1)/D]$ are $(1 \geq 2, 1)$ and $(2 \geq 3, 2)$. It is found that at least four beds must be used to accommodate the given sequence. The operations are divided into three blocks; each lasts for an integer multiple of D. The timetable for the case of (1, 2, 1) is given in Figure 1. The rate of each operation may then be considered to choose the best schedule from the possible soltuions.

Example 2. To better utilize the partially separated gases in a high-pressure bed, one may want to equalize it with a series of progressive lower-pressure beds. In addition, purge with the initial blowdown gas would be cheaper than that with the product gas. Thus, one may consider a design as follows:

1) Pressure equalization with a high-pressure bed (O_1)
2) Pressure equalization with other higher pressure bed (O_2)
3) Repressurizing with low-quality product from other bed (O_3)
4) Repressurization with feed (O_4)
5) Adsorption and production (O_5)
6) Repressurization of another bed with part or all of its product (O_3')
7) Equalization of its pressure with another bed (O_2')
8) Partial depressurization using the off gas to purge another bed (O_6)
9) Equalizing rest pressure with a freshly purged bed (O_1')
10) Vent (O_7)
11) Purge with off gas of another bed (O_6')

If all the product in operation O_3' are used to pressurize another bed, one would write $S_5 \geq D$. Again, by taking $S_j \leq D$ for all other operations, the following relations can be written:

$$D \cdot J_1 = S_1 + 2S_2 + 2S_3 + S_4 + S_5 + S_6 > D$$
$$D \cdot J_2 = S_2 + 2S_3 + S_4 + S_5 > D$$
$$D \cdot J_3 = S_3 + S_4 + S_5 > D$$
$$3D \geq D \cdot J_6 = S_1 + S_6 + S_7 > 0.$$

Rearranging the relations one gets

$$3D \geq D(J_1 - J_2) = S_1 + S_2 + S_6 > 0 \quad (5)$$

$$2D \geq D(J_2 - J_3) = S_2 + S_3 > 0 \quad (6)$$

$$-D < D(J_6 + J_2 - J_1) = S_7 - S_2 < D,$$
$$\text{or } 3D \geq D \cdot J_6 = D(J_1 - J_2) = S_1 + S_6 + S_7 > 0 \quad (7)$$

$$D(2J_3 - J_2) = S_5 + (S_4 - S_2) > 0,$$
$$\text{or } J_3 > (J_2 - J_3) \text{ or } S_3 + S_4 + S_5 > S_2 + S_3 \quad (8)$$

$$2D > D(J_6 - J_2 + J_3) = S_1 + S_6 - S_3 > -D \quad (9)$$

The possible combinations of $(J_6, J_1 - J_2, J_3, J_2 - J_3)$ or $[(S_6 + S_1 + S_7)/D, (S_6 + S_1 + S_2)/D, (S_3 + S_4 + S_5)/D, (S_2 + S_3)/D]$ are $(1, 1 \geq 2, 1)$, $(2, 2 \geq 2, 1)$, $(2, 2 \geq 3, 2)$, or $(3, 3 \geq 3, 2)$. Since $T/D = N$, the total number of the beds can be calculated by the sum of the numbers in the bracket. At least five beds are needed for this sequence. The operations are

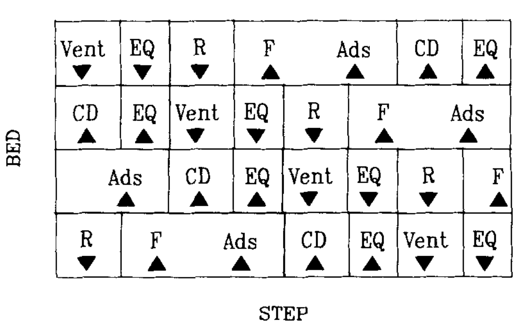

Figure 1. Four-bed schedule for the operation sequences in example 1.

▲, ▼, flow direction; EQ, equalization; R, repressurization; Ads, adsorption; CD, countercurrent depressurization.

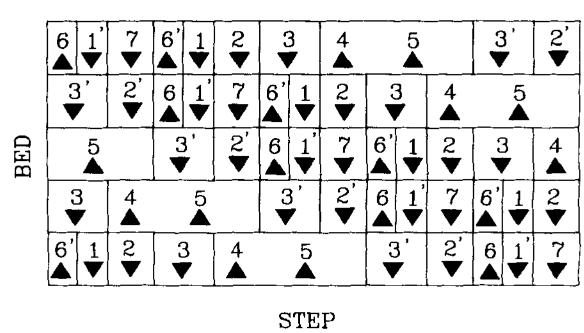

Figure 2. Five-bed schedule for the operation sequences in example 2.

The step number corresponds to that given in the text. ▲, ▼, indicates the flow direction.

divided into four blocks. Each lasts for an integer multiple of D. The possible multiplication factors are limited except the block containing the production step. A time table based on the five bed case is shown in Figure 2.

If only part of the product in operation O_3' is used to pressurize the other bed, instead of $S_5 \geq D$ one would use $S_5 + S_3 \geq D$ to ensure a continuous production. Furthermore, we will assume that operation O_4 is eliminated or $S_4 = 0$. For such a sequence, the analysis will be similar except for Eq. 8. Since $D(2J_3 - J_2) = S_5 - S_2 > -D$ in this case, one may use $J_3 \geq J_2 - J_3$ in place of Eq. 8. The permissible solution for $(J_6, J_1 - J_2, J_3, J_2 - J_3)$ will be $(1, 1 \geq 1, 1)$, $(2, 2 \geq 1, 1)$, $(2, 2 \geq 2, 2)$, and $(3, 3 \geq 2, 2)$. The minimum number of beds needed is four in this case. The schedule of a four-bed system is exactly the same as that given by Cassidy and Holmes (1984).

Summary

Since all beds are operated with the same repeating sequence, each bed must be initiated with a shift of $D = T/N$ time interval. By recognizing that dual-bed operations must be initiated simultaneously in different beds, a relation can be established for each pair of such operations. A sequence with L pairs of dual-bed operations will then be divided into L blocks. The above relations specify the number of beds needed to accomplish a balanced cycle and the ratios between the duration of such operation blocks. If no operation were allowed to last longer than one shift, only a limited number of schedules will be possible for a given sequence. Otherwise, there will be infinite possibility.

Thus, by following such a simple analysis, one can easily establish the permissible schedules for a given PSA operation sequence. This practice will greatly accelerate the design of a PSA process.

Notation

D = T/N, duration between the sequence initiation of successive beds
J_i = number of shifts between a pair of dual-bed operations O_i and O_i'
L = number of dual-bed operation pairs in the given sequence
M = number of operations in a given sequence
N = number of adsorption beds in a PSA system
O_i = ith PSA operation
S_i = duration of ith operation
T = duration of the entire PSA operation sequence

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