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Tuning of Pressure Swing Adsorption Systems Based on Differential Pressure Profile*

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Abstract. A method for tuning a Pressure Swing Adsorption (PSA) system aimed to achieve symmetrical operating conditions based on pressure differential in the adsorption vessels is developed in this study. Simulation of an oxygen Pressure-Vacuum Swing Adsorption (PVSA) process indicates that the pressure drop inside the adsorption vessel is closely related to the nitrogen concentration and gas velocity. The technique is applied to the tuning of an oxygen PVSA process. Adsorbent vessels of the PSA system are monitored and tuned by making corrective adjustments in each of the steps in a PSA cycle in response to imbalances in the differential pressure profiles in each of the adsorbent vessels. The method developed in this study provides a faster, easier, and more effective way to bring a PSA plant to its symmetrical, optimal state than those based on other parameters such as concentration, temperature, and pressure profile.

Keywords: PSA, VSA, PVSA, oxygen, plant, tuning, control, and pressure differential

1. Introduction

For a PSA system with more than one adsorption bed to be operated optimally, it is necessary to adjust the equalization, backfill, or purge flows for each of the adsorbent vessels in the system to ensure that each of the adsorbent beds produces a product of the same purity. This has typically been done by measuring the product-gas breakthrough purity with a product-purity analyzer connected to the downstream of the product-withdrawal line. Once the breakthrough purity is balanced, the process is said being "tuned", and maximum product-gas capacity would be produced at the lowest unit power consumption.

Abel et al. (1991) described the control of the product flow from an adsorption-separation system when the downstream customer has a discontinuous use pattern by monitoring the differential pressure in a product pipeline. Schebler et al. (1986) used a small bleeding valve in conjunction with an oxygen partial pressure monitor to control the partial pressure of oxygen in the product stream. In Gunderson's patent (Gunderson, 1988), the inlet feed flows were changed in response to the purity levels in the product stream. Grader (1987) reported a PSA system that supplies oxygen under variable demand conditions by varying the oxygen product to feed air ratio. Miller and Gary (1987) disclosed a method for controlling the purity of

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*This paper is dedicated to the memory of Professor Wolfgang Schirmer.

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a gas component in a PSA-product stream. Co-current depressurization gas is analyzed to determine whether a product-purity problem exists.

Schaub et al. (1995) introduced a method for tuning the PSA system by adjusting the pressure equalization and repressurization steps in response to imbalance in the temperature profiles of the vessels. However, bed temperature is a less sensitive parameter compared to pressure gradient when a PSA system is subject to any processing disturbance. Making corrective adjustments in response to an imbalance in bed temperature requires a relatively long period of time before a PSA system can be brought to its balanced state.

It is of great practical importance to compensate for any process inefficiencies before they can negatively impact the performance of a PSA plant. Product purity and bed temperature are 'slow' process indicators, which do not change significantly with respect to time. Monitoring quantities such as product-stream flow, purity, or bed temperature would not be effective in determining whether there is a process problem that needs to be corrected. This is due to the fact that the state of the adsorption beds has already been altered when a change in product flow, product purity, or bed temperature is detected. Solving potential process problems before they occur is inherently a more advantageous way to control PSA processes.

Differential-pressure transmitters are widely used in PSA plants to ensure that the adsorption beds operate below the fluidization limit. Tuning of a PSA system can be targeted to eliminating imbalances in the differential-pressure profiles of the adsorbent vessels by making corrective adjustments in each of the steps in the PSA cycle (such as pressure equalization, evacuation, purge, backfill, repressurization, and/or production steps). Using the profile of differential pressure, rather than temperature, product purity, or process performance in each of the PSA beds, as reference parameter or indicator, a PSA system could be tuned more quickly and easily to its symmetrical, optimal state. The method developed in this study extends the functions of differential-pressure transmitters and provides a much more efficient and effective way in tuning PSA plants.

2. Simulation Study

2.1. The PSA Model

A PSA-process simulator, DAPS (Dynamic Adsorption Process Simulator), described by Doong and Propsner (1998), was adapted to study the symmetrical and non-symmetrical O_2-VPSA process. The simulation program comprises a rigorous mathematical model that embraces mass and energy balances, adsorption equilibrium, mass and heat transfer, etc., which, in particular, enables a description of the transport phenomena in adsorption columns.

The following assumptions were made for model derivation: (i) the ideal-gas law applies to all the gases; (ii) no radial-pressure gradient exists across the bed; (iii) thermal equilibrium exists between the fluid and solid phases; and (iv) there is no radial variation in both concentration and temperature.

The current study employs a two-bed O_2-PVSA cycle with equalization, purge, and backfill. The cycle steps considered are as follows:

(i) *Adsorption step*: air is introduced into the bed from the feed end of the bed, and O_2 product is drawn from its product end;
(ii) *Equalization* (−) *step*: feed supply is terminated, and the bed is depressurized by transferring the O_2-rich gas through the product end to the other bed, which is at lower bed pressure;
(iii) *Vent step*: the bed is connected to a vacuum pump from the feed end and further depressurized;
(iv) *Purge step*: the bed is regenerated by receiving a portion of the O_2 product at the product end from the other bed, which is undergoing Step (i), while the feed end still being connected to the vacuum system;
(v) *Equalization* (+) *step*: the bed is re-pressurized from the product end using the depressurization gas from the other bed, which is undergoing Step (ii);
(vi) *Backfill step*: the bed is pressurized with product from the product end; and
(vii) *Feed-pressurization step*: the bed is pressurized by feed gas.

The mass balances for the gas species in a packed bed read as follows:

$$\varepsilon \frac{\partial C_i}{\partial t} + \frac{\partial u C_i}{\partial z} - D_L \frac{\partial^2 C_i}{\partial z^2} - s_i = 0 \quad i = 1, \ldots, n \tag{1}$$

where ε is the inter-particle void-volume fraction; C_i is the concentration of component i in the gas phase; u is the superficial gas velocity; z is the bed distance; D_L is the axial-dispersion coefficient; and s_i is the sorption rate of component i per unit volume of the bed.

The energy balance in the bed is given as follows:

$$\frac{\partial}{\partial t}\left\{\left(\varepsilon C_{pg}C + \rho_B C_{ps} + \rho_B C_{pg}\sum_{j=1}^{n} q_j\right)T\right\} + \frac{\partial\left(uC_{pg}CT\right)}{\partial z} - K_L\frac{\partial^2 T}{\partial^2 z} - \sum_{j=1}^{n}\Delta H_j\frac{\partial q_j}{\partial t}\rho_B + \frac{4h_w}{d_i}(T - T_w) = 0 \tag{2}$$

where C_{pg} is the heat capacity of the gas; C is the overall gas concentration in the gas phase; ρ_B is the bulk density of the adsorbent; C_{ps} is the heat capacity of the adsorbent; q_j is the adsorbed amount of component j in the solid phase; ΔH_j is the adsorption heat of component j; h_w is the heat-transfer coefficient between the packed bed and the wall; K_L is the axial thermal conductivity; d_i is the inside diameter of the bed; and T_w is the average wall temperature.

Another energy-balance equation can be written for the wall of the bed:

$$A_w\rho_w C_{pw}\frac{\partial T_w}{\partial t} = \pi d_i h_w(T - T_w) - \pi d_o h_o(T_w - T_a) + K_w A_w\frac{\partial^2 T_w}{\partial z^2}, \tag{3}$$

where A_w is the cross-section area of the wall; ρ_w is the density of the wall; C_{pw} is the heat capacity of the wall; d_o is the outside diameter of the bed; K_w is the thermal conductivity of the wall; T_a is ambient temperature; and h_o is the heat-transfer coefficient between wall and surroundings.

A *Glueckauf* model of linear-driving force, LDF, is used to describe the mass-transfer resistance of adsorbent particles. The sorption rate is expressed as follows:

$$\begin{aligned} S_i &= -\rho_B\frac{q_{io}RT_o}{P_o}\frac{\partial Q_i}{\partial\tau} \\ &= -\rho_B k\frac{L}{u_o}\frac{q_{io}RT_o}{P_o}\left(Q_i^s - Q_i\right), \end{aligned} \tag{4}$$

where k represents the LDF-rate coefficient; and Q_i^s is the equilibrium value of adsorbed amount at gas-phase composition Y_i.

Complete model equations and a list of parameters used in the simulation can be found in the paper by Doong and Propsner (1998). A finite-difference method is employed to convert the model equations into ordinary differential equations. Backward difference for the first-order derivative with respect to the bed distance was used to ensure numerical stability. For O_2-PVSA systems, where gas velocities tend to be very high, the dispersion term is much smaller than the convection term. Therefore, central difference was used for the second-order derivative with respect to the bed distance without any numerical difficulty. A standard-time integrator, the Runge-Kutta method, is then used to solve those equations. Boundary and initial conditions can be written based on PSA-process steps. Although the gas-flow direction can alter in a PSA bed depending on step sequence, the condition at one end of the bed is always known.

2.2. *Correlation between PSA Performance and Adsorbent-Vessel Pressure Gradients*

The pressure drop at the top region (cells 22 to 27, total number of cells are 30) of Bed A and the bed pressure profiles of both beds (Bed A and Bed B) in a two-bed oxygen VPSA system calculated from the simulation are given in Fig. 1. The pressure drop profile at the top region based on the simulation agrees well with what was observed in the experimental study shown in Figs. 3 through 8. The pressure drop increases slightly towards the end of the adsorption step as the nitrogen front moves up to the top region of the adsorbent bed. A peak in pressure drop appears at the beginning of the equalization step when the bed-pressure difference between the sending bed and the receiving bed is the largest. A sharp negative pressure drop always occurs in the purge-receiving bed at the beginning of the purge step.

The purity of the product that comes from each of the adsorbent vessels is directly related to the bed-concentration profile that is determined by the flow-rate (or velocity) profiles inside the vessel in each of the steps of a PSA cycle. Figure 2 shows the profiles of nitrogen concentration, gas velocity, and pressure gradient along the length of the adsorbent bed at the beginning ($t = 0.64$ sec) and end ($t = 16$ sec) of the adsorption step. As seen from Fig. 2, at different stages of an O_2-PVSA cycle, the concentration profiles coincide with the velocity profiles. As the strongly adsorbed component in the feed continues being adsorbed at the concentration front, the velocity in front of the concentration plateau is lower than that inside the plateau. The velocity profile, $u(x)$, along the

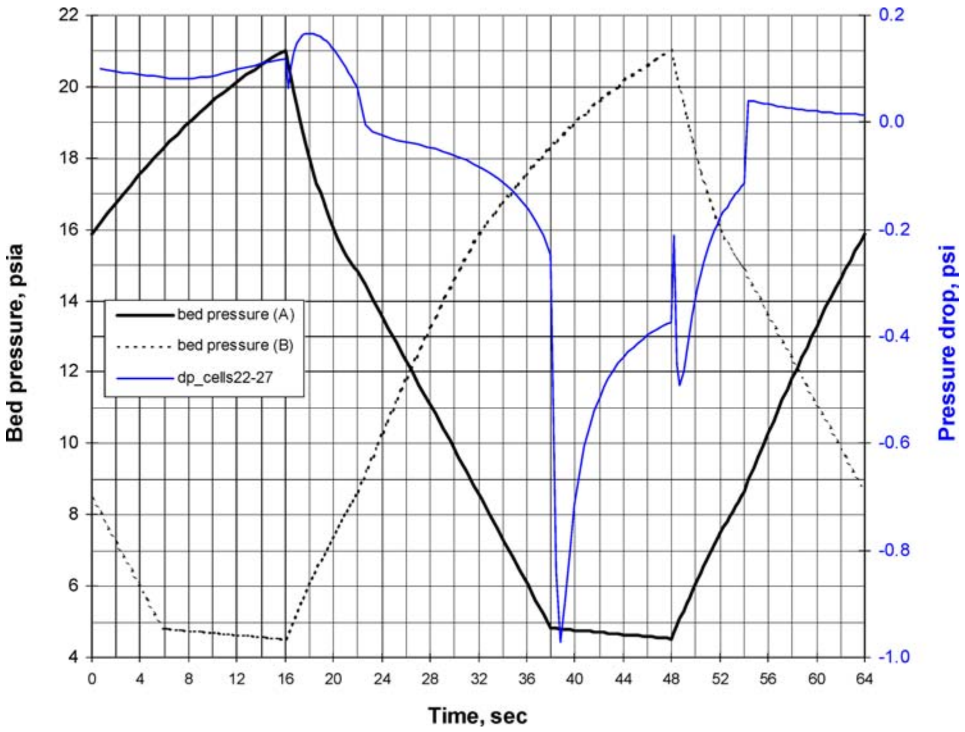

Figure 1. Bed pressure and pressure-differential profiles from the simulation results of a two-bed oxygen-PVSA plant.

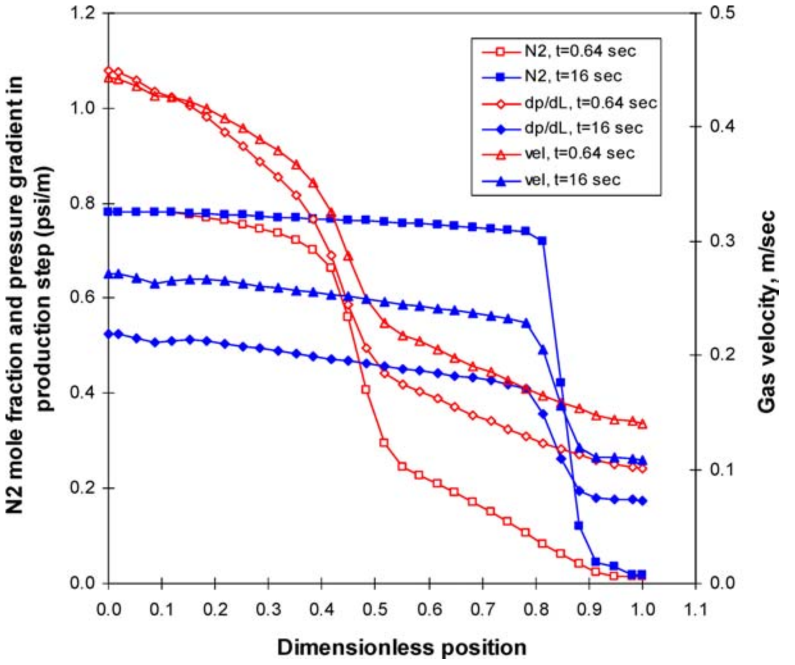

Figure 2. Profiles of N_2 concentration, gas velocity, and pressure-gradient from the simulation results for a two-bed oxygen-PVSA plant.

length of the adsorbent vessel is related to the pressure gradient, $\frac{\partial p}{\partial x}$, by the Ergun equation:

$$\frac{\partial p}{\partial x} = Au(x) + Bu(x)^2 \tag{5}$$

Whenever the adsorbent vessels became "unbalanced", the concentration profiles inside the vessels would be different. This causes the "asymmetrical" behavior in velocity profiles of the vessels, which can then be detected by measuring the pressure-gradient profiles of the vessels. When an imbalance in the process occurs, which can be determined immediately by a variation in the bed-pressure-gradient profile, each vessel would start producing different purity levels of product at different flow rates.

In the practice of this study, it is not necessary to measure the entire pressure gradient for the vessel. Monitoring the pressure drop in a small section of the adsorption beds will provide sufficient information for the tuning of a PSA plant. While this section of the bed can be at any location of the bed, it is preferred to monitor the pressure drop about 6 to 12 inches below the product end of the bed. At the end of the production step of a PSA cycle, the concentration front reaches a position close to the outlet of the product end. Therefore, pressure-drop measurement at this location will indicate whether the concentration front reaches this point at the end of the production step. If it does, a peak in the pressure-drop profile will show up, indicating an increase in the flow or velocity at this location. The vessel that produces lower-purity product would develop a peak in the pressure-gradient profile earlier than the vessel that produces higher-purity product.

One way to correct such imbalance is to change the relative amounts of product flow from each vessel. However, this would require additional control and flow-measurement equipment. Instead, the relative amounts of equalization gas, backfill gas, or purge gas entering each vessel can be adjusted. A suitable control process that compares the pressure drop profiles of both adsorption vessels can be employed to adjust the equalization, purge, or backfill flows. The difference in bed-pressure-drop profiles between the vessels is used to calculate a new pressure equalization, purge, or backfill setting for the control valves at the product end of each of the adsorbent vessels.

3. Experimental Study

3.1. Experimental Set-Up and PVSA Cycle

The experimental set-up and the adsorbent material used was reported earlier (Lü et al., 2004). The oxygen-PVSA unit consisted of two adsorbent beds, each having an inner diameter of 6.7 cm and length of 85 cm, and was operated between 4 psi and 21 psi at cycle time of 64 seconds.

The cycle comprised seven (7) steps: pressurization, production, sending equalization, sending equalization with evacuation (i.e., sending equalization through the production end while being evacuated from the feed end), evacuation, purge with evacuation, and receiving equalization. The step times in half of the PVSA cycle are given in Table 1.

3.2. Tuning of an Oxygen-PVSA System Based on Differential-Pressure Profile

Ideally, the separation performance of both adsorption beds is expected to be the same. To this end, a PSA plant would require a symmetrical setup for the plant piping, valves, adsorbent packing, etc. From an operational point of view, gas flow, pressure and temperature need to be balanced in each bed and during every cycle. Due to the dynamic nature of the PSA process, these variables tend to be very difficult to control or measure. Physical/geometrical differences in the adsorption beds, piping, valves, adsorbent loading, and how the adsorbent is packed can all result in unbalanced performance in adsorption beds. In addition, any disturbance in the system, such as ambient temperature, ambient pressure, switching valve position, etc., could tip the balance and result in an asymmetrical operation for a PSA plant. As a consequence, each PSA bed may no longer run at the same pressure swing or process the same amount of gas.

Table 1. Cycle features of the O_2-PVSA process for the experimental study.

Actions in Bed A	Actions in Bed B	Step time (sec)
Pressurization	Evacuation	13
Production	Purge-evacuation	10
Sending equalization	Receiving equalization	6
Evacuation-equalization	Receiving equalization	3
Half-cycle time (sec)		32

For example, if a two-bed PSA process is operated in an asymmetrical way, one bed may produce higher purity than the other bed. Consequently, there will be a mixing of product gas streams with different purities, which will cause the separation efficiency to drop. Not only is the net product purity lower than the case of symmetrical operation, but both beds also generate lower purity individually.

To effectively maintain stable operation of PSA systems, it is essential to detect the asymmetrical problems as soon as possible and to make corrective adjustment accordingly. Conventionally, the bed pressure profile has been used as an indicator of the imbalance between the adsorbent vessels. However, it is difficult to detect any symmetry problem from the pressure profile alone. As will be shown later, the bed pressure is not sensitive enough to reflect any imbalance of the PSA system and therefore is not useful for the plant tuning and process control. Other parameters, such as product purity and bed temperature, are slow in response to the system change.

The pressure drop was measured between two points located at 12 inches and 24 inches from the bottom of the two beds. With purge flow kept at zero, the equalization flow was adjusted such that the equalization sending from Bed A to Bed B was less than that sending from Bed B to Bed A. The bed pressure profiles (P_A and P_B) and the pressure drops (dp_A and dp_B) are given in Fig. 3, where the pressure drop for Bed B was shifted by 32 sec (half cycle time) for comparison purpose.

During the pressurization and equalization step, the pressure drop measured in Bed B is about 0.05 psi higher than that in Bed A. The product flow and oxygen purity were 8.31 slpm and 89.8%, respectively. When the equalization from Bed A to Bed B was increased such that the difference in pressure drop measured between the two beds was reduced to about 0.01 psi as shown in Fig. 4, the performance was improved significantly with product flow of 8.78 slpm and purity of 92.1%. It can be seen from Fig. 3 that the imbalance between the two beds is shown much more clearly in the pressure-drop profiles than in the pressure profiles. The largest difference in the pressure drop can be observed in the equalization-receiving bed at the beginning of the equalization step. The oxygen-PVSA performances

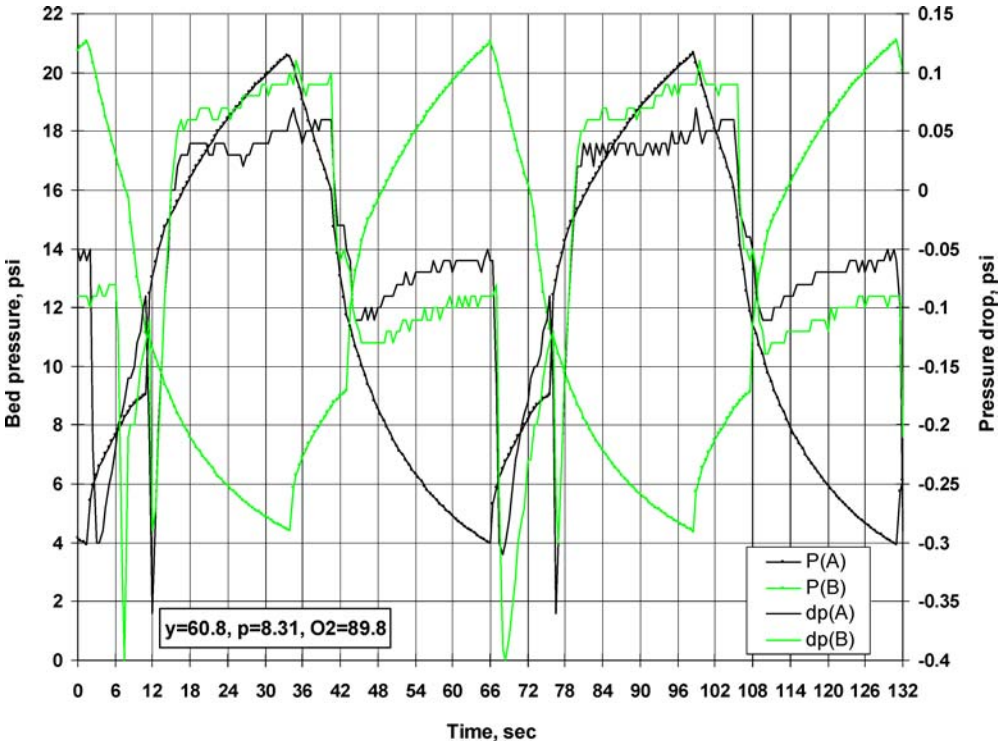

Figure 3. Bed pressure and pressure-differential profiles of an oxygen-PVSA plant with unbalanced equalization (pressure drop difference = 0.05 psi).

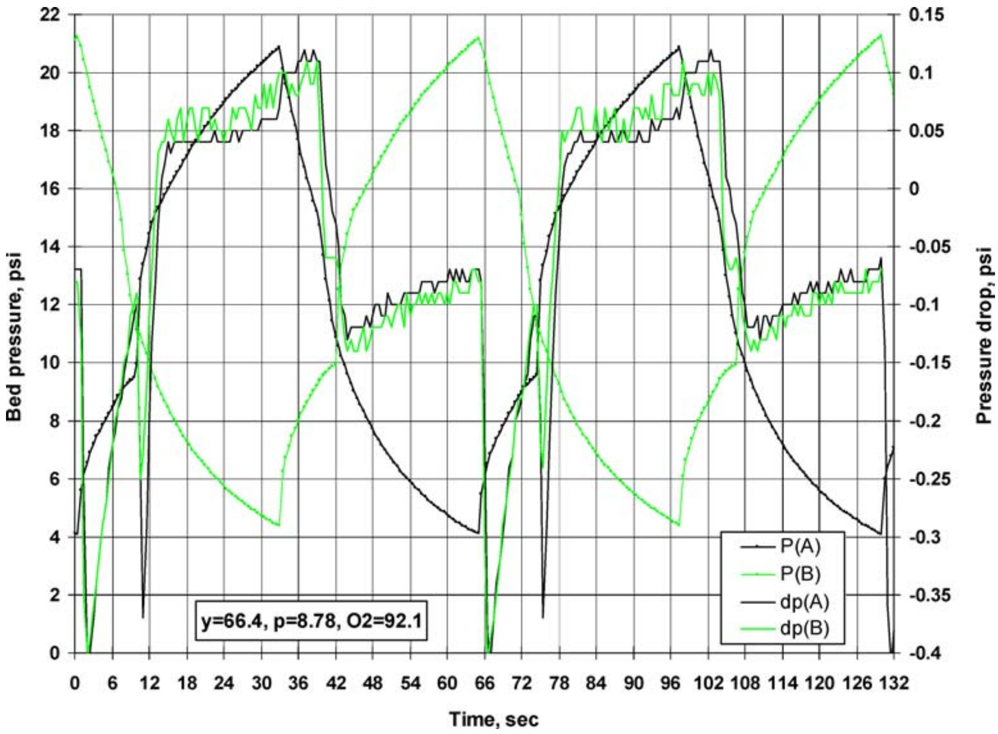

Figure 4. Bed pressure and pressure-differential profiles of an oxygen-PVSA plant with balanced equalization (pressure drop difference = 0.01 psi).

observed in the two cases shown in Figs. 3 and 4 are given in Table 2.

With the setting as shown in Fig. 4, unbalanced purges were introduced with Bed A receiving less purge than Bed B. As shown in Fig. 5, the maximum difference in pressure drop during production and equalization between Bed B and Bed A was 0.1 psi. The performance observed was 7.26 slpm product flow and 90.2% oxygen purity. As the purge flows were adjusted towards a more balanced state, the maximum pressure-drop difference was reduced to 0.05 psi (see Fig. 6). Accordingly, the product flow was increased by 0.29 slpm and oxygen purity by 2.9%.

Table 2. Performance comparison of unbalanced and balanced equalization.

	Unbalanced equalization (Fig. 3)	Balanced Equalization (Fig. 4)
Pressure drop (psi)	0.05	0.01
Oxygen purity (%)	89.8%	92.1%
Oxygen yield (%)	60.8%	66.4%
Product flow (slpm)	8.31	8.78

Further reducing the pressure-drop difference between the two beds to about 0.01 psi (see Fig. 7) increased the product flow by 0.25 lpm and purity by 0.8%. Further attempt to make the pressure profiles of the two beds more symmetrical by adjusting the purge flow only resulted in slightly lower performance, as the pressure-drop difference increases from 0.01 psi to 0.02 psi (see Fig. 8). While other minor factors such as bed-geometric difference and pressure-meter accuracy should be considered, the oxygen-PVSA performance data in Figs. 7 and 8 suggest that the pressure differential is a more sensitive indicator than the pressure profile. Table 3 summarizes the oxygen-PVSA performances observed in the four cases for different purges as discussed above.

It must be pointed out that the method reported in this study can be applied to tuning PSA systems in which the adsorbed species is the major component(s). For PSA systems where the concentration of the adsorbed component(s) is small, the adsorbent-bed pressure drop is not significant enough to be used as an indicator for PSA-plant tuning.

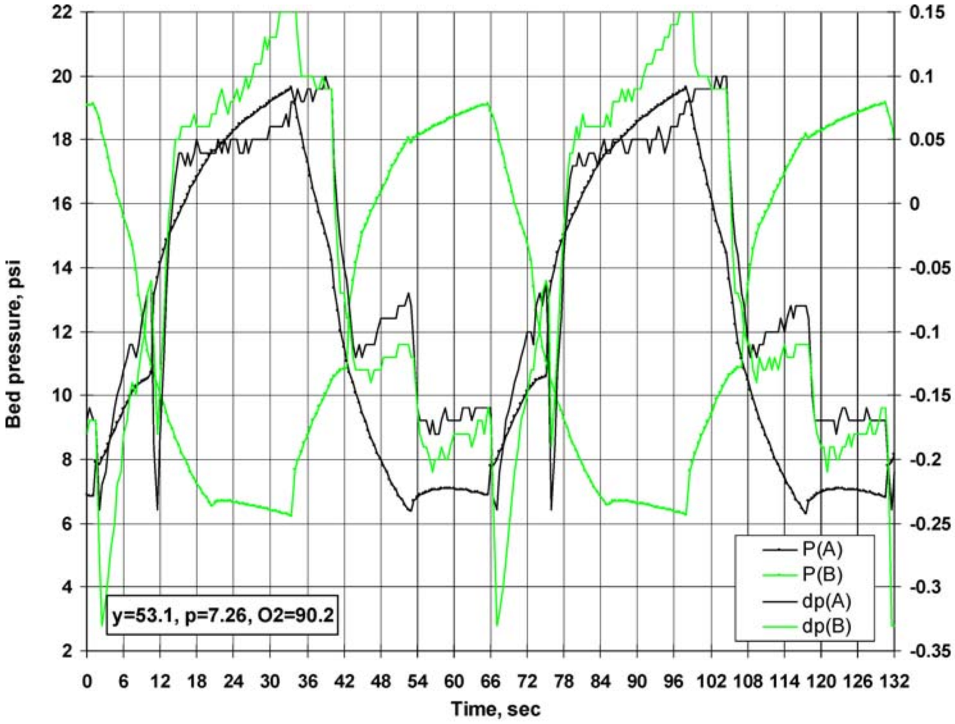

Figure 5. Bed pressure and pressure-differential profiles of an oxygen-PVSA plant with unbalanced purge (pressure drop difference = 0.10 psi).

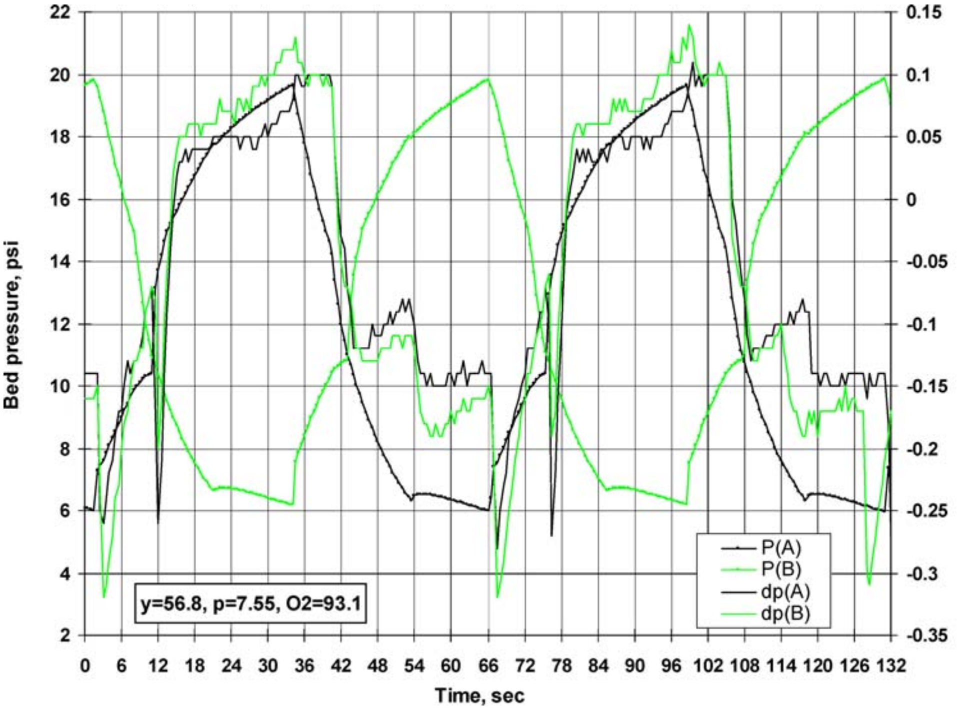

Figure 6. Bed pressure and pressure-differential profiles of an oxygen-PVSA plant with unbalanced purge (pressure drop difference = 0.05 psi).

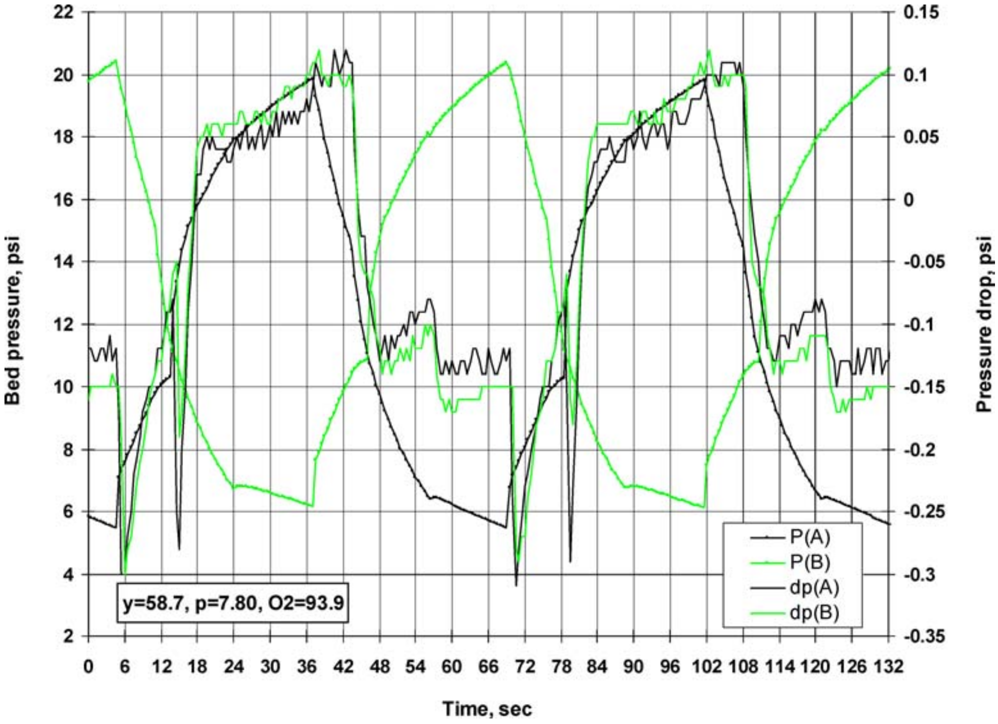

Figure 7. Bed pressure and pressure-differential profiles of an oxygen-PVSA plant with balanced purge (pressure drop difference = 0.01 psi).

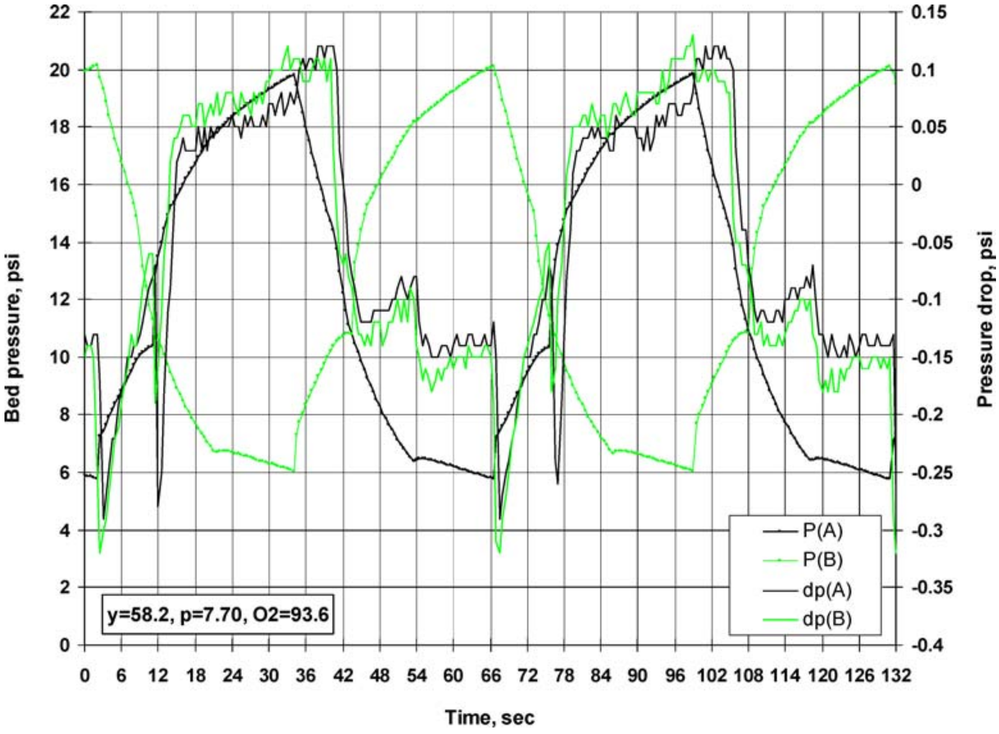

Figure 8. Bed pressure and pressure-differential profiles of an oxygen-PVSA plant with balanced purge (pressure drop difference = 0.02 psi; more symmetrical in pressure profile).

Table 3. Comparison of oxygen PVSA performance with unbalanced and balanced purge.

	Unbalanced purge (Fig. 5)	Unbalanced purge (Fig. 6)	Balanced purge (Fig. 7)	More symmetrical pressure profile (Fig. 8)
Pressure drop (psi)	0.10	0.05	0.01	0.02
Oxygen purity (%)	90.2%	93.1%	93.9%	93.6%
Oxygen yield (%)	53.1%	56.8%	58.7%	58.2%
Product flow (slpm)	7.26	7.55	7.80	7.70

4. Conclusions

The tuning of pressure swing adsorption processes is developed to achieve stable operation and high performance. The adsorbent-vessel pressure gradients are used as the indicator in determining whether an imbalance exists as a result of asymmetrical process parameters and operating conditions between the adsorption beds. Adjustments are made in equalization flow, backfill flow, and purge flow, pertaining to each of the vessels in order to balance the pressure-gradient profiles in each bed. In doing so, the imbalance in the gases transferred between the adsorbent vessels and between the vessels and machines (feed and product compressors and vacuum machines) and process inefficiencies are compensated.

Equalization flow, backfill flow, and purge flow are not only the variables which can be adjusted to keep a PSA system in balance, these variables should all be optimized in tuning a PSA plant. Before an optimization of a PSA plant can be performed, any of these variables should be kept in balanced state between the adsorbent beds by using pressure gradient as a reference. Therefore, any change made to any of these variables in the optimization has to be done in such a way that adsorbent beds are balanced with respect to the variable. As a result, tuned performance and optimal flow rates are achieved at any particular product-purity level, with the lowest power consumption for the process.

The method developed in this study enables one to make adjustments to solve potential process problems before they occur, which minimizes any undesired effects on desired product flow and/or purity values. The use of pressure-gradient profiles in adsorbent vessels for the tuning of PSA processes offers a faster and more efficient way to maintain stable and symmetrical operation of the PSA processes than those based on purity, temperature, or pressure profile.

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