Adsorption 6, 233–240, 2000

Performance of a Two-Bed Pressure Swing Adsorption Process with Incomplete Pressure Equalization

HEUNG-SOO SHIN* AND DONG-HO KIM
Department of Chemical System Engineering, Hong-Ik University, Chocheewon, Cheungnam, South Korea 339-800
shinhs@wow.hongik.ac.kr

KEE-KAHB KOO
Department of Chemical Engineering, Sogang University, Seoul, South Korea

TAE-SOO LEE
Department of Mechanical Engineering, Sogang University, Seoul, South Korea

Received September 9, 1999; Revised April 20, 2000; Accepted May 15, 2000

Abstract. Incomplete pressure equalization (PE) is practiced in a commercial oxygen concentrator for medical use by adopting simultaneous PE and feed-pressurization for pressurizing an adsorption bed. In such a cycle configuration, extent of equalization during PE affects process performance. In order to assess the effect, performance of pressure swing adsorption (PSA) process with incomplete PE was determined by both simulations and experiments. In simulations, an equilibrium model was used with the assumptions of multicomponent Langmuir isotherms, isothermal operation, and no pressure drop through a bed. The required parameters for simulations were measured in separate experiments. PSA experiments were performed for a two-bed cycle with PE. Two kinds of pressurization, feed and product, were examined. Effects of purge amount and extent of equalization on process performance were assessed in view of productivity and light-component recovery. From the obtained results performance contours were constructed. 95 oxygen mole percent production from air with zeolite 13× was considered as a case study. In both pressurizations, an optimal specific purge and an extent of equalization for the productivity and recovery were observed, but with a different level of equalization. For a maximum productivity feed-pressurization favored incomplete PE, while a maximum recovery occurred at complete PE for both pressurizations. The simulations depicted well existence of optimum conditions, though they showed quantitative disagreement with experiments.

Keywords: PSA, pressure equalization, extent of equalization, simulation, experiment

Introduction

Pressure equalization (PE) has been widely employed in pressure swing adsorption (PSA) processes ranging from a small-scale unit for medical oxygen to a large-scale hydrogen production unit. Inclusion of PE steps into a PSA cycle can enhance recovery of component as well as mechanical energy contained in a high-pressure gas (Ruthven et al., 1994). Normally, PE is achieved by connecting two beds, one of which has been purged and the other has completed a high-pressure feed step, through their product ends to

*Author to whom correspondence should be addressed.

equalize a pressure. Following PE the partially pressurized bed is finally pressurized to an adsorption pressure with a feed or a product. In this configuration, the final pressures of connected beds become nearly equal, and then so called complete PE approaches. On the other hand, when PE and final feed-pressurization take place simultaneously, only a fraction of the amount for complete PE can transfer from a depressurizing bed to a pressurizing one during PE. Thus, incomplete PE occurs. The latter configuration is used in a commercial oxygen concentrator (Devilbiss, USA) for medical use. The extent of incompleteness during PE is expected to affect process performance and its effect needs to be assessed for optimum process design.

Previous works usually analyzed PSA processes with PE for complete equalization (Hwang and Suh, 1996; Shin, 1996) or with the unrealistic assumption of frozen-adsorbed phase concentration profiles during PE steps (Hassan et al., 1987). Several related works examined the effect of incomplete equalization on process performance, but only fragmentary results were reported (Lemcoff et al., 1993; Doong, 1996; Doong and Propsner, 1998). In this paper, performance of PSA process with incomplete equalization was investigated by both simulations and experiments. Contours of performance variables were constructed and analyzed for a two-bed PSA process. The simulations were performed to predict experimental results.

Simulation

Process Description

The process considered in this study is a two-bed cycle with PE steps as illustrated in Fig. 1. The cycle consists of six steps: 1) high-pressure feed, 2) depressurization for pressure equalization, 3) blowdown, 4) purge, 5) repressurization by pressure equalization, 6) final pressurization with a feed or a product. Detailed operation of each step is described elsewhere (Ruthven et al., 1994). Pressure equalization is achieved by connecting the product ends of both beds. Product-pressurization and purging a bed is fulfilled by using a product storage vessel.

Mathematical Model for a Single Bed

Due to its nature of a PSA process, each bed behaves in the same way. Thus, a mathematical model will be developed for a single bed under the assumption of an isothermal bed, an ideal gas, a negligible pressure drop through the bed, multicomponent Langmuir isotherms, and instantaneous equilibrium between gas and adsorbent. The isothermal assumption is justified by the small temperature fluctuations (±3°C) inside a bed observed during experiment. The negligible pressure drop is acceptable because its experimental value between the feed end of a bed and the product tank was less than 6% of a feed pressure. The equilibrium between gas and adsorbent is approximated by allowing enough step durations.

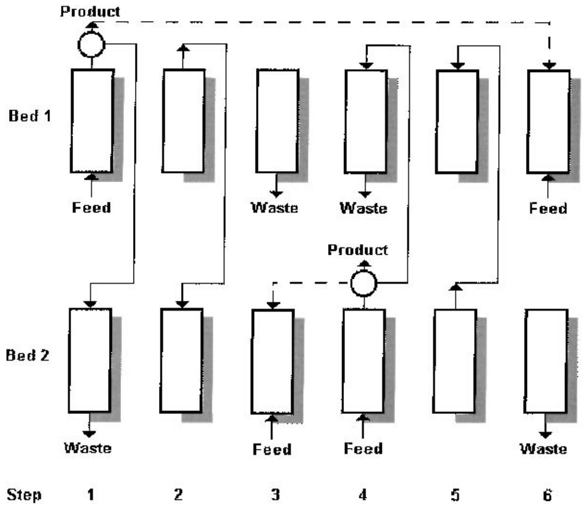

Figure 1. Two-bed PSA process with pressure equalization. Dot line = product pressurization.

The material balance for component A and overall material balance are given by:

$$\frac{\partial C_A}{\partial t} + \frac{\rho}{\varepsilon}\frac{\partial q_A}{\partial t} + \frac{\partial}{\partial z}(UC_A) = 0 \qquad (1)$$

$$\frac{\partial C}{\partial t} + \frac{\rho}{\varepsilon}\frac{\partial}{\partial t}(q_A + q_B) + \frac{\partial}{\partial z}(UC) = 0 \qquad (2)$$

Stipulated boundary conditions for each step are obtained from the operating policy.

For a high-pressure feed step:

$$C_A|_{Z=0} = C_{A,F} \qquad (3)$$

$$U|_{Z=0} = U_H \qquad (4)$$

For a cocurrent depressurization step for pressure equalization:

$$U|_{Z=0} = 0 \qquad (5)$$

For a countercurrent blowdown step:

$$U|_{Z=L} = 0 \tag{6}$$

For a purge step:

$$C_A|_{Z=L} = C_{A,P} \tag{7}$$
$$U|_{Z=L} = U_P \tag{8}$$

For a countercurrent pressurization step:

$$C_A|_{Z=L} = C_{A,P} \quad \text{(with product)} \tag{9}$$
$$C_A|_{Z=L} = C_{A,E} \quad \text{(with effluent from other bed)} \tag{10}$$
$$U|_{Z=0} = 0 \tag{11}$$

Initial condition:

$$\text{At } t = 0, C_A = C_{A,F} \quad \text{for all } Z \tag{12}$$

Multicomponent Langmuir isotherm is given by:

$$q_i = q_{si} \frac{b_i P_i}{1 + \sum_j b_j P_j} \quad (i = \text{ A or B}) \tag{13}$$

Finite difference method was applied to the partial differential equations along an axial direction. The resulting ordinary differential equations were integrated by Gear's method (Gear, 1971). Average concentrations of effluents were used for all steps in the simulations. Pressures were assumed to change linearly with respect to time during all pressure-changing steps and to remain constant during high-pressure feed and purge steps. Under the assumption of equilibrium gas and adsorbent, the PSA performance is independent of the type of pressure change and only depends on a pressure ratio between feed and purge pressures. The extent of pressure equalization were adjusted by changing the pressure of a depressurizing bed during PE step. Complete pressure equalization was recognized when the final pressures of two-connected beds during PE step became identical. The final pressure of a repressurized bed during PE step was determined so as to satisfy the material balance between connected beds. Spatial points were adjusted for approximating experimental results. Cyclic steady state is assumed to reach when the absolute difference of average mole fraction of product between two adjacent cycles is less than 2×10^{-4}.

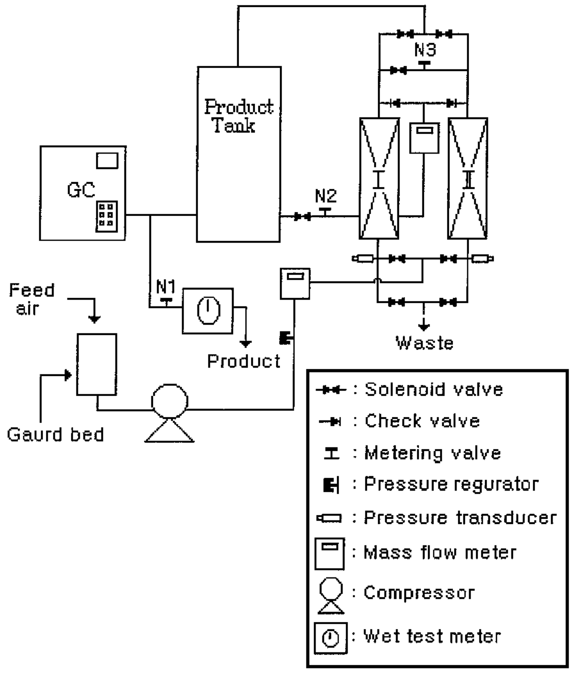

Figure 2. Experimental apparatus.

Experimental

A two-bed apparatus set for this study is shown in Fig. 2. The system consisted of two adsorption columns, each 100 cm long and 2.54 cm I.D. The columns were packed with zeolite 13× ($PSAO_2$ type, 0.4–1.0 mm, UOP). Mass flow meters (Aalborg Inc.) were used to measure air feed and purge flow rates and a wet test meter was used to measure a net product flow rate. Product purity was analyzed by a gas chromatography (Hewlett-Packard Model 6980). Two pressure transducers were located at the bottom of the beds and a thermocouple was inserted into a bed at the middle location of a bed. Feed air was supplied to adsorption beds after predried in a guard bed packed with silica gel and activated alumina. Zeolite 13× was pretreated before its use. Its adsorption and physical properties were measured in separate experiments and directly used in simulations (Kim, 1999).

Experiments were performed at a feed pressure of 3.2 atm and a regeneration pressure of 1 atm. Metering valve N1 was used to adjust a net product flow rate, consequently a product purity. The purge step was implemented by using the stored gas in a product tank and its flow rate was adjusted by the metering valve N2. In order to maintain a constant purge rate and minimize a pressure decrease in the product tank, a large volume (20 L) of a tank was used. During PE steps the extent of equalization was adjusted by using the needle valve N3. Data acquisition system (Work bench, Strawberry Tree Inc.) was used to control the cycle sequence and to store the measured data from mass flow meters.

PSA performance was determined in terms of product productivity and component recovery following attainment of cyclic steady state. The productivity is defined as the amount of net product per unit time per unit amount of an adsorbent and component recovery is defined as the ratio of an amount of component in a net product to that introduced to a bed as a fresh feed. Normally, PSA operation of more than 24 hours was allowed to ensure a cyclic steady state due to a transient effect in the product tank.

Results and Discussion

Determination of Step Durations

In order to specify step durations experiments were performed for various step times. Step durations were decided to ensure equilibrium between gas and adsorbent phases as possible. By doing so, any kinetic effects were eliminated and the effect of an extent of pressure equalization could be only observed. In addition, an equilibrium model could be applied to the system of study. Recently, it was shown that asymmetrical equalization could occur due to different flow characteristics of a needle valve when the flow was reversed (Doong and Propsner, 1998). Such asymmetrical equalization can be avoided by allowing enough duration during a PE step as made in this study. Figures 3–5 show the

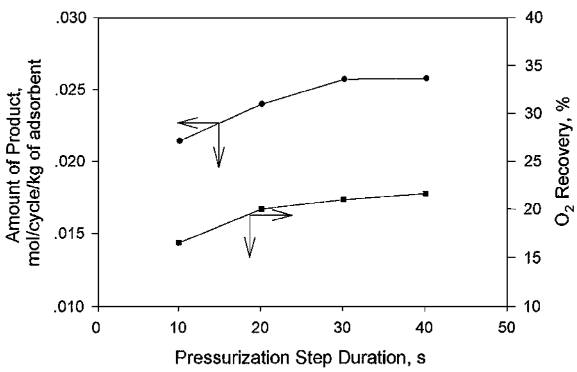

Figure 3. Effect of pressurization step duration on productivity and recovery.

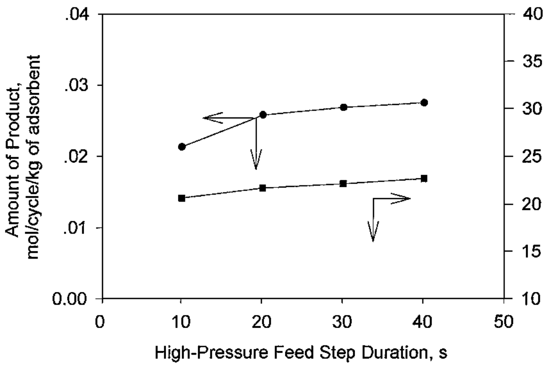

Figure 4. Effect of high-pressure feed step duration on productivity and recovery.

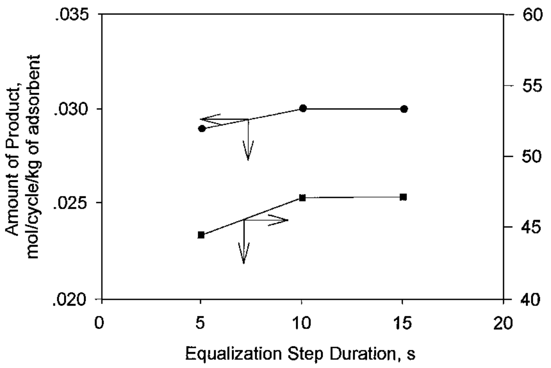

Figure 5. Effect of pressure equalization step duration on productivity and recovery.

effects of durations for three steps. Based on the results, 40, 30, and 10 seconds of durations were specified for pressurization, high-pressure feed, and pressure equalization steps, respectively. For synchronizing the cycle sequence, the durations of blowdown and purge steps were set to those for pressurization and high-pressure feed steps, respectively.

Contours for Productivity and Recovery

Contours for productivity and recovery were formulated from the experimental results obtained by varying purging amount and extent of equalization. In formulating contours, product purity was fixed at 95 oxygen mole percent. 95% purity was achieved by controlling carefully a product flow rate from the product tank. Since argon was produced with oxygen, it was considered as a product. The extent of equalization is defined as the ratio of pressure decrease of the depressurized bed during a PE step to that for complete pressure equalization. Thus, the extent of equalization is 1.0 for complete equalization. The definition in a term of pressure decrease does not seem to be reasonable since it does not indicate an actually transferred fraction. Instead, the expression in a term of moles transferred from one bed to the other is more acceptable. However, pressure can be measured more accurately than an amount of moles. Fortunately, it was experimentally observed that the final pressure of connected beds for complete equalization did not deviate much from an average value of initial pressures of beds. This fact suggests that nonlinearity and coupling of isotherms are not significant over the operating condition of this work. As a result, both definitions give a similar extent of equalization in this study. This fact was also confirmed in simulation.

Productivity and recovery contours in the case of feed-pressurization are shown in Figs. 6 and 7. Maximum productivity is observed at around the specific purge of 2.0 mol/hr kg of adsorbent and the extent of equalization of 0.75, and it is about 8% higher than the productivity at complete equalization and more than 20% than at no equalization. Specific purge is defined as the amount of purge per unit time per unit amount of an adsorbent. Optimum purging for the productivity appears independent of the extent of equalization, while that for the recovery decreases gradually for increase in an equalization level. The existence of optimum purging for a 4-step PSA cycle was already reported in previous works (Ruthven et al., 1994). Concerning the effect of equalization level, a higher extent of equalization results in a higher productivity in the range below the optimum equalization level. When a PE step is included into a PSA cycle, the penetration of nitrogen into the product end of a bed during the subsequent feed-pressurization step is retarded due to a partial pressurization with the effluent from the depressurizing bed, which has a fairly high purity. Then, more amount of a feed can be treated, resulting in a higher productivity. This is the same reason for productivity improvement for a product-pressurization (Ruthven et al., 1994). However, too high level of equalization results in contamination of the product side of a bed due to the low purity of effluent from the depressurizing bed, and consequently reduces a feed amount to be treated. The optimum equalization level was also observed in the previous works (Doong, 1996; Doong and Propsner, 1998). Contrary to the productivity, maximum recovery occurs at complete equalization as seen in Fig. 7. Apparently, productivity and recovery increase simultaneously up to the optimum equalization level at optimum purging and after that level a trade-off between two parameters exists. For a small-scale unit for medical oxygen a high recovery is not a matter of primary concern. Thus, operation at the optimum equalization level is desirable, where a productivity is highest. In addition, by employing simultaneous PE and feed-pressurization the productivity can be increased more due to a shorter cycle.

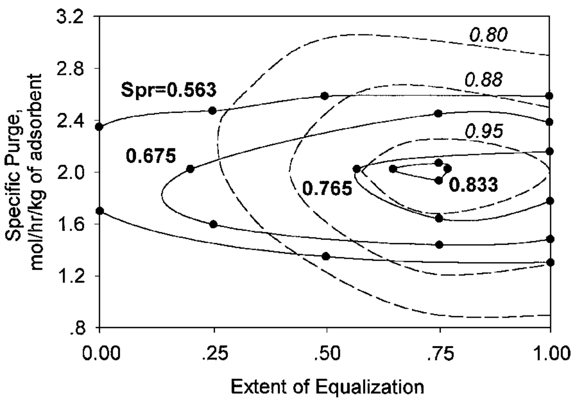

Figure 6. Experimental and theoretical productivity contour for different specific purge and equalization levels in case of feed-pressurization at 20°C. Spr = productivity, mol/hr/kg of adsorbent. Solid lines and bold digits = experiment, short-dashed lines and italic digits = simulation.

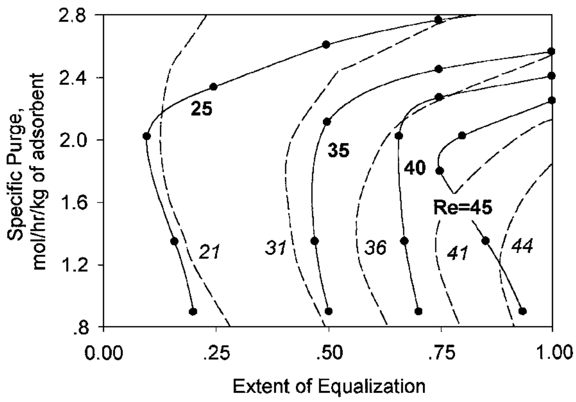

Figure 7. Experimental and theoretical recovery contour for different specific purge and equalization levels in case of feed-pressurization at 20°C. Re = percent oxygen recovery. Solid lines and bold digits=experiment, short-dashed lines and italic digits = simulation.

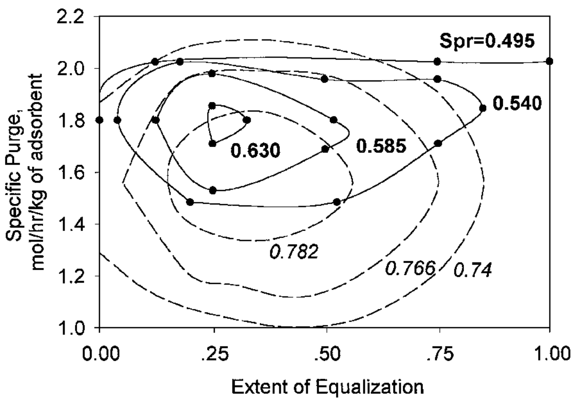

Figure 8. Experimental and theoretical productivity contour for different specific purge and equalization levels in case of product-pressurization at 30°C.

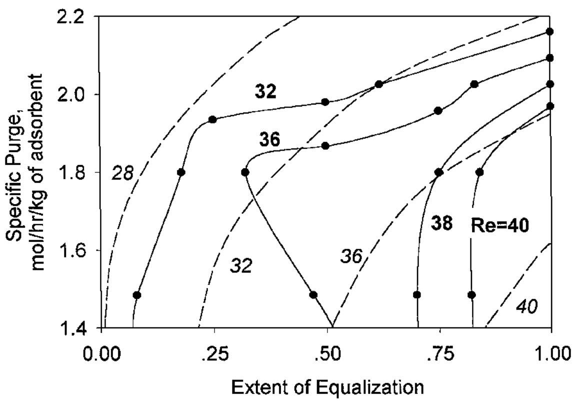

Figure 9. Experimental and theoretical recovery contour for different specific purge and equalization levels in case of product-pressurization at 30°C.

The corresponding contours in the case of product-pressurization are shown in Figs. 8 and 9. As for the feed-pressurization, there exists an optimum purging and an equalization level for the productivity as shown in Fig. 8 and the productivity at the optimal condition increases more than 15% than at complete and no equalization. Also, a maximum recovery is observed at full equalization as seen in Fig. 9 and optimum purging for the productivity is not affected by the extent of equalization, with a slightly lower value than that for the feed-pressurization. However, two differences are apparent. One is the lower maximum values of productivity and recovery for the product-pressurization. On the contrary, it is known that the product-pressurization gave a better performance. The possible explanation is a higher temperature during experiments of the product-pressurization. Due to insufficient facility, the laboratory could not be maintained at constant temperature. The room temperature was higher by about 10°C while conducting experiments of the product-pressurization due to hot summer weather. The assertion was confirmed by simulations, as described in the next section. The other is the shift of an optimum equalization level for the productivity to a lower value for the product-pressurization.

Simulation Results

Simulations were performed using the parameters in Table 1, which were measured in separate experiments. The adsorption pressure was set to 3 atm by considering pressure drop through a bed. Preliminary simulation studies showed that use of large spatial points in order to approximate equilibrium assumption resulted in a significant overestimation of performance. That implies that a process did not operate under the instantaneous equilibrium, even though step durations were determined to ensure equilibrium as possible. Especially, fast pressurization during an initial stage of pressurization steps and the resulting dispersion might contribute the deviation. In order to account for the effect, the number of spatial points was adjusted so as to fit experimental results. All of kinetic and dispersive effects were included implicitly into the effect of a number of

Table 1. Parameters used in simulations.

Adsorption pressure	3 atm	
Purge pressure	1 atm	
Bulk density	771 kg/m^3	
Bed void fraction	0.375	
Step durations(s)		
High-pressure feed: 30		
Cocurrent depressurization for pressure equalization: 10		
Countercurrent blowdown: 40		
Purge: 30		
Countercurrent pressurization for pressure equalization: 10		
Final pressurization: 40		
	at 293 K	303 K
$q_{s,O2}$ (mol/kg of adsorbent)	4.15	2.83
$q_{s,N2}$ (mol/kg of adsorbent)	2.88	2.74
b_{O2} (atm^{-1})	0.0283	0.0354
b_{N2} (atm^{-1})	0.126	0.104

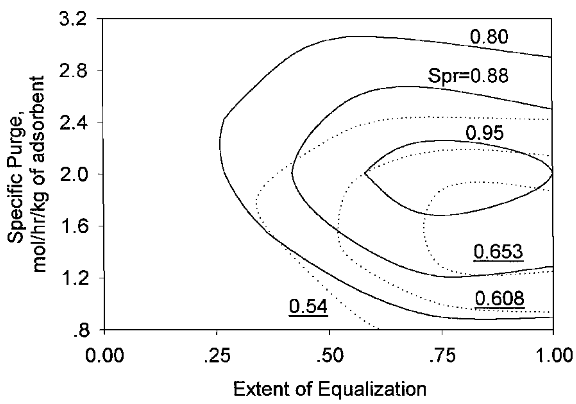

Figure 10. Theoretical productivity contour for different specific purge and equalization levels in case of feed-pressurization at 20 and 30°C. Solid lines = 20°C, dotted lines and underlined digits = 30°C.

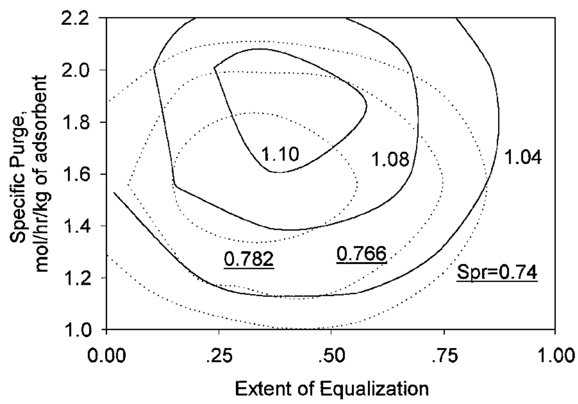

Figure 12. Theoretical productivity contour for different specific purge and equalization levels in case of product-pressurization at 20 and 30°C.

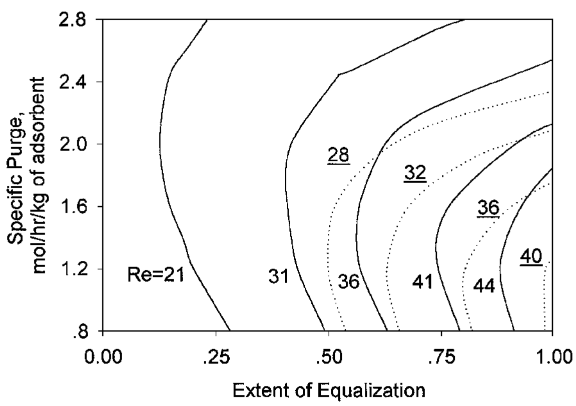

Figure 11. Theoretical recovery contour for different specific purge and equalization levels in case of feed-pressurization at 20 and 30°C. Solid lines = 20°C, dotted lines and underlined digits = 30°C.

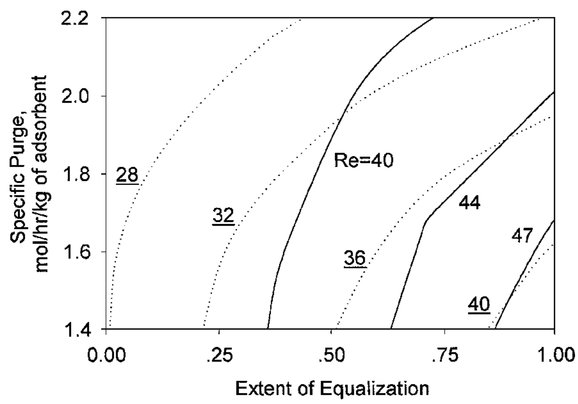

Figure 13. Theoretical recovery contour for different specific purge and equalization levels in case of product-pressurization at 20 and 30°C.

points. Even though this approach is purely empirical, it has advantage that no kinetic data is required. The selected number of points was 22. The simulated results for the feed-pressurization are shown in Figs. 6 and 7. The qualitative agreement between simulation and experiment is fairly good. Especially, the model predicted correctly existence of optimum conditions for the productivity and recovery; however, slight quantitative discrepancy was noticed.

Figures 8 and 9 illustrate the corresponding contours for the product-pressurization. The agreement is not as good as for the feed-pressurization. Despite quantitative disagreement, an optimum equalization level for the productivity was also predicted without significant discrepancy. The effect of temperature on process performance was examined by simulating processes at two different temperatures, 20 and 30°C. The results are shown in Figs. 10–13. At the identical temperature, the product-pressurization resulted in a better performance. Like in the experiment, the feed-pressurization at 20°C showed better results than the product-pressurization at 30°C. The optimum conditions were affected slightly by the temperature. For both pressurizations the optimum purging decreased by a small amount at higher temperature and the optimum equalization level changed slightly.

Conclusions

Through an intensive investigation of a two-bed PSA process with incomplete PE, optimum conditions for the productivity and recovery were indicated. Use of incomplete PE improved the productivity for feed-pressurization. For product-pressurization a maximum productivity was also observed at incomplete equalization level, but with a lower level than that for the feed pressurization. On the other hand, maximum recovery occurred at complete equalization for both pressurizations. The simulation predicted well existence of optimal conditions for productivity and recovery, but with qualitative discrepancy.

Nomenclature

- b Langmuir constant (atm^{-1})
- C Concentration of sorbate in gas phase (mol/cm^3)
- P Pressure of a bed (atm)
- q Concentration of sorbate in solid phase (mol/kg of adsorbent)
- q_s Saturated concentration of sorbate in solid phase (mol/kg of adsorbent)
- T Absolute temperature (K)
- t Time (s)
- U Interstitial gas velocity (cm/s)
- z Axial distance (cm)

Greek Symbols

- ε Bed void fraction
- ρ Bulk density (kg/m^3)

Subscripts

- A Light component
- B Heavy component
- E Effluent from other bed
- F Feed
- H High-pressure feed step
- i A or B
- L Bed length
- P Purge step

Acknowledgment

This study was supported by a grant (HMP-95-G-2-26) of the 1995 Highly Advanced National Projects on the development of Biomedical Engineering and Technology, Ministry of Health and Welfare, R.O.K.

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