

Novel simulated moving-bed adsorber for the fractionation of gas mixtures

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Abstract

The separation of propylene–propane mixture is an energy intensive operation commercially practiced using cryogenic distillation. The separation by pressure swing adsorption has been studied as an alternative. A fixed-bed pressure swing adsorption yields the heavy component as a pure product. The product recovery and the productivity are not high. In a moving-bed process, because of the counter-current solid–gas contact, the separation achieved is similar to that of the fractionation by distillation. Although the moving-bed operation offers the upper limit for the performance of a cyclic adsorptive process, due to mechanical complexities in the handling of solids the ‘simulated’ moving-bed is preferred. By moving the inlet and outlet ports of streams located along the length of the bed, a moving-bed process can be realized in a fixed bed. We describe here a ‘moving-port’ system which permits injection or withdrawal of the fluid along the axial direction in a fixed bed. A fixed bed embedded with the moving-port systems emulates a simulated moving-bed adsorber. The proposed adsorber can fractionate a binary gas mixture into two product streams with high purities. It is similar to the Sorbex process of UOP but does not have the eluent as an additional separating agent. A parametric study indicates that high purity products and a higher productivity by an order of magnitude can be achieved with simulated moving-beds compared to the fixed beds.

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1. Introduction

Adsorption, unlike distillation, is mostly carried out in a fixed bed or a multitude of fixed beds, as a batch or a cyclic process. In the fixed-bed adsorption, a sharp mass-transfer zone is formed and it traverses from one end of the bed to the other. The driving force for the mass transfer in this zone is small and it is virtually negligible on either side of the zone, as the flowing fluid is almost in equilibrium with the solid phase. As a consequence, the amount of stationary (solid) phase required is very high compared to that of a continuous counter-current process [1].

A moving-bed permits the counter-current contact of the solid and the gas, which enables to achieve a high driving force for interphase mass transfer, which in turn leads to high product purities and productivities. Berg [2] proposed a

moving-bed process which he called as hypersorption. In the hypersorption process the regeneration was done by thermal swing and it was used for recovering ethylene from refinery off gases. The hypersorption process can fractionate a binary mixture into two nearly pure products as in distillation. Kapfer et al. [3] carried out experimental studies on the fractionation of a gas mixture in a moving-bed adsorber. Szirmai [4] proposed a moving-bed process similar to the hypersorption but with batchwise desorption for the separation of the ethylene–ethane mixture. The desorption of the adsorbent by vacuum, direct heating or steam heating was proposed. He showed that the fractionation in a moving-bed is economical compared to distillation. However, the problems associated with the solid handling and the loss of adsorbent by attrition has made the moving-bed contactors less attractive.

The ‘simulated’ moving-bed (SMB) can overcome these difficulties associated with the moving-beds. UOP (Des Plaines, USA) successfully commercialized the SMB technology for the separation of liquid mixtures. These processes

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are known by the generic name Sorbex processes. The Sorbex process employs two separating agents, namely, the eluent and the adsorbent. The eluent can either be a gas or a liquid. Both products are diluted with the eluent and additional separation processes, like flash or fractional distillation, are required to get pure products.

In principle, the Sorbex process could be adopted for the separation of a gas or vapor mixture. However, it is mostly used to separate liquid mixtures since its commercialization in 1963. Storti et al. [5] used a six-port SMB for the vapor phase separation of a mixture of *m*-xylene and *p*-xylene. They used isopropyl benzene as the eluent and KY-Zeolite as the adsorbent. Morbidelli and coworkers [6] demonstrated the separation of a *n*-pentane and *iso*-pentane mixture in a six-port vapor phase SMB pilot plant using *n*-heptane as the eluent and 5A-Zeolite as the adsorbent. They reported that the separation efficiency is higher in a vapor-phase SMB unit compared to the liquid phase separation. Raghuram and Wilcher [7] compared and contrasted the separation of *n*-alkanes from a mixture of alkanes by the UOP's liquid-phase Sorbex process and the Union Carbide's vapor-phase Isosiv process. They concluded that the determination of the technology that best suits a particular situation needs an evaluation on a case-by-case basis. Ruthven and Ching [8] presented a state-of-art review of the moving-bed and simulated moving-bed adsorbers.

In the above processes an eluent has been used to regenerate the adsorbent. However, LaCava [9] used the principles of pressure swing to regenerate the adsorbent in a continuous counter-current adsorber. Only one separating agent, i.e. the adsorbent was employed. This process was named continuous counter-current pressure difference-driven adsorption processes (CCPDDAP). The production of high purity oxygen from an oxygen-rich mixture was studied. The advantages of these processes over the conventional PSA in terms of specific production and power requirements have been reported.

The advent of the Skarstrom cycle for air drying [10] is considered to be a milestone in the adsorptive separation.

Pressure swing was employed for the regeneration of the adsorbent and is referred to as pressure swing adsorption (PSA). It led to a phenomenal growth of the adsorptive gas separation. The original PSA cycle proposed by Skarstrom is for drying of air. Later he used the same cycle for recovering oxygen from air [11]. In the former process, there is only one component, namely moisture, which is transferred from one phase to the other, whereas in the other both oxygen and nitrogen are exchanged between the two phases. The drying of air is similar to absorption and the separation of air by adsorption is similar to distillation. The recognition of this distinction is important in the process design.

The propylene–propane mixture is difficult to separate by ordinary distillation. Cryogenic distillation is used to separate this mixture using a large reflux ratio in the range of 10–20, and the number of trays is in excess of 100. It is one of the most costly separations practiced in the chemical process industry. Alternately, several variants of the Skarstrom cycle have been employed for the separation of propylene–propane gas mixture [12–16]. Table 1 presents the experimental studies on the separation of propylene–propane mixture by PSA in fixed beds. These studies indicate that propylene of about 99.0 mol.% purity can be obtained. However, the product recovery and productivity are low. The separation achieved using the ‘ π -complexed adsorbents’ (*AgNO₃ dispersed on SiO₂ substrate*) developed by Rege and Yang [15] showed improvement in the product recovery. Though there is enhancement in product recovery, both the products are not of high purities.

In this work, we:

- (1) Classify adsorptive separation processes into absorption-like and distillation-like processes.
- (2) Describe a moving-port system to simulate a moving-bed operation in a fixed bed.
- (3) Present simulated moving-bed processes to achieve sharp separation.
- (4) Assess the potential of the proposed processes for the separation of the propylene–propane mixture.

Table 1
Compendium of the literature on the fixed-bed PSA separation of propylene/propane

Ref.	Adsorbent	Pressure (bar)		Bed parameters		Step time (s)	<i>T</i> (°C)	<i>F</i> ‘SLPM’	C ₃ H ₆		Productivity (mol kg (ads.) ⁻¹ h ⁻¹)
		<i>P_H</i>	<i>P_L</i>	<i>L</i> (m)	<i>D</i> (m)				Purity (%)	Recovery (%)	
[16]	Z 4A Z 13X	1.7	0.1	–	–	100	90.0	6.13	96.0	97.4	1.817
[12]	Ag ⁺ resin in packed bed	1.01	0.03	3.5	2.0		25.0	11855	90.0	87.6	2.744
	Ag ⁺ resin in magnetically stabilized bed			2.0	2.0	4800		12000	>99.0	<1.0	
[13]	AgNO ₃ /SiO ₂	1.0	0.1	3.0	1.0	1600	70.0	3770	99.05	43.58	0.015
	Z 4A					2400	100.0	1885	99.98	27.29	0.0035
[14]	Z 13X	5.0	0.5/0.1	0.8	0.016	480	150.0	2	99.3	12.5	0.822
[15]	AgNO ₃ /SiO ₂	7.09	0.20	3.0	0.50	240	120.0	235.6	98.52	71.65	0.062
	AlPO ₄ -14							1178.0	98.65	63.91	0.014

2. Mechanism of fractionation with pressure swing regeneration

In the following section, we bring out the salient differences between distillation-like and absorption-like adsorptive processes to understand the mechanism of adsorptive separations.

2.1. Distillation-like processes

Consider the adsorption equilibria of a gas mixture of components A and B in which both the components get adsorbed. At saturation, the amount of A in the adsorbate influences the amount of B that can get adsorbed. Fig. 1a depicts the equilibria on the x - y diagram, where x and y are the mole or mass fractions of the gas and the adsorbate, respectively. To completely represent the adsorption data, we need an additional diagram, i.e. q_T^c versus y or x diagram which is similar to the enthalpy-concentration diagram. We can define the separation factor as $\alpha = (y_A/x_A)(x_B/y_B)$ and it is analogous to the relative volatility. The separation of such a gas mixture in a moving-bed adsorber and in a distillation column is shown in Fig. 1b and c. To bring out the similarities, the solids were shown to flow upwards. Refluxes are required at both ends of the adsorber as in the distillation column. The enriching and stripping zones are similar to the enriching and stripping sections of a distillation column. The adsorbent can be regenerated in desorption section by applying vacuum or heating. The desorption section is similar to the condenser in its function. A part of the gas stream is drawn from the desorption section as extract product and the rest is refluxed to the enriching zone. This reflux is identical to the reflux at the top of a distillation column. A part of the gas is drawn from the stripping zone as the raffinate product and the rest is refluxed to presaturate the fresh adsorbent with the light component (less adsorbable component) before it enters the stripping zone. This flow of the light component

as adsorbate to the stripping zone is similar to the vapor flow from the reboiler to the column. The role of these refluxes in separation processes has been discussed by Rao [17].

In distillation-like processes, if the amount of adsorbate is constant, then equimolar counter exchange of A and B takes place. Further, near isothermal conditions prevail in the enriching and the stripping zones even in the absence of a provision for cooling or heating of the beds, if the heats of adsorption of both components are equal. Szirmay [4] has also discussed this aspect. On the other hand, there would be considerable cooling in the desorption section and heating in the presaturation section.

2.2. Absorption-like process

Now consider that only B is adsorbed. The adsorption equilibrium is similar to the absorption where only one component gets adsorbed. The equilibrium diagram can be represented in terms of X and Y as shown in Fig. 2a. Here, X is the mass or mole fraction of B in the gas phase and Y is the mass or mole fraction of B in the solid phase (or mol/kg of adsorbate may be used). It can be shown that the separation factor is infinite for such gas mixtures.

The similarity of a moving-bed adsorber with an absorber is shown in Fig. 2b and c. For the absorption-like process, there is only adsorption section and the refluxes at the ends of the adsorber are not required to obtain high purities. There can be a rise in temperature in the adsorption zone due to the heat of adsorption and an isothermal operation is not possible without cooling. The desorption section is similar to a solvent regenerator used to regenerate the solvent. However, there is no need to saturate the adsorbent that is being recycled as in the distillation-like process.

Identifying the nature of the adsorption equilibria and the classification into distillation-like and absorption-like processes helps in the design of the adsorber.

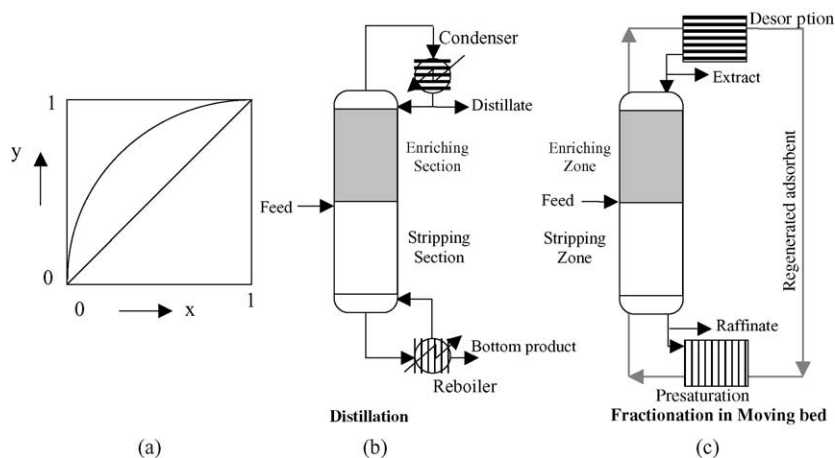


Fig. 1. Similarity of fractionation of gas mixtures in moving-bed adsorber with pressure swing and distillation.

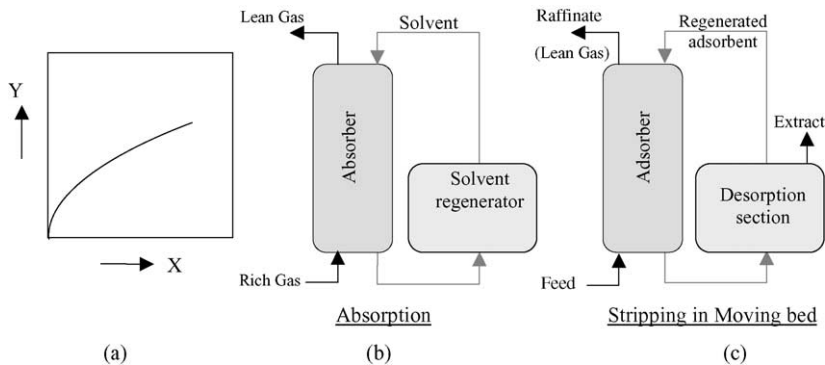


Fig. 2. Similarity of gas stripping in a moving-bed adsorber and absorption.

3. Moving-bed adsorber

In this section, we describe as to how one can achieve simulated moving-bed processes for carrying out the distillation-like and the absorption-like processes. Consider a circular moving-bed adsorber as shown in Fig. 3. A true counter-current contact can be achieved when the circular bed is rotated as a whole in the direction opposite to the flow of the fluid, holding the inlet and the outlet ports stationary. Thereby the different zones within the bed can be made stationary. In accomplishing a distillation-like process four zones are formed as depicted in Fig. 3. On the other hand, only the adsorption and desorption zones are formed in an absorption-like adsorptive process.

Alternately, we can achieve the same counter-current effect if the bed is held stationary and the ports are moved in the direction of flow of the fluid. In this mode of operation, the different zones move along with the ports. A circular bed is rather difficult to construct as compared to a straight bed. We propose to move the inlet and the outlet ports along the axial direction of a fixed bed to simulate the moving-bed operation. The movement of the ports is achieved using devices, hereafter; referred to as moving-port systems. We describe below one such moving-port system.

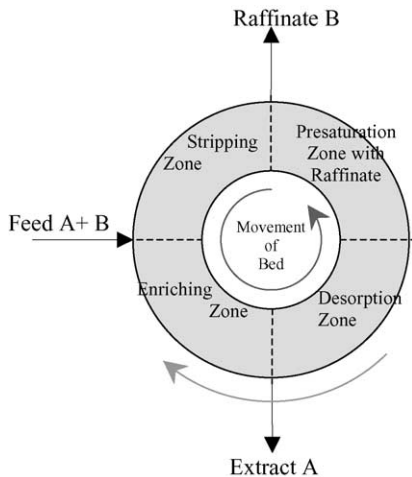


Fig. 3. Conceptual simulated moving-bed adsorber.

3.1. Moving-port systems

A sketch of a moving-port system is given in Fig. 4. It consists of two closely fitting circular tubes. The outer one has a straight slot along its length and the inner one a helical slot. A diamond-shaped port is formed where the slots cross each other. If either one of the tubes is rotated, the port moves from the left to the right or the other way depending on the direction of rotation. The speed of rotation sets the port velocity. When the port reaches one end of the slot, it abruptly shifts to the other end and continues to move in the same direction. It is possible to introduce or withdraw a fluid from a bed of solids if the moving-port system is embedded in the bed. By connecting the inner tubes of the systems to a train of gears driven by a motor or to individual stepper motors, the movement of ports could be synchronized. A suitable sealant has to be used to prevent the leakage of fluids into or out of the bed along the slots. It appears that several variants of moving-port systems are possible which facilitates the uniform injection or withdrawal across the cross section of the bed (a patent pending on the variants and the applications of the moving-port systems). Using these moving-port systems we can construct simulated moving-bed adsorbers of different configurations.

3.2. Single-bed configuration

A conceptual simulated moving-bed adsorber suitable for the fractionation of a gas mixture by distillation-like process is depicted in Fig. 5. There are five moving-port systems embedded in a fixed bed, one each for the inlet and the exit

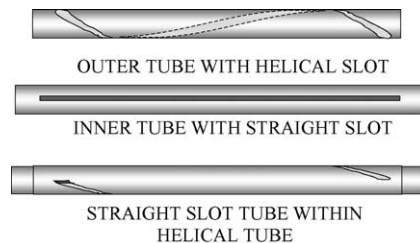


Fig. 4. Moving-port system with straight and helical slots.

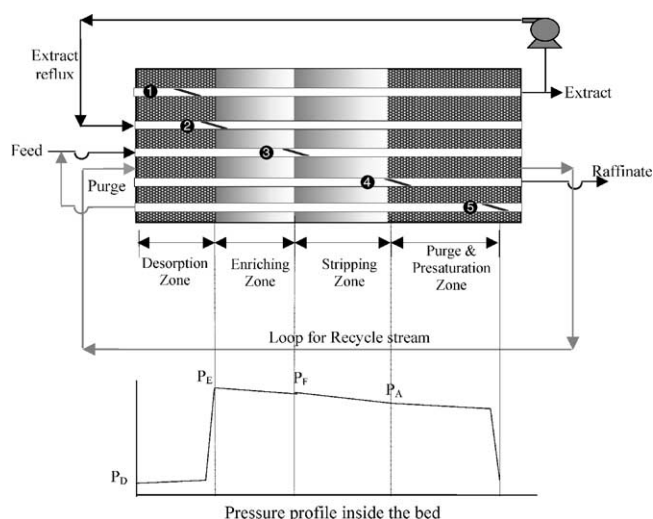


Fig. 5. Adsorptive fractionation of a gas mixture in a fixed bed adsorber embedded with moving ports.

streams. The moving-port systems are depicted as lines and the ports as thick slanted lines. The feed is introduced through port 3 at a pressure P_F . The zones between the ports 2 and 4 correspond to the stripping and the enriching zones. The feed flows towards port 4 due to the high pressure in the enriching zone. In the desorption zone, the desorbed gas is drawn through port 1. A part of the extract product is compressed and refluxed back at a pressure P_E , which is slightly higher than P_F to the enriching section through port 2. These zones move with the same velocity from the left to the right and the gas in the opposite direction. A part of the gas from the stripping section is drawn as the raffinate and the rest is used to purge and to presaturate the purge section. The loop line for the flow of the gas shown in the figure ensures smooth transfer of the sections from one end to the other. The pressure profile along the adsorber is shown in Fig. 5. Due to the adverse pressure difference present in a single bed, it is difficult to realize such operation. However, this configuration can be used to assess the potential for realizing high product purities and productivities.

3.3. Two-bed configuration

In order to overcome the difficulty mentioned above, we propose a two-bed scheme which can be realized in practice as shown in Fig. 6. Each bed has three moving-port systems. In the regeneration section, the moving-ports are inactive and they have not been shown for clarity.

The bed in front of the stripping zone is saturated with the raffinate and that behind the enriching zone is saturated with the extract. The raffinate product is withdrawn using the moving port 3. The moving ports 2 and 1 are used for introducing the feed and the extract reflux streams, respectively. When the stripping zone is about to move out of the bed, the raffinate withdrawal is stopped and the zone is allowed to move into the other bed which was saturated with

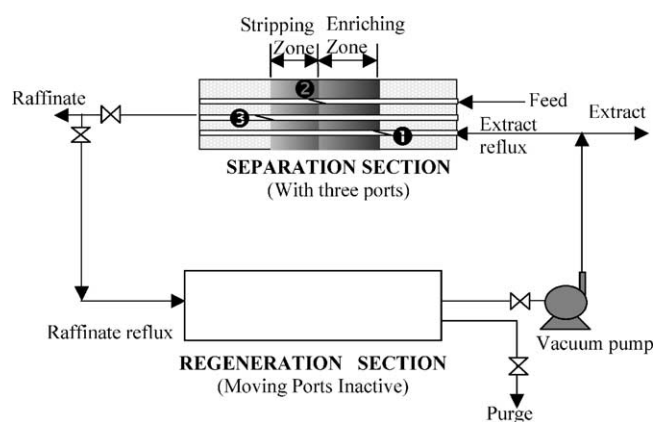


Fig. 6. Configuration of adsorber with moving ports for fractionation and pressure swing regeneration.

the raffinate. As the enriching zone leaves the bed, it is set for regeneration, purge and presaturation. From the regeneration section, the gas is withdrawn as the extract product by reducing the pressure using a vacuum pump and a part is sent to the other bed as the extract reflux after compression. A part of the raffinate stream is used to purge the regenerated bed. The purge effluent can be recycled along with the fresh feed. The regenerated bed is then presaturated by pressurizing the bed with the raffinate to the adsorption pressure. The stripping, enriching, regeneration by pressure swing, purge and pressurization steps are staggered in between the two beds. The switching of the streams in between the two beds can be accomplished using solenoid valves.

Rao et al. [18] discussed the thermal regeneration in SMB with moving-port systems. The thermal regeneration can be accomplished in a shorter time compared to fixed beds because of the moving-port systems. The direction of gas withdrawal in the regeneration step can be done either in a co-current or counter-current to the direction of the gas flow. The latter mode appears to have advantage and requires evaluation. It may be mentioned that it is feasible to carry out continuous distillation-like process using four fixed beds [19].

For the absorption-like process only two moving-ports are required in each bed and only the stripping zone is formed.

To assess the potential of the proposed adsorber in achieving high product purities with an increased productivity, we have used the separation of the propylene–propane mixture using silica gel as adsorbent. The adsorption phase equilibria indicate that the separation has to be carried as a distillation-like process. We have employed the single-bed configuration adsorber for the modeling and simulation studies and the details are given below.

4. Mathematical model

Fig. 7 shows the process steps involved and the notation employed in the modeling and simulation. The gas and adsorbate flow rates are represented by L and V , respectively,

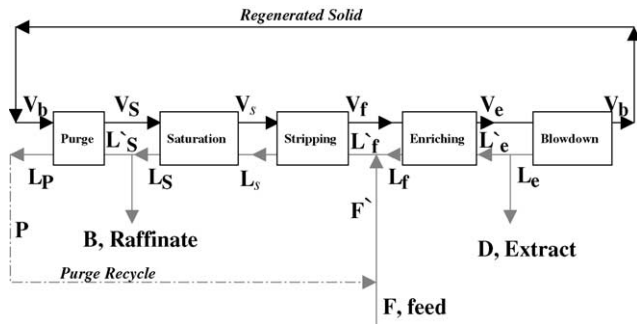


Fig. 7. Schematic of the SMB adsorber.

and their subscripts indicate the streams entering and leaving the various sections. The stripping, enriching and the purge sections are considered to be counter-current contactors.

The following assumptions are used:

- (i) Steady-state operation.
- (ii) Isothermal conditions.
- (iii) Plug flow of gas.
- (iv) Purge, stripping and enriching sections are at uniform pressure and the adsorbent is at saturated condition.
- (v) The “linear driving force” (LDF) approximation is applicable [20].

Fig. 8 shows a differential volume of length ‘dz’ in the bed. A mass balance of component ‘i’ in the solid phase gives:

$$v_s \frac{dq_i}{dz} = N_i \quad \text{for } i = 1, 2 \quad (1)$$

and

$$N_i = x_i N_T + J_i \quad \text{for } i = 1, 2 \quad (2)$$

where, N_i is the interphase transfer rate (taken as positive if the transfer is from the gas to the solid) and N_T (i.e. $\sum_{i=1}^n N_i$) is the net rate of moles exchanged across the interphase and is determined as given below:

$$N_T = v_s \frac{dq_T^e}{dz} \quad (3)$$

Under the saturated condition, strictly speaking, a single mass-transfer coefficient has to be used in estimating J_i (in Eq. (2)) for the binary system as is done for distillation. However, in the literature two mass-transfer coefficients have been

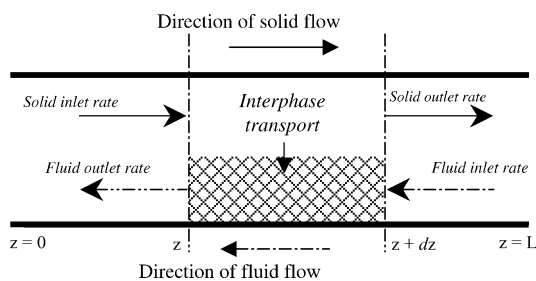


Fig. 8. Differential volume of a counter-current bed adsorber.

used, one for each component. This amounts that the adsorption of one component is unaffected by the other which is contrary to what is implied in the use of the extended Langmuir equation. Which of these is valid in reality requires an evaluation based on the carefully designed experimental investigation.

To evaluate the diffusional flux J_i , we have assumed that the pore diffusion is rate controlling, and the flux for the adsorption in a particle can be satisfactorily represented by the LDF model and the expression is given below:

$$J_i = k_q(q_i^e - \bar{q}_i) \quad \text{for } i = 1, 2 \quad (4)$$

where

$$k_q = \frac{15\epsilon_p D_c}{r_p^2 \tau_p} \frac{c_T}{q_T^e} \frac{\Delta x}{\Delta y} \quad (5)$$

In Eq. (5), D_c is the combined diffusivity and is given as a combination of the molecular diffusivity, D_m and the Knudsen diffusivity, D_k as given below:

$$\frac{1}{D_c} = \frac{1}{D_m} + \frac{1}{D_k} \quad (6)$$

Similarly, a mass balance of component ‘i’ in the gas phase yields

$$\frac{d(vc_i)}{dz} - \frac{(1 - \epsilon_b)}{\epsilon_b} (x_i N_T + J_i) = 0 \quad \text{for } i = 1, 2 \quad (7)$$

Summing up for all the components, we get

$$v \frac{dc_T}{dz} + c_T \frac{dv}{dz} - \frac{(1 - \epsilon_b)}{\epsilon_b} N_T = 0 \quad \text{for } i = 1, 2 \quad (8)$$

When the pressure is uniform across a section, Eq. (5) reduces to

$$\frac{dv}{dz} = \frac{1}{c_T} \frac{(1 - \epsilon_b)}{\epsilon_b} N_T \quad (9)$$

Substituting Eq. (9) in Eq. (8), we get

$$\frac{dc_i}{dz} = \frac{1}{v} \frac{(1 - \epsilon_b)}{\epsilon_b} J_i, \quad i = 1, 2 \quad (10)$$

To obtain the interphase transfer rates, velocity and the composition profiles of the gas and the solid phase in the stripping, enriching and purge sections, Eqs. (1), (9) and (10) are to be solved with the initial conditions given below:

Stripping section :

$$\text{I.C. at } z = 0, \quad x = x_{si}, y = y_{si}, v = v_0 \quad (11)$$

Enriching section :

$$\text{I.C. at } z = 0, \quad x = x_{fi}, y = y_{fi}, v = v_0 \quad (12)$$

Purge section :

$$\text{I.C. at } z = 0, \quad x = x_{pi}, y = y_{bi}, v = v_0 \quad (13)$$

The saturation by pressurization and the evacuation can be rigorously modeled as transient process. For the sake of simplicity, we have considered these processes as similar to flash distillation or a single equilibrium stage process. Therefore, the streams leaving the stage are considered to be in equilibrium.

The solid-phase equilibrium concentration q_i^e can be estimated by the extended Langmuir isotherm given below.

$$q_i^e = \frac{q_{si} b_i P_i}{1 + \sum_{j=1}^n b_j P_j} \quad i = 1, 2 \text{ and } n = 2 \quad (14)$$

5. Simulation of the SMB adsorber

We have simulated the performance of the SMB adsorber for the two cases as given below:

- (i) Complete regeneration.
- (ii) Partial regeneration with a raffinate purge.

The parameters used in the simulations are given in Table 2. The specification variables for the simulation are: F , x_F , x_E , v_s , P_H , P_L , R_P , T .

5.1. Complete regeneration

In this case there is no need of purge, and blowdown section is equivalent to a total condenser. We have set the V_b to be zero and the streams B and D were calculated from the overall material balance. The V_S was estimated by considering the adsorbent is saturated with the gas of composition x_B . Using the V_S , L_S as the initial conditions, Eqs. (1), (9) and (10) were solved till the gas composition reached the feed composition to obtain the stripping length, the gas and the adsorbate flow rates and the compositions using the fourth order Runge–Kutta method [21]. Using the V_f , L_f as the ini-

tial conditions the enriching section zone length, flow rates and the compositions were obtained by integrating the equations till x_D is reached.

5.2. Partial regeneration with a raffinate purge

In the case of partial regeneration the bed is not completely regenerated. V_b was computed by setting the adsorbate composition y_B to be in equilibrium with the extract composition x_D . We require the initial conditions and the V_S and L_S' to solve the purge section. We have found L_S' from the purge ratio. Setting their compositions as x_B , we have found the L_p and x_p from the material balance. Using the V_b , y_b , L_p and x_p as the initial conditions, the end streams of the purge section were found by solving Eqs. (1), (9) and (10) by the fourth order Runge–Kutta method. The material balance around the saturation section was made as mentioned earlier to obtain the initial conditions of the stripping section. The integration was performed using the fourth order Runge–Kutta method to simulate the stripping and enriching sections. The recycle and the feed streams have been added into the calculations at appropriate locations as shown in Fig. 7.

The productivity is calculated as the amount of extract obtained per unit weight of the adsorbent per unit time. The theoretical energy requirements are calculated based on adiabatic compression and the method is outlined by Kota [22].

6. Results and discussions

6.1. Complete regeneration

We have set the desired purities of the extract and the raffinate products as 99.0 mol.% propylene and 99.0 mol.% propane and simulated the performance of the adsorber.

The flow rates and compositions of the streams in different sections can be graphically depicted on the well known McCabe–Thiele diagram [23]. Fig. 9 depicts the performance of the adsorber on the McCabe–Thiele diagram. The operating lines for the enriching and the stripping sections were plotted from the mole fractions of propylene in the gas and the solid phases computed along these sections as discussed in the previous section. It can be seen that both the operating lines meet on the vertical line passing through the feed composition x_F . It is the 'q-line' for adsorption. It may be noted that the operating lines are not straight lines, as to be expected, since q_T^e varies with the mole fraction of propylene. They would have been straight lines had q_T^e been constant. However, the operating lines are nearly constant and the McCabe–Thiele assumptions appear to hold good for this system. With increase in the extract reflux ratio, the operating lines moved towards the x – y line. It is possible to operate the adsorber at total reflux as in the case of distillation.

Fig. 10 shows the variation of the mass-transfer zone lengths with the extract reflux ratio. It can be seen that the zone lengths pass through minima. It is counter intuitive

Table 2
Parameters used for the fractionation of propylene–propane on silica gel [24]

Physical properties of adsorbent	
Bulk density of adsorbent	1260 kg/m ³
Bed diameter	0.035 m
Bed void fraction	0.4
Tortuosity factor	2.5
Particle radius	0.5 mm, 0.25 mm
Particle porosity	0.4
Langmuir isotherm model parameters	
$b_{C_3H_6}$	0.2778 m ³ /mol
$b_{C_3H_8}$	0.1307 m ³ /mol
$q_{sC_3H_6}$	2000 mol/m ³
$q_{sC_3H_8}$	1429 mol/m ³
Operating variables	
Feed composition	50% C ₃ H ₆
Extract composition	99% C ₃ H ₆
Raffinate composition	99% C ₃ H ₈
Temperature	303 K
Adsorption pressure	1.0 atm
Molecular diffusivity	6.0 × 10 ⁻⁶ m ² /s at 1 atm
Knudsen diffusivity	5.6 × 10 ⁻⁷ m ² /s

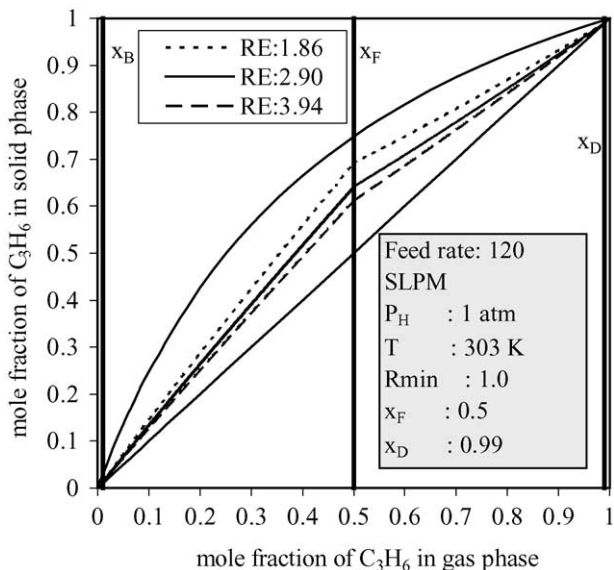


Fig. 9. Performance of the adsorber in the McCabe–Thiele diagram.

because the McCabe–Thiele diagram indicates the required number of stages or transfer units is infinite for the minimum reflux and decreases monotonically as the reflux approaches the total reflux. But, the implicit assumption is that the stages are equilibrium stages or the height of the transfer unit is held constant by varying the diameter. In the present case, the diameter is held constant. Therefore, as the reflux increased from the minimum reflux, the flow rate of gas increased and the number of transfer units decreased but the height transfer unit increased even more. Therefore, the zone lengths passed through a minimum. A similar trend is expected for distillation in a packed column.

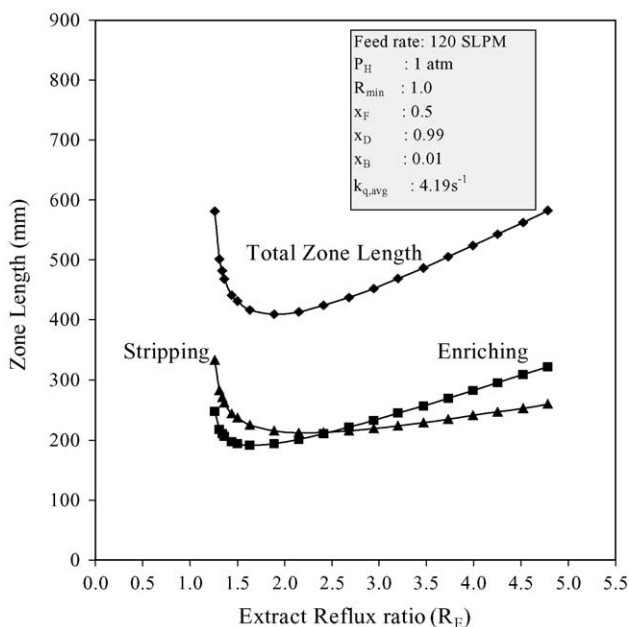


Fig. 10. Effect of the extract reflux ratio on zone lengths.

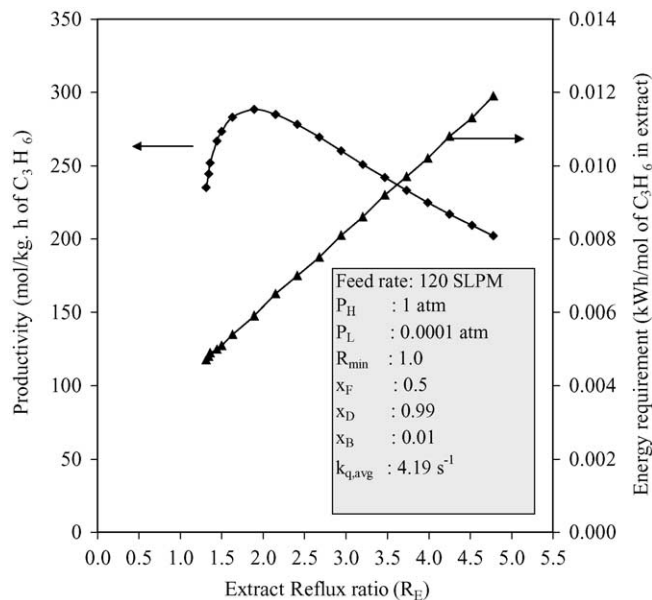


Fig. 11. Effect of extract reflux ratio on productivity and energy requirement.

Fig. 11 shows the variation of productivity and the theoretical energy requirements. The latter has been computed by setting $P_L = 0.0001$ atm at which the bed is almost free from the adsorbate (1 atm = 101,325 Pa). The productivity is in the range of 100–300 mol kg⁻¹ h⁻¹, whereas the productivity in conventional PSA is 3 mol kg⁻¹ h⁻¹ or less. This is because of the driving force with the counter-current flow is higher than the one in the conventional PSA.

6.2. Partial regeneration with a raffinate purge

The regeneration at high vacuum is not cost effective. As the regeneration pressure increases, a significant amount of propylene is carried by the adsorbent to the saturation section. This leads to the lowering of the raffinate purity and hence the recovery of propylene. We have explored how the regeneration pressure affects the product purities. The recovery of propylene can be increased purging the bed with propane as shown Fig. 7. Fig. 12 shows the operating lines on the McCabe–Thiele diagram. The purge operating lines are above the x - y line because the propylene is getting stripped from the bed using the raffinate as eluent. It can also be seen that the lines are highly curved indicating that the gas and the adsorbate flow rates vary substantially along the purge section. The end of the stripping operating line is away from the diagonal as the adsorbent retained propylene even after the purge.

The effect of the extract reflux ratio on the performance of the adsorber with purge at a regeneration pressure of 0.01 atm has been shown in Figs. 13 and 14. For the particle diameter of 1 mm, the zone lengths were in the range of 3700–5800 mm and the productivities were in the range of 20–32 mol kg⁻¹ h⁻¹.

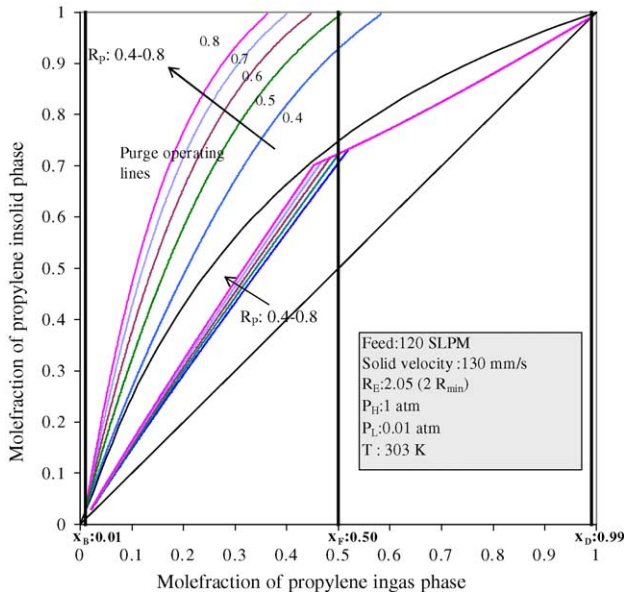


Fig. 12. Performance of the adsorber with purge in the McCabe–Thiele diagram.

As the zone lengths were very high, we have examined if these zone lengths could be decreased by decreasing the particle diameter. Figs. 15 and 16 present the variation of the zone lengths with the reflux and purge ratios for the particle diameters of 1 mm and 0.5 mm at three different P_L . For both ratios the zone lengths exhibited minima. The total zone lengths (sum of the enriching, stripping and purge zones) for the lower size particle were smaller than the larger size particle since the mass-transfer coefficient increased with the decrease in the particle size. For the particle size of 0.5 mm, the zone lengths became smaller by four times. The pressure drop for smaller size was found to be lower as zone length

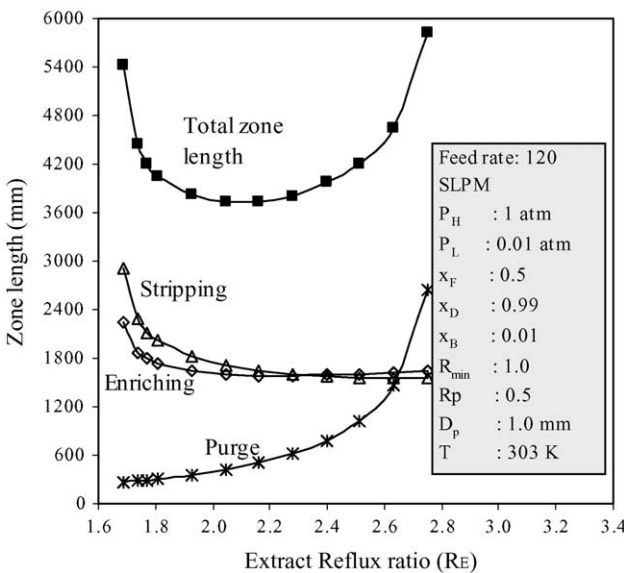


Fig. 13. The effect of extract reflux ratio on zone length.

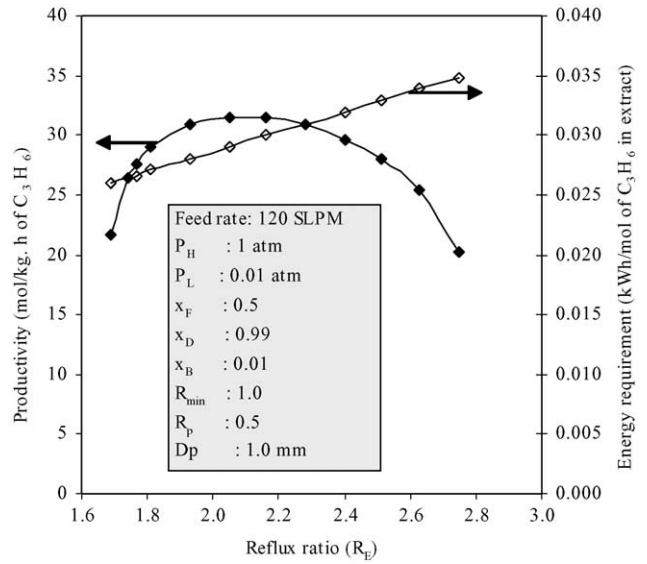


Fig. 14. The effect of the extract reflux ratio on productivity and the energy requirement for the adsorber with purge.

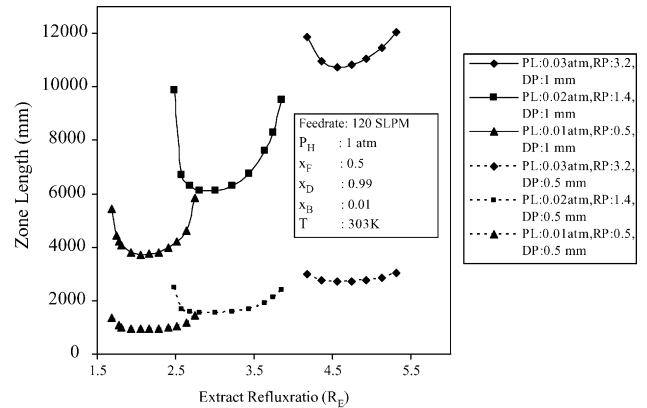


Fig. 15. Effect of extract reflux ratio on total zone length with varying P_L and particle diameters.

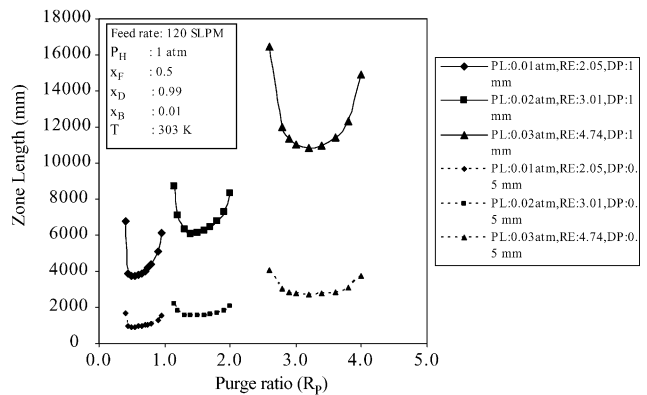


Fig. 16. Effect of purge ratio on total zone length with varying P_L and particle diameters.

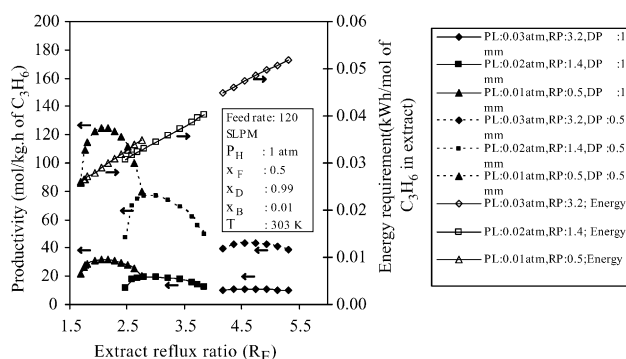


Fig. 17. Effect of reflux ratio on productivity and energy requirement.

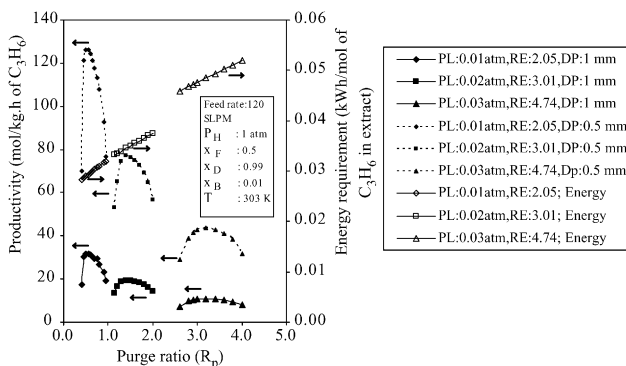


Fig. 18. Effect of purge ratio on productivity and energy requirement.

was lower though the pressure drop per unit length was larger with smaller size particles.

The effect of the extract reflux ratio and the purge ratio on productivity and the energy requirement are shown in Figs. 17 and 18. The productivity exhibits a maximum with the variation of both purge and reflux ratios. We did not consider the pressure drop across the sections in the energy requirement calculations. Therefore, the energy requirement calculated was independent of the particle diameter. For realistic case, the optima of reflux ratio, purge ratio, particle diameter and P_L have to be determined considering the pressure drop across the zones as well. The purge ratio increased with increase in P_L to obtain the specified separation. With the increase in purge ratio the energy requirement increased and the productivity decreased. It is desirable to employ as high a P_L though its optimum value has to be determined based on economic considerations. It was found that we can employ 0.03 atm to get desired separation. The pressure higher than 0.03 atm led to lower values of purity of the products.

7. Conclusions

We have presented a moving-port system which, when embedded into a fixed bed, facilitates the continuous movement of the port along the bed for the injection and withdrawal of a

fluid. We have described how to realize the simulated moving-bed process in practice for fractionation of a gas mixture using pressure swing for regeneration. To assess the performance of the idealized simulated moving-bed adsorber, we studied the fractionation of the propylene–propane mixture. It is shown that it is possible to achieve clean separation of the mixture. The productivity of the idealized adsorber is a few orders of magnitude compared to the conventional PSA process. The proposed adsorber appears to hold high promise as an alternative to conventional PSA and cryogenic distillation.

8. Nomenclature

A	cross-sectional area of the adsorber bed (m^2)
B	moles of the raffinate (mol/s)
b_i	Langmuir constant of component i (mol/m^3) ⁻¹
c_T	total gas-phase molar concentration (mol/m^3)
c_i	gas-phase molar concentration of component i (mol/m^3)
D	moles of the extract (mol/s)
D_c	combined diffusivity (m^2/s)
D_k	Knudsen diffusivity (m^2/s)
D_M	molecular diffusivity (m^2/s)
D	extract flow rate (mol/s)
F	feed flow rate (mol/s)
J_i	diffusional flux of component i (mol/s)
k_q	mass-transfer coefficient (s^{-1})
L	molar flow rate of the gas in the adsorber (mol/s)
N_i	molar rate of interfacial transfer for component i (mol/s)
N_T	total molar flux (mol/s)
n	number of moles in the gas phase (mol)
P_A	stripping section pressure (atm)
P_E	enriching section pressure (atm)
P_D	desorption section pressure (atm)
P_F	feed gas pressure (atm)
P_H	high pressure (atm)
P_L	low pressure (atm)
P	total pressure in the fluid phase (atm), moles of purge effluent (mol/s)
q_i	solid-phase molar concentration of component i (mol/m^3)
\bar{q}_i	average solid-phase molar concentration of component i (mol/m^3)
q_i^e	solid-phase molar concentration in equilibrium with c_i (mol/m^3)
q_{si}	saturation constant of component i (mol/m^3)
q_{T_s}	total solid-phase molar concentration at saturation (mol/m^3)
R	universal gas constant ($atm\ m^3\ gmol^{-1}\ K^{-1}$)
R_E	extract reflux ratio
R_p	purge ratio
r_p	radius of the adsorbent particle (m)
T	temperature (K)

V	molar flow rate of the adsorbate in the adsorber (mol/s)
v	interstitial fluid velocity (m/s)
v_0	local interstitial fluid velocity (m/s)
v_s	solid velocity (m/s)
X	mole (mol/kg adsorbate) or mass fraction (kg/kg adsorbate) in the gas phase
x	mole fraction of heavy component in gas phase
x_D	extract purity
x_B	raffinate purity
Y	mole (mol/kg adsorbate) or mass fraction (kg/kg adsorbate) in the solid phase
y	mole fraction of heavy component in solid phase
y_i	mole fraction of the adsorbed component 'i' in gas phase
Z_T	total zone length (mm)
z	axial distance (m)

Greek letters

α	separation factor
ϵ_b	bed voidage
ϵ_p	particle voidage
μ	viscosity of the fluid phase ($\text{kg m}^{-1} \text{s}^{-1}$)
ρ	density of the fluid phase (kg/m^3)
τ_p	tortuosity factor

Superscripts

e	equilibrium condition
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Subscripts

B	raffinate
b	blowdown
D	extract
e	enriching
F	fresh feed
F'	fresh feed + recycle
f	enriching gas outlet/solid inlet
i	number of components
j	number of components

n	number of components
p	purge
S	saturation
s	stripping

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