A Short Note
The Optimal Design of Pressure Swing
Adsorption Systems: Part II

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Introduction

A previous paper (Smith and Westerberg, 1991) detailed primarily the second step in a proposed three step design scenario for pressure swing adsorption (PSA) separation system design. This paper presents the details the third step and presents an example of the use of this methodology in the design of a PSA system.

The problem decomposition strategies previously given will first be used to illustrate the design decisions better and then to help facilitate the solution of the design problem. The resulting design is simulated rigorously to assure feasibility.

1. Proposed Design Scenario

Suppose that PSA is being considered as a potential method to perform a necessary separation task. The feed stream conditions (i.e. temperature, pressure, and composition) as well as a number of possible adsorbents are assumed to be specified. Also, it is assumed that the minimum separation task (i.e. the minimum acceptable purity of the product stream) to be performed is known. It has been proposed (Smith and Westerberg, 1991) that the design procedure for such a PSA system can be performed by the following approach:

1. Perform preliminary experiments and/or simulations to determine the values of some of the key parameters of the system.

2. Make appropriate model simplifications and perform a design optimization.

3. Perform additional experiments and/or simulations to verify that the structure and operating conditions obtained is correct If it is not correct, then modify the parameter values and return to step 2.

This method is basically an inside-out optimization procedure since a simplified model is being used in a small region to approximate rigorous hard-to-calculate models. Care must be taken so that information is not overlooked that leads to a suboptimal solution point (Biegler et al., 1985).

By the use of this approach, it is hoped that the number and amount of both laboratory and

parameter studies necessary to determine the correct operating structure and conditions can be reduced. The use of this procedure will be illustrated by an example problem.

Example Problem Specification

The example problem below is similar to that given previously (Smith and Westerberg, 1991) with only slight differences in the parameter values. It is desired to continuously produce a purified hydrogen stream from a stream of hydrogen and methane. A PSA system is being considered as one of the alternatives to perform this separation task. The given specifications for the feed stream, the adsorbent, and the process economics are presented in Table 1-1, where component A is Methane. The methane concentration can be considered to be trace, and the hydrogen can be considered to be inert to the adsorbent.

Preliminary woric suggests considering a PSA system with operations similar to the Skarstrom cycle (Skarstrom, 1960) with the possibility of including either zero, one, two, or three pressure equalization operations in the sequence. Thus, the overall operation sequence that contains all these possible operations is:

1: O_x (Adsorption and production of product gas)
2: O_2 (Pressure equalization with low pressure operation O_8)
3: O_3 (Pressure equalization with low pressure operation 0_7)
4: O_4 (Pressure equalization with low pressure operation $O^\wedge$
5: O_5 (Blowdown and counter-current purge with product gas)
6: O_6 (Pressure equalization with high pressure operation OJ
7: O_7 (Pressure equalization with high pressure operation O_3)
8: O_8 (Pressure equalization with high pressure operation O_2)
9: O_9 (Repressurize with feed gas)

It will be prespecified that operations O_v O_5, and O_9 must always occur, whereas, operations O_v O_v O_4, $\langle 9_6$, O_v and $O_\%$ are allowed to vary since they determine the above specification of either zero, one, two, or three pressure equalization operations in the sequence.

Before continuing with the overall design of the system, a detailed analysis will be performed on the three major components of cyclic scheduling, dynamic simulation, and optimization. The insight gained from these analyses will allow the solution of the problem to be determined more easily.

$c_{p,A}$	3.68 x 10^4 $\frac{-gJ}{Kgmole\,K}$
c_{pB}	2.93 x 10^4 $\frac{J}{Kgmole\,K}$
$c_{p,ads}$	8.04 x 10^5 $\frac{J}{m^3\,K}$
dr	0.125 $\frac{1}{-}$
Ft''_{18}	3.111 x 10^{-2} $\frac{Kgmole}{sec}$
H_A	8.90 x 10^8 $\frac{J}{Kgmole}$
tiD_{tf}	Z.oO X 1U $\frac{.}{Kgmole}$
Pr_B	3.5 $\frac{\$}{Kgmole}$
tg''	350 AT
r_A	298 JC
P_A	2.45 x 10^6 Fa
r_{pfr}	2 yr*
fax	0.4
^	0.05
e	0.44
Pa^	**800** $\frac{\$}{m}$

Table 1-1: Modeling Parameters used for Example Problem

Cyclic Scheduling

The cyclic scheduling problem given above may be formulated and solved separately from the overall optimization problem by using reasonable estimates for the operation times and other design variables that need to be fixed for this analysis (Smith and Westerberg, 1990). The scheduling of this problem was previously given (Smith and Westerberg, 1991). A possible schedule that results from this analysis for each of the four sequences is shown in Figure 1-1.

2,0,0,0

#			
1	01	05	09
2	O5	O9	01

3,1,0,0

#					
1	01	O2	O5	08	09
2	08	09	01	02	05
3	O2	05	08	09	01

4,2,1,0

#							
1	01	02	03	05	07	08	09
2	08	09	01	02	03	05	07
3	05	07	O8	O9	01	02	O3
4	02	03	05	07	08	09	01

5,3,2,1

#									
1	01	02	03	04	05	06	07	08	09
2	O8	09	01	02	03	04	05	06	07
3	06	07	O8	09	01	02	03	04	05
4	04	05	06	07	08	09	01	02	03
5	02	03	O4	05	06	O7	08	09	01

Figure 1-1: Possible Schedules for Four Operation Cases

Dynamic Simulation

For this process it is assumed that methane can be considered a trace component and that all operations are isothermal. A mathematical model of the Skarstrom PSA system similar to that of Raghavan et al. (Raghavan et al., 1985) with the following approximations will be used:

1. The feed consists of a single trace component in an inert carrier.

2. The system is isothermal with negligible axial pressure drop.

3. The concentration of the solid phase is frozen during the depressurization and repressurization operations.

4. Axial dispersion is negligible.

The dimensionless component mass balance equation for this problem becomes:

$$\frac{\partial Y_i}{\partial \tau} = - \frac{}{L} \frac{}{dY} - \frac{(1-\varepsilon)}{\varepsilon} \frac{RTq_{scale}}{Pt_{end}} \frac{\partial \overline{q}_i}{\partial \tau} \tag{1}$$

where r_{end} is the duration of the operation and q_{scale} is the solid concentration in equilibrium with the feed gas. The dimensionless parameters are:

$$x = \frac{t}{\tau} \qquad \overline{z} = \frac{z}{j} \qquad \overline{q}_i = \frac{q_i}{} \tag{2}$$

The mass transport processes are assumed to be well described by the linear driving force (LDF) model so the solid phase concentration is modeled by:

$$\frac{\wedge}{\partial \tau} = \frac{KpKnd_i}{q_{scale}} (q_i^* - q_{scale}\overline{q}_i) \tag{3}$$

where k_{o_p} is the LDF mass transfer coefficient for the modeled operation. The equilibrium isotherm is assumed to be given by a loading ratio correlation (LRC) equilibrium isotherm with the constants given by Cen and Yang (Cen and Yang, 1986).

The boundary condition for the adsorption and purge operations were respectively:

$$Y_i(\overline{z}=0,\tau) = Y_i^o \tag{4}$$

$$Y_i(\overline{z}=1,\tau) = 0 \tag{5}$$

In the depressurization and repressurization operations, the solid phase concentration of the adsorbable component, $''\overline{q}_{i\%}$ is assumed not to change (frozen solid assumption) during the operation. For the depressurization and repressurization operations, the gas phase concentration, $Y_{i\%}$ is averaged across the whole bed at the end of the operation.

Values for the linear driving force (LDF) mass transfer coefficients for the adsorption and purge operations, k_{op}, are important to the final solution and must be estimated well. The larger the coefficients the closer the system will be to equilibrium and the smaller the mass transfer zone (MTZ).

Figures 1-2 and 1-3 show the solid and gas concentration profiles respectively after the adsorption and desorption operations for the system parameters given in Table 1-2 and the operation parameters given in Table 1-3 for the system using three pressure equalization operations.

An initial guess of the bed utilization and efficiency parameters can be calculated from this simulation. Since the majority of adsorption occurs at equilibrium, from Figure 1-2, the adsorption efficiency is $r^\wedge = 1$. By integrating the solid concentration profiles, the moles of methane adsorbed or desorbed during an operation, $m\pounds>$ can be calculated.

$$m_A^{s,e} = (1 - \varepsilon)\, q_{scale} \frac{\pi d^2 L}{4} \int_0^1 \overline{q}\, d\overline{z} \tag{6}$$

The integration of the solid profiles after adsorption and desorption, Figure 1-2, gives ty_{Ads} and $\S_{Des}$ to be 0.88 and 0.99, respectively. The efficiency of desorption, $r|_{Des}$, is calculated as the ratio of the amount of incoming hydrogen during desorption to the amount of methane removed from the bed to be 1.26.

Optimization

Due to the shape of the concentration profiles, the time integrated mass and energy balances given previously (Smith and Westerberg, 1991) without any modifications should sufficiently describe the behavior of this system. All binary and integer scheduling variables are fixed at the values determined above. Thus the design optimization problem can be solved by the solution of four nonlinear optimization problems (NLP).

Solid Concentration   (q/q*)

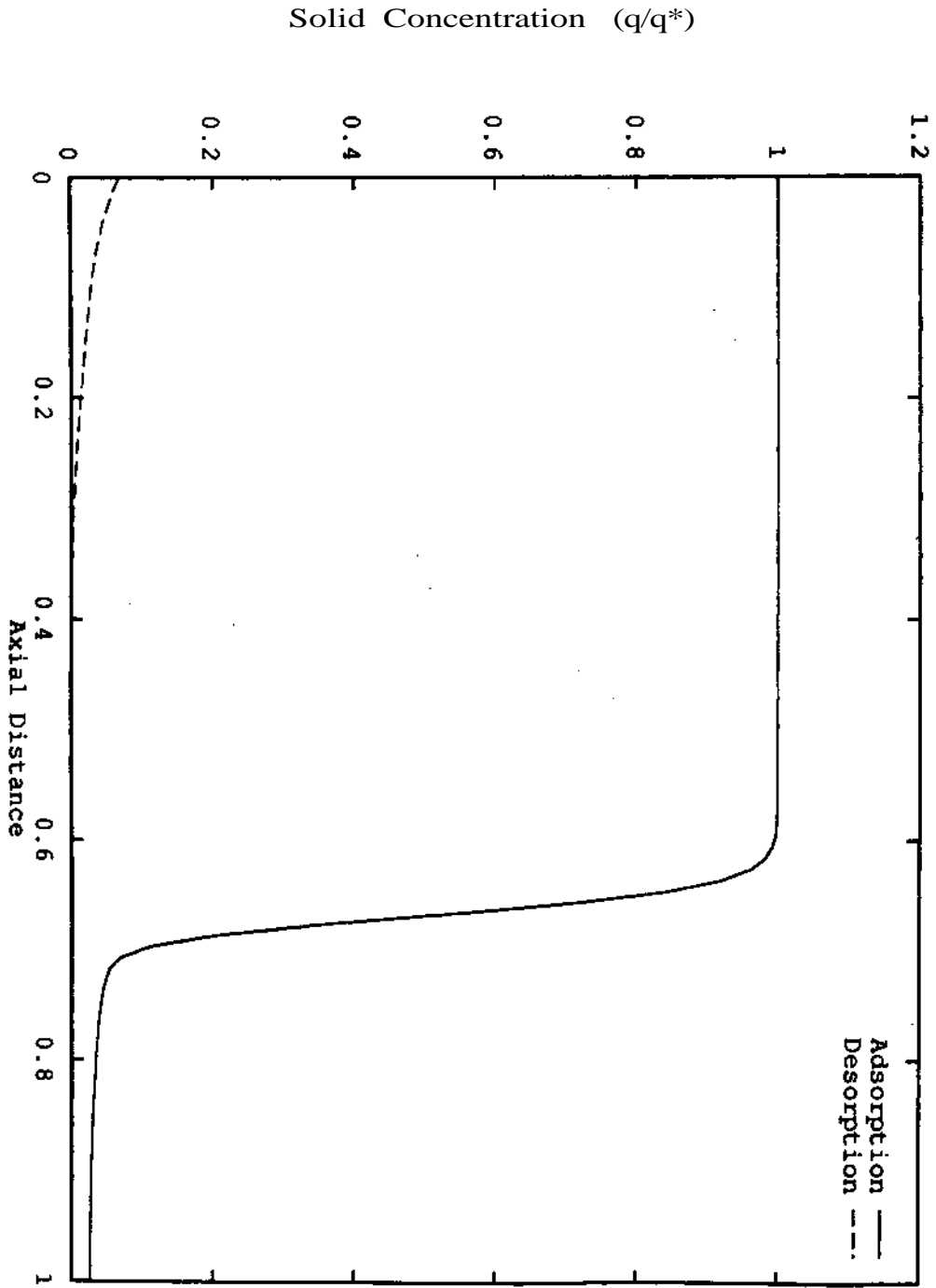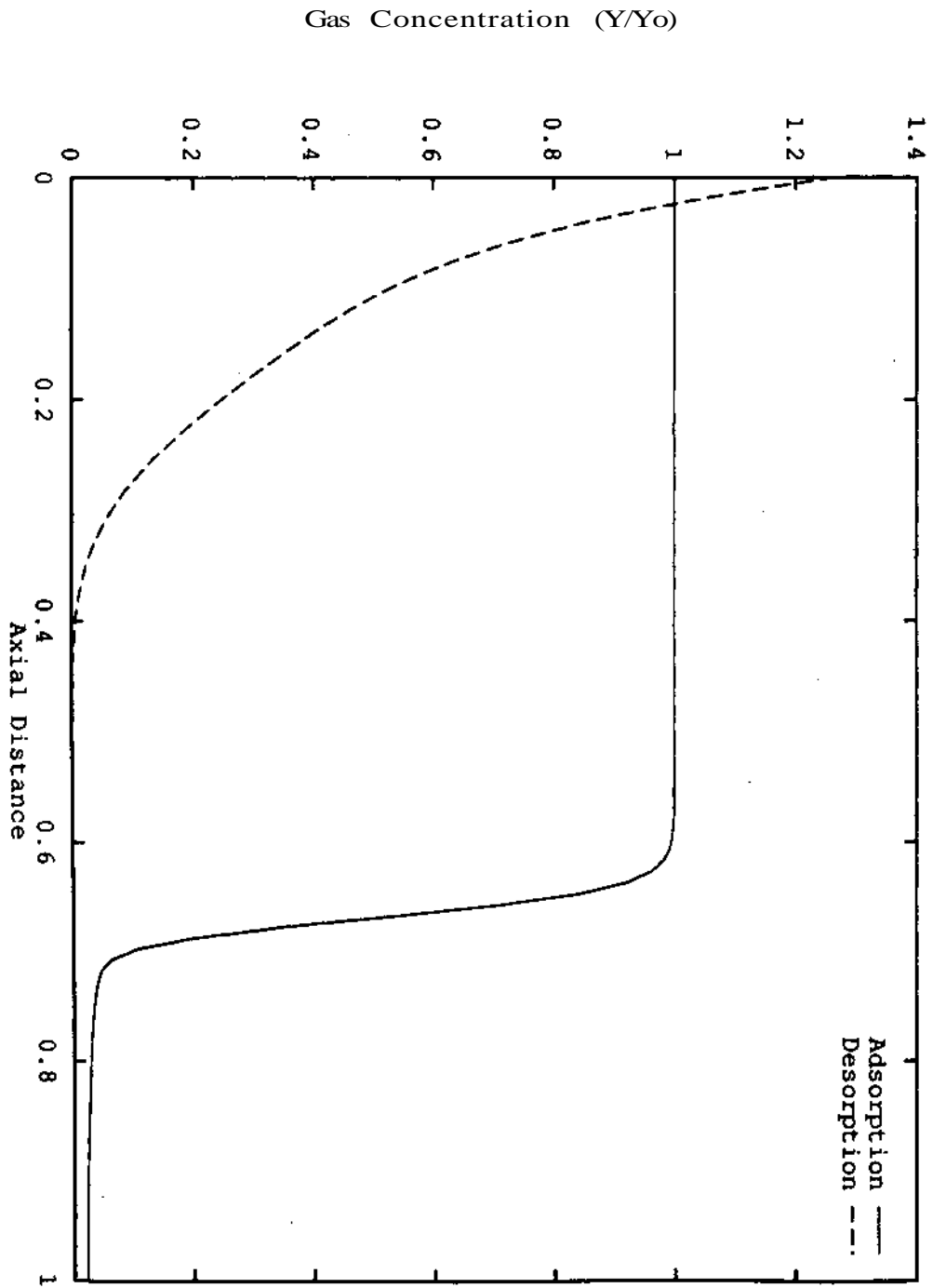Adsorption ———
Desorption —·—·

Figure I-3: Gas Concentration ESS Profiles

Gas Concentration (Y/Yo)

[a]$CH4$	-0.76
[b]$CH4$	$40539\,K$
B_{CH4}	$0.0129\,\text{-i.-}$ *psia*
d	$0.396\,m$
e	0.4
L	1.982 m
n_{CH4}	1.0
T	299 AT

Table 1-2: System Parameters

	Adsorption	Purge
k_{op}	**4.0į**	**4.0į**
t_{end}	69 *s*	31 *s*
F^{in}	$3.11 \times 10^{-2}\,\frac{Kgmole}{s}$	$4.21 \times 10^{-3}\,\frac{Kgmole}{s}$
P	355 *psia*	15 *psia*

Table 1-3: Model Parameters

Implementation of Design Scenario

The three step design scenario can now be implemented using the following steps:

1. Estimate values **for ϕ_{Ads}, $\$_{Des}$, r i ^ , and** $r|_{Des}$.
2. Perform the NLP design optimization using the utilization and efficiency parameters to determine the system design parameters.
3. Perform a dynamic simulation with the determined system design parameters to determine product purity and also to estimate (t ^ , ty_{Des}, $r|_{Ads}$, and $T|_{Des}$.

4. If the product purity constraint is met and the predicted and calculated values of (f)^, ty_{Des}, η_{Ads}'*and ^Dts ᵃgrec. then stop, else reestimate 0^ , $_{Des}$, $r|_{A\pounds is9}$ and $r|_{Des}$ and go to step 2.

Table 1-4 shows the iteration steps taken for the one pressure equalization operating sequence. The purity constraint used to determine termination was 0.9989. It should be mentioned that due to the averaging of the gas phase concentration profiles after depressurization, pressure equalization, and repressurization, the simulated product purity is expected to be a valid lower bound. It is a bound because real fixed-beds will not operate with infinite axial dispersion during these operations (what the above assumption maintains) but with a finite amount of dispersion. Any finite dispersion would tend to sharpen the MTZ and allow higher product purity.

An explanation of this table is warranted. The design optimization NLP was solved with $\S Ads = {}_{\circ}\text{-}^{90}$, $\$ Des = {}_{\circ}\text{-}^{98}$, $^\land Ads = {}^{10}$, and $^\land Des = {}^{125}$. The solution yielded the following values for some of the design parameters $d = 0.396$ m, $L = 1.982$ m, $P_{Ads} = 355$ psia, $x_x = 69.4$ s, and $x_5 = 43.8$ s. These design parameters were then used in the dynamic simulation of the system which predicted a purity of 0.9988 and the utilization and efficiency parameters to be $\$_{Ads} = 0.81$, $\$_{Des} = 0.98$, $r|_{Ads} = 1.0$, and $r|_{Des} = 1.25$. These values are essentially those guessed at the start, but the desired purity is not obtained. Since the purity constraint is not satisfied, the ty_{Ads} parameter must be lowered or the $\$_{Des}$ parameter must be raised for the next iteration. For this example, $\$_{Des}$ is already so high that all adjustments due to purity constraints are made on $\$_{Ads}$. Therefore, $\S_{Ads}$ is lowered to 0.80, and then the above iteration is performed again until both the parameters and the purity constraint are in agreement.

Table 1-5 lists the optimal values of some of the important design variables, such as the operation durations, pressures, and gas flowrates, for each of the four systems considered. The specified parameters used are those given in Table 1-1. As can be seen from Table 1-5, the largest profit is obtained from the configuration using two pressure equalization operations, but the profits from the three and one pressure equalization configurations are very close. All four configurations adsorb at the inlet pressure of 355 psia and desorb at the low pressure limit of 15 psia, and thus all the bed diameters and lengths are the same.

T-ble 1-4: luAon Iteratioo r O PE 00 u? 8

	Φ_{A}	4>Dc.	TlA*	HDe«	Purity	d (m)	L(m)	PA* (psia)	ti(s)	ts(s)
NLPl	0.90	0.98	1.00	1.25	n.a. -J^	0.396	1.982	355	69.4	43.8
Simulation 1	0.81	0.98	1.00	1.25	0.9988-4-	0.396	1.982	355	70	40
NLP2	0.80	0.98	1.00	1.25	n.a. -^»	0.396	1.982	355	62.0	43.4
Simulation 2	0.81	0.98	1.00	1.25	0.9988-4-	0.396	1.982	355	62	43
NLP3	0.78	0.98	1.00	1.25	n.a. -^	0.396	1.982	355	60.5	50.0
Simulation 3	0.77	0.98	1.00	1.26	0.9989-^-	0.396	1.982	355	60	50

Variable	5,3,2,1	4,2,1,0	3,1,0,0	2,0,0,0
$C^{\wedge\wedge}miin$	**-1.3643**	**-1.3653**	**-1.3588**	-1.3234
ϕ_{Ads}	0.90	0.85	0.78	0.75
D	68.6	65.3	60.5	58.1
d	0.396	0.396	0.396	0.396
1	1.98	1.98	1.98	1.98
x_1	68.6	65.3	60.5	58.1
x_2	31.4	32.6	30.3	**n.a.**
x_3	31.4	32.6	**n.a.**	**n.a.**
x_4	31.4	**n.a.**	**n.a.**	**n.a.**
x_5	31.4	32.6	30.3	29.1
x_9	31.4	32.6	30.3	29.1
P_2 (psia)	257.3	230.3	195.1	**n.a.**
P_3 (psia)	183.1	117.3	**n.a.**	**n.a.**
P_4 (psia)	95.8	**n.a.**	**n.a.**	**n.a.**
P_5 (psia)	15.0	15.0	**15.0**	15.0
P_9 (psia)	355.0	355.0	355.0	355.0
$m_{fg,Ads}^{in}$	2099	1986	1825	1703
$m_{fg,FR}^{in}$	**35.8**	43.7	58.0	103.2
$m_{B,Ads}$	1999	1891	1738	1622
$m_{B,Des}^{in}$	135.4	128.6	118.3	115.5
Rec_B	0.90	0.89	0.88	0.86

Table 1-5: Optimal Design Variables for the Four Cases Considered

Discussion

The three step design scenario was used above to design an industrial PSA separation system. Initially, a few parameters are fixed in the NLP design optimization problem which when solved gives the structure (such as operation sequence) and design variables (such as size and pressure) of the system.

Since simplified models were used in the NLP, the resulting design must be verified by either additional experiments and/or more detailed simulations, the emphasis being to ensure that the given structure and operating conditions meet the product purity and recovery specifications. For this work, the design was verified by performing additional detailed simulations. The results of these simulations were then used to recalculate the parameters that were fixed in the design optimization NLP. An optimal design is achieved when a feasible design has been determined and convergence of the above parameters is obtained.

Nomenclature

a,b,B **isotherm parameters**

c_p **heat capacity** $- \frac{J}{g \cdot K}$

d **bed diameter -** m

dr **depreciation rate - dimensionless**

F **molar flowrate** $- \frac{Kmol}{sec}$

H **heat of adsorption -** $\frac{J}{gmol}$

k **linear driving force coefficient -** sec^{-1}

L **bed length -** m

m **moles -** *Kgmole*

O_k **operation k**

P **pressure -** *Pa*

q_i **amount adsorbed on solid phase -** $\frac{1}{Bads}$

q_i^* **equilibrium amount adsorbed on solid phase -** $\frac{kg_i}{kg_{ads}}$

$\overline{q}_i$ **dimensionless amount adsorbed on solid phase**

R **gas constant-** $\frac{m^3 Pa}{Kgmole\,K}$

Rec **product recovery - dimensionless**

t **time -** *sec*

T **temperature -** *K*

tax **tax rate - dimensionless**

u **velocity -** $\frac{m}{j}$

Y **mole fraction - dimensionless**

F **dimensionless axial distance**

Greek letters

e **void fraction - dimensionless**

•	**bed** utilization
η	efficiency
P	density $-\frac{k}{m}-|$
τ	**dimensionles time - *sec***

Superscripts

e	end (or final)
in	into operation
out	out of operation
s	solid (or adsorbent) phase and slack time

Subscripts

A	**component A**
ads	adsorbent
Ads	Adsorption operation
B	**component B (product)**
Des	Desorption operation
fg	feed gas
FR	**Feed Repressurization operation**
k	operation *k*
pb	pay back

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