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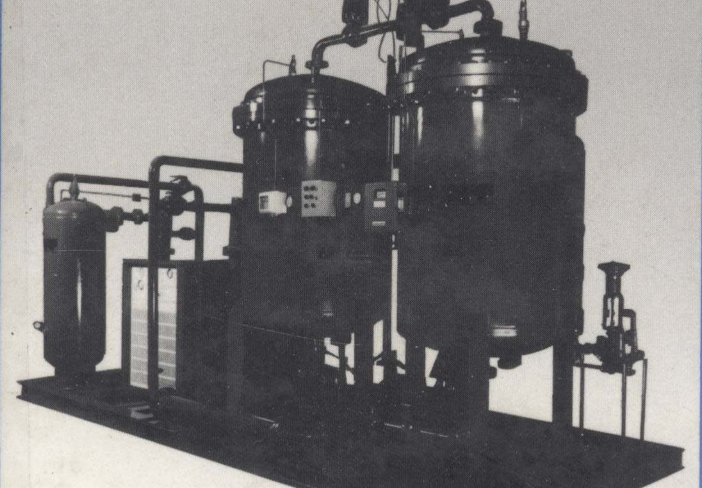

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Pressure Swing Adsorption

Preface

Although pressure swing adsorption (PSA) is not a new process, it is really only during the past decade that such processes have achieved widespread commercial acceptance as the technology of choice for more than a few rather specific applications. Nowadays, however, PSA processes are widely used, on a very large scale, for hydrogen recovery and air separation, and further important applications such as recovery of methane from landfill gas and production of carbon dioxide appear to be imminent. The suggestion for a book on this subject came from Attilio Bisio, to whom we are also indebted for his continuing support and encouragement and for many helpful comments on the draft manuscript.

The authors also wish to acknowledge the seminal contributions of two pioneers of this field, the late Frank B. Hill and Robert L. Pigford. Several of their publications are cited in the present text, but their influence is far broader than the citations alone would suggest. Suffice it to say that much of the book would not have been written without their encouragement and the stimulus provided by their widsom and insight. Several graduate students and post-doctorals have made major contributions, most of which are recognized explicitly by citations. However, they, as well as others whose work may not have been directly referenced, also contributed in a very real way by helping the authors, through discussion and argument, to understand and appreciate some of the subtleties of PSA systems. It would be remiss not to mention by name M. M. Hassan, J. C. Kayser, N. S. Raghavan, and H. S. Shin.

This book is not intended as an exhaustive review of PSA technology, neither is it a design manual. Rather, we have attempted to present a coherent general account of both the technology and the underlying theory. Perhaps more than in other processes the rational design and optimization of a pressure swing adsorption process requires a reasonably detailed mathematical model. The two commonly used approaches to PSA modeling, equilibrium theory, and dynamic numerical simulation are discussed in some detail in Chapters 4 and 5. Inevitably these chapters are somewhat mathematical in approach. The details may be important only to those who are involved in process design and optimization but we hope that the more general reader will still be able to gain some insight concerning the underlying principles and the strengths and limitations of the various approaches.

A three-way collaboration between authors inevitably raises some difficulties since it becomes hard to maintain consistency in style and emphasis and to avoid repetition between different sections of the text. We hope, however, that the advantages of a more authoritative treatment of the subject will more than compensate for any such deficiencies. From our perspective the collaboration has proved interesting and instructive, and we have encountered no serious disagreements amongst ourselves.

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June 1993

List of Symbols

a	sorbate activity; external area per unit volume for adsorbent sample (Eq. 2.46)
A	adsorbent surface area per mole (Eq. 2.10); $A_{cs} + A'$ (Table 5.10); membrane area (Eq. 8.1)
A'	cross-sectional area of column wall (Table 5.10)
A_{cs}	internal cross-sectional area of column
A_s	Helmholtz free energy (Eq. 2.11)
$A(k, i)$	collocation coefficient for internal (intraparticle) concentration profile (Appendix B)
$AH(j, i)$	collocation coefficient for velocity profile during pressurization (Appendix B)
$Ax(j, i)$	collocation coefficient for the external (fluid-phase) concentration profile (Appendix B)
b	Langmuir constant
b_o	pre-exponential factor ($b = b_o e^{-\Delta U/RT}$)
B	mobility coefficient (Eq. 2.29); constant in Eq. 4.76
$B(k, i)$	collocation coefficient for the intraparticle (internal) phase Laplacian
$Bx(j, i)$	collocation coefficient for the external fluid-phase Laplacian
c	sorbate concentration in gas phase
c_o	sorbate concentration in feed
C	total gas-phase concentration
C_g	volumetric heat capacity of gas (ρC_p)

C_s	volumetric heat capacity of solid (ρC_p)
$C_{p\,\mathrm{steel}}$	heat capacity of steel wall (mass basis) (Table 5.10)
d	internal diameter of adsorbent column
D	diffusivity
D_c	micropore or intracrystalline diffusivity
D_e	effective diffusivity
D_K	Knudsen diffusivity
D_L	axial dispersion coefficient
D_m	molecular diffusivity
D_p	pore diffusivity
E	diffusional activation energy
E_A	enrichment of heavy component ($\bar{y}/y_{AF}$)
$f_{i,j}$	isotherm function for component i at composition j
f'_j	isotherm slope (dq^*/dc) at composition j
F	total feed volume
F_s	free energy of adsorbed phase (Eq. 2.11)
F_A, F_B	fractions of components A, B desorbed from column during depressurization
G	purge-to-feed velocity ratio
G_s	Gibbs free energy of adsorbed phase (Eq. 2.8)
h	overall heat transfer coefficient
ΔH	enthalpy change on adsorption
J	flux of sorbate
k	overall mass transfer (LDF) rate coefficient based on adsorbed phase concentration
K	adsorption equilibrium constant or isotherm slope; constant in Eq. 7.5
K_c	adsorption equilibrium constant on crystal (microparticle) volume
K'	adsorption equilibrium constant or isotherm slope based on sorbate pressure
K_o, K'_o	pre-exponential factors (Eq. 2.2)
K_L	effective thermal conductivity of steel wall (Table 5.10)
L	adsorbent bed length
L_B, L_A	phenomenological coefficients
M	molecular weight; constant in quadratic isostherm expression
n	exponent in Freundlich isotherm expression
n_a	moles of adsorbable component (Eq. 2.8)
n_s	moles of solid adsorbent (Eq. 2.8)
N	flux relative to fixed frame of reference (Eq. 2.26); total moles (gaseous and adsorbed) in bed at time t
p	partial pressure of sorbate
p_s	saturation vapor pressure
P	absolute pressure (in column)
P'	rate of change of pressure during feed step (Eq. 4.35)

P_H	high pressure (at end of pressurization)
P_F	feed pressure
P_L	low pressure (during purge step)
P_{cH}	high pressure for compressor
P_{cL}	low pressure for compressor
Pe	Peclet number ($v_{oH}L/D_L$)
$\wp$	absolute pressure ratio P_H/P_L
$\wp_1$	pressure ratio P_H/P_F
$\wp_F$	pressure ratio P_F/P_L
$\wp_H$	pressure ratio P_H/P_L (end of pressurization versus end of blowdown)
$\wp_c$	absolute compression ratio P_{cH}/P_{cL}
q	adsorbed phase concentration
q^*	equilibrium value of q
q_o	value of q at equilibrium with feed (concentration c_o)
$\bar{q}$	value of q averaged over an adsorbent particle
q_s	saturation limit
Q	molar gas flow rate
r	radial coordinate in microparticle
r_c	microparticle radius
r_{in}, r_{out}	inner and outer radii of column
R	radial coordinate in a microparticle; gas constant (R_g); product recovery
R_p	macroparticle radius
S_E	equilibrium selectivity K_A/K_B
S_k	kinetic selectivity D_A/D_B
Sh	Sherwood number $2R_pk_f/D_m$
t	time
t^*	adsorption or desorption time
T	temperature
T_o	feed temperature
ΔU	internal energy change or adsorption
v	interstitial gas velocity
v_o	interstitial gas velocity at inlet
$\bar{v}$	dimensionless interstital gas velocity v/v_{oH}
V	volume
w_c	velocity of concentration front
w_t	velocity of temperature front
w'_c	velocity of shock front
x	mole fraction (of component A) in adsorbed phase; dimensionless adsorbed phase concentration averaged over a macroparticle $\bar{q}_i/\bar{q}_{is}$
x_c	dimensionless adsorbed phase concentration averaged over a microparticle (q/q_s)

X	fraction of complete purge
y	mole fraction of A in gas phase
$\bar{y}_{bd}$	average mole fraction (of raffinate product B) in blowdown gas
$\bar{y}_{pdt}$	average mole fraction (of raffinate product B) in high-pressure product stream
z	axial distance
Z	dimensionless axial distance z/L

Greek Symbols

α permeability ratio (intrinsic separation factor); $t_H/(t_H + t_L)$ (in Table 5.9)

α' separation factor $x(1-y)/y(1-x)$ or $y(1-x)/x(1-y)$

α_k kinetic selectivity (effective)—see Eq. 2.46

β parameter characterizing heat effect $[(\Delta H/C_s)(\partial q^*/\partial T)_p]$ in Eq. 2.46; adsorption selectivity parameter β_A/β_B; b_iC

β_i ratio of hold-up component i in void space as fraction of total hold-up $[1 + ((1-\varepsilon)/\varepsilon)K_i]^{-1}$

γ ratio of gas heat capacities at constant pressure and constant volume

γ_E ratio of Langmuir constants b_B/b_A

γ_k ratio of micropore diffusivities D_{cB}/D_{cA}

γ_s ratio of saturation capacities q_{Bs}/q_{As}

Γ dimensionless parameter $(r_c^2/D_{Ac})(3k_f/R_p)(C/q_{As})$

Γ' dimensionless parameter $(r_c/D_{Ac})(C/q_{As})k_f$

ε voidage of adsorbent bed

ϵ_p porosity of adsorbent particle

ζ $[1 + \xi P_H y_F \beta_{A_0}(1-\beta)]^{-1}$ (Chapter 4)

η mechanical efficiency of compression; dimensionless radial coordinate R/R_p

θ adsorption selectivity parameter θ_A/θ_B

θ_i dimensionless concentration q_i/q_{is} (Chapters 2 and 5); parameter $\theta_i\,(P, y_1, y_2) = [1 + ((1-\varepsilon)/\varepsilon)((f_{i2} - f_{i1})/(y_{i2} - y_{i1}))(RT/P_H)]^{-1}$, where 1 and 2 refer to arbitrary states (Chapter 4)

θ_c dimensionless adsorption or desorption time $(\epsilon_p D_p/R_p^2)(c_0/q_0)\ t^*$ (for macropore control) or $D_c t^*/r_c^2$ for micropore control
λ ratio of dead volume to column volume; non-linearity parameter q_o/q_s
μ chemical potential; viscosity; mean residence time in column
Ξ parameter $((1-\varepsilon)/\varepsilon)\,(M_A/RT)$
ξ $(1-\varepsilon)M_A/\varepsilon R$
ρ density
σ^2 variance of pulse response
τ dimensionless time variable, tv_{OH}/L (LDF model); tD_c/r_c^2 (pore diffusion model)
ϕ parameter $\epsilon A_{cs} L P_L/\beta_A RT$
Φ surface potential
Ω parameter defined by Eq. 5.16; integral function used in determining recovery for pressurization with feed

Subscripts

A, B	components A (more strongly adsorbed) and B (less strongly adsorbed)
B	blowdown step
c	micropore or intracrystalline
ci	component i in microparticle
C	column
DV	dead volume
ei	equivalent value (for component i) in countercurrent flow model
F	feed or feed end
G	purge-to-feed ratio
H, OH, iH	high-pressure step, at inlet during high-pressure step, and for component i during high-pressure step
i	refers to species i (A or B).
ip, is	species i in microparticle, species i at saturation
I	intermediate
L, oL, iL	low-pressure (purge) step, at inlet during low-pressure step, and for component i during low-pressure step
o, oi	limiting or reference value, limiting or reference value for component i
O	outlet or effluent
p	macropore or macroparticle
P	product end or pressurization step
PU	purge step

R	rinse step
s	saturation value
S	condition following pressurization step
SH	shock wave
w	at wall
W	combined blowdown and purge step effluent; waste or byproduct
0, 1, 2	initial state, ahead of shock, and behind shock
Superscript	* is sometimes used to denote and emphasize "equilibrium value"

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