This article was downloaded by:
On: *25 January 2011*
Access details: *Access Details: Free Access*
Publisher *Taylor & Francis*
Informa Ltd Registered in England and Wales Registered Number: 1072954 Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK

Separation Science and Technology

Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713708471

Column Dynamics for Multicomponent Adsorption-Constant Pattern Formation

Ravi Kumar[a]
[a] AIR PRODUCTS AND CHEMICALS, INC., ALLENTOWN, PENNSYLVANIA

To cite this Article Kumar, Ravi(1986) 'Column Dynamics for Multicomponent Adsorption-Constant Pattern Formation', Separation Science and Technology, 21: 10, 1039 — 1046
To link to this Article: DOI: 10.1080/01496398608058395
URL: http://dx.doi.org/10.1080/01496398608058395

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: http://www.informaworld.com/terms-and-conditions-of-access.pdf

This article may be used for research, teaching and private study purposes. Any substantial or systematic reproduction, re-distribution, re-selling, loan or sub-licensing, systematic supply or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand or costs or damages whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

SEPARATION SCIENCE AND TECHNOLOGY, **21**(10), pp. 1039-1046, 1986

Column Dynamics for Multicomponent Adsorption—Constant Pattern Formation

RAVI KUMAR

AIR PRODUCTS AND CHEMICALS, INC.
ALLENTOWN, PENNSYLVANIA 18105

Abstract

A mathematical model for predicting adsorption breakthrough time for an N-component mixture from a carrier gas is described. Formation of constant pattern fronts is assumed, and the model accounts for roll-up of each species. Mixture equilibrium isotherms for all the species and length of the mass transfer zone, only for the least strongly adsorbed component, are needed for prediction.

INTRODUCTION

Adsorption is the preferred technology for removing trace quantities of contaminants from liquid or gas streams. If each of the adsorbate species acts independently, i.e., linear isotherms, the adsorber can be designed by determining the behavior of the least strongly adsorbed species (*1*). However, nonlinear equilibrium isotherms lead to adsorbate concentrations inside the column being higher than the feed concentration due to strong interactions. This is known as the "roll-up" effect. Three approaches may be used to design such adsorption systems. In the first approach, the effect of roll-up is neglected and the adsorbent requirement for each single adsorbate species is calculated by adding its individual equilibrium section length and the corresponding length of the unused bed (*LUB*) at the inlet feed concentration (*2*). The total bed length is obtained by adding individual adsorbent requirements for each of the adsorbate species. This approach is very simple to use and requires only pure component data. However, it may lead to considerable overdesign.

0149-6395/86/2110-1039$3.50/0

The second approach uses computer simulation to solve the relevant mass balance and mass transfer rate expressions along with appropriate equilibrium isotherms (*3–9*). This approach can be used for designing adiabatic as well as isothermal systems and can be extended to systems where the column is not long enough for the formation of stable fronts. However, the computation time for any realistic system makes the use of this approach prohibitive.

Another approach (*10*) is to assume constant pattern fronts for all the adsorbate species in an isothermal, isobaric system. The present study extends and generalizes this approach to a multicomponent (N adsorbate species in a carrier) system. Simple algebraic equations are given to calculate the roll-up concentrations for all the species. This information, along with *LUB*, only for the least strongly adsorbed species, are needed to accurately determine the breakthrough time from an adsorber. These equations provide a simple and accurate method for the design of a multicomponent trace removal adsorber.

MATHEMATICAL MODEL

Figure 1 shows the mass transfer profiles at a fixed time in an N-component system with an inert carrier. There are N-equilibrium and N-mass transfer sections. Adsorption affinity follows the order: Component $1 > 2 > \cdots > i > i + 1 > \cdots > N$. The flow rate, pressure, and temperature are assumed to be constant. It should be noted that

$$n_i^j, y_i^j = 0, \qquad \text{for } i < j \tag{1a}$$

$$\neq 0, \qquad \text{for } i \geqslant j \tag{1b}$$

Figure 1 shows that for a breakthrough time t, the column length L is given by

$$L = \sum_{j=1}^{N} Ls_j + LUB_N \tag{2}$$

where

$$Ls_j = \frac{Gt}{\rho_b} \frac{y_i^1}{n_i^j} - \frac{1}{n_i^j} \sum_{j=1}^{(j-1)} Ls_j n_i^j \tag{3}$$

Ls_j is the length of the jth equilibrium section in which the jth species is removed. Subscript i in Eq. (3) is numerically the same as subscript j.

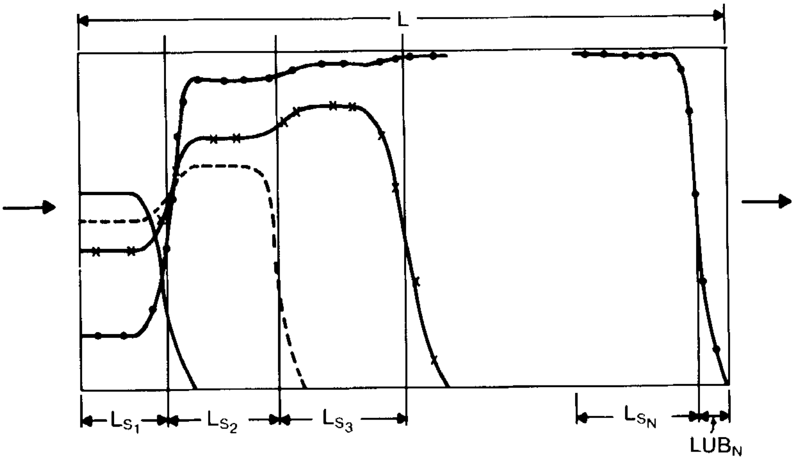

FIG. 1. Gas-phase concentration profiles inside the column at breakthrough time: (——) Component 1; (- -) Component 2; (×) Component 3; (●) Component N. Mole fractions of N species in the feed gas are $y_1, y_2, y_3, \ldots, y_N$.

Equation (3) assumes negligible gas-phase accumulation and is obtained from a mass balance on each component. For example, the length of the first equilibrium section ($j = 1 = i$) is

$$Ls_1 = \frac{Gt}{\rho_b} \frac{y_1^1}{n_1^1} \tag{4a}$$

The length of the second equilibrium section ($j = 2 = i$) is

$$Ls_2 = \frac{Gt}{\rho_b} \frac{y_2^1}{n_2^2} - Ls_1 \frac{n_2^1}{n_2^2} \tag{4b}$$

The length of the third equilibrium section ($j = 3 = i$) is

$$Ls_3 = \frac{Gt}{\rho_b} \frac{y_3^1}{n_3^3} - Ls_1 \frac{n_3^1}{n_3^3} - Ls_2 \frac{n_3^2}{n_3^3} \tag{4c}$$

For known feed conditions (n_1^1, y_1^1, G), the length of the first equilibrium section (Ls_1) can be calculated from Eq. (4a). The remaining equilibrium section lengths (Ls_2, Ls_3, · · ·, Ls_N) can be obtained from Eq. (3) in a manner described above (Eqs. 4b, 4c, etc.). However, the roll-up gas-phase concentrations (y_i) and the corresponding solid-phase loadings

(n_i) in equilibrium sections 2, 3, . . . , N are needed before Eq. (3) may be used for calculating equilibrium section lengths $Ls_2, Ls_3, Ls_4, \cdots, Ls_N$. A procedure for obtaining these is now outlined.

The mass balance for isobaric, isothermal adsorption of component i from an inert carrier is given by

$$\varepsilon\rho_g \left.\frac{\partial y_i}{\partial t}\right|_x = -G \left.\frac{\partial y_i}{\partial x}\right|_t - \rho_b \left.\frac{\partial n_i}{\partial x}\right|_t, \qquad i = 1, 2, 3, \ldots, N \tag{5}$$

If it is further assumed that all the N-interfering species form constant pattern fronts, Eq. (5) reduces to (*11*):

$$\frac{\partial}{\partial t}\left[\varepsilon\rho_g y_i - \frac{G y_i}{\beta} + \rho_b n_i\right] = 0 \tag{6}$$

Since the velocity of each element (β) in a constant pattern front is independent of gas-phase or solid-phase composition, Eq. (6) may be integrated across each of the (N − 1) mass transfer zones. Neglecting gas-phase accumulation, the above integration gives the following equation across the jth ($j = 1, 2, \cdots, (N-1)$) mass transfer front:

$$\frac{n_i^{j+1} - n_i^j}{y_i^{j+1} - y_i^j} = \frac{n_j^j}{y_j^j} \tag{7}$$

where, $i = (j + 1), (j + 2), \ldots, N$.

For example, across the first mass transfer zone ($j = 1$):

$$i = 2: \quad \frac{n_2^2 - n_1^1}{y_2^2 - y_2^1} = \frac{n_1^1}{y_1^1} \tag{8a}$$

$$i = 3: \quad \frac{n_3^2 - n_3^1}{y_3^2 - y_3^1} = \frac{n_1^1}{y_1^1} \tag{8b}$$

and so on.

Therefore, Eq. (7) provides (N − 1) independent equations, similar to Eqs. (8a), (8b), etc., across the first mass transfer zone. The equilibrium relationships

$$n_i = n_i(y_1, y_2, y_3, \cdots, y_N), \qquad i = 1, 2, 3, \ldots, N \tag{9}$$

provide another set of N − 1 nontrivial, independent equations relating the gas-phase and solid-phase compositions in the second equilibrium section (n_i^2, y_i^2, $i = 2, 3, \ldots, N$). Since the gas-phase and solid-phase loadings in the first equilibrium section (n_i^1, y_i^1, $i = 1, 2, 3, \ldots, N$) are known from the feed composition and equilibrium relationships, Eqs. (8) and (9) provide $(2N - 2)$ independent equations relating $(2N - 2)$ unknowns. A unique solution may, therefore, be obtained by simultaneous solution of the algebraic Eqs. (7) and (9).

In a similar manner, Eqs. (7) and (9) provide $(2N - 4)$ equations across the 2nd mass transfer zone ($j = 2$) relating $(2N - 4)$ unknowns. This set of equations can again be solved and a unique solution obtained for gas-phase compositions and solid-phase loadings in the 3rd equilibrium section (n_i^3, y_i^3, $i = 3, 4, \ldots, N$). This method is continued till $j = N - 1$ and roll-up gas-phase compositions and corresponding solid-phase loadings in all the N equilibrium sections are determined.

*N*TH MASS TRANSFER ZONE

Length of the unused bed (LUB_N) for the most weakly adsorbed species (N) can be measured either experimentally by carrying out a breakthrough experiment with only the Nth species in the carrier gas or, for a Langmurian system, from the following equation (*11*):

$$LUB_N = \frac{1}{2} \frac{G y_N^N b_N}{\rho_b n_N^N (1 + b_N)} \frac{1}{k_N} \left(\frac{2}{\lambda} - 1\right) \ln\left(\frac{y_N^N}{y_N^*} - 1\right) \tag{10}$$

where the Langmuir model is given as:

$$n = \frac{mby}{1 + by} \tag{10a}$$

and

$$\lambda = n_N^N / m \tag{10b}$$

EXPERIMENTAL DATA

Necessary information for multicomponent ($N > 2$) adsorption systems is not readily available in the literature. Therefore, sorption of a binary mixture of toluene (1) and benzene (2) from N_2 carrier gas on activated carbon was used to compare the predicted and observed breakthrough times. Necessary data for this sytem has been published (*12*). The operating conditions are summarized in Table 1.

In this case, $N = 2$, therefore Eq. (7) gives

$$j = 1, i = 2: \qquad \frac{n_2^2 - n_2^1}{y_2^2 - y_2^1} = \frac{n_1^1}{y_1^1} \tag{11}$$

Binary equilibrium isotherms plotted in Figs. 6 and 7 of Ref. *12* and the feed inlet concentrations are used to obtain n_1^1 ($= 5.3 \times 10^{-4}$ g-mol/g) and n_2^1 ($= 6.2 \times 10^{-5}$ g-mol/g). These are substituted in Eq. (11) to give one equation with two unknowns: n_2^2 and y_2^2. The equilibrium isotherm for pure benzene (Table 1, Eq. 10a) provides another independent equation. These two are simultaneously solved to obtain

$$n_2^2 = 2.75 \times 10^{-4} \text{ g-mol/g}$$

$$y_2^2 = 5.27 \times 10^{-4}$$

Therefore, Eq. (3) gives

$$Ls_1 = 2.06 \times 10^{-4}\, t \tag{12a}$$

and

$$Ls_2 = 2.52 \times 10^{-4}\, t \tag{12b}$$

The experimental breakthrough curve for benzene (Component 2) adsorption from N_2 carrier gas (Fig. 15 of Ref. *12*) at $G = 3.97 \times 10^{-4}$ g-mol/cm^2/s and $y_2 = 2.12 \times 10^{-4}$ and Eq. (10) are used to calculate a mass transfer coefficient $k_2 = 1.83 \times 10^{-2}$ S^{-1}.

This mass transfer coefficient gives

$$LUB_2 = 0.224 \text{ cm} \tag{13}$$

for the present example (Table 1).

Equations (2), (12a), (12b), and (13) therefore reduce to

$$L = 4.58 \times 10^{-4}\, t + 0.224$$

Therefore, the present model predicts the breakthrough time $t = 21$ min for $L = 0.8$ cm. The match with the experimentally observed breakthrough time, $t = 19$ min, is excellent.

TABLE 1[a]

Adsorbate	Toluene (1)	Benzene (2)
y_i^1, g-mol/cm^3	4.58×10^{-4}	3.44×10^{-4}
Langmuir parameters (pure component):		
m, g-mol/g	10.11×10^{-4}	6.74×10^{-4}
b, dimensionless	5.10×10^3	1.31×10^3

[a] Adsorbate = activated carbon. $\rho_b = 0.638$ g/cm^3. Carrier gas = N_2. $G = 1.52 \times 10^{-4}$ g-mol/cm^2/s. $L = 0.8$ cm. $T = 423.15$ K. $P = 1$ atm.

SYMBOLS

b	Langmuir constant (dimensionless)
G	molar flow rate based upon empty cross-section area (g-mol/cm^2/s)
k_N	mass transfer coefficient for the Nth component (s^{-1})
L	column length (cm)
Ls_j	length of the jth equilibrium section in which the jth adsorbate species is removed ($j = 1, 2, \ldots, N$) (cm)
LUB_N	length of the unused bed for the most weakly adsorbed species, N (cm)
m	Langmuir saturation capacity (g-mol/g)
n	solid phase equilibrium loading (g-mol/g)
N	number of adsorbing species in a carrier stream
t	time (s)
x	distance variable (cm)
y	gas-phase mole fraction of an adsorbate (dimensionless)
y_N^*	gas-phase mole fraction of the Nth component at breakthrough time (dimensionless)

Greek Symbols

ρ_b	bulk density of the adsorbent (g/cm^3)
ε	total void fraction in the column (dimensionless)
ρ_g	carrier-phase density (g-mol/cm^3)
β	velocity of an element in the mass transfer front (cm/s)

Subscript

$i = 1, 2, 3, \ldots, N$, adsorbate species

Superscript

$j = 1, 2, 3, \ldots, N$, equilibrium section

Acknowledgment

The author is thankful to Air Products and Chemicals, Inc. for their kind permission to publish this paper.

REFERENCES

1. D. O. Cooney and E. N. Lightfoot, *Ind. Eng. Chem., Process Des. Dev.*, *5*(1), 25 (1966).
2. J. J. Collins, *Chem. Eng. Prog., Ser.*, *74*(63), 31 (1967).
3. M. W. Balzli, A. I. Liapis, and D. W. T. Rippin, *Trans. Inst. Chem. Eng.*, *56*, 145 (1978).
4. M. Morbidell, A. Servida, G. Stortl, and S. Carra, *Ind. Eng. Chem., Fundam.*, *21*, 123 (1982).
5. K. Miura, H. Kurahashi, Y. Inokuchi, and K. Hashimoto, *J. Chem. Eng. Jpn.*, *12*(4), 281 (1979).
6. A. Liapis and R. J. Litchfield, *Chem. Eng. Sci.*, *35*, 2366 (1980).
7. Y. W. Wong and J. L. Niedzwiecki, Presented at the AIChE Meeting, Orlando, February 28–March 4, 1982.
8. J. W. Carter and H. Husain, *Chem. Eng. Sci.*, *29*, 267 (1974).
9. A. Mansour, D. U. von-Rosenberg, and N. D. Sylvester, *AIChE J.*, *28*(5), 765 (1982).
10. Y. Takeuchi, Y. Suzuki, and E. Furuya, *J. Chem. Eng. Jpn.*, *12*(6), 486 (1979).
11. S. Sircar and R. Kumar, *Ind. Eng. Chem., Process Des. Dev.*, *22*(2), 271 (1983).
12. W. J. Thomas and J. L. Lombardi, *Trans. Inst. Chem. Eng.*, *49*, 240 (1971).

Received by editor March 17, 1986