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Ho-Ming Yeh^a; Chin-Fwu Chiou^a

^a CHEMICAL ENGINEERING DEPARTMENT, NATIONAL CHENG KUNG UNIVERSITY, TAINAN, TAIWAN, REPUBLIC OF CHINA

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NOTE

Comparison of Various Methods of Calculating a Separation Factor in Thermal Diffusion

 HO-MING YEH and CHIN-FWU CHIOU

 CHEMICAL ENGINEERING DEPARTMENT
 NATIONAL CHENG KUNG UNIVERSITY
 TAINAN, TAIWAN, REPUBLIC OF CHINA

Abstract

An improved equation of separation applicable to the whole range of concentration in flat-plate thermal diffusion columns has been derived by the least squares method. Separations calculated from this equation are more accurate than those from the generalized equation obtained by Yeh and Chu, particularly for low flow-rate operations and equifraction solution.

INTRODUCTION

The first complete presentation of the separation theory in thermal diffusion columns was that of Furry et al. (2, 3). They obtained two ordinary differential equations by integrating the transport equations

$$H \left[c(1 - c) - \frac{\sigma}{H}(c_T - c) \right] = K \frac{dc}{dz} \quad (1)$$

for the enriching section and

$$H \left[c(1 - c) + \frac{\sigma}{H}(c_B - c) \right] = K \frac{dc}{dz} \quad (2)$$

for the stripping section. The transport constants in Eqs. (1) and (2) are defined by

$$H = \alpha \beta_T \rho g (2\omega)^3 B (\Delta T)^2 / (6! \mu \bar{T}) \quad (3)$$

$$K = \beta_T^2 \rho g^2 (2\omega)^7 B (\Delta T)^2 / (9! D \mu^2) + 2\omega D B \rho \quad (4)$$

The product form of the concentration dependence of the thermal diffusion effect incorporated in Eqs. (1) and (2) introduces nonlinearity into the differential equations which makes the solution so complicated and implicit that meaningful interpretation and further application of the results are difficult:

$$\begin{aligned}\Delta_{\text{exact}} &= c_T - c_B \\ &= \frac{2c_i(1 - c_i)}{\frac{\sigma}{H} - 1 + 2c_i + \left[\left(1 + \frac{\sigma}{H}\right)^2 - 4\frac{\sigma c_T}{H} \right]^{1/2}} \\ &\quad \times \coth \left\{ \frac{HL}{4K} \left[\left(1 + \frac{\sigma}{H}\right)^2 - 4\frac{\sigma c_T}{H} \right]^{1/2} \right\} \\ &= - \frac{2c_i(1 - c_i)}{-\frac{\sigma}{H} - 1 + 2c_i + \left[\left(1 - \frac{\sigma}{H}\right)^2 + 4\frac{\sigma c_B}{H} \right]^{1/2}} \\ &\quad \times \coth \left\{ -\frac{HL}{4K} \left[\left(1 - \frac{\sigma}{H}\right)^2 + 4\frac{\sigma c_B}{H} \right]^{1/2} \right\} \quad (5)\end{aligned}$$

Note that the above equation satisfies the following boundary conditions:

$$z = 0 \quad c = c_i \quad (6)$$

$$= L/2 \quad = c_T \quad (7)$$

$$= -L/2 \quad = c_B \quad (8)$$

Furry et al. obtained a simple explicit solution of Eqs. (1) and (2) with the same boundary conditions and under the following assumption:

$$c(1 - c) = \text{constant} = 0.25$$

The solution is

$$\Delta_2 = c_T - c_B = \frac{H}{2\sigma} \left[1 - \exp \left(-\frac{\sigma L}{2K} \right) \right] \quad (9)$$

Numerous investigators (1, 4, 6-13, 15, 16) have made attempts to improve upon the application of theory. However, the product form of the concentration dependence of the thermal diffusion effect incorporated in Eqs. (1) and (2) was also assumed to be constant in all these works, and the results obtained under this assumption are still not valid for $c < 0.3$ or $c > 0.7$.

In 1975, Yeh and Chu (14) derived a generalized equation of separation

applicable to the whole range of concentrations in thermal diffusion columns by the method of linear approximation. Later, this equation was checked with the experimental data of Yeh and Lu (17). The results showed that Yeh and Chu's work is in good agreement with the experimental results, particularly for high flow-rate operations and high or low values of feed concentration. It is the purpose of this work to improve the separation theory to make it applicable to any flow-rate operation and to any value of feed concentration.

LINEAR APPROXIMATION

Yeh and Chu (14) suggested that the product form of concentration dependence of the thermal diffusion effect incorporated in Eqs. (1) and (2) can be approximated by a straight line over the whole range of concentration

$$c(1 - c) \approx a_1 + b_1c \quad (10)$$

with the appropriate choice of constants:

$$a_1 = c_i^2 - \frac{\Delta_1^2}{8} \quad (11)$$

$$b_1 = 1 - 2c_i \quad (12)$$

Substituting Eq. (10) into Eqs. (1) and (2), integrating, and making use of the boundary conditions of Eqs. (6), (7), and (8) give

$$\begin{aligned} \Delta_1 &= c_T - c_B \\ &= -S + \sqrt{S^2 + 8c_i(1 - c_i)} \end{aligned} \quad (13)$$

in which

$$S = \frac{2\{\sigma'L' + 2(1 - 2c_i)L'e^{-[2(1-2c_i)L' + \sigma'L']}\} \times \{\sigma'L' - 2(1 - 2c_i)L'e^{[2(1-2c_i)L' - \sigma'L']}\}}{L'\{2\sigma'L' + [2(1 - 2c_i)L' - \sigma'L']e^{-[2(1-2c_i)L' + \sigma'L']} - [2(1 - 2c_i)L' + \sigma'L']e^{[2(1-2c_i)L' - \sigma'L']}\}} \quad (14)$$

$$\sigma' = 2\sigma/H \quad (15)$$

$$L' = HL/4K \quad (16)$$

Equation (13) is an explicit form of separation and is much more simple and convenient for application than Eq. (5).

Yeh and Lu (17) compared Eqs. (9) and (13) with their experimental results and found that Yeh and Chu's work is in good agreement with the experimental data, while the agreement of Furry et al.'s work with the experimental results is fair for equifraction solutions and miserable for high and low values of feed concentration.

LEAST SQUARES METHOD

The values of a_1 and b_1 in Eqs. (11) and (12) were determined by taking the arithmetic mean (14). This is correct only for a low degree of separation. For any degree of separation, the values of a_1 and b_1 must be selected more logically.

Let

$$c(1 - c) \approx (a_3 + b_3c)$$

and define

$$I = \int_{c_B}^{c_T} [c(1 - c) - (a_3 + b_3c)]^2 dc \quad (17)$$

in which

$$c_T \approx c_i + \frac{\Delta_3}{2}$$

and

$$c_B \approx c_i - \frac{\Delta_3}{2}$$

The necessary conditions for I having a minimum value are

$$\partial I / \partial a_3 = 0 \quad (18)$$

and

$$\partial I / \partial b_3 = 0 \quad (19)$$

thus

$$a_3 = c_i^2 - \frac{\Delta_3^2}{12} \quad (20)$$

$$b_3 = 1 - 2c_i = b_1 \quad (21)$$

and

$$c(1 - c) \approx a_3 + b_3c = \left(c_i^2 - \frac{\Delta_3^2}{12}\right) + (1 - 2c_i)c \quad (22)$$

Finally, the separation equation thus obtained is

$$\begin{aligned}\Delta_3 &= c_T - c_B \\ &= -\frac{3}{2}S + \sqrt{\frac{9}{4}S^2 + 12c_i(1 - c_i)}\end{aligned}\quad (23)$$

DISCUSSION AND CONCLUSION

The improvement in separation theory of thermal diffusion by using the least squares method is best illustrated by calculating the percentage error in separation based on the exact solution. The exact solution was calculated from Eq. (5) with a computer by the New-Raphson method. The results are presented in Table 1. It is shown from this table that Δ_3 is much better than Δ_1 , particularly for low flow-rate operations and equifraction solution.

The experimental data obtained by Lu (5) were also employed to check Eqs. (13) and (23) by following the same procedure used by Yeh and Lu (17). Although the values of Δ_1 and Δ_3 are very close in the particular range of experimental work studied by Lu, the values of Δ_3 are closer to the experimental results, especially for low flow-rate operations and equifraction solution, as shown in Table 2.

On the basis of the results of this study, we conclude that separations calculated from Eq. (23) are more accurate than those from Eq. (13), particularly for low flow-rate operations and equifraction solution.

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SYMBOLS

a_1, a_3	constant defined by Eqs. (8) and (20)
B	column width
b_1, b_3	constant defined by Eqs. (9) and (21)
c	fraction of Component 1 in a binary solution
c_B, c_T	fraction of Component 1 in the product stream exiting from the stripping, enriching section
c_i	fraction of Component 1 in the feed stream
D	ordinary diffusion coefficient

TABLE 1
Comparison of Δ_1 and Δ_3 based on Δ_{exact}

c_i	σ'	$L' = 0.4$			$L' = 1.0$			$L' = 5.0$		
		$\frac{\Delta_1 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_3 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_1 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_3 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_1 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_3 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_1 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_3 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$	$\frac{\Delta_3 - \Delta_{\text{exact}}}{\Delta_{\text{exact}}} (\%)$
0.1	1.0	0.94	0.30	4.39	2.44	6.10	3.20			
0.1	3.0	0.65	0.33	1.44	0.89	1.92	1.25			
0.1	7.0	0.29	0.18	0.35	0.23	0.36	0.24			
0.3	1.0	1.87	0.50	7.28	3.52	14.1	8.15			
0.3	3.0	1.44	0.73	3.45	2.22	4.28	2.93			
0.3	7.0	0.67	0.42	0.84	0.56	0.84	0.57			
0.5	1.0	2.11	0.53	7.52	3.25	23.4	17.2			
0.5	3.0	1.69	0.85	4.15	2.71	5.01	3.45			
0.5	7.0	0.80	0.51	1.00	0.67	1.00	0.67			

TABLE 2
Comparison of Separation Obtained from Experimental Work and Theoretical Equations

g/min	Δ_0 (%)	Δ_1 (%)	Δ_3 (%)	Conditions and quantities	
0.079	13.5	10.5	10.6	$c_t = 0.1$ $(T_1 + T_2)/2 = 588.5^\circ\text{R}$ $\rho = 0.817 \text{ g/cm}^3$ ^a $H = 0.1676 \text{ g/min}$	$T = 58^\circ\text{F}$ $D = 2.65 \times 10^5 \text{ cm}^2/\text{sec}^a$ $K = 11.187 \text{ (g)(cm)/min}$
0.162	10.5	8.6	8.6		
0.320	7.2	6.7	6.7		
0.641	4.8	4.3	4.3		
1.305	2.5	2.3	2.3		
2.011	1.5	1.5	1.5		
0.073	36.0	29.8	30.3	$c_t = 0.3$ $(T_1 + T_2)/2 = 588.5^\circ\text{R}$ $\rho = 0.773 \text{ g/cm}^3$ ^a $H = 0.101 \text{ g/min}$	$T = 58^\circ\text{F}$ $D = 2.7 \times 10^5 \text{ cm}^2/\text{sec}^a$ $K = 4.214 \text{ (g)(cm)/min}$
0.149	30.0	21.9	22.1		
0.300	18.0	13.4	13.4		
0.603	9.6	7.0	7.0		
1.237	4.5	3.4	3.4		
1.913	2.2	2.2	2.2		
2.865	1.1	1.1	1.1		
0.067	39.5	37.0	37.8	$c_t = 0.5$ $(T_1 + T_2)/2 = 588.5^\circ\text{R}$ $\rho = 0.733 \text{ g/cm}^3$ ^a $H = 0.105 \text{ g/min}$	$T = 58^\circ\text{F}$ $D = 3.05 \times 10^5 \text{ cm}^2/\text{sec}^a$ $K = 4.252 \text{ (g)(cm)/min}$
0.135	29.5	28.3	28.7		
0.270	19.0	18.0	18.1		
0.551	9.6	9.5	9.5		
1.167	4.7	4.5	4.5		
2.443	2.2	2.1	2.1		
3.665	1.3	1.4	1.4		

^a These physical properties are taken from the *Journal of Chemical Engineering Data*, 16(4), 425 (1971).

- g gravitational acceleration
- H system constant evaluated by Eq. (3)
- K system constant evaluated by Eq. (4)
- L total column length
- L' dimensionless column length, $HL/4K$
- S system constant defined by Eq. (14)
- T absolute temperature
- T_1, T_2 temperature of cold and hot wall
- \bar{T} reference temperature
- ΔT $T_2 - T_1$
- z transport direction

Greek Letters

α	thermal diffusion constant
β_T	$-(\partial\rho/\partial T)$
Δ	$c_T - c_B$
Δ_0	Δ obtained from experimental work
$\Delta_1, \Delta_2, \Delta_3$	Δ obtained from Eqs. (13), (9), and (23)
μ	viscosity
ρ	mass density
ω	one-half of the distance between the plates of a thermal diffusion column
σ	mass flow rate
σ'	$2\sigma/H$

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