LETTERS TO THE EDITOR

To the Editor:

The note titled "Approximate Models for Nonlinear Adsorption in a Packed-Bed Adsorber" by Lai and Tan (March, 1991, Vol. 37, p. 461) contains a rather serious error in time scales. Thus, their transformation from Eq. (32) to Eq. (33) required the introduction of relative time scale:

$$T = t - z/v \tag{1}$$

where $v = u/\epsilon_b$ is the interstitial fluid velocity (cf. Rice, *Chem. Eng. Sci.*, Vol. 37, p. 84, 1982). Thus, the time scales for their diffusion equation (Eq. 31) must also be changed to read:

$$\begin{aligned}\theta &= T \cdot D_e/(R^2K) \\ &= D_e(t - z/v)/(R^2K) = \tau/K \end{aligned}\tag{2}$$

and similarly their original scale τ must be:

$$\tau = T \cdot D_e/R^2 = D_e(t - z/v)/(R^2) \tag{3}$$

Thus, both θ and τ are misrepresented.

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Reply:

Indeed, we need to explain Eqs. 32 and 33 of our recent note further to avoid readers' confusion. To obtain Eq. 33 from Eq. 32, it requires to define a time variable θ' as:

$$\theta' = \frac{De}{R^2K}\left(t - \frac{z\epsilon_b}{u}\right) = \theta - \frac{De\epsilon_b z}{R^2uK} \tag{1}$$

With this definition and $Z = (z/L)$, Eq. 32 becomes

$$\frac{L}{u}\frac{\partial C_B}{\partial Z} = \frac{3(1-\epsilon_b)}{R}k_f(C_s - C_B) \tag{2}$$

After rearrangement, we have

$$\frac{\partial C_B}{\partial Z} = \alpha Bi(C_s - C_B)$$

which is Eq. 33 in the note.

The above derivation is similar to that proposed by Masamune and Smith (1965). For Figures 1 to 3 in the note, we calculated along the θ' and Z coordinates and transformed the calculated exit concentration from the θ' coordinate to the θ coordinate. Because θ' did not appear elsewhere in the note, the above derivation and the relevant literature were not mentioned. We would like to express our thanks to Prof. R. G. Rice for pointing out this omission. Incidentally, another point needs to be raised. During our calculation, we observed that almost the same results could be obtained using the pseudosteady-state approximation which neglects the transient term in Eq. 32 (Tan, 1986). This means that C_B at $Z = 1$ could be calculated by using either θ or θ'.

Literature cited

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To the Editor:

In the note titled "Batch Distillation of Binary Mixtures at Minimum Reflux," Bauerle and Sandall (June 1987, Vol. 33, p. 1034) found analytical solutions to the integration of the Rayleigh (1902) and the Bogart (1937) equations for the case of minimum reflux. We have found that these results are far from original. Additionally, we have derived an original approximate solution to the integration of the Rayleigh equation at any fixed reflux ratio. For clarity, all formulas are expressed using the same nomenclature as in the note by Bauerle and Sandall.

Rayleigh's famous equation for constant reflux operation is:

$$\ln\frac{W_2}{W_1} = \int_{x_{w1}}^{x_{w2}} \frac{dx_w}{x_D - x_w}. \tag{1}$$

Bauerle and Sandall integrated this for the case of constant minimum reflux to give:

$$\ln\frac{W_2}{W_1} = \frac{1}{R+1}\left[\frac{1}{\alpha-1}\ln\left(\frac{1-x_{w1}}{1-x_{w2}}\right)\frac{x_{w2}}{x_{w1}} + \ln\left(\frac{1-x_{w1}}{1-x_{w2}}\right)\right]. \tag{2}$$

Exactly the same equation, albeit in a slightly different form, due to changes in nomenclature, is given by Robinson and Gilliland (1950, p. 378). Furthermore, an equivalent equation is given by Bowman and Cichelli (1949):

$$\ln\frac{W_2}{W_1} = \frac{1}{R+1}\left[\frac{\alpha}{\alpha-1}\left(\ln\frac{1-x_{w1}}{1-x_{w2}}\right) - \frac{1}{\alpha-1}\ln\frac{x_{w1}}{x_{w2}}\right]. \tag{3}$$

Simple rearrangement of Eq. 3 gives Eq. 2. An earlier article by Colburn and Stearns (1941) is cited in both of the above. This article wrongly states the result as:

$$\ln\frac{W_2}{W_1}=(1-R)\left[\frac{1}{\alpha-1}\ln\left(\frac{1-x_{w1}}{1-x_{w2}}\right)\frac{x_{w2}}{x_{w1}}+\ln\left(\frac{1-x_{w1}}{1-x_{w2}}\right)\right]. \quad (4)$$

A simple mistake in the development of this equation was made in which R was used instead of $R/(R+1)$.

Bogart's equation for operation at constant overhead product composition is:

$$V=W_1(x_D-x_{w1})\times\int_{x_{w1}}^{x_{w2}}\frac{dx_w}{(x_d-x_w)^2\left(1-\dfrac{dL}{dV}\right)}. \quad (5)$$

Bauerle integrated this for the case of minimum reflux to give:

$$V=\frac{W_1(x_D-x_{w1})}{x_D(1-x_D)(\alpha-1)}\times\left[(1-x_D)\ln\left(\frac{x_D-x_{w2}}{x_D-x_{w1}}\right)\frac{x_{w1}}{x_{w2}}+x_D\alpha\ln\left(\frac{x_D-x_{w2}}{x_D-x_{w1}}\right)\left(\frac{1-x_{w1}}{1-x_{w2}}\right)\right]. \quad (6)$$

This same formula has been stated wrongly in two previous references. Perry and Green (1963, § 13, p. 31) offered the same equation as the above except that the factor α of the second term in the brackets on the righthand side is omitted. The equation is also stated incorrectly on p. 379 of Robinson and Gilliland (1950). In this case, an error probably has been made while developing the equation. Both of these references cite an earlier article by Edgeworth-Johnstone (1944), in which the original equation was developed correctly. This equation is given as:

$$V=\frac{W_1(x_D-x_{w1})}{x_D(1-x_D)(\alpha-1)}\left[(1-x_D)\ln\frac{1}{1-y_r}+x_D\alpha\ln\frac{x_D(1-x_{w2})}{x_D(1-x_{w2})-y_rx_{w2}(1-x_D)}\right], \quad (7)$$

where y_r is the final yield fraction. A simple material balance gives the yield fraction as:

$$y_r=\frac{x_D(W_1-W_2)}{x_{w1}W_1}=\frac{x_D(x_{w2}-x_{w1})}{x_{w1}(x_{w2}-x_D)}.$$

Substituting this into Eq. 7 yields Eq. 6.

An anonymous referee once advised one of us (WRP) that "the grand universal heuristic for researchers in distillation is 'someone has probably done it before'." WRP is happy to learn that he is not the only researcher subject to this doctrine.

We agree with Bauerle and Sandall on the advantages of approximate analytical solutions to batch distillation problems, avoiding tedious graphical and numerical procedures. It has long been known that an analytic solution to the integration of the Rayleigh equation, using the Smoker (1938) equation to relate x_p to x_s, is not available (Rose and Long, 1941). For high-purity separations ($x_d\approx 1$), however, we now offer an equation that we believe to be new. Jafarey et al. (1979) have shown that for such separations the Smoker equation for the rectification section of a column reduces to:

$$N=\frac{\ln\left(\dfrac{1-x_w}{1-x_D}\right)\left[\dfrac{R(\alpha-1)x_D-1}{R(\alpha-1)x_w-1}\right]}{\ln\left(\dfrac{\alpha R}{R+1}\right)}, \quad (8)$$

where N is the total number of theoretical plates (including the still pot). This may be written:

$$P=\left(\frac{1-x_w}{1-x_D}\right)\left(\frac{x_D-k}{x_w-k}\right), \quad (9)$$

where

$$P=\left(\frac{\alpha R}{R+1}\right)^N \text{ and } k=\frac{1}{R(\alpha-1)}.$$

Putting $x_D'=x_D-k$ and $x_w'=x_w-k$, and rearranging gives:

$$x_D'=\frac{Px_w'(1-k)}{1-k-x_w'}. \quad (10)$$

Table 1. Equation 12 (a) vs. Numerical Results (b)

α	N	R	$\frac{W_2}{W_1}$ (a)	$\frac{W_2}{W_1}$ (b)	$\overline{x_D}$
1.5	13	10	0.641	0.651	0.966
1.5	13	15	0.654	0.658	0.981
2.0	8	5	0.642	0.653	0.970
2.0	8	7.5	0.656	0.659	0.983

The Rayleigh equation may now be expressed as:

$$\ln\frac{W_2}{W_1}=\int_{x_{w1}'}^{x_{w2}'}\frac{dx_w'}{x_D'-x_w'}. \quad (11)$$

Substituting Eq. 10 into Eq. 11 yields eventually the tidy form:

$$\frac{W_2}{W_1}=\left[\left(\frac{1-x_{w1}}{1-x_{w2}}\right)^P\left(\frac{x_{w2}-k}{x_{w1}-k}\right)\right]^{\frac{1}{P-1}}. \quad (12)$$

Table 1 shows the results of calculating W_2/W_1 for four operating conditions. In all four cases, $x_{w1}=0.5$ and $x_{w2}=0.25$. The results from Eq. 12 are compared with those obtained when the Smoker equation is substituted into the Rayleigh equation and the result integrated numerically. The specifications were chosen to illustrate how the accuracy of the equation is affected by deviation from the assumption that the average distillate composition $\overline{x_D}\approx 1$. The equation is seen to be more accurate for the cases where the average distillate composition $\overline{x_D}$ is higher. For the cases in Table 1, agreement is to better than approximately 1.5% and roughly proportional to $1-\overline{x_D}$.

Literature cited

Bauerle, K. L., and O. C. Sandall, "Batch Distillation of Binary Mixtures at Minimum Reflux," *AIChE J.*, **33**, 1034 (1987).

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