The object of this column is to enhance our readers' collection of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested as well as those that are more traditional in nature, which elucidate difficult concepts. Please submit them to Professor James O. Wilkes and Professor T. C. Papanastasiou, ChE Department, University of Michigan, Ann Arbor, MI 48109.

AMUNDSON'S MATRIX METHOD FOR BINARY DISTILLATION REVISITED

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Amundson[1] expressed the binary distillation problem as a matrix difference equation. In this paper, matrix power equations will be used to solve and simplify the same problem, making it suitable for illustrating the application of matrices in courses of engineering mathematics or separations processes.

SOME RELATIONSHIPS IN MATRICES

Consider the matrix A of order 2:

$$A = \begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix} \tag{1}$$

whose characteristic equation, $|A - rI| = 0$, is

$$\begin{vmatrix} a_1 - r & a_2 \\ b_1 & b_2 - r \end{vmatrix} = 0 \tag{2}$$

or

$$r^2 - (a_1 + b_2)r + (a_1 b_2 - a_2 b_1) = 0 \tag{3}$$

where I is the unit matrix of the order of A. From the Cayley-Hamilton theorem, the matrix A also satisfies its own characteristic equation. Thus

$$A^2 - (a_1 + b_2)A + (a_1 b_2 - a_2 b_1)I = 0 \tag{4}$$

where O is the zero matrix of the order of A.

By using equations like Eq. (4) for higher powers and substituting from the lower power equations, it can be shown that

$$A^p = \alpha A + \beta I \tag{5}$$

where α and β are numerical constants which depend on the matrix A and exponent p.

Further, r_1 and r_2, the roots of Eq. (3), will also satisfy Eq. (5). Thus

$$r_1^p = \alpha r_1 + \beta \tag{6}$$

$$r_2^p = \alpha r_2 + \beta \tag{7}$$

Eqs. (5), (6), and (7) will be applied to binary distillation. However, first we need to formalize some of Amundson's treatment.

BINARY DISTILLATION

Following Amundson, by assuming constant volatility, the equilibrium line is

$$y = \frac{x}{A + Bx} \tag{8}$$

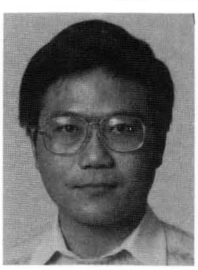
and the operating line is

$$y = mx + b \tag{9}$$

Taking the top product composition as d, the use of a total condenser gives $y_1 = d$. The plate numbers are counted from top to bottom. The liquid leaving plate 1 is obtained from Eq. (8). Thus

$$x_1 = \frac{Ay_1}{-By_1 + 1} \tag{10}$$

and y_2, obtained from the substitution of x_1 from Eq.



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(10) into the operating line equation [Eq. (9)], is

$$y_2 = mx_1 + b \qquad (11a)$$

Simplifying

$$y_2 = \frac{(mA - Bb)y_1 + b}{-By_1 + 1} \qquad (11b)$$

Now we can define y_{p+n}, the composition of the vapour leaving the $(p+n)^{th}$ plate, as

$$y_{p+n} = \left(y^*_{p+n} / y^{**}_{p+n}\right) \qquad (12a)$$

where

$$\begin{bmatrix} y^*_{p+n} \\ y^{**}_{p+n} \end{bmatrix} = \begin{bmatrix} a_1 & a_2 \\ b_1 & b_2 \end{bmatrix}^p \begin{bmatrix} y_n \\ 1 \end{bmatrix} \qquad (12b)$$

The plate number from which we begin the stepping-off process is n. The value of y_{p+n} when p = 1 (*i.e.*, y_{1+n}), is thus given by

$$y_{1+n} = \frac{y^*_{1+n}}{y^{**}_{1+n}} = \frac{a_1 y_n + a_2}{b_1 y_n + b_2} \qquad (13)$$

By comparing Eqs. (11b) and (13), where p = 1 and n = 1,

$$a_1 = mA - Bb \qquad (14a)$$

$$a_2 = b \qquad (14b)$$

$$b_1 = -B \qquad (14c)$$

$$b_2 = 1 \qquad (14d)$$

Thus

$$\begin{bmatrix} y^*_2 \\ y^{**}_2 \end{bmatrix} = \begin{bmatrix} (mA - Bb) & b \\ -B & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ 1 \end{bmatrix} \qquad (15)$$

With reference to Eq. (12b), it may be shown by induction that

$$\begin{bmatrix} y_{p+n^*} \\ y_{p+n^{**}} \end{bmatrix} = \begin{bmatrix} (mA - Bb) & b \\ -B & 1 \end{bmatrix}^p \begin{bmatrix} y_n \\ 1 \end{bmatrix} \qquad (16)$$

Applying Eq. (5), Eq. (16) may be re-written as

$$\begin{bmatrix} y_{p+n^*} \\ y_{p+n^{**}} \end{bmatrix} = \begin{bmatrix} \alpha(mA - Bb) & \alpha b \\ -\alpha b & \alpha \end{bmatrix} \begin{bmatrix} y_n \\ 1 \end{bmatrix} + \begin{bmatrix} \beta & O \\ O & \beta \end{bmatrix} \begin{bmatrix} y_n \\ 1 \end{bmatrix} \qquad (17)$$

The composition of vapour leaving the $(p+n)^{th}$ plate may then be written in terms of the vapour leaving the n^{th} plate as

$$y_{p+n} = \left(\frac{y_{p+n^*}}{y_{p+n^{**}}}\right) = \frac{\left[\alpha(mA - Bb) + \beta\right] y_n + \alpha b}{-\alpha B y_n + \alpha + \beta} \qquad (18)$$

In Eq. (18), given a binary distillation problem and assuming constant volatility and molal overflow, the only unknowns are α and β. Furthermore, β may be solved explicitly in terms of α by using Eq. (18). Thus

$$\beta = \frac{\left[-By_n y_{p+n} + y_{p+n} - (mA - Bb)y_n - b\right]\alpha}{y_n - y_{p+n}} \qquad (19)$$

It is now possible to eliminate α and β in Eqs. (6) and (7), and to evaluate p, the number of plates. The factors r_1 and r_2 are the roots of the characteristic equation of the square matrix given in Eq. (16), and they may be readily shown to be

$$r_1, r_2 = \frac{1}{2}\left[(mA - Bb + 1) \pm \sqrt{(mA - Bb + 1)^2 - 4mA}\right] \qquad (20)$$

Dividing Eq. (6) and Eq. (7), substituting the value for β from Eq. (19), and eliminating α

$$\left(\frac{r_1}{r_2}\right)^p = \frac{r_1(y_n - y_{p+n}) + \left[y_{p+n}(1 - By_n) - (mA - Bb)y_n - b\right]}{r_2(y_n - y_{p+n}) + \left[y_{p+n}(1 - By_n) - (mA - Bb)y_n - b\right]} \qquad (21)$$

Thus, the number of plates p betwen tray number (p+n) and n is given by

$$p = \frac{\ell n \dfrac{r_1(y_n - y_{p+n}) + \left[y_{p+n}(1 - By_n) - (mA - Bb)y_n - b\right]}{r_2(y_n - y_{p+n}) + \left[y_{p+n}(1 - By_n) - (mA - Bb)y_n - b\right]}}{\ell n \dfrac{r_1}{r_2}} \qquad (22)$$

APPLICATION

We shall now apply Eq. (22) to the same problem considered by Amundson in solving the distillation of a 0.40 mole fraction benzene mixed with toluene introduced at its bubble point. The equilibrium curve is given by

$$y = \frac{x}{0.41 + 0.59x} \qquad (23)$$

The top produce is 0.995 benzene, and the bottom is 0.005 benzene. The operating lines above and below the feed are, respectively

$$y = 0.75x + 0.249 \qquad (24)$$

$$y = 1.3773x + 0.001886 \qquad (25)$$

The roots for the characteristic equations for above and below the feed are, respectively

$$r_1 = 0.75130 \qquad r_2 = 0.40920 \qquad (26)$$

and

$$r_1 = 0.99744 \qquad r_2\,0.56615 \tag{27}$$

Applying Eq. (22) to above the feed position, $n = 1$, $y_1 = 0.995$, inserting the appropriate values for A, B, m, and b from Eqs. (23) and (24) with reference to Eqs. (10) and (11), and using $r_1 = 0.75130$ and $r_2 = 0.40920$, we obtain y_{n+1} by substituting the feed composition into the operating line as the feed is introduced at its bubble point. Thus $y_{n+1} = 0.549$ (or 0.553 using the lower operating line).

Applying the values

$$r_1 = 0.75130 \qquad r_2 = 0.40920$$
$$y_1 = 0.995 \qquad y_{p+1} = 0.549$$
$$B = 0.59 \qquad m = 0.75$$
$$A = 0.41 \qquad b = 0.249$$

results in 9.54 plates above feed position.

Below the feed position, Eq. (22) may be applied by taking $n = 9.54$, *i.e.*, $y_{9.54} = 0.549$. We obtain $y_{p+9.54}$ by substituting values for A, B, m, and b from Eqs. (23) and (25), and using $r_1 = 0.99744$ and $r_2 = 0.56615$. We obtain $y_{p+9.54}$ by substituting $x = 0.005$ into the equilibrium line to give $y_{p+9.54} = 0.0121$. Thus

$$r_1 = 0.99744 \qquad r_2 = 0.56615$$
$$y_{9.54} = 0.549 \qquad y_{p+9.54} = 0.0121$$
$$B = 0.59 \qquad m = 1.3773$$
$$A = 0.41 \qquad b = 0.001886$$

These values, when substituted into Eq. (22) yield 9.91 plates below feed position.

CONCLUSIONS

The binary distillation problem considered by Amundson was re-examined, and a simpler method involving powers of matrices has been given and an explicit solution obtained. This approach is suitable for use in engineering mathematics or separation processes courses to illustrate the application of matrices to engineering problems.

ACKNOWLEDGEMENTS

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POWER OF SPREADSHEETS

Continued from page 49.

students. Insight into the relative importance of variables and sensitivity of results to changes in the input can be gathered from such an exercise. The ease of changing input data also allows instructors to efficiently check calculations made with different combinations of independent variables.

CONCLUSIONS

Our experience with spreadsheet computing has proved to us that it is feasible to provide instruction on spreadsheet use as part of the mass and energy balances class. Within a time-frame of approximately two hours, students can learn sufficient fundamentals to use spreadsheets as a tool for solving a variety of problems in the class. After solving five to eight problems, most of them have enough confidence and experience to apply the techniques in future engineering classes.

The use of spreadsheets also encourages organization in problem solving which hopefully will carry through to the student's non-computer work. The flexibility and convenience of spreadsheets allows students to solve more meaningful problems and to examine the solutions in detail by manipulating independent variables to determine their effect. The built-in graphics capability also helps to tie together graphical and algebraic solution techniques when such alternate methods exist for a given problem.

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