ChE class and home problems

The object of this column is to enhance our readers' collections 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 and that elucidate difficult concepts. Manuscripts should not exceed ten double-spaced pages if possible and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

THE SHERRY SOLERA

An Application of Partial Difference Equations

CAMERON M. CROWE

McMaster University • Hamilton, Ontario, Canada L8S 4L7

In Andalucia in Spain, sherry is made using a system called the *solera*. The sherry *solera* is a sequential batch-mixing process in a collection of barrels that is designed to produce sherry with uniform quality from year to year. Each year the sherry product is removed from the set of barrels containing the oldest sherry, which is then replenished by the same amount of sherry from the set of barrels holding the next oldest sherry. This is repeated for sets of successively younger barrels until finally the set of barrels containing the youngest sherry is topped off with fresh sherry from the current vintage. This process has been called "fractional blending" by Baker, *et al*. [2]

PROBLEM STATEMENT

Don Juan de Amontillado y Fino, whose name is well known in the sherry world, wishes to set up a new *solera*. He has told us that Baker, *et al.*, published tables of the fractions of sherry of given ages in a given set of barrels after a specific number of years, but he would like to have a general formula showing how the number of barrels and the fraction withdrawn from a barrel would affect the average age of the sherry and the time to achieve steady state. Señor de Amontillado plans to start by accumulating P sets of barrels of sherry, each of whose ages initially equals the index, p=1,2,..., of that set of barrels. Then for each successive year, n=0,1,2,..., he will remove in turn a fraction α of each set of barrels, p=P,P-

1,...,3,2,1, and replace it from the next younger set, p=P-1,P-2,...,2,1,0, respectively. Here, p=0 represents the freshly produced sherry from the current vintage of age zero.

With A_{pn} representing the average age of barrel set p at year n, the equations can be written

$$\begin{split} A_{1,n+1} &= (1-\alpha) \big(A_{1n}+1\big) \\ A_{p+1,n+1} &= (1-\alpha) \big(A_{p+1,n}+1\big) + \alpha \big(A_{pn}+1\big) \qquad (p \geq 1) \\ A_{0n} &= 0; \qquad A_{p0} &= p-\alpha \qquad \text{for} \qquad p = 1, 2, ..., P \end{split} \tag{1}$$

The initial average ages are found by the sum

$$A_{p0} = (1-\alpha)p + \alpha(p-1) = p - \alpha$$

Equations (1) can be written in a standard form as



Cameron Crowe obtained his undergraduate degree from McGill University and his PhD from the University of Cambridge. He is a former Chair of Chemical Engineering at McMaster University and is now Professor Emeritus. His interests include data reconciliation and applied mathematics.

$$A_{1,n+1} - (1-\alpha)A_{1n} = 1 - \alpha$$

$$A_{p+1,n+1} - (1-\alpha)A_{p+1,n} - \alpha A_{pn} = 1 \quad (p \ge 1)$$
(2)

These are linear partial difference equations since there are two discrete indices, n and p, and the coefficients are constants. They are first order because the maximum difference in each subscript is unity.^[3] They can be solved by several different methods. First we will use recursion, starting with p=1. For simplicity, we will consider only one barrel in each set.

SOLUTIONS

#1. Recursive Solution

The solution of Eq. (2) for the first barrel can be written as the sum of the solution to the homogeneous equation (right side equal to zero) and a particular solution to the actual right side. The homogeneous solution is

$$A_{1n}^{H} = C_{1}(1-\alpha)^{n}$$

and the particular solution is a constant, namely

$$A_{1n}^{P} = \frac{(1-\alpha)}{\alpha}$$

Combining the two and inserting the initial condition $A_{10}=1-\alpha$, we get the solution

$$A_{1n} = \frac{(1-\alpha)}{\alpha} \left[1 - (1-\alpha)^{n+1} \right]$$
 (3)

We can now turn to the second difference equation (2) with p=1. This becomes

$$A_{2,n+1} - (1-\alpha)A_{2n} = 1 + \alpha A_{1n}$$
 (4)

The homogeneous solution has the same form as for $A_{\rm in}$, but the right side now involves not only a constant but also the same function as the homogeneous solution. The trial particular solution would then be

$$A_{2n}^{P} = a + bn(1-\alpha)^{n}$$

where a and b are unknowns to be found. The particular solution is then

$$A_{2n}^{P} = \frac{(2-\alpha)}{\alpha} - n(1-\alpha)^{n+1}$$
 (5)

The solution for A_{2n} can be written as

$$A_{2n} = \frac{(2-\alpha)}{\alpha} - \frac{2(1-\alpha)^{n+2}}{\alpha} - (n+1)(1-\alpha)^{n+1}$$
 (6)

The general solution can be obtained by continuing recursively until a pattern becomes clear. Using the notation for the binomial coefficient (read as "n choose j")

$$\binom{n}{j} \equiv \frac{n(n-1)(\cdots)(n-j+1)}{j!} = \frac{n!}{(n-j)!j!}$$
(7)

we find that

$$A_{pn} = \frac{(p-\alpha)}{\alpha} - \sum_{j=0}^{p-1} {n+1 \choose j} (p-j)(1-\alpha)^{n-j+2} \alpha^{j-1}$$
 (8)

We see that the steady-state average age of the p^{th} barrel is $(p-\alpha)/\alpha$.

This solution can be written in a different form by extending the summation to j=n+1 and subtracting the added terms. This allows us to use the binomial theorem

$$(x+y)^{m} = \sum_{j=0}^{m} {m \choose j} x^{j} y^{m-j}$$
 (9)

to obtain

$$A_{pn} = (p-\alpha) + n(1-\alpha) - \sum_{j=p}^{n} {n+1 \choose j+1} (j-p+1)(1-\alpha)^{n-j+1} \alpha^{j}$$
(10)

Here we can see that the summation is zero as long as n<p, so that for this case, the average age of a barrel is a linear function of n. It is only when n=p that the influence of the constant zero age of the fresh sherry addition is first felt in the pth barrel. This "shock wave" progresses through the barrels at the rate of one barrel per year and offers an interesting analogy to the shock wave traversing a tube at a fixed velocity in a first-order linear partial differential equation with constant coefficients.

#2. Use of z-Transforms

The partial difference equations (2) can also be solved by using the z-transform. The z-transform of A_{pn} is defined as

$$\sigma_{p} = \sum_{n=0}^{\infty} \frac{A_{pn}}{z^{n}} \tag{11}$$

The transforms of the partial difference equations (2) are obtained by dividing by z^n and adding over n=0 to infinity. We find that the transformed equations become

$$z\sigma_{1} - zA_{10} - (1 - \alpha)\sigma_{1} = \frac{(1 - \alpha)z}{(z - 1)}$$

$$z\sigma_{p+1} - zA_{p+1,0} - (1 - \alpha)\sigma_{p+1} - \alpha\sigma_{p} = \frac{z}{(z - 1)}$$
(12)

The transformed equations have become ordinary difference equations that can be solved directly. First, we can write the transform for the first Eq. (12), which becomes a boundary condition on the general equation

$$\sigma_1 = \frac{(1-\alpha)z^2}{(z-1)(z-1+\alpha)}$$
 (13)

It is easy to verify that this is indeed the transform of the previously obtained solution (3) for $A_{\rm ln}$. The general transformed equation can be put in standard form as

$$(z-1+\alpha)\sigma_{p+1} - \alpha\sigma_p = \frac{z}{(z-1)} + z(p+1-\alpha)$$
 (14)

The homogeneous solution to this equation is

$$\sigma_p^{H} = \frac{C\alpha^p}{(z-1+\alpha)^p} \tag{15}$$

Its particular solution is of the form ap+b and is

$$\sigma_{p}^{P} = \frac{pz}{(z-1)} + \frac{(z - \alpha z^{2})}{(z-1)^{2}}$$
 (16)

Adding these two terms and applying the boundary condition for p=1, we obtain the solution to the transformed difference equation as

$$\sigma_{p} = \frac{-(1-\alpha)z^{2}\alpha^{p}}{(z-1)^{2}(z-1+\alpha)^{p}} + \frac{pz}{z-1} + \frac{(z-\alpha z^{2})}{(z-1)^{2}}$$
(17)

To invert the transformed solution, we need to know the inverses of the components of Eq. 17. These inverses are listed in Table 1. The inverse of a product of two transforms is the convolution sum of their inverses. Thus, if σ is the transform of x_n and θ is the transform of y_n , then $\sigma\theta$ is the transform of

$$\sum_{k=0}^{n} x_k y_{n-k} \tag{18}$$

Then the inverted transform solution is

$$A_{pn} = p - \alpha + n(1 - \alpha) - \alpha^{p} \sum_{k=p}^{n} {k-1 \choose p-1} (n-k+1)(1-\alpha)^{k-p+1}$$
(19)

This solution is similar to the recursive Eq. (10), but differs notably in that the summation in the recursive solution changes the lower index of the binomial coefficient, whereas the transform solution changes the upper index. The question immediately arises as to whether or not these solutions are identical. The direct proof of their identity is somewhat laborious and is presented in Appendices 1 and 2 (which are available as an MS Word file from the author at crowe@mcmaster.ca). There is a simpler approach, however. If we can verify that *each* solution satisfies the partial difference equations, then it is sufficient to show that the solution is unique in order to prove their identity.

TABLE 1 List of inverses

Transform, σ z/(z-1) $z/(z-1)^2$ $z^2/(z-1)^2$ $\beta/(z-\beta)^p$ Inverse $1 \qquad n \qquad n+1 \qquad \binom{n-1}{p-1}\beta^{n-p+1}$

Proof of Identity of the Recursive and Transform Solutions

By setting n=0 in Eqs. (10) and (19), we can verify that the initial condition is satisfied by both. Further, by setting p=1, the solution for the first barrel (3) is found for both solutions. Then by substituting the recursive solution, Eq. (10), into the partial difference Eq. (2), we obtain

$$1 - \sum_{j=p+1}^{n+1} {n+2 \choose j+1} (j-p)(1-\alpha)^{n-j+2} \alpha^{j} +$$

$$\sum_{j=p+1}^{n} {n+1 \choose j+1} (j-p)(1-\alpha)^{n-j+2} \alpha^{j} +$$

$$\sum_{j=n}^{n} {n+1 \choose j+1} (j-p+1)(1-\alpha)^{n-j+1} \alpha^{j+1} = 1$$
(20)

The upper limit of the second summation can be increased to (n+1) since the added term is zero and the dummy variable in the third summation can be changed to i=j+1. Then the identity^[4]

$$\binom{n+2}{j+1} = \binom{n+1}{j+1} + \binom{n+1}{j}$$
 (21)

makes the three summations vanish together, thus satisfying the partial difference equation, Eq. (2).

Inserting the transform solution (Eq. 19) into the partial difference equation (2), we get

$$1+\alpha^{p+1}(1-\alpha)^{-p}\begin{bmatrix} -\sum_{k=p+1}^{n+1} \binom{k-1}{p} (n-k+2)(1-\alpha)^k + \\ \sum_{k=p+1}^{n} \binom{k-1}{p} (n-k+1)(1-\alpha)^{k+1} + \\ \sum_{k=p}^{n} \binom{k-1}{p-1} (n-k+1)(1-\alpha)^{k+1} \end{bmatrix} = 1$$
(22)

With arguments similar to those for Eq. (20), we find that the three bracketed summations also vanish here.

Thus, it remains only to prove that the solution is unique. Assume that there are two different solutions, A_{pn} and B_{pn} , both of which satisfy the partial difference equations and the

initial conditions. Then, if $\Delta_{pn} = B_{pn} - A_{pn}$, Eqs (2) imply that

$$\Delta_{1,n+1} - (1-\alpha)\Delta_{1n} = 0$$

$$\Delta_{p+1,n+1} - (1-\alpha)\Delta_{p+1,n} - \alpha\Delta_{pn} = 0$$
 (23)

But since $\Delta_{p0} = 0$ for all p, the only solution is $\Delta_{pn} = 0$, so that the solution is unique and the two forms of the solution are indeed identical.

#3. Matrix Solution

We rewrite the difference equations in matrix form and use matrix algebra to obtain another solution. If we define

$$\mathbf{A}_{n} = \begin{bmatrix} \mathbf{A}_{1n} & \mathbf{A}_{2n} & \dots & \mathbf{A}_{Pn} \end{bmatrix}^{\mathrm{T}} \tag{24}$$

then the difference equations (2) can be written as

$$\mathbf{A}_{n+1} - \mathbf{M} \mathbf{A}_n = \mathbf{b} \tag{25}$$

where

$$\mathbf{M} = \begin{bmatrix} (1-\alpha) & & & \\ \alpha & (1-\alpha) & & \\ & \ddots & \ddots & \\ & & \alpha & (1-\alpha) \end{bmatrix}$$
 (26)

M is bidiagonal with uniform elements on the diagonal and also on the sub-diagonal.

The right side of Eq. (25) is

$$\mathbf{b} = \begin{bmatrix} (1 - \alpha) \ 1 \ \dots \ 1 \end{bmatrix}^{\mathrm{T}} \tag{27}$$

and the initial condition is

$$\mathbf{A}_0 = \begin{bmatrix} (1 - \alpha) & (2 - \alpha) & \dots & (P - \alpha) \end{bmatrix}^{\mathrm{T}}$$
 (28)

The particular solution to Eq. 25 can be written as

$$\mathbf{A}_{n}^{P} = (\mathbf{I} - \mathbf{M})^{-1} \mathbf{b} = \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix}^{-1} \frac{\mathbf{b}}{\alpha} = \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ \vdots & \vdots & \ddots & \\ 1 & 1 & \dots & 1 \end{bmatrix} \frac{\mathbf{b}}{\alpha} = \frac{\mathbf{A}_{0}}{\alpha}$$
(29)

whereas the homogeneous solution is $\mathbf{A}_n^H = \mathbf{M}^n \mathbf{A}_0$.

Then the general solution is

$$\mathbf{A}_{n} = \mathbf{A}_{n}^{P} + \mathbf{C}\mathbf{A}_{n}^{H} = \frac{\mathbf{A}_{0}}{\alpha} + \mathbf{C}\mathbf{M}^{n}\mathbf{A}_{0}$$
 (30)

with **C** as a diagonal matrix of constants to force the solution to fit the initial conditions. Thus, with n=0 we find that

$$\mathbf{C} = \left[\operatorname{diag} \left(- \left(\frac{1 - \alpha}{\alpha} \right) \right) \right]$$

Therefore, the solution becomes

$$\mathbf{A}_{n} = \frac{\left[\mathbf{I} - (1 - \alpha)\mathbf{M}^{n}\right]\mathbf{A}_{0}}{\alpha} \tag{31}$$

Now the n^{th} power of \mathbf{M} can be seen by direct multiplication to be a lower triangular matrix with uniform elements on the diagonal and on each sub-diagonal. When n < P, there are n non-zero sub-diagonals, whereas for $n \ge P$, all the sub-diagonals are non-zero. We find that the j^{th} sub-diagonal of \mathbf{M}^n is uniformly equal to

$$\binom{n}{j} \alpha^{j} (1-\alpha)^{n-j} \tag{32}$$

and the diagonal elements are given by setting j=0 in this expression.

We can then write Eq. (31) for a particular barrel p and year n as

$$A_{pn} = \frac{(p-\alpha)}{\alpha} - \sum_{j=0}^{p-1} {n \choose j} (p-j-\alpha) (1-\alpha)^{n-j+1} \alpha^{j-1}$$
 (33)

As with the recursive solution, Eq. (10), we can add and subtract the terms in the summation for j going from p to n. Using the binomial theorem, we can show that the solution also takes the form

$$A_{pn} = (p-\alpha) + n(1-\alpha) - \sum_{j=0}^{n} {n \choose j} (j-p+\alpha) \alpha^{j-1} (1-\alpha)^{n-j+1}$$
 (34)

This solution is very similar to the recursive solution Eq. (10), but is not the same. We can again show that it satisfies the difference equations (2), the initial conditions, and the solution for p=1 and is thus the same unique solution in a slightly different form. The direct proof that the matrix solution and the recursive solution are identical is available as Appendix 3 from the author.

#4. Forward Shift Operator Method

We define the forward shift operators, E_1 and E_2 , by the operator equations^[3]

$$E_1 A_{pn} = A_{p+1,n}$$
 and $E_2 A_{pn} = A_{p,n+1}$ (35)

Then the difference equations (2) can be written as

$$\left[E_2 - (1 - \alpha)\right]A_{1n} = 1 - \alpha \tag{36}$$

$$[E_1E_2 - (1-\alpha)E_1 - \alpha]A_{pn} = 1$$
 (37)

The particular solution for Eqs. (36) and (37) can be written as before as

$$A_{pn}^{P} = \frac{(p-\alpha)}{\alpha} \tag{38}$$

For Eq. (36), the homogeneous solution is

$$A_{1n}^{H} = C_1 (1 - \alpha)^n \tag{39}$$

Winter 2002

which gives the same general solution as in Eq. (3). For the homogeneous solution to Eq. (37), we can operate on it with E_1^{-1} to get

$$E_2 A_{pn}^{H} = \left[\alpha E_1^{-1} + (1 - \alpha) \right] A_{pn}^{H}$$
 (40)

Since the operator on the right side has no effect on the subscript n, the homogeneous solution takes the form

$$A_{pn}^{H} = \left[\alpha E_{1}^{-1} + (1 - \alpha)\right]^{n} B_{p}$$
 (41)

where B_p is an unknown function of p. We can expand the operator expression with the binomial theorem, but we need to remember that $A_{nn}=0$ for p<1. Then

$$A_{pn}^{H} = \sum_{j=0}^{p-1} {n \choose j} \alpha^{j} (1-\alpha)^{n-j} B_{p-j}$$
 (42)

and with Eq. (38)

$$A_{pn} = A_{pn}^{P} + A_{pn}^{H} = \frac{(p - \alpha)}{\alpha} + A_{pn}^{H}$$
 (43)

When n=0, A_{p0} =p- α so that we see that

$$B_{p} = -\frac{(p-\alpha)(1-\alpha)}{\alpha} \tag{44}$$

We can then recover the same solution as we did using matrix algebra.

COMMENTS

To calculate most easily the numerical solution to the partial difference equations (2), we can use a spreadsheet by entering the initial conditions at n=0 on the worksheet. Then the recursive equations (1) can be entered in the cells n=1 and for p=1 and 2, respectively, and then copied over the desired ranges of p and n. The values for five barrels are shown in Figure 1, with α =0.25. The number of years needed to reach 90% of the steady-state average ages for two values of α are shown in Table 2.

The effect of the fraction withdrawn, α , on the average age of the sherry in the fifth barrel is shown in Figure 2.

The actual number of years to reach any particular average barrel age is the number of years since the startup of the *solera* plus the number of barrels, since that many additional years had to pass before the *solera* could be started. From Figures 1 and 2 and Table 2, it is evident that the steady state is reached earlier, the higher is the fraction α removed from each barrel, but the steady-state average age of each barrel is also reduced by increasing the fraction removed. This would affect the quality of the sherry product.

The linear partial difference equations that describe the sherry *solera* can be solved in different ways. Four different theoretical methods have been applied to obtain the unique solution, even though three superficially different forms of the solution were obtained. The fact that each solution satis-

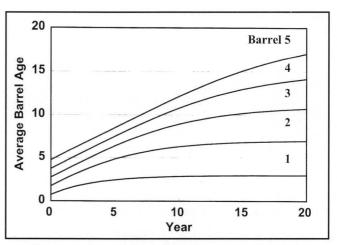
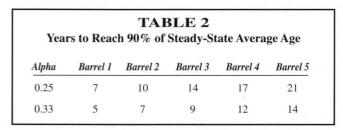


Figure 1. Average barrel age versus year; $\alpha = 0.25$.



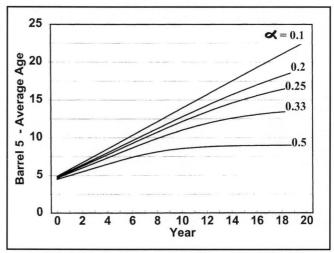


Figure 2. Effect of α on the average age of barrel 5.

fies the equations and the initial conditions, and that the solution was shown to be unique, prove that the apparently different solutions are indeed the same. For the numerical solution, a spreadsheet is the most convenient tool to use.

REFERENCES

- 1. Jeffs, J., Sherry, 3rd ed., Faber and Faber, London (1982)
- Baker, G.A., M.A. Amerine, and E.B. Roessler, "Theory and Application of Fractional-Blending Systems," *Hilgardia*, 21, 383 (1952)
- Mickens, R.E., Difference Equations: Theory and Applications, 2nd ed., Van Nostrand Reinhold, New York, NY (1990)
- Graham, R.L., D.E. Knuth, and O. Patashnik, Concrete Mathematics, Addison-Wesley Publishing Company, Reading, MA (1989) □