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@engin.umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

USE OF THE RESIDUE THEOREM TO INVERT LAPLACE TRANSFORMS

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Chemical engineers are quite familiar with the use of the Laplace transform method for solving linear ordinary differential equations. Usually, the differential equation is converted to an equivalent algebraic equation, then the appropriate initial conditions are applied, and the resulting algebraic equation is prepared for inversion in order to recover the sought-after solution.

Frequently, the techniques to invert the resulting algebraic equation involve the use of a table of Laplace transforms. Most practitioners of this approach develop devices to extend their table of Laplace transforms when their particular inversion is not listed.

There is an alternate technique, however, that is especially useful when a difficult inversion is to be performed. This method employs a concept that is fundamental in the theory of functions of a complex variable—namely the *residue theorem.*

Following Mickley, Sherwood, and Reed,[1] Churchill and Brown,[2] and Dettman,[3] the variable s in

$$F(s)=\int_0^\infty e^{-st}f(t)dt \tag{1}$$

can be interpreted as a complex number. Here, F(s) is the Laplace transform of f(t). Further, except for singularities, F(s) is usually analytic (has a Taylor series expansion).

A frequently encountered class of problems in chemical engineering are the Sturm-Liouville problems, and it is useful to know that the transform of a solution to a Sturm-Liouville equation is analytic for all finite s except at the singularities (poles) of the system.

When F(s) is analytic, except for poles, the inverse transform is given by

$$f(t)=L^{-1}\{F(s)\}=\sum_{n=0}^{\infty}\rho_n(t) \tag{2}$$

where $\rho_n(t)$ is the residue of F(s) at the pole s_n. Even though this concept is firmly grounded in the theory of functions of a complex variable, direct use of complex variables is not always required. A procedure is given below that avoids the direct use of complex variables.

PROCEDURE

Rewrite F(s) as a quotient

$$F(s)=\frac{P(s)}{Q(s)} \tag{3}$$

which enables us to quickly identify the singular points (poles) of F(s) and to determine if the degree of Q(s) is at least one greater than that of P(s). This procedure may require power series expansions of both P(s) and Q(s). If the degree of the denominator is at least one greater than that of the numerator, and the poles are simple (singularities of order one), then

$$\rho_n(t)=\frac{P(s_n)}{Q'(s_n)}e^{s_n t} \tag{4}$$

where $Q'(s_n)$ is the derivative of Q(s) evaluated at the simple pole s_n.

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If the poles are of order m (multiple pole), then

$$\rho_n(t)=e^{s_n t}\left[A_1+tA_2+\frac{t^2}{2!}A_3+\ldots+\frac{t^{m-1}A_m}{(m-1)!}\right]=e^{s_n t}\sum_{j=1}^{m}A_j\frac{t^{j-1}}{(j-1)!} \tag{5}$$

The A's are defined by

$$A_j=\frac{1}{(m-j)!}\frac{d^{m-j}}{ds^{m-j}}\left[(s-s_n)^m F(s)\right]_{s=s_n} \qquad j=1,2,\ldots,m \tag{6}$$

Three examples are presented below. Examples 1 and 2 are elementary problems that can be quickly inverted by use of tables; they are presented here to illustrate the concept of the residue method. The third example demonstrates a more appropriate application of the method.

EXAMPLE PROBLEMS

1. Simple Poles

Suppose we need to invert

$$F(s)=\frac{5s^2-7s+17}{(s-1)(s^2+4)}=\frac{P(s)}{Q(s)} \tag{7}$$

Here,

$$P(s)=5s^2-7s+17, \quad Q(s)=(s-1)(s^2+4), \quad Q'(s)=s^2+4+(s-1)2s \tag{8}$$

The roots of Q(s) are the simple poles of F(s). Therefore, Eq. (4) is the appropriate form with which to evaluate the residues since the poles are not repeated; that is

$$\rho_1(t)=\frac{P(1)}{Q'(1)}=3e^t \tag{9}$$

$$\rho_{2i}(t)=\frac{P(2i)}{Q'(2i)}e^{2it}=\left(1+\frac{5i}{4}\right)e^{2it} \tag{10}$$

$$\rho_{-2i}(t)=\frac{P(-2i)}{Q'(-2i)}e^{-2it}=\left(1-\frac{5i}{4}\right)e^{-2it} \tag{11}$$

so that use of Eq. (2) results in

$$f(t)=\rho_1(t)+\rho_{2i}(t)+\rho_{-2i}(t) \tag{12}$$

That is

$$f(t)=3e^t+2\cos 2t-\frac{5}{2}\sin 2t \tag{13}$$

2. Multiple Poles

Suppose we wish to invert

$$F(s)=\frac{s}{\left(s^2+1\right)^2} \tag{14}$$

for which

$$P(s)=s \quad \text{and} \quad Q(s)=\left(s^2+1\right)^2 \tag{15}$$

Q(s) has repeated roots at ±i,±i, so that the multiplicity, m, of each root is two. Therefore, as singularities of F(s), these are poles of order 2. Then using Eq. (5) with s=-i,

$$\rho_{-i}(t)=e^{-it}(A_1+tA_2) \tag{16}$$

since m = 2. Also,

$$(s+i)^2\frac{s}{(s-i)^2(s+i)^2}=\frac{s}{(s-i)^2} \tag{17}$$

Application of Eq. (6) gives

$$A_1=\frac{1}{(2-1)!}\frac{d}{ds}\left[\frac{s}{(s-i)^2}\right]=\frac{1}{2}\left[\frac{-i-s}{(s-i)^3}\right]_{s=-i}=0 \tag{18}$$

and

$$A_2=\frac{1}{1!}\left[\frac{s}{(s-i)^2}\right]_{s=-i}=\frac{i}{4} \tag{19}$$

Therefore

$$\rho_{-i}(t)=\frac{it}{4}e^{-it} \tag{20}$$

Similarly

$$\rho_i(t)=-\frac{it}{4}e^{it} \tag{21}$$

such that Eq. (2) results in

$$f(t)=\rho_{-i}(t)+\rho_i(t)=\frac{t}{2}\left(\frac{e^{it}-e^{-it}}{2i}\right)=\frac{1}{2}t\sin t \tag{22}$$

in which use of the identities

$$\cos\theta=\frac{e^{i\theta}+e^{-i\theta}}{2} \quad \text{and} \quad \sin\theta=\frac{e^{i\theta}-e^{-i\theta}}{2i} \tag{23}$$

are employed to express the final results of both examples.

3. Diffusivities of Gases in Polymers

Consider a model of diffusion through a membrane that separates two compartments of a continuous-flow permeation chamber. Then, following Felder, Spence, and Ferrell,[4] at time t=0, a penetrant is introduced into one compartment (the upstream compartment) and permeates through the membrane into a stream flowing through the other (downstream) compartment. Further, this model includes the following assumptions:

- *Diffusion of the penetrant in the gas phase and absorption at the membrane surface are instantaneous processes.*
- *Diffusion in the membrane is Fickian with a constant diffusivity.*
- *The concentration of dissolved gas at the downstream surface of the membrane is always sufficiently low compared to that at the upstream surface, such that the downstream surface concentration may be set equal to zero.*

Then, diffusion through a flat membrane of thickness h is described by

$$\frac{\partial C(t,x)}{\partial t}=D\frac{\partial^2 C(t,x)}{\partial x^2} \tag{24}$$

subject to

$$C(0,x)=0 \tag{25}$$

$$C(t,0)=C_1 \tag{26}$$

$$C(t,h)=0 \tag{27}$$

Application of Eq. (1) to transform Eqs. (24 - 27) results in the second-order constant-coefficient homogeneous differential equation

$$0=\frac{d^2y(s,x)}{dx^2}-\frac{sy}{D} \tag{28}$$

subject to

$$y(s,0)=\frac{C_1}{s} \tag{29}$$

and

$$y(s,h)=0 \tag{30}$$

The solution to the boundary-value problem described by Eqs. (28-30) is

$$y(s,x)=C_1\left[\frac{\sinh\left(\sqrt{\frac{s}{D}}h\right)\cosh\left(\sqrt{\frac{s}{D}}x\right)-\cosh\left(\sqrt{\frac{s}{D}}h\right)\sinh\left(\sqrt{\frac{s}{D}}x\right)}{s\sinh\left(\sqrt{\frac{s}{D}}h\right)}\right] \tag{31}$$

Then, applying Eqs. (2-4) to invert y(s,x), we get

$$L^{-1}[y(s,x)]=C(t,x)=C_1\sum_{n=0}^{\infty}\frac{P(s_n,s)}{Q'(s_n)}\exp(s_n t)=$$

$$C_1 L^{-1}\left[\frac{\sinh(h-x)\sqrt{\frac{s}{D}}}{s\sinh\left(\sqrt{\frac{s}{D}}h\right)}\right] \tag{32}$$

Recall that

$$\frac{P(s_n)}{Q'(s_n)}=\lim_{s\to s_n}\frac{P(s)}{\left[\frac{Q(s)-Q(s_n)}{s-s_n}\right]}=\lim_{s\to s_n}(s-s_n)\frac{P(s)}{Q(s)} \tag{33}$$

such that for $s_0=0$

$$\rho_0(t)=\frac{P(0)}{Q'(0)}=\lim_{s\to 0}s\frac{P(s)}{Q(s)} \tag{34}$$

Then for

$$y(s,x)=\frac{P(s,x)}{Q(s)} \tag{35}$$

where

$$P(s,x)=\sinh(h-x)\sqrt{\frac{s}{D}} \tag{36}$$

and

$$Q(s)=s\sinh\left(\sqrt{\frac{s}{D}}h\right) \tag{37}$$

$$\rho_0(t)=\lim_{s\to 0}s\frac{P(s)}{Q(s)}=\lim_{s\to 0}s\frac{\sinh(h-x)\sqrt{\frac{s}{D}}}{s\sinh\left(\sqrt{\frac{s}{D}}h\right)}=\frac{h-x}{h} \tag{38}$$

gives the residue at s=0 using l'Hospital's rule. for $s_n \neq 0$,

$$Q'(s_n)=\sinh\left(\sqrt{\frac{s}{D}}h\right)+s\left[\frac{h}{2\sqrt{sD}}\cosh\left(\sqrt{\frac{s}{D}}h\right)\right] \tag{39}$$

The simplifying substitution $i\lambda=\sqrt{s/D}$ results in

$$\lambda=n\frac{\pi}{h},\qquad n=1,2,\cdots \tag{40}$$

$$s_n=-\lambda_n^2 D \tag{41}$$

That is, when Eq. (37) is set equal to zero, either s=0 or $\sinh\sqrt{s/D}\,h=0$. The case s=0 results in the residue $\rho_0(t)$ given above (Eq. 38), while the case s≠0 gives $\sinh i\lambda=0$, a condition that is satisfied for the values of λ as given in Eq. (40). Finally, after performing the necessary algebra, we get the result

$$\rho_n(t,x)=\frac{P(s_n,x)}{Q'(s_n)}e^{s_n t}=-\frac{2}{n\pi}\sin\left(\frac{n\pi x}{h}\right)e^{-\lambda_n^2 Dt} \tag{42}$$

and the concentration profile is

$$C(t,x)=C_1\left[\frac{h-x}{h}-\frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\exp\left(\frac{n^2\pi^2 tD}{h^2}\right)\sin\left(\frac{n\pi x}{h}\right)\right] \tag{43}$$

Then, the rate of penetrant across the surface x=h is given by

$$J(t)=-DA\left(\frac{\partial C}{\partial x}\right)_{x=h}=\frac{DAC_1}{h}\left[1+2\sum_{n=1}^{\infty}(-1)^n\exp\left(-\frac{n^2\pi^2 Dt}{h^2}\right)\right] \tag{44}$$

for a flat membrane with a surface area A. Also notice that the steady-state rate, J_{ss}, is given by

$$J_{ss}=D\frac{AC_1}{h} \tag{45}$$

For an example involving cylindrical geometry, the reader is directed to the recent literature where a model based on membrane separation is treated by Ramraj, Farrell, and Loney.[5] Also, a model involving membrane separation with chemical reaction in a flowing system is treated by Loney.[6]

Inversion by the residue method is not a new concept; however, it can be very useful in efficiently solving systems of non-homogeneous linear partial differential equations.

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