LETTERS TO THE EDITOR

To the Editor:

In a recent R&D note by Huang et al. (1984), an analytical solution for a packed bed reactor with a first-order reaction is derived. The solution is obtained by the Laplace-transform method and by inversion in the complex plane. Since the transform contains branch points a, so called second Bromwich contour (McLachlan, 1953) is used to obtain the solution in the time domain.

Some criticism is also made of an earlier analytical solution of the same problem (but without chemical reaction) given by Rasmuson and Neretnieks (1980). We are supposed to have used the first Bromwich contour (McLachlan, 1953) in our derivation. Since the Laplace transform contains branch points, they contend, this procedure is not valid. This statement is correct. However, in our analytical inversion, neither the first nor second Bromwich contour is used. Instead, we integrate along the imaginary axis. This integration path follows direct application of the complex inversion integral for the Laplace transform. We would like to clarify our analytical inversion of the Laplace transform and discuss relative merits of various methods.

Under very general conditions, the inversion integral of the Laplace transform is given (Churchill, 1972; Doetsch, 1976) by:

$$f(t) = \frac{1}{2\pi i} \int_{\alpha - i\infty}^{\alpha + i\infty} e^{st} \bar{f}(s)\, ds \qquad (1)$$

The integration is to be performed along the straight line $Re(s) = \alpha$ parallel to the imaginary axis. The real number α is chosen so that $s = \alpha$ lies to the right of all the singularities of the integrand but is otherwise arbitrary. At this stage, it should be stressed that Eq. 1 defines the inversion operation. Bromwich contours, on the other hand, are methods of evaluating Eq. 1 by closing the integration path in the left half-plane. This is done in various ways depending on the type of singularities of $\bar{f}(s)$.

In contrast, the method we use directly evaluates Eq. 1. This is done by using the fact that for any real function $f(t)$:

$$\overline{\bar{f}(s)} = \bar{f}(\bar{s}) \qquad (2)$$

i.e. the complex conjugate of the Laplace transform of $f(t)$ is equal to the Laplace-transform of the complex conjugate of the independent variable s (principle of reflection, Churchill, p. 188). Then, although the inversion integral is an integral in the complex plane, we can write it as a real improper integral (Churchill, p. 194). In our derivation, we take the path of integration along the imaginary axis with a small semicircle Γ of radius $\epsilon \to 0$ excluding the origin (where there is a simple pole). Details are given in the original paper (Rasmuson and Neretnieks, 1980). The evaluation of the square root in the Laplace transform can cause no ambiguities. Of the two possible roots, that one is to be picked for which $\bar{f}(s)$ tends to zero as $s \to +\infty$.

It is not surprising that our solution and the solution of Huang *et al.* have different structures. They have been obtained using different integration paths in the complex plane, and any function can be represented in many ways. Our method of analytical inversion has the advantage that the exact locations of the singularities of $\bar{f}(s)$ are not needed. It is necessary only to show that the integration path is to the right of all of them.

However, the ultimate test of formal analytical solutions of this kind is how they perform numerically. We have devised a method where the integration of the real improper integral is performed over each half-period of the oscillatory integrand (Rasmuson and Neretnieks, 1981). The convergence of the alternating series obtained, which may be very slow, is then accelerated by repeated averaging of the partial sums (Dahlquist and Björck, 1974). Convergence is usually very rapid.

Furthermore, an upper bound of the truncation error is obtained. Using this numerical method, our solution has been evaluated over a wide range of parameter values (Rasmuson and Neretnieks, 1981, 1982; Rasmuson, 1983). In addition, the solution has, numerically, been compared with the analytical solution by Rosen (1952, 1954) when $D_L \to 0$ (D_L longitudinal dispersion coefficient); Lapidus and Amundson (1952) for the case of negligible external and internal diffusion resistance but D_L finite; Carslaw and Jaeger (1959, p. 396) for short contact times, $D_L \to 0$, negligible external diffusion resistance but with internal diffusion; with excellent agreement. Moreover, the solution has been favorably compared with various numerical codes (e.g., INTRACOIN, 1984; Raghavan and Ruthven, 1983; Rasmuson et al. (1982)).

The problem treated by Huang et al. (1984), including chemical reaction, is essentially a special case of a problem treated by Rasmuson (1982) concerning conversion in catalytic reactors.

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Reply:

We agree with Rasmuson and Neretnieks regarding our paper (1984) and the earlier paper by Rasmuson and Neretnieks (1980). Their procedure is correct and represents a different approach for obtaining solutions to problems of this type. We thank Rasmuson and Neretnieks for clarifying our misconceptions regarding their work.

Equation 17 of Huang et al. (1984) should read:

$$Y_D(s) = \frac{3K_s}{\sigma^2}(\sigma \coth \sigma - 1) + \lambda K$$

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