

$u$	= velocity component along x-co-ordinate
$u_1$	= dimensionless velocity component defined in Equation (3)
$U$	= velocity component outside the boundary layer
$U_1$	= dimensionless velocity component defined in Equation (3)
$U_\infty$	= velocity of free stream
$Wi$	= Weissenberg number defined by Equations (4) and (39)
$x$	= distance along the curved surface
$x_1$	= dimensionless distance defined in Equation (3)
$y$	= distance normal to the curved surface
$y_1$	= dimensionless distance defined in Equation (3)

#### Greek Letters

$\alpha_F$	= ratio of the thermal boundary layer thickness to the momentum boundary layer thickness for pure forced convection
$\alpha_N$	= ratio of the thermal boundary layer thickness to the momentum boundary layer thickness for pure free convection
$\beta$	= expansion coefficient of the fluid
$\delta$	= momentum boundary layer thickness
$\delta_1$	= dimensionless momentum boundary layer thickness defined in Equation (3)
$\delta_T$	= thermal boundary layer thickness

$\delta_{T1}$	= dimensionless thermal boundary layer thickness defined in Equation (3)
$\eta$	= similarity variable defined in Equation (9)
$\eta_T$	= similarity variable defined in Equation (9)
$\theta$	= dimensionless temperature difference defined in Equation (3)
$\mu$	= viscosity of the second order fluid
$\rho$	= density of the fluid

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Manuscript received August 13, 1979; revision received October 31, and accepted November 2, 1979.

## Exact Solution of a Model for Diffusion in Particles and Longitudinal Dispersion in Packed Beds

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The problem of mass and heat transfer during flow through a packed bed has numerous applications in the chemical process industries. Theoretical studies of longitudinal dispersion, of either thermal energy or component concentration, in fixed-bed systems are readily available in the literature, and the analogy between heat conduction and component diffusion renders the analyses interchangeable. The following set of equations, which go back to the work by Deisler and Wilhelm (1953), has been employed by several authors

$$\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial z} - D_L \frac{\partial^2 C}{\partial z^2} = -\frac{1}{m} \left( \frac{\partial q}{\partial t} \right) \quad (1)$$

$$\frac{\partial q_i}{\partial t} = D_s \left( \frac{\partial^2 q_i}{\partial r^2} + \frac{2}{r} \frac{\partial q_i}{\partial r} \right) \quad (2)$$

The terms in the first equation stand for accumulation in the fluid phase, convective transport, transport by axial dispersion and volume-averaged accumulation in the spherical porous particles. In the second equation, the terms give accumulation in the particles and radial diffusion respectively. The assumptions leading to these equations have been discussed by Babcock et al. (1966) and by Pellett (1966). The boundary conditions commonly used are

$$C(0, t) = C_o \quad (3)$$

$$C(\infty, t) = 0 \quad (4)$$

$$C(z, 0) = 0 \quad (5)$$

$$q_i(0, z, t) \neq \infty \quad (6)$$

$$q_i(b, z, t) = q_s(z, t) \text{ given by } \frac{\partial q}{\partial t} = \frac{3k_f}{b} \left( C - \frac{q_s}{K} \right) \quad (7)$$

$$q_i(r, z, 0) = 0 \quad (8)$$

The boundary condition (7) is the link between Equations (1) and (2). It states mathematically that the mass entering or leaving the particles must equal the flow of mass transported across a stagnant fluid film at the external surface.

For the case with no dispersion ( $D_L = 0$ ), a classical solution of Equations (1) and (2) subject to the boundary conditions (3)-(8) was given by Rosen (1952) in terms of an infinite integral. Babcock et al. (1966) and Pellett (1966) have presented analytical solutions for the case including dispersion. Approximate solutions have been given by Radeke et al. (1976).

The solution of Babcock et al. (1966) was found to be in error for  $D_L > 0$ . For short times, values of  $C/C_o$  are predicted that are independent of time (Figure 1). It is to be shown below that Babcock's solution is actually a limiting solution for low values of

$D_L$ . For  $D_L = 0$  the solution is identical to that given by Rosen (1952). The solution of Pellett (1966) is an infinite integral, where the integrand is a function of two infinite sums. This solution is difficult to evaluate in the general case. A solution was therefore developed (Appendix) based on the work by Rosen, where the infinite sums are given as explicit functions. The numerical evaluation is thereby considerably simplified.

The simultaneous solution for Equations (1) and (2), with the boundary conditions indicated, involves the following steps. The details are presented in Appendix.

The solution of Equation (2) is available (Carslaw and Jaeger 1959, Rosen 1952) in a form that expresses the concentration distribution within the solid particles as a function of the variable surface concentration  $q_s(z, t)$ . This expression is first averaged by integration over the entire volume of the particle. It is then differentiated with respect to time to yield an expression for  $\partial \bar{q}/\partial t$ , the rate of change of average concentration within the solid. The expression for  $\partial \bar{q}/\partial t$  is introduced into Equation (1) and the Laplace transform with respect to time is taken. When one makes use of the Faltung integral theorem, uses Equation (7) in the Laplace domain to express the surface concentration  $q_s(z, t)$  in terms of  $\partial \bar{q}/\partial t$ , expresses the result as the left hand side of Equation (1), and substitutes the entire group back into the transformed equation, an ordinary, second-order linear differential equation results. It has the transformed variable  $\bar{C}$  as the dependent variable. Solving the ordinary differential equation and taking the inverse transform in the complex domain one finally obtains

$$u(z, t) = \frac{C(z, t)}{C_0} = \frac{1}{2} + \frac{2}{\pi} \int_0^\infty \exp\left(\frac{Vz}{2D_L} - z \sqrt{\frac{x'(\lambda)^2 + y'(\lambda)^2 + x'(\lambda)}{2}}\right) \sin\left(\sigma\lambda^2 t - z \sqrt{\frac{x'(\lambda)^2 + y'(\lambda)^2 - x'(\lambda)}{2}}\right) \frac{d\lambda}{\lambda} \quad (9)$$

with

$$x'(\lambda) = \frac{V^2}{4D_L^2} + \frac{\gamma}{mD_L} H_1 \quad (10)$$

$$y'(\lambda) = \frac{\sigma\lambda^2}{D_L} + \frac{\gamma}{mD_L} H_2 \quad (11)$$

$H_1$  and  $H_2$  are complicated hyperbolic functions of  $\lambda$  and  $\nu$

$$H_1(\lambda, \nu) = \frac{H_{D1} + \nu(H_{D1}^2 + H_{D2}^2)}{(1 + \nu H_{D1})^2 + (\nu H_{D2})^2} \quad (12)$$

$$H_2(\lambda, \nu) = \frac{H_{D2}}{(1 + \nu H_{D1})^2 + (\nu H_{D2})^2} \quad (13)$$

$H_{D1}$  and  $H_{D2}$  are defined as

$$H_{D1}(\lambda) = \lambda \left( \frac{\sinh 2\lambda + \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda} \right) - 1 \quad (14)$$

$$H_{D2}(\lambda) = \lambda \left( \frac{\sinh 2\lambda - \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda} \right) \quad (15)$$

For small values of  $\lambda$  Equations (14) and (15) simplify (for  $\lambda < 0.1$  the relative error is less than  $10^{-3}$ ) to

$$H_{D1} = \frac{4\lambda^4}{45} \quad (16)$$

$$H_{D2} = \frac{2\lambda^2}{3} \quad (17)$$

It follows that  $\lim_{\lambda \rightarrow 0} H_{D1} = 0$  and  $\lim_{\lambda \rightarrow 0} H_{D2} = 0$ . For high values of  $\lambda$  Equations (14) and (15) simplify (for  $\lambda > 5$  the relative error is less than  $10^{-3}$ ) to

$$H_{D1} = \lambda - 1 \quad (18)$$

$$H_{D2} = \lambda \quad (19)$$

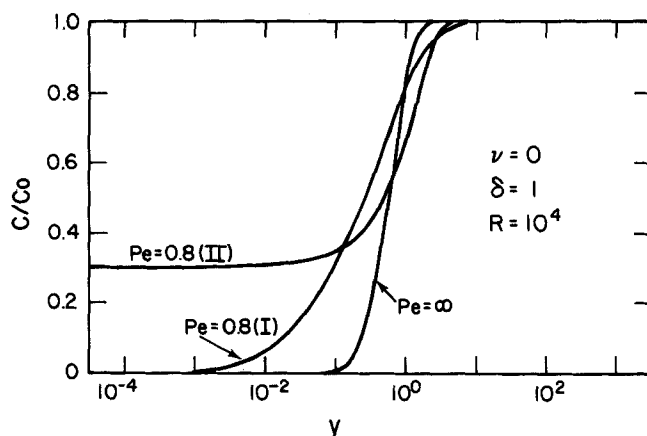


Figure 1. Comparison of breakthrough curves. I. This paper, II. Babcock et al. (1966).

It is interesting to note that in the case of a finite step boundary condition

$$\begin{aligned} C'(0, t) &= C_0 & t < t_0 \\ C'(0, t) &= 0 & t > t_0 \end{aligned} \quad (20)$$

the Laplace transform becomes

$$\tilde{u}'(z, s) = (1 - e^{-t_0 s}) \tilde{u}(z, s) \quad (21)$$

and

$$u'(z, t) = u(z, t) - u(z, t - t_0) H(t - t_0) \quad (22)$$

where  $H$  is Heaviside's step function.

The following dimensionless quantities are introduced

$$\delta = \frac{\gamma z}{mV} \quad \text{bed length parameter}$$

$$R = \frac{K}{m} \quad \text{distribution ratio}$$

$$Pe = \frac{zV}{D_L} \quad \text{Peclet number}$$

$$y = \sigma t \quad \text{contact time parameter}$$

Equation (9) now becomes

$$u(z, t) = \frac{1}{2} + \frac{2}{\pi} \int_0^\infty \exp\left(\frac{1}{2} Pe - \sqrt{\frac{(z^2 x')^2 + (z^2 y')^2 + z^2 x'}{2}}\right) \sin\left(y\lambda^2 - \sqrt{\frac{(z^2 x')^2 + (z^2 y')^2 - z^2 x'}{2}}\right) \frac{d\lambda}{\lambda} \quad (23)$$

with

$$z^2 x' = Pe \left( \frac{1}{4} Pe + \delta H_1 \right) \quad (24)$$

$$z^2 y' = \delta Pe \left( \frac{2}{3} \frac{\lambda^2}{R} + H_2 \right) \quad (25)$$

For high values of  $Pe$  ( $D_L \rightarrow 0$ ), disregarding all terms of order  $1/Pe^2$  and less, Equation (23) becomes

$$\begin{aligned} u(z, t) &= \frac{1}{2} + \frac{2}{\pi} \int_0^\infty \exp \\ &\quad - \left[ \delta H_1 + \frac{\delta^2}{Pe} \left( \frac{4}{9} \frac{\lambda^4}{R^2} + \frac{4}{3} \frac{\lambda^2 H_2}{R} + H_2^2 - H_1^2 \right) \right] \\ &\quad \sin \left[ \sigma \theta \lambda^2 - \delta H_2 + \frac{2\delta^2}{Pe} \left( \frac{2}{3} \frac{\lambda^2 H_1}{R} + H_1 H_2 \right) \right] \frac{d\lambda}{\lambda} \end{aligned} \quad (26)$$

where  $\theta = t - \frac{z}{V}$ .

This is the solution Babcock et al. (1966) claimed to be exact, but obviously a limiting solution for high values of  $Pe$ . Røsen's (1952) solution for  $D_L = 0$  is obtained from Equation (26) by letting  $Pe \rightarrow \infty$ .

Another case, which could easily be obtained, is when the component is subject to radioactive decay. We add  $-\lambda_d C$  and  $-\lambda_d q_i$  on the right-hand sides of Equations (1) and (2) respectively, and modify the boundary condition (3)

$$C(0, t) = C_0 e^{-\lambda_d t} \quad (3a)$$

This boundary condition simulates a constant leach rate of a body containing a decaying nuclide. For this case the Laplace transform of  $C$  becomes a function of  $s + \lambda_d$  instead of  $s$ . Hence, due to the properties of the Laplace transform, the solution becomes

$$u(\lambda_d > 0) = e^{-\lambda_d t} u(\lambda_d = 0) \quad (27)$$

Because of the complicated nature of the integral expression for  $u(z, t)$ , numerical integration must be performed. The integrand is the product of an exponential decaying function and a periodic sine function. The total function is thus a decaying sine wave, in which both the period of oscillation and the degree of decay are functions of the system parameters. Due to the very rapid oscillation of the integrand for certain parameter values, a straightforward integration method may fail. In some instances, the magnitude of the integrand is not negligible, even after a thousand oscillations of the wave.

Furthermore, with ordinary integration methods, one must choose a step size which is small with respect to the wave length. A special integration method was therefore developed, where the oscillatory behavior of the integrand is utilized. The integration is performed over each half-period of the sine-wave, respectively. The convergence of the alternating series obtained is then accelerated by repeated averaging of the partial sums. The solution was checked against the analytical solution of Lapidus and Amundson (1952) for the case of negligible external and internal diffusion resistance. The agreement was excellent.

## ACKNOWLEDGMENT

This work was supported by the project "Nuclear Fuel Safety" in Sweden and performed at Lawrence Berkeley Laboratory.

## NOTATION

$b$	= particle radius, m
$C$	= concentration in fluid, mol/m <sup>3</sup>
$C_0$	= inlet concentration in fluid, mol/m <sup>3</sup>
$D_L$	= longitudinal dispersion coefficient, m <sup>2</sup> /s
$D_s$	= diffusivity in solid phase, m <sup>2</sup> /s
$H_1$	= see Equation (12)
$H_2$	= see Equation (13)
$H_{D1}$	= see Equation (14)
$H_{D2}$	= see Equation (15)
$K$	= volume equilibrium constant, m <sup>3</sup> /m <sup>3</sup>
$k_f$	= mass transfer coefficient, m/s
$m$	= $\epsilon/1 - \epsilon$
$Pe$	= $zV/D_L$ , Peclet number
$\bar{q}$	= volume averaged concentration in particles, mol/m <sup>3</sup>
$q_i$	= internal concentration in particles, mol/m <sup>3</sup>
$q_s$	= $q_i(b, z, t)$ , mol/m <sup>3</sup>
$R$	= $K/m$ , distribution ratio
$R_F$	= $b/3k_f$ , film resistance, s
$r$	= radial distance from center of spherical particle, m
$s$	= Laplace transform variable
$t$	= time, s
$u$	= $C/C_0$ , dimensionless concentration in fluid
$V$	= average linear pore velocity, m/s
$x'$	= see Equation (10), m <sup>-2</sup>
$y$	= $\sigma t$ , contact time parameter

$y'$  = see Equation (11), m<sup>-2</sup>  
 $z$  = distance in flow direction, m

## Greek Letters

$\gamma$	= $3D_s K/b^2$ , s <sup>-1</sup>
$\delta$	= $\gamma z/mV$ , bed length parameter
$\epsilon$	= porosity, m <sup>3</sup> /m <sup>3</sup>
$\lambda$	= variable of integration
$\lambda_d$	= decay constant of radionuclide, s <sup>-1</sup>
$\nu$	= $\gamma R_F$
$\sigma$	= $2D_s/b^2$ , s <sup>-1</sup>

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## APPENDIX

Differential equations:

$$\frac{\partial C}{\partial t} + V \frac{\partial C}{\partial z} - D_L \frac{\partial^2 C}{\partial z^2} = - \frac{1}{m} \left( \frac{\partial \bar{q}}{\partial t} \right) \quad (1)$$

$$\frac{\partial q_i}{\partial t} = D_s \left( \frac{\partial^2 q_i}{\partial r^2} + \frac{2}{r} \frac{\partial q_i}{\partial r} \right) \quad (2)$$

Boundary conditions:

$$C(0, t) = C_0 \quad (3)$$

$$C(\infty, t) = 0 \quad (4)$$

$$C(z, 0) = 0 \quad (5)$$

$$q_i(0, z, t) \neq \infty \quad (6)$$

$$q_i(b, z, t) = q_s(z, t) \text{ given by } \frac{\partial \bar{q}}{\partial t} = \frac{3k_f}{b} \left( C - \frac{q_s}{K} \right) \quad (7)$$

$$q_i(r, z, 0) = 0 \quad (8)$$

The boundary condition (7) is the linking equation between Equations (1) and (2).

Carslaw and Jaeger (1959) solved Equation (2) for the special case of a constant value of  $q_s$ . By applying Duhamel's theorem to the solution of Carslaw and Jaeger, Rosen (1952) obtained an expression for  $q_i(r, z, t)$  in terms of the surface concentration  $q_s(z, t)$

$$q_i(r, z, t) = 2D_s \sum_{n=1}^{\infty} \left\{ (-1)^{n+1} \sigma_n \frac{\sin(\sigma_n r)}{r} \int_0^t q_s(z, \lambda) \exp[-D_s \sigma_n^2 (t - \lambda)] d\lambda \right\} \quad (9)$$

where  $\sigma_n = n\pi/b$ .

The average concentration in the particles is given by

$$\bar{q}(z, t) = \frac{3}{b^3} \int_0^b q_i(r, z, t) r^2 dr \quad (10)$$

If Equations (9) and (10) are combined and the order of integration and

summation is changed we get

$$\hat{q}(z, t) = \frac{6D_s}{b^2} \sum_{n=1}^{\infty} \left\{ \int_0^t q_s(z, \lambda) \exp[-D_s \sigma_n^2(t - \lambda)] d\lambda \right\} \quad (11)$$

Taking the derivative of  $\hat{q}$  with respect to time, integrating by parts and making use of the fact that  $q_s(z, 0) = 0$ , we obtain

$$\frac{\partial \hat{q}}{\partial t} = \frac{6D_s}{b^2} \sum_{n=1}^{\infty} \left\{ \int_0^t \frac{\partial q_s(z, \lambda)}{\partial \lambda} \exp[-D_s \sigma_n^2(t - \lambda)] d\lambda \right\} \quad (12)$$

This expression for  $\partial \hat{q} / \partial t$  is introduced into Equation (1) and the Laplace transform with respect to time is taken

$$s\tilde{C} + V \frac{\partial \tilde{C}}{\partial z} - D_L \frac{\partial^2 \tilde{C}}{\partial z^2} = -\frac{6D_s}{mb^2} \sum_{n=1}^{\infty} L \left\{ \int_0^t \frac{\partial q_s(z, \lambda)}{\partial \lambda} \exp[-D_s \sigma_n^2(t - \lambda)] d\lambda \right\} \quad (13)$$

$L$  is the Laplace transform operator.

The Laplace transform of the integral on the right-hand side of Equation (13) may be evaluated with the Faltung integral theorem as  $L\{f_1\}L\{f_2\}$  where  $f_1 = \partial q_s / \partial t$  and  $f_2 = \exp[-D_s \sigma_n^2 t]$ . Using the boundary condition (7) and Equation (1),  $L\{\partial q_s / \partial t\} = s\tilde{q}_s$  can be expressed as

$$s\tilde{q}_s = sK \left[ \tilde{C} + \frac{bm}{3k_f} \left( s\tilde{C} + V \frac{\partial \tilde{C}}{\partial z} - D_L \frac{\partial^2 \tilde{C}}{\partial z^2} \right) \right] \quad (14)$$

and furthermore we have

$$L\{\exp[-D_s \sigma_n^2 t]\} = \frac{1}{s + D_s \sigma_n^2} \quad (15)$$

With these substitutions and the following notation

$$\gamma = \frac{3D_s K}{b^2}$$

$$R_f = \frac{b}{3k_f}$$

$$Y_D(s) = 2\gamma \sum_{n=1}^{\infty} \frac{s}{s + D_s \sigma_n^2}$$

$$Y_T(s) = \frac{Y_D(s)}{R_f Y_D(s) + 1}$$

Equation (13) becomes

$$\frac{\partial^2 \tilde{C}}{\partial z^2} - \frac{V}{D_L} \frac{\partial \tilde{C}}{\partial z} - \left( \frac{s}{D_L} + \frac{Y_T(s)}{mD_L} \right) \tilde{C} = 0 \quad (16)$$

Equation (16) may be treated as an ordinary, second-order, linear differential equation whose solution after applying the boundary conditions is

$$\tilde{u}(z, s) = \tilde{C}(z, s)/C_o = \frac{1}{s} \exp \left\{ \left( \frac{V}{2D_L} - \sqrt{\frac{V^2}{4D_L^2} + \frac{s}{D_L} + \frac{Y_T(s)}{mD_L}} \right) z \right\} \quad (17)$$

The desired result  $u(z, t)$  is given by the contour integral representing the inverse transform of  $\tilde{u}(z, s)$

$$u(z, t) = C(z, t)/C_o = \exp \left( \frac{V}{2D_L} z \right) \frac{1}{2\pi i} \int_{\alpha-i\infty}^{\alpha+i\infty} \frac{1}{s} \exp(st - zY_T'(s)) ds \quad (18)$$

where

$$Y_T'(s) = \sqrt{\frac{V^2}{4D_L^2} + \frac{s}{D_L} + \frac{Y_T(s)}{mD_L}} \quad (19)$$

The integration is to be performed along the straight line  $Re(s) = \alpha$  parallel to the imaginary axis. The real number  $\alpha$  is chosen so that  $s = \alpha$  lies to the right of all the singularities of the integrand but is otherwise arbitrary.

The infinite sum  $Y_D(s)$  (Rosen 1952) could be written as

$$Y_D(s) = \gamma(w \cot w - 1) \quad (20)$$

where

$$w = w(s) = ib(s/D_s)^{1/2} = i(2s/\sigma)^{1/2} \\ \sigma = 2D_s/b^2$$

The principle properties of the functions  $Y_D(s)$  and  $Y_T(s)$  have been evaluated by Rosen. It can readily be seen from its series form that  $Y_D(s)$  has an infinite number of first-order poles along the negative real axis at the points  $s = -D_s \sigma_n^2$ ,  $n = 1, 2, \dots$ . Except for these poles  $Y_D(s)$  is analytic throughout the  $s$ -plane. The essential singularities of  $Y_T(s)$  are given by

$$R_f Y_D(s) + 1 = 0$$

or using Equation (20), the singularities are  $s = -\alpha_i$ , where the  $\alpha_i$  are the roots of

$$(2\alpha/\sigma)^{1/2} \cot(2\alpha/\sigma)^{1/2} + 1/\nu - 1 = 0$$

Since the roots are real and positive, the corresponding singularities are along the negative real axis. Because of the properties of  $Y_T(s)$ , it can easily be shown that  $Y_T'(s)$  only have branch points for  $Re(s) < 0$ . In view of these properties the function  $\tilde{u}(z, s)$  has the above mentioned singularities and in addition a simple pole at  $s = 0$ .

Following Rosen (1952), since  $\tilde{u}(z, s)$  is analytic for  $Re(s) \geq 0$  except at  $s = 0$ , we can take the path of integration to be along the imaginary axis with a small semicircle  $\Gamma$  of radius  $\epsilon \rightarrow 0$  excluding the origin. Then

$$u(z, t) \exp \left( -\frac{V}{2D_L} z \right) = \frac{1}{2\pi i} \lim_{\epsilon \rightarrow 0} \left[ \int_{-i\epsilon}^{-i\infty} + \int_{\Gamma} + \int_{+i\epsilon}^{+i\infty} \right] \frac{1}{s} \exp(st - zY_T'(s)) ds = I_1 + I_2 + I_3 \quad (21)$$

To evaluate the integral around  $\Gamma$  transform to polar coordinates and use  $Y_T'(s) \rightarrow V/2D_L$  as  $|s| \rightarrow 0$ . Then it readily follows that for  $\epsilon \rightarrow 0$  the second integral is

$$I_2 = \frac{1}{2} \exp \left( -\frac{V}{2D_L} z \right) \quad (22)$$

The first and last integrals can be combined by making the substitution  $s = -i\beta$  and  $s = i\beta$ , respectively, and taking the limit. This gives

$$I_4 = I_1 + I_3 = \frac{1}{2\pi} \int_0^{\infty} [e^{-i\beta t} \tilde{u}(z, -i\beta) + e^{i\beta t} \tilde{u}(z, i\beta)] d\beta$$

where

$$\tilde{u}(z, i\beta) = \frac{1}{i\beta} \exp[-zY_T'(i\beta)]$$

For any complex quantity  $F$  we have  $F + \bar{F} = 2 Re(F)$ , where the bar indicates the complex conjugate. Furthermore, since  $\tilde{u}(z, s)$  is a Laplace transform  $\tilde{u}(z, \bar{s}) = \bar{\tilde{u}}(z, s)$ . Hence

$$I_4 = \frac{1}{\pi} \int_0^{\infty} Re[e^{i\beta t} \tilde{u}(z, i\beta)] d\beta \quad (23)$$

To proceed we have to evaluate  $Y_T'(i\beta)$

$$Y_T'(i\beta) = \sqrt{\frac{V^2}{4D_L^2} + \frac{i\beta}{D_L} + \frac{Y_T(i\beta)}{mD_L}}$$

$Y_T(i\beta)$  is given by Rosen (1952) as

$$Y_T(i\beta) = \gamma[H_1(\lambda, \nu) + iH_2(\lambda, \nu)] \quad (24)$$

with

$$\lambda = \left( \frac{\beta}{\sigma} \right)^{1/2} \\ \nu = \gamma R_f$$

$$H_1(\lambda, \nu) = \frac{H_{D_1} + \nu(H_{D_1}^2 + H_{D_2}^2)}{(1 + \nu H_{D_1})^2 + (\nu H_{D_2})^2}$$

$$H_2(\lambda, \nu) = \frac{H_{D_2}}{(1 + \nu H_{D_1})^2 + (\nu H_{D_2})^2}$$

$$H_{D_1}(\lambda) = \lambda \left( \frac{\sinh 2\lambda + \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda} \right) - 1$$

$$H_{D_2}(\lambda) = \lambda \left( \frac{\sinh 2\lambda - \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda} \right)$$

Accordingly

$$Y_T(i\beta) = \sqrt{\frac{V^2}{4D_L^2} + \frac{i\beta}{D_L} + \frac{\gamma}{mD_L} [H_1(\lambda, \nu) + iH_2(\lambda, \nu)]}$$

The square-root is evaluated by writing the quantity under the square-root sign on polar form

$$Y_T(i\beta) = \sqrt{r'(\cos \theta + i \sin \theta)}$$

where

$$r' = \sqrt{x'^2 + y'^2}$$

$$\theta = \arctan \frac{y'}{x'}$$

$$x' = \frac{V^2}{4D_L^2} + \frac{\gamma}{mD_L} H_1$$

$$y' = \frac{\beta}{D_L} + \frac{\gamma}{mD_L} H_2$$

Applying de Moivre's theorem we get

$$Y_T(i\beta) = r'^{1/2} \left( \cos \frac{\theta}{2} + i \sin \frac{\theta}{2} \right)$$

Using trigonometric formulas we find that

$$\cos \frac{\theta}{2} = \sqrt{\frac{1 + \frac{x'}{r'}}{2}}$$

$$\sin \frac{\theta}{2} = \sqrt{\frac{1 - \frac{x'}{r'}}{2}}$$

It follows that

$$Y_T(i\beta) = \sqrt{\frac{r' + x'}{2}} + i \sqrt{\frac{r' - x'}{2}} \quad (25)$$

We are now ready to obtain

$$\begin{aligned} \operatorname{Re}[e^{i\beta t} \tilde{u}(z, i\beta)] &= \operatorname{Re} \left\{ \frac{1}{i\beta} \exp \left[ i\beta t - z \left( \sqrt{\frac{r' + x'}{2}} + i \sqrt{\frac{r' - x'}{2}} \right) \right] \right\} \\ &= \operatorname{Re} \left\{ -\frac{i}{\beta} \exp \left( -z \sqrt{\frac{r' + x'}{2}} \right) \left[ \cos \left( \beta t - z \sqrt{\frac{r' - x'}{2}} \right) \right. \right. \\ &\quad \left. \left. + i \sin \left( \beta t - z \sqrt{\frac{r' - x'}{2}} \right) \right] \right\} = \frac{1}{\beta} \exp \left( -z \sqrt{\frac{r' + x'}{2}} \right) \\ &\quad \sin \left( \beta t - z \sqrt{\frac{r' - x'}{2}} \right) \end{aligned}$$

and

$$I_4 = \frac{1}{\pi} \int_0^\infty \exp \left( -z \sqrt{\frac{r' + x'}{2}} \right) \sin \left( \beta t - z \sqrt{\frac{r' - x'}{2}} \right) \frac{d\beta}{\beta} \quad (26)$$

From (21), (22) and (26) making the substitution  $\beta = \sigma \lambda^2$  we finally obtain

$$\begin{aligned} u(z, t) &= C(z, t)/C_0 \\ &= \frac{1}{2} + \frac{2}{\pi} \int_0^\infty \exp \left( \frac{Vz}{2D_L} - z \sqrt{\frac{\sqrt{x'(\lambda)^2 + y'(\lambda)^2} + x'(\lambda)}{2}} \right) \\ &\quad \sin \left( \sigma \lambda^2 t - z \sqrt{\frac{\sqrt{x'(\lambda)^2 + y'(\lambda)^2} - x'(\lambda)}{2}} \right) \frac{d\lambda}{\lambda} \quad (27) \end{aligned}$$

with

$$x'(\lambda) = \frac{V^2}{4D_L^2} + \frac{\gamma}{mD_L} H_1$$

$$y'(\lambda) = \frac{\sigma \lambda^2}{D_L} + \frac{\gamma}{mD_L} H_2$$

Manuscript received August 13, 1979; revision received November 26, and accepted December 21, 1979.

## Hydrodesulfurization of Benzo[b]naphtho[2,3-d]thiophene Catalyzed by Sulfided CoO-MoO<sub>3</sub>/γ-Al<sub>2</sub>O<sub>3</sub>: The Reaction Network

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The need for clean-burning fuels and the depletion of petro-

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leum reserves are dictating the development of catalytic hydrodesulfurization processes for the heaviest petroleum fractions and for coal-derived liquids. These feedstocks require processing conditions much more severe than those used for