SKBF TEKNISK
KBS RAPPORT

80-23

Exact solution of a model for diffusion in particles and longitudinal dispersion in packed beds

Anders Rasmuson
Ivars Neretnieks

Royal Institute of Technology, August 1979

SVENSK KÄRNBRÄNSLEFÖRSÖRJNING AB / PROJEKT KÄRNBRÄNSLESÄKERHET

POSTADRESS: Kärnbränslesäkerhet, Box 5864, 102 48 Stockholm, Telefon 08-67 95 40

EXACT SOLUTION OF A MODEL FOR DIFFUSION IN PARTICLES AND LONGITUDINAL DISPERSION IN PACKED BEDS

Anders Rasmuson
Ivars Neretnieks

Royal Institute of Technology, August 1979

This report concerns a study which was conducted for the KBS project. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

A list of other reports published in this series is attached at the end of this report. Information on KBS technical reports from 1977-1978 (TR 121) and 1979 (TR 79-28) is available through SKBF/KBS.

EXACT SOLUTION OF A MODEL FOR DIFFUSION IN PARTICLES AND LONGITUDINAL DISPERSION IN PACKED BEDS

Anders Rasmuson
Ivars Neretnieks

July 1979

Department of Chemical Engineering
Royal Institute of Technology
S - 100 44 Stockholm
Sweden

Published in AIChE Journal
Vol. 26, No. 4, 686-690 (July 1980)

SUMMARY

An analytical solution of a model for diffusion in particles and longitudinal dispersion in porous media is derived. The solution is obtained by the method of Laplace transform. The result is expressed as an infinite integral of five dimensionless quantities. The extension for a decaying species is given.

EXACT SOLUTION OF A MODEL FOR DIFFUSION IN PARTICLES AND LONGITUDINAL DISPERSION IN PACKED BEDS

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:

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

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

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:

$$C(0,t) = C_o \tag{3}$$

$$C(\infty,t) = 0 \tag{4}$$

$$C(z,0) = 0 \tag{5}$$

$$q_i(0,z,t) \neq \infty \tag{6}$$

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

$$q_i(r,z,0) = 0 \tag{8}$$

The boundary condition (7) is the link between the 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 given in the form of 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 $\partial\overset{\Delta}{q}/\partial t$, the rate of change of average concentration within the solid. The expression for $\partial\overset{\Delta}{q}/\partial t$ 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 $\partial\overset{\Delta}{q}/\partial t$, 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 $\tilde{C}$ as the dependent variable. Solving the ordinary differential equation and taking the inverse transform in the complex domain one finally obtains:

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

with:

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

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

H_1 and H_2 are complicated hyperbolic functions of λ and ν:

$$H_1(\lambda,\nu) = \frac{H_{D_1} + \nu(H_{D_1}^2 + H_{D_2}^2)}{(1 + \nu H_{D_1})^2 + (\nu H_{D_2})^2} \qquad (12)$$

$$H_2(\lambda,\nu) = \frac{H_{D_2}}{(1 + \nu H_{D_1})^2 + (\nu H_{D_2})^2} \qquad (13)$$

H_{D_1} and H_{D_2} are defined as:

$$H_{D_1}(\lambda) = \lambda \left(\frac{\sinh 2\lambda + \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda}\right) - 1 \qquad (14)$$

$$H_{D_2}(\lambda) = \lambda \left(\frac{\sinh 2\lambda - \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda}\right) \qquad (15)$$

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

$$H_{D_1} = \frac{4\lambda^4}{45} \qquad (16)$$

$$H_{D_2} = \frac{2\lambda^2}{3} \qquad (17)$$

It follows that $\lim_{\lambda \to 0} H_{D_1} = 0$ and $\lim_{\lambda \to 0} H_{D_2} = 0$. For high values of λ equations (14) and (15) simplify (for $\lambda > 5$ the relative error is less than 10^{-3}) to:

$$H_{D_1} = \lambda - 1 \tag{18}$$

$$H_{D_2} = \lambda \tag{19}$$

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

$$C'(0,t) = C_o \qquad t < t_o \tag{20}$$
$$C'(0,t) = 0 \qquad t > t_o$$

the Laplace transform becomes:

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

and

$$u'(z,t) = u(z,t) - u(z,t-t_o)\ H(t-t_o) \tag{22}$$

where H is Heaviside's step function.

The following dimensionless quantities are introduced:

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

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

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

$y = \sigma t$ contact time parameter

Equation (9) now becomes:

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

with:

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

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

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

$$u(z,t) = \frac{1}{2} + \frac{2}{\pi} \int_0^{\infty} \exp - \left[\delta H_1 + \frac{\delta^2}{Pe}\left(\frac{4}{9}\,\frac{\lambda^4}{R^2} + \frac{4}{3}\,\frac{\lambda^2 H_2}{R} + H_2^2 - H_1^2\right)\right] \sin\left[\sigma\theta\lambda^2 - \delta H_2 + \frac{2\delta^2}{Pe}\left(\frac{2}{3}\,\frac{\lambda^2 H_1}{R} + H_1H_2\right)\right] \frac{d\lambda}{\lambda} \qquad (26)$$

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. Rosen's (1952) solution for $D_L = 0$ is obtained from equation (26) by letting $Pe \to \infty$.

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):

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

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:

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

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.

Acknowledgements: 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^3
C_o	inlet concentration in fluid	mol/m^3
D_L	longitudinal dispersion coefficient	m^2/s
D_s	diffusivity in solid phase	m^2/s
H_1	see equation (12)	
H_2	see equation (13)	
H_{D_1}	see equation (14)	
H_{D_2}	see equation (15)	
K	volume equilibrium constant	m^3/m^3
k_f	mass transfer coefficient	m/s
m	$= \frac{\varepsilon}{1-\varepsilon}$	
Pe	$= \frac{zV}{D_L}$, Peclet number	
$\hat{q}$	volume averaged concentration in particles	mol/m^3
q_i	internal concentration in particles	mol/m^3
q_s	$= q_i\ (b,z,t)$	mol/m^3
R	$= \frac{K}{m}$, distribution ratio	
R_F	$= \frac{b}{3k_f}$, film resistance	s
r	radial distance from center of spherical particle	m
s	Laplace transform variable	

t	time	s
u	$= C/C_o$, dimensionless concentration in fluid	
V	average linear pore velocity	m/s
x'	see equation (10)	m^{-2}
y	$= \sigma t$, contact time parameter	
y'	see equation (11)	m^{-2}
z	distance in flow direction	m

Greek letters

γ	$= \dfrac{3D_s K}{b^2}$	s^{-1}
δ	$= \dfrac{\gamma z}{mV}$, bed length parameter	
ε	porosity	m^3/m^3
λ	variable of integration	
λ_d	decay constant of radionuclide	s^{-1}
ν	$= \gamma R_F$	
σ	$= \dfrac{2D_s}{b^2}$	s^{-1}

References

Babcock, R.E., D.W. Green and R.H. Perry: Longitudinal dispersion mechanisms in packed beds. AIChE J. 12, 922 (1966)

Carslaw, H.S. and J.C.Jaeger: Conduction of heat in solids, Oxford Univ. Press, New York (1959)

Deisler, P.F. Jr., and R.H. Wilhelm: Diffusion in beds of porous solids. Measurement by frequency response techniques. Ind. Eng. Chem. 45, 1219 (1953)

Lapidus, L. and N.R. Amundson: Mathematics of adsorption in beds. VI. The effect of longitudinal diffusion in ion exchange and chromatographic columns. J. Phys. Chem. 56, 984 (1952)

Pellett, G.L.: Longitudinal dispersion, intraparticle diffusion and liquid-phase mass transfer during flow through multiparticle systems. Tappi 49 (2), 75 (1966)

Radeke, K.-H., K. Wiedemann and D. Gelbin: Näherungslösung zur Berechnung und Auswertung von Durchbruchskurven bei linearer Isotherme. Chem. Techn. 28, 476 (1976)

Rosen, J.B.: Kinetics of a fixed bed system for solid diffusion into spherical particles. J. Chem. Phys. 20, 387 (1952).

Figure caption

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

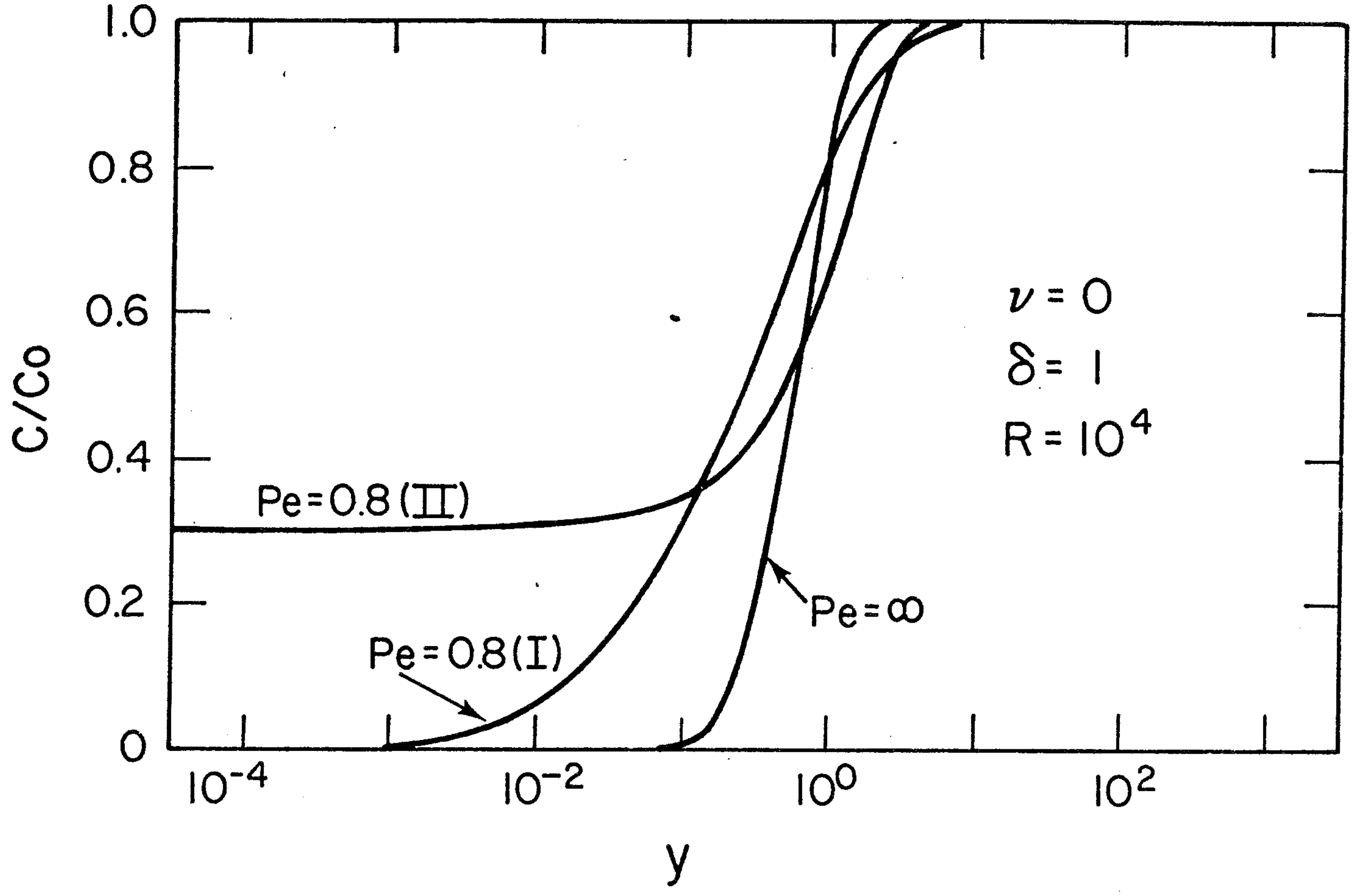

FIGURE 1

APPENDIX

Differential equations:

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

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

Boundary conditions:

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

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

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

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

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

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

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 $q_s(z,t)$:

$$q_i(r,z,t) =$$

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

where $\sigma_n = n\pi/b$

The average concentration in the particles is given by:

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

If equations (9) and (10) are combined and the order of integration and summation is changed we get:

$$\overset{\Delta}{q}(z,t) =$$

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

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

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

This expression for $\frac{\partial \overset{\Delta}{q}}{\partial t}$ is introduced into equation (1) and the Laplace transform with respect to time is taken:

$$s\tilde{C} + V\frac{\partial \tilde{C}}{\partial z} - D_L \frac{\partial^2 \tilde{C}}{\partial z^2} =$$

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

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 $L\left\{f_1\right\} \; L\left\{f_2\right\}$ where $f_1 = \frac{\partial q_s}{\partial t}$ and $f_2 = \exp\left[-D_s \sigma_n^2 t\right]$. Using the boundary condition (7) and equation (1), $L\left\{\frac{\partial q_s}{\partial t}\right\} = s\tilde{q}_s$ can be expressed as:

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

and furthermore we have:

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

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:

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

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

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

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

$$u(z,t) = C(z,t)/C_o =$$

$$\exp\left(\frac{V}{2D_L} z\right) \frac{1}{2\pi i} \int_{\alpha-i\infty}^{\alpha+i\infty} \frac{1}{s} \exp\left(st - zY_T'(s)\right) ds \tag{18}$$

where:

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

The integration is to be performed along the straight line Re(s) = α 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.

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

$$Y_D(s) = \gamma\,(w \cot w - 1) \tag{20}$$

where:

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

$$\sigma = 2D_s/b^2$$

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 $s = -D_s\sigma_n^2$, $n = 1,2...$ 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 α_i are the roots of:

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

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 $\mathrm{Re}(s) < 0$. 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 $\mathrm{Re}(s) \geq 0$ except at s=0, we can take the path of integration to be along the imaginary axis with a small semicircle Γ of radius $\varepsilon \to 0$ excluding the origin. Then:

$$u(z,t) \exp\left(-\frac{V}{2D_L} z\right) =$$

$$\frac{1}{2\pi i} \lim_{\varepsilon \to 0} \left[\int_{-i\infty}^{-i\varepsilon} + \int_{\Gamma} + \int_{+i\varepsilon}^{+i\infty} \right] \frac{1}{s} \exp(st - zY_T'(s))\, ds = I_1 + I_2 + I_3 \quad (2$$

To evaluate the integral around Γ transform to polar coordinates and use $Y_T'(s) \to \frac{V}{2D_L}$ as $|s| \to 0$. Then it readily follows that for $\varepsilon \to 0$ the second integral is:

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

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

$$I_4 = I_1 + I_3 =$$

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

where:

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

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

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

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:

$$Y_T(i\beta) = \gamma \left[H_1(\lambda,\nu) + i\, H_2(\lambda,\nu)\right] \tag{24}$$

with:

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

$$\nu = \gamma\, R_f$$

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

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

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

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

Accordingly:

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

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:

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

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:

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

We are now ready to obtain:

$$\mathrm{Re}\left[e^{i\beta t}\,\tilde{u}(z,i\beta)\right] =$$

$$\mathrm{Re}\left\{\frac{1}{i\beta}\exp\left[i\beta t - z\left(\sqrt{\frac{r'+x'}{2}} + i\sqrt{\frac{r'-x'}{2}}\right)\right]\right\} =$$

$$\mathrm{Re}\left\{-\frac{i}{\beta}\exp\left(-z\sqrt{\frac{r'+x'}{2}}\right)\left[\cos\left(\beta t - z\sqrt{\frac{r'-x'}{2}}\right) + i\sin\left(\beta t - z\sqrt{\frac{r'-x'}{2}}\right)\right]\right\}$$

$$= \frac{1}{\beta}\exp\left(-z\sqrt{\frac{r'+x'}{2}}\right)\sin\left(\beta t - z\sqrt{\frac{r'-x'}{2}}\right)$$

and:

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

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

$$u(z,t) = C(z,t)/C_o =$$

$$\frac{1}{2} + \frac{2}{\pi}\int_0^\infty \exp\left(\frac{Vz}{2D_L} - z\sqrt{\frac{\sqrt{x'(\lambda)^2 + y'(\lambda)^2} + x'(\lambda)}{2}}\right)$$

$$\sin\left(\sigma\lambda^2 t - z\sqrt{\frac{\sqrt{x'(\lambda)^2 + y'(\lambda)^2} - x'(\lambda)}{2}}\right)\frac{d\lambda}{\lambda} \qquad (27)$$

with:

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

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

FÖRTECKNING ÖVER KBS TEKNISKA RAPPORTER

1977-78

TR 121 KBS Technical Reports 1 - 120.
Summaries. Stockholm, May 1979.

1979

TR 79-28 The KBS Annual Report 1979.
KBS Technical Reports 79-01--79-27.
Summaries. Stockholm, March 1980.

1980

TR 80-01 Komplettering och sammanfattning av geohydrologiska undersökningar inom sternöområdet, Karlshamn
Lennart Ekman
Bengt Gentzschein
Sveriges geologiska undersökning, mars 1980

TR 80-02 Modelling of rock mass deformation for radioactive waste repositories in hard rock
Ove Stephansson
Per Jonasson
Department of Rock Mechanics
University of Luleå

Tommy Groth
Department of Soil and Rock Mechanics
Royal Institute of Technology, Stockholm
1980-01-29

TR 80-03 GETOUT - a one-dimensional model for groundwater transport of radionuclide decay chains
Bertil Grundfelt
Mark Elert
Kemakta konsult AB, January 1980

TR 80-04 Helium retention
Summary of reports and memoranda
Gunnar Berggren
Studsvik Energiteknik AB, 1980-02-14

TR 80-05 On the description of the properties of fractured rock using the concept of a porous medium
John Stokes
Royal Institute of Technology, Stockholm
1980-05-09

TR 80-06 Alternativa ingjutningstekniker för radioaktiva jonbytarmassor och avfallslösningar
Claes Thegerström
Studsvik Energiteknik AB, 1980-01-29

TR 80-07 A calculation of the radioactivity induced in PWR cluster control rods with the origen and casmo codes
Kim Ekberg
Studsvik Energiteknik AB, 1980-03-12

TR 80-08 Groundwater dating by means of isotopes
A brief review of methods for dating old groundwater by means of isotopes
A computing model for carbon - 14 ages in groundwater
Barbro Johansson
Naturgeografiska Institutionen
Uppsala Universitet, August 1980

TR 80-09 The Bergshamra earthquake sequence of December 23, 1979
Ota Kulhánek, Norris John, Klaus Meyer, Torild van Eck and Rutger Wahlström
Seismological Section, Uppsala University
Uppsala, Sweden, August 1980

TR 80-10 Kompletterande permeabilitetsmätningar i finnsjö-området
Leif Carlsson, Bengt Gentzschein, Gunnar Gidlund, Kenth Hansson, Torbjörn Svenson, Ulf Thoregren
Sveriges geologiska undersökning, Uppsala, maj 1980

TR 80-11 Water uptake, migration and swelling characteristics of unsaturated and saturated, highly compacted bentonite
Roland Pusch
Luleå 1980-09-20
Division Soil Mechanics, University of Luleå

TR 80-12 Drilling holes in rock for final storage of spent nuclear fuel
Gunnar Nord
Stiftelsen Svensk Detonikforskning, september 1980

TR 80-13 Swelling pressure of highly compacted bentonite
Roland Pusch
Division Soil Mechanics, University of Luleå
Luleå 1980-08-20

TR-80-14 Properties and long-term behaviour of bitumen and radioactive waste-bitumen mixtures
Hubert Eschrich
Eurochemic, Mol, October 1980

TR 80-15 Aluminium oxide as an encapsulation material for unreprocessed nuclear fuel waste - evaluation from the viewpoint of corrosion
Final Report 1980-03-19
Swedish Corrosion Institute and its reference group

TR 80-16 Permeability of highly compacted bentonite
Roland Pusch
Division Soil Mechanics, University of Luleå
1980-12-23

TR 80-17 Input description for BIOPATH
Jan-Erik Marklund
Ulla Bergström
Ove Edlund
Studsvik Energiteknik AB, 1980-01-21

TR 80-18 Införande av tidsberoende koefficientmatriser i BIOPATH
Jan-Erik Marklund
Studsvik Energiteknik AB, januari 1980

TR 80-19 Hydrothermal conditions around a radioactive waste repository
Part 1 A mathematical model for the flow of groundwater and heat in fractured rock
Part 2 Numerical solutions
Roger Thunvik
Royal Institute of Technology, Stockholm, Sweden
Carol Braester
Israel Institute of Technology, Haifa, Israel
December 1980

TR 80-20 BEGAFIP. Programvård, utveckling och benchmarkberäkningar
Göran Olsson
Peter Hägglöf
Stanley Svensson
Studsvik Energiteknik AB, 1980-12-14

TR 80-21 Report on techniques and methods for surface characterization of glasses and ceramics
Bengt Kasemo
Mellerud, August 1980

TR 80-22 Evaluation of five glasses and a glass-ceramic for solidification of Swedish nuclear waste
Larry L Hench
Ladawan Urwongse
Ceramics Division
Department of Materials Science and Engineering
University of Florida, Gainesville, Florida
1980-08-16

TR 80-23 Exact solution of a model for diffusion in particles and longitudinal dispersion in packed beds
Anders Rasmuson
Ivars Neretnieks
Royal Institute of Technology, August 1979

TR 80-24 Migration of radionuclides in fissured rock - The influence of micropore diffusion and longitudinal dispersion
Anders Rasmuson
Ivars Neretnieks
Royal Institute of Technology, December 1979

TR 80-25 Diffusion and sorption in particles and two-dimensional dispersion in a porous media
Anders Rasmuson
Royal Institute of Technology, January 1980