c' = RMS concentration fluctuation
$\bar{c}$ = average concentration
d = transverse jet orifice diameter
d = tube diameter
f,g = functions
I = impulse
J = ratio of transverse to axial momentum
K_i = unknown constants (i = 1,2,3)
t = time after injection
U = pipe velocity
V_j = jet velocity
x = distance downstream of injection point
ρ = density
Ω = global vorticity

LITERATURE CITED

Broadwell, J. E., and R. E. Breidenthal, "A Simple Model of Mixing and Chemical Reaction in a Turbulent Shear Layer," *J. Fluid Mech.*, **125**, 397 (1982).

———, "Structure and Mixing of a Transverse Jet in Incompressible Flow," *J. Fluid Mech.*, **148**, 405 (1984).

Brown, G. L., and M. R. Rebollo, "A Small, Fast-Response Probe to Measure Composition of a Binary Gas Mixture," *AIAA J.*, **10**, no. 5, 49–652 (1972).

Hartung, H. K., and J. W. Hiby, "Acceleration of Turbulent Mixing in Tubes," *Chem. Ing. Tech.*, **18**, 1051 (1972).

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Exact Solution of a Model for Diffusion in Particles and Longitudinal Dispersion in Packed Beds: Numerical Evaluation

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In an earlier paper (Rasmuson and Neretnieks, 1980) an analytical solution of a model for flow and longitudinal dispersion in beds of spherical particles, coupled with diffusion and linear sorption in the particles, was given. The solution is derived for a step inlet concentration and is in the form of an infinite integral:

$$C/C_o = \frac{1}{2} + \frac{2}{\pi}\int_o^\infty \exp[g(\delta,Pe,R,\nu,\lambda)] \times \sin[h(\delta,Pe,R,\nu,y,\lambda)]\frac{d\lambda}{\lambda} \quad (1)$$

The entities g and h are complicated functions of the variable of integration λ and of the following dimensionless parameters:

$\delta = \frac{3D_p\epsilon_p}{b^2}\frac{z}{mV}$ bed length parameter

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

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

$\nu = \frac{D_p\epsilon_p}{k_f b}$ film resistance parameter

$y = \frac{2D_p\epsilon_p}{Kb^2}t$ contact time parameter

The integrand is oscillatory. Due to the very rapid oscillation of the integrand for certain parameter values, especially for longer times, a straightforward integration will fail. To overcome this difficulty a special integration method was developed. In this method the integration is performed over each half-period of the sine wave separately. The convergence of the alternating series obtained is then accelerated by repeated averaging of the partial sums.

For the case where the film resistance is negligible ($\nu = 0$), the method was utilized in a computer program for the prediction of the migration of radionuclides in fissured rock (Rasmuson and Neretnieks, 1981).

The main problem is the calculation of the zeros of

$$\sin[h(\lambda_n)] = 0 \qquad n = 1,2\ldots \quad (2)$$

A combination of limiting expressions and Newton-Raphson's iteration is used.

The effect of ν has now been incorporated into the numerical scheme. Apart from the fact that H_1 and H_2 now are different from H_{D_1} and H_{D_2} (Rasmuson and Neretnieks, 1980) the procedure for solving Eq. 2 is modified. For $\nu > 0$ the calculations of the roots are done in two steps. First the old method is used as if $\nu = 0$. This value is then taken as the starting value for a new Newton-Raphson iteration. The convergence is then very rapid.

Some minor changes were also introduced into the code. First, the integral is calculated up to $\lambda = \lambda_{10}$ (10th root of Eq. 2). The magnitude of the integrand is then checked at the point halfway between λ_9 and λ_{10}. If the absolute value is less than 10^{-10} the integration is stopped; if not, the averaging procedure is entered. Twenty terms of the alternating series are calculated up to λ_{30}. The averaging procedure is continued until an absolute accuracy of 10^{-6} is obtained.

Some examples, showing the influence of ν, are given in Figures 1–3. Typical computing times on a CDC Cyber 170-720 are in the range of 10–35 s for 20–40 points on the concentration-time curve. The operation time for one multiplication on this computer is 4.0 μs. The running times are somewhat higher for $\nu > 0$ as compared to the case for which $\nu = 0$.

The solution was checked against the tabulated values by Rosen (1954) for $Pe = \infty$. Note that the contact time y in Rosen's notation is related to our y by

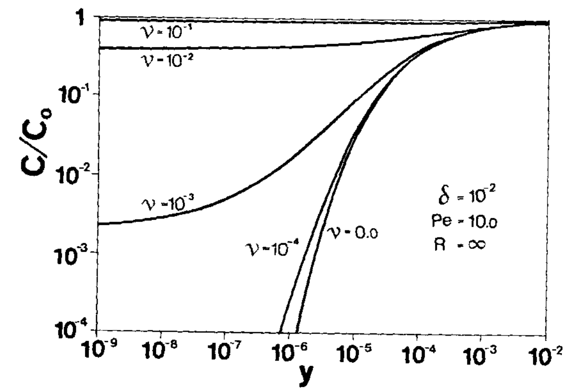

Figure 1. Breakthrough curves, C/C_o versus y, for $\delta = 10^{-2}$, $Pe = 10.0$, $R = \infty$, and $\nu = 0.0, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}$.

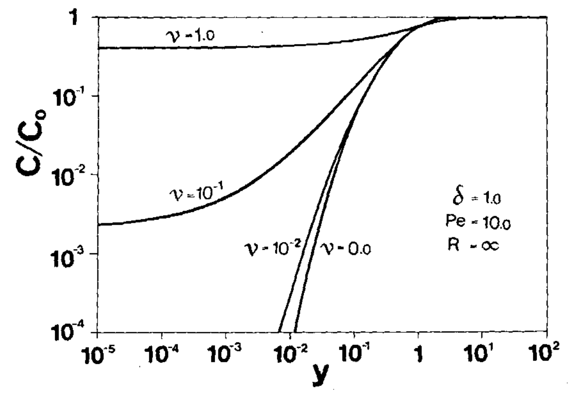

Figure 2. Breakthrough curves, C/C_o versus y, for $\delta = 1.0$, $Pe = 10.0$, $R = \infty$, and $\nu = 0.0, 10^{-2}, 10^{-1}, 1.0$.

$$y_{\text{Rosen}} = y - y_w$$

where

$$y_w = \frac{2}{3}\frac{\delta}{R}$$

Taking $R = \infty$ we get $y_{\text{Rosen}} = y$.

Some minor discrepancies were noted especially for $\delta = 0.2$ (x in Rosen's notation) at the lower end of y. Similar discrepancies were noted by Weber and Chakravorti (1974) in checking their numerical solution. An example is given in Table 1 for $\delta = 0.2$ and $\nu = 0.005$. For $\delta = 0.2$ and $\nu = 0.02$ and 0.04, Rosen had difficulties in evaluating the integral. These difficulties are eliminated using the averaging technique. For example, calculation of C/C_o for $\delta = 0.2$ and $\nu = 0.04$ at the seven values of y given by Rosen required 4.5 CPU seconds on the CDC Cyber 170-720.

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_p = diffusivity in fluid in intrapores, m^2/s
K = volume equilibrium constant, m^3/m^3
k_f = mass transfer coefficient, m/s
m $= \dfrac{\epsilon}{1-\epsilon}$
Pe $= \dfrac{zV}{D_L}$, Peclet number
R $= \dfrac{K}{m}$, distribution ratio
t = time, s
V = average linear pore velocity, m/s
y $= \dfrac{2D_p\epsilon_p}{Kb^2}t$, contact time parameter
z = distance in flow direction, m

Greek Letters

δ $= \dfrac{3D_p\epsilon_p}{b^2}\dfrac{z}{mV}$, bed length parameter
ϵ = void fraction of bed, m^3/m^3
ϵ_p = void fraction of particle, m^3/m^3
λ = variable of integration
ν $= \dfrac{D_p\epsilon_p}{k_f b}$, film resistance parameter

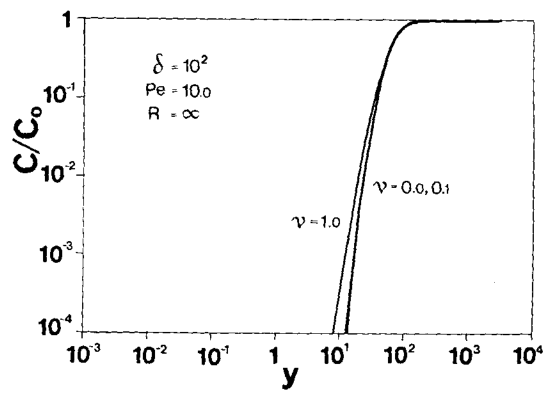

Figure 3. Breakthrough curves, C/C_o versus y, for $\delta = 10^2$, $Pe = 10.0$, $R = \infty$, and $\nu = 0.0, 0.1, 1.0$.

TABLE 1. COMPARISON OF BREAKTHROUGH CURVE C/C_o FOR $\delta = 0.2$, $PE = \infty$, AND $\nu = 0.005$ ($R = \infty$).

y	Rosen (1954)	Weber and Chakravorti (1974) C/C_o	This Paper
0.02	0.200	0.221	0.212
0.0295	0.312	0.315	0.312
0.04	0.403	0.396	0.397
0.06	0.506	0.508	0.510
0.10	0.642	0.642	0.645
0.20	0.799	0.797	0.799
0.40	0.915	0.915	0.916

LITERATURE CITED

Rasmuson, A., and I. Neretnieks, "Exact Solution of a Model for Diffusion in Particles and Longitudinal Dispersion in Packed Beds," *AIChE J.*, **26**, 686 (1980).

———, "Migration of Radionuclides in Fissured Rock: The Influence of Micropore Diffusion and Longitudinal Dispersion," *J. Geophys. Res.*, **86**, 3749 (1981).

Rosen, J. B., "General Numerical Solution for Solid Diffusion in Fixed Beds," *Ind. Eng. Chem.*, **46**, 1590 (1954).

Weber, T. W., and R. K. Chakravorti, "Pore and Solid Diffusion Models for Fixed-Bed Adsorbers," *AIChE J.*, **20**, 228 (1974).

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