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STEADY-STATE DIFFUSION THROUGH A FINITE PORE
INTO AN INFINITE RESERVOIR: AN EXACT SOLUTION*

by

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ABSTRACT

An outline is given of an analysis that leads to an exact solution for the problem of steady-state diffusion through a finite thick pore into an infinite region surrounding the mouth of the pore. From this exact formula a simple expression for the flux is derived. This expression approximates the flux with a relative error of less than 3.42% independently of the ratio l/a where l is the length of the pore and a its radius. If desired more accurate expressions for the flux can be obtained from the exact solution.

1. <u>Introduction</u>. Diffusion in biological systems is often characterized
by what, from a mathematical point of view, are difficult geometries
(Rashevsky, 1960, Section I). In such geometries although the methods
of finite differences may be numerically useful, it is often difficult
with these procedures to obtain rigorous and realistic error estimates
since even simple irregularities of the geometry (e.g. a right angle in
a boundary surface) often imply large absolute values of the higher
derivatives, and practically all rigorous error estimates depend on
estimates of these higher order derivatives (Forsythe,1958). Thus there
is a distinct need for exact solutions in such a form that biologically
useful data can be computed with useful and rigorous error estimates.
Although these exact solutions will be applicable to only a limited
number of situations, they serve as indispensable benchmarks for gauging
the credibility of approximate procedures. Compare Stoker (1962) where
a similar situation is described in the physical sciences.

With this in mind the writer (Kelman,1963a,b) has begun the task
of widening the class of three-dimensional geometries in which explicit
solutions are available for Laplace's equation--the equation governing
steady-state diffusions. These solutions are being developed in such
a way that they yield formulas for the flux of solute with rigorous and
realistic estimates of the relative error. The emphasis on relative
error is especially important in biological applications since models are
often constructed for distinguishing "passive" from "active" transport
(see, e.g., Csáky (1963), Hogben (1960)).

Because of the mathematical complexity of these developments it seems best that they be presented fully in the mathematical literature and that appropriate resumés be given in the biological literature. This paper is the first such resumé. The reader interested only in the formulas derived for the flux can proceed directly to $\lozenge$ 3.

2. <u>Background and method of solution</u>. There is a class of steady-state diffusion problems of biological interest (Patlack, 1959) which is characterized by diffusional flow from a region, say on the left, through a right cylinder (or cylinders), called pore(s), into a large surrounding region on the right, called the reservoir. Gray, Mathews and MacRobert (1931) have given an exact solution for a zero thick pore with an infinite region above it and have given an approximate analysis for a zero thick pore centered on the face of a cylinder where the radius of the cylinder is much larger than the height of the cylinder which in turn is much larger than the radius of the pore. Smythe (1953a,b), Cooke and Tranter (1959), Collins (1960), and Williams (1962) have performed analyses for a zero thick pore centered on the face of a cylinder of infinite height. Cooke (1956,1958)and Collins (1960a,b) and Williams (1962) have studied a zero thick pore opening into a cylinder of infinite radius and finite height. Also in the above mentioned papers are analyses applicable to diffusion from a spherical cap into a cylindrical region (cf. Collins (1962), Knight (1936), Smythe (1960)).

Our extension (Kelman,1963a,b) consists of an exact solution for a pore of finite thickness with an infinite region above the pore--a useful

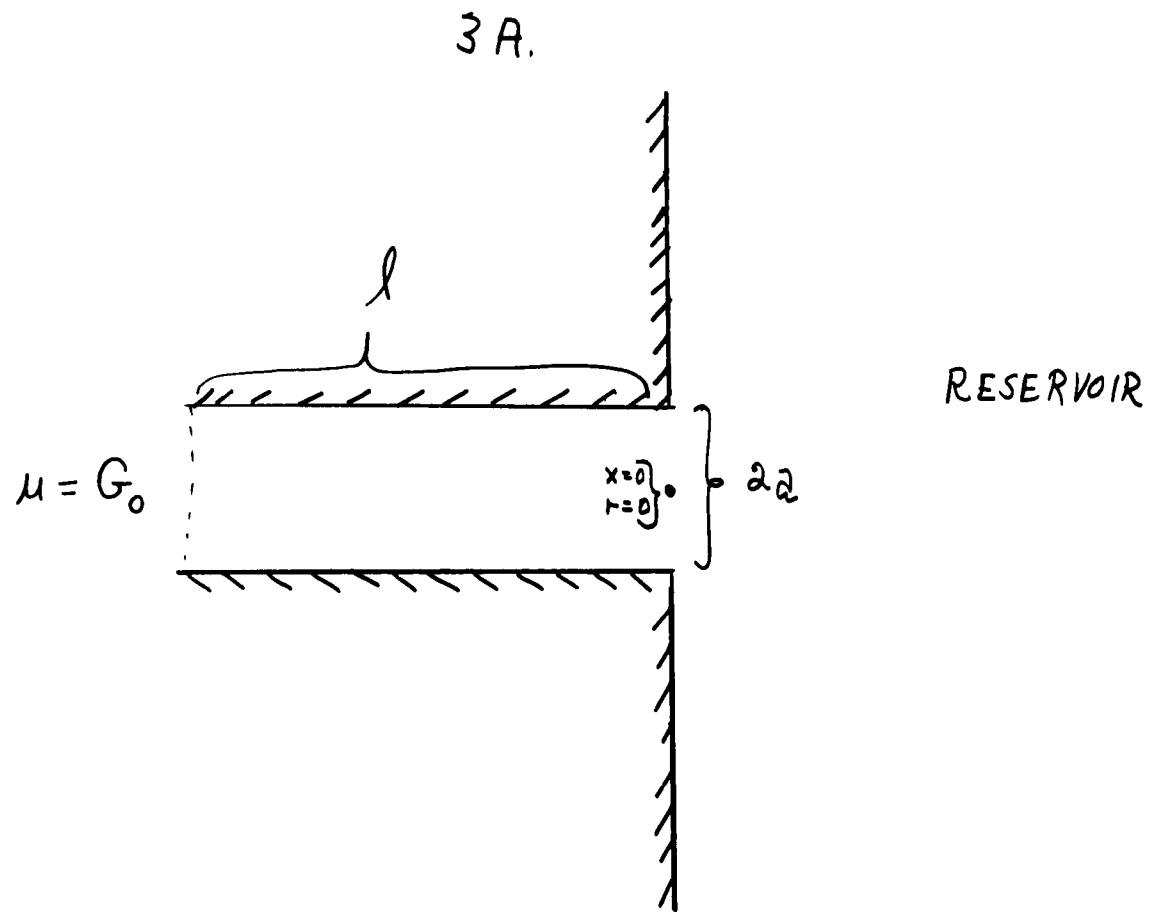3 A.

$\mu = G_o$

ℓ

RESERVOIR

$x=0$
$r=0$

$2a$

FIG 1.   Cross section of pore opening into reservoir.

model for example for water loss through a plant pore. The writer
(Kelman,1963c) was, however, originally led to study this problem by
considering the time dependent, longitudinal diffusion of inulin through
a nephron.

Let $\underline{r}$, $\underline{x}$, and θ denote cylindrical coordinates, $\underline{a}$ the radius of
the pore, $\underline{\ell}$ its length, G_0 the concentration at the base of the pore,
$\underline{F}$ the flux (i.e. the amount of solute entering the reservoir per unit
of time), and $u(r,x)$ the concentration of solute. The axis of the pore
(see Fig.1) coincides with the $\underline{x}$-axis. One of its faces is centered at
the origin and the other face at $r = 0$ and $x = -\ell$. The lateral walls
of the pore and the wall of the reservoir (i.e. the area $r > a$ and
$x = 0$) are assumed to be impervious to the solute. Then we seek $\underline{u}$ and
$\underline{F}$ from the system (1) of equations ($\underline{n}$ denotes outward drawn normal):

$$r\frac{\partial^2 u}{\partial r^2} + r\frac{\partial^2 u}{\partial x^2} + \frac{\partial u}{\partial r} = 0 \,, \quad \begin{cases} 0 < r < a \text{ and } -\ell < x \leq 0 \\ r > 0 \quad \text{and } x > 0 \end{cases} \,, \quad (1a)$$

$$u(r,x) = G_0 \qquad\qquad x = 0 \text{ and } 0 \leq r < a \,, \quad (1b)$$

$$u(r,x) = 0 \qquad\qquad x > 0 \text{ and } r + x = \infty \,, \quad (1c)$$

$$\frac{\partial u}{\partial n} = 0, \quad \begin{cases} r = 0 \quad \text{and } x > -\ell \\ r = a \quad \text{and } -\ell < x < 0 \\ r > a \quad \text{and } x = 0 \end{cases} \,. \quad (1d)$$

Equation (1a) is Laplace's equation in cylindrical coordinates for the region under consideration. Equation (1b) gives the boundary condition at the left face of the pore. Equation (1c) expresses the fact that the concentration is finite at the far reaches of the reservoir. If one wished it to have a value other than 0, say G_1 at $r+x = \infty$, one would make the change of dependent variable $v(r,x) = G_1 + u(r,x)$. In the case of water loss through a plant pore the value $u = 0$ at infinity can be realized by placing anhydrous sulfuric acid in the chamber in which the plant leaf is located. Equation (1d) is the mathematical expression that: (i) the line $r = 0$ and $x > -l$ is the axis of symmetry and hence there is no flow across it; (ii) $r = a$ and $-l < x < 0$ is the impervious lateral surface of the pore; (iii) $r > a$ and $x = 0$ is the impervious surface surrounding the mouth of the pore.

We now briefly describe the method of solution. Since Bessel functions are used in solving Laplace's equation in cylindrical regions (Carslaw and Jaeger, 1959) one formally expands $u(r,x)$ on $0 \leqslant r \leqslant a$ and $x = 0$ as follows

$$u(r,0) = j_0 \sqrt{2} + \sum_{n=1}^{\infty} \frac{j_n J_2(\alpha_n r/a) \sqrt{2}}{J_0(\alpha_n)} \tag{2}$$

where J_0 is a Bessel function of the first kind, α_n is the nth positive root of $J_1(r)$ and where the coefficients $\{j_n: n = 0,1,\ldots\}$ are unknowns. Technically, we regard $j = \{j_n\}$ as an element in the Hilbert space of square summable column vectors (Riesz and Nagy, 1952). On the basis of

equation (2) one can write down a formal solution, say u_p, to hold inside the pore (Carslaw and Jaeger, 1959, p.218).

$$U_p(r,x) = \left(J_0 - \left(J_0 - \frac{C_0}{\sqrt{2}} \right) \frac{x}{\ell} \right) \sqrt{2}$$
$$+ \sum_{n=1}^{\infty} \frac{d_n \sinh \alpha_n (\ell + x)/a}{\sinh \alpha_n \ell/a} \cdot \frac{\sqrt{2} \, J_0(\alpha_n r/a)}{J_0(\alpha_n)} \quad .$$

Now if $\ell = 0$ it is known that the surfaces of equiconcentration are oblate spheroids (Tranter, 1959, p.100). Therefore we introduce oblate spheroidal coordinates (η , ϕ) in the reservoir. These are given by (Hobson, 1955, p.421)

$$r = \cosh \eta \, \sin \phi \qquad , \quad x = \sinh \eta \, \cos \phi$$

Then separating variables in the reservoir leads to Legendre's differential equation (Hobson, 1955) with $\sqrt{1-r^2}$ as the independent variable. This suggests expanding $u(r,0)$ in even order Legendre polynomials $P_{2n}(\sqrt{1-r^2})$ as follows

$$U(r,0) = \sum_{n=0}^{\infty} p_n (4n+1)^{1/2} P_{2n}(\sqrt{1-r^2})$$

where $p = \left\{ p : n = 0, 1, \ldots \right\}$ is unknown. Then a formal solution, say U_R , can be written for the reservoir in terms of p (Hobson, 1955, 252)

$$u_R(\eta, \phi) = \sum_{n=0}^{\infty} p_n (4n+1)^{1/2} P_{2n}(\cos \phi) \frac{Q_{2n}(i \sinh \eta)}{Q_{2n}(0)}$$

where Q_{2n} is a Legendre function of the second kind.

These two solutions are matched on the interface in the following way.

We set

$$U_P(r,x)\Big|_{x=0} = U_R(n,\phi)\Big|_{n=0}, \quad r = \sin\phi \qquad (3)$$

Both sides of (3) are then multiplied by $(4n+1)^{\frac{1}{2}} P_{2n}(\cos\phi)\sin\phi$ and integrated with respect to ϕ over $0 \leqslant \phi \leqslant \pi/2$. Using the orthogonality property of the Legendre polynomials (Hobson, 1955), i.e.

$$(4n+1)\int_0^{\pi/2} P_{2n}(\cos\phi)\, P_{2m}(\cos\phi)\sin\phi\, d\phi = 1, \quad n = m$$
$$= 0, \quad n \neq m,$$

we obtain from (3) an expression for p_n in terms of j. To obtain a second system of equations we set

$$\frac{\partial U_P}{\partial x}\Big|_{x=0} = \frac{\partial U_R}{\partial x}\Big|_{n=0}, \quad r = \sin\phi \qquad (4)$$

Both sides of (4) are then multiplied by

$$\sqrt{2}\, J_0(\alpha_n \sin\phi)\sin\phi\cos\phi / J_0(\alpha_n)$$

and integrated with respect to ϕ over $0 \leqslant \phi \leqslant \pi/2$. Using the orthogonality property (Carslaw and Jaeger, 1959)

$$\frac{2}{J_0(\alpha_n) J_0(\alpha_m)} \int_0^{\pi/2} J_0(\alpha_n \sin\phi)\, J_0(\alpha_m \sin\phi)\sin\phi\cos\phi\, d\phi = 1, \quad n = m$$
$$= 0, \quad n \neq m$$

we obtain from (4) an expression for j_m in terms of p. From these
two systems of equations between j and p one is able to obtain an
explicit and remarkably useful formula for j (Kelman,1963a,b). Knowing
j one can then determine p and u.

3. Flux. From the solution u found above the following exact expression
can be obtained for the amount of solute entering the reservoir per unit
of time in terms of the dimensionless parameter $\lambda = l/a$ (Kelman,1963a).

$$F = \frac{4KG_0 a}{1 + \frac{4\lambda}{\pi}} \left[1 - \frac{1}{1 + \frac{4\lambda}{\pi}} \sum_{k=2}^{\infty} d_{00}^{(k,+)} \right] \tag{5}$$

where

$$d_{00}^{(k,+)} = \sum_{n_1, n_2, \cdots, n_{k-1} = 0}^{\infty} d_{0n_1}^* d_{n_1 n_2} d_{n_2 n_3} \cdots d_{n_{k-2}, n_{k-1}} d_{n_{k-1}, 0}^* , \quad k = 2, 3, \cdots$$

$$d_{kk} = 0, \qquad\qquad\qquad\qquad k = 0, 1, \cdots$$

$$d_{0n} = -\frac{2}{\sqrt{\pi}} \left(\frac{4\lambda \gamma_n}{\pi + 4\lambda} \right)^{1/2} \frac{\sin \alpha_n}{\alpha_n^{3/2} J_0(\alpha_n)} , \quad n = 1, 2, \cdots,$$

$$d_{kn} = \frac{-2(\gamma_k \gamma_n)^{1/2}}{\pi (\alpha_k \alpha_n)^{1/2} J_0(\alpha_n) J_0(\alpha_k)} \left[\frac{\sin(\alpha_k + \alpha_n)}{\alpha_k + \alpha_n} + \frac{\sin(\alpha_k - \alpha_n)}{\alpha_k - \alpha_n} \right],$$
$$k \neq n; \ k, n = 1, 2, \cdots,$$

$$d_{0n}^* = \left(\frac{\pi + 4\lambda}{\pi \lambda} \right)^{1/2} d_{0n} , \qquad n = 0, 1, \cdots,$$

$$\gamma_n = \tanh \alpha_k \lambda \left[1 + \frac{2 \tanh \alpha_k \lambda}{\pi \alpha_k J_0^2(\alpha_k)} \left(1 + \frac{\sin 2\alpha_k}{2\alpha_k} \right) \right]^{-1}, \quad k = 1, 2, \cdots .$$

By estimating the sum in (5) the following approximation and error estimate is obtained where $\widetilde{F}$ denotes an approximation to F and $\delta F = \widetilde{F} - F$ (Kelman, 1963a).

$$\widetilde{F} = \frac{4 K G_0 a}{1 + \frac{4\lambda}{\pi}} \left[1 - \frac{0.0449}{1 + \frac{4\lambda}{\pi}} \right], \quad 0 \leq \lambda < \infty, \quad (6)$$

$$\frac{|\delta F|}{F} \leq \frac{0.0353}{0.715 + \lambda}, \quad 0 \leq \lambda < \infty$$

Thus F is approximated with a relative of less than 5% uniformly in λ $(0 \leq \lambda < \infty)$ while for the range $\lambda > 2.82$ the relative error is less than 1%. In the range $0 \leq \lambda \leq \pi^{-1}$ a more accurate approximation is (Kelman, 1963a)

$$\widetilde{F} = \frac{4 K G_0 a}{1 + \frac{4\lambda}{\pi}} \left[1 - \frac{0.8432 \delta^2}{1 + \frac{4\lambda}{\pi}} \right], \quad 0 \leq \lambda \leq 1/\pi \quad (7)$$

where

$$\delta^2 = \frac{0.0566 \tanh \alpha_1 \lambda}{1 + 1.156 \tanh \alpha_1 \lambda} + \frac{0.0183 \tanh \alpha_2 \lambda}{1 + 1.079 \tanh \alpha_2 \lambda} + \zeta(\lambda)$$

and where

$$\zeta(\lambda) = 0.02052 \quad , \quad 4/9\pi \leq \lambda \leq 1/\pi$$

$$= \lambda \left[0.3196 \ln\left(\frac{4 + 9\pi\lambda}{18\pi\lambda} \right) + \frac{0.1594(1 + 2\lambda\pi)}{(1 + \lambda\pi)^2} \right],$$

$$0 \leq \lambda \leq 4/9\pi.$$

In this case

$$\frac{|\delta F|}{F} \leq \frac{0.662\delta^2}{0.785 - 1.33\delta^2 + \lambda} , \qquad 0 \leq \lambda \leq 1/\pi . \quad (8)$$

Now the right hand side of (8) decreases to 0 as λ goes for $1/\pi$ to 0 (Kelman, 1963a). For $\lambda = 1/\pi$ its value is 0.0341. Thus (6) combined with (7) gives an approximation to F such that the relative error is less than 3.41% uniformly in λ ($0 \leq \lambda < \infty$) and moreover this error tends to 0 as $\lambda \to 0$ and as $\lambda \to \infty$.

These approximations seem adequate for most biological applications If, however, the need arose for formulas of greater accuracy one could achieve this by computing the terms $d_{00}^{(k,+)}$. This is comparatively easy to do because of the availability of asymptotic formulas for the quantities entering the sum giving F. Each pair of terms $d_{00}^{(2k,+)}$ and $d_{00}^{(2k+1,+)}$ thus computed can be shown to reduce the relative error by about 0.407 (Kelman, 1963a).

Applying Patlak's (1959) variant of Landahl's (1953) method to the system (1) gives the approximation

$$\widetilde{F} = \frac{4KG_0a}{1 + \frac{4\lambda}{\pi}} ,$$

i.e. the first term in the series in (5).

It can be shown that for this approximation (Kelman, 1963a)

$$\frac{|\delta F|}{F} \leq \frac{0.705}{0.715 + \lambda} , \qquad 1/\pi \leq \lambda < \infty$$

$$\leq \frac{1.33\delta^2}{0.785 - 1.33\delta^2 + \lambda} , \qquad 0 \leq \lambda \leq 1/\pi$$

and that the relative error is less than 6.82% uniformly in λ . This particular approximation was used by Brown and Escombe (1900) in their study of water loss through a plant pore.

LITERATURE

Brown, H. T. and F. Escombe. 1900. "Static Diffusion of Gases and
Liquids in Relation to the Assimilation of Carbon and Translocation
in Plants." Phil. Trans. Roy. Soc. (Lond.) B, 193, 223-291.

Carslaw, H. S. and J. C. Jaeger. 1959. Conduction of Heat in Solids,
2nd. ed. Oxford: Clarendon Press.

Collins, W. D. 1960a. "On the Solution of Some Axisymmetric Boundary
Value Problems By Means of Integral Equations III. Some Electrostatic
and Hydrodynamic Problems For Two Spherical Caps." Proc. Lond. Math.
Soc., 10, 428-460.

_____. 1960b. "On the Solution of Some Axisymmetric
Boundary Value Problems by Means of Integral Equations. IV. The
Electrostatic Potential Due to a Spherical Cap Between Two Infinite
Conducting Planes." Proc. Edin. Math. Soc., 12, 95-106.

_____. 1962. "On the Solution of Some Axisymmetric
Boundary Value Problems by Means of Integral Equations VII. The
Electrostatic Potential Due to a Spherical Cap." ibid., 13, 13-24.

Cooke, J. C. 1956. "A Solution of Tranter's Dual Integral Equation
Problem." Quart. J. Mech. Appl. Math., 9, 103-110.

_____. 1958. "The Coaxial Circular Disc Problem." Z.
Angew. Math. Mech., 38, 349-356.

Cooke, J. D. and J. C. Tranter. 1959. "Dual Fourier Bessel Series."
Quart. J. Mech. Appl. Math., 12, 379-386.

Csáky, T. Z. 1963. "A Possible Link Between Active Transport of
Electrolytes and Nonelectrolytes." Fed. Proc., 22, 3-7.

Forsythe, G. E. 1958. Numerical Analysis and Partial Differential
Equations, New York: J. Wiley.

Gray, A., B. B. Mathews, and T. M. MacRobert. 1931. A Treatise on
Bessel Functions and Their Applications to Physics. London: Macmillan
and Co., Ltd.

Hobson, E. W. 1955. The Theory of Spherical and Ellipsoidal Harmonics,
reprint. New York: Chelsea Pub. Co.

Hogben, C. A. M. 1960. "Movement of Material Across Cell Membranes." Physiologist, 3, 56-62.

Kelman, R. B. 1963a. "Axisymmetric Potentials in Composite Geometries: Finite Cylinder and Half Space." Contrib. Diff. Eqs., to appear.

_____. 1963b. "Axisymmetric Potentials Arising From Biological Considerations." Bull. Amer. Math. Soc., to appear.

_____. 1963c. "Longitudinal Diffusion Along the Nephron During Stop Flow." Bull. Math. Biophysics, this issue.

Knight, R. C. 1936. "The potential of a sphere inside an infinite circular cylinder." Quart. J. Math., 7, 124-133.

Landahl, H. D. 1953. "An Approximation Method For Diffusion and Related Problems." Bull. Math. Biophysics. 15, 49-61.

Patlak, C. S. 1959. "A Contribution to the Study of the Diffusion of Neutral Particles Through Pores." Bull. Math. Biophysics, 21, 129-140.

Rashevsky, N. 1960. Mathematical Biophysics, Vol.1, 3rd and Rev. Ed. New York: Dover Publications, Inc.

Riesz, F. and B. Sz-Nagy. 1952. Leçons d'Analyse Fonctionelle. Budapest: Akadémia Kiado.

Smythe, W. R. 1953a. "Current Flow in Cylinders." J. Appl. Physics, 24, 70-73.

_____. 1953b. "Charged Disc in Cylindrical Box." ibid., 773-775.

_____. 1960. "Charged Sphere in a Cylinder." ibid., 31, 553-556.

Stoker, J. J. 1962. "Some Observations on Continuum Mechanics with Emphasis on Elasticity." Bull. Amer. Math. Soc., 68, 239-278.

Tranter, C. J. 1959. Integral Transforms in Mathematical Physics, 2nd ed. London: Metheun.

Williams, W. E. 1962. "The Reduction of Boundary Value Problems to Fredholm Integral Equations of the Second Kind." Z. Angew. Math. Phys., 13, 133-152.