Exact Solution of the Diffusion-Convection Equation in Cylindrical Geometry

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Introduction

The diffusion-convection arises in a number of biological transport problems in which a bulk fluid like water transports a solute or even a drug with concentration C_0. As shown in Eq. 1, the species transport occurs due to *diffusion*, with diffusion coefficient D, and *convection*, due to the velocity vector $\vec{V}$, of the bulk fluid flow

$$\frac{\partial C}{\partial t} + \vec{V}(r)\nabla C = \nabla(D\nabla C) \tag{1}$$

Solution of this equation is invaluable for validating the accuracy of numerical techniques as well, especially in complex biological systems.[1–7] Several analytical techniques such as the method of characteristics or the Laplace transformation can be applied to find an analytical solution.[8–13] In a one-dimensional (1-D) linear medium with continuous infusion at one boundary, i.e., constant convection velocity, the exact solution is simple.[14] We are interested in obtaining analytical solutions in cylindrical and spherical domains, where the convection velocity varies radially. Such solutions are very useful in studying drug distribution during convection enhanced drug delivery in human brain. A cylindrical or spherical infusion source occurs due to the choice of the infusion catheter, which may be single port or a porous membrane catheter. Unfortunately, analytical solutions of only certain particular problems in which the diffusivity can be expressed as a power function of the Peclet numbers have been presented.[8] We present an analytical solution for the convection diffusion problem in a cylindrical domain. Assuming symmetry with central source a desired concentration field C_S (r,t), would be a function of one spatial coordinate r, and time t. For convenience, we use normalized species concentration $C(r,t) = C_S/C_0$, ranging from zero to unity, where C_0 is the inlet concentration at the source.

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General solution

The diffusion-convection equation in polar coordinates is given by Eq. 2, with the boundary condition described by Eq. 3, and initial condition by Eq. 4, q is a volumetric bulk flow rate

$$\frac{\partial C}{\partial t} + \frac{V_0}{r}\frac{\partial C}{\partial r} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right);\ V(r) = \frac{q}{2\pi r} = \frac{V_0}{r} \tag{2}$$

Boundary conditions

$$\text{Boundary Conditions}: C(r=0,t) = C_0(\textit{finite});\quad C(r=L,t) = 0 \tag{3}$$

Initial condition

$$\text{Initial Condition}: C(r,t=0) = f(r) \tag{4}$$

For the general solution for the normalized species concentration profile $C(r,t)$, we first use the variable separation

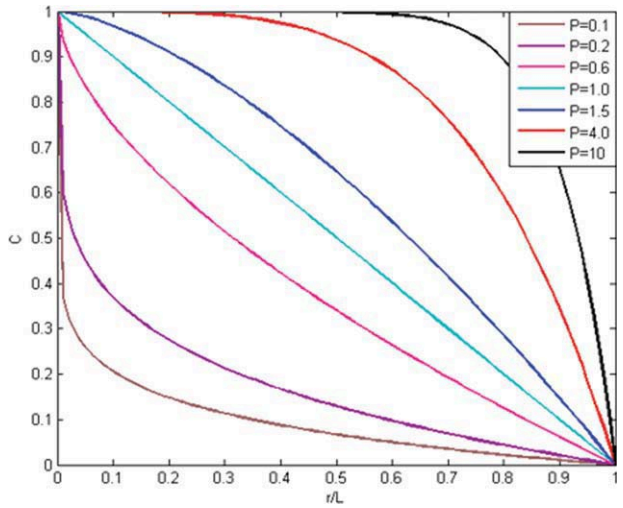

Figure 1. The dimensionless concentration profiles at steady state for a range of Peclet numbers.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

technique.[15–17] The procedure is shown in Eqs. 5–7. Here λ is the separation constant

$$\frac{1}{D\cdot T}\cdot\frac{\partial T}{\partial t}=\frac{1}{R}\cdot\left[\frac{\partial^2 R}{\partial r^2}+\frac{q}{r}\cdot\frac{\partial R}{\partial r}\right]=-\lambda; \tag{5}$$

Substituting $\mu = 1\text{-}V_0/D$ yields the system of Eqs. 6–8

$$\dot{T}+\lambda\cdot D\cdot T=0 \tag{6}$$

$$R+\frac{\mu}{r}R'+\lambda\cdot R=0 \qquad r\cdot R+\mu\cdot R'+r\cdot\lambda\cdot R=0 \tag{7}$$

$$R(L)=0 \tag{8}$$

The time function, $T(t)$, for Eq. 6 has well known exponential solution shown in Eq. 9

$$T_i(t)=\exp(-\lambda_i D t) \tag{9}$$

The solution for the spatial function $R(r)$, given in Eq. 10 follows from power series method in the same procedure adopted for the solution of the well-known Bessel equation[15–16]

$$R_i(r)=\sum_{n=0}^{\infty}\frac{(-1)^n\left(r\sqrt{\lambda_i}\right)^{2n}}{2^{2n-\gamma}n!\cdot\Gamma(v-\gamma+1)\cdot\lambda_i^{\gamma/2}} \text{ with}$$

$$\gamma=\frac{1-\mu}{2}=\frac{V_0}{2D} \tag{10}$$

This solution can be represented using a negative γ-order Bessel function $J_{-\gamma}$, of the first kind given in Eq. 11. Equation 11 also allows to determine the separation constant λ_i, in relation to the roots of the Bessel function s_i. The separation constant λ_i of a specific problem is a scaled version of the general Bessel function roots to accommodate to the boundary condition at the outer dimension of the domain L

$$R_i(r)=r^{\gamma}\cdot J_{-\gamma}\left(r\sqrt{\lambda_i}\right)\underset{r=L}{=}0; \quad \sqrt{\lambda_i}=\frac{s_i}{L} \tag{11}$$

Combining the spatial and temporal components $R(r)$ and $T(t)$, gives the desired solution as an infinite sum of eigenfunctions as in Eq. 12

$$C(r,t)=\sum_{i=0}^{\infty}\left[A_i\cdot r^{\gamma}\cdot J_{-\gamma}\left(r\sqrt{\lambda_i}\right)\cdot\exp(-\lambda_i D t)\right] \tag{12}$$

To accommodate initial condition, the coefficients A_i, can be adjusted using a Fourier-Bessel decomposition as in Eq. 13. The orthogonal base functions correspond to the weights r^{μ}, according to the Sturm-Liouville theory

$$A_i=\frac{\int_0^L f(r)\cdot J\left(\frac{s_i}{L}r\right)\cdot r^{\gamma+\mu}\cdot dr}{\int_0^L\left[J\left(\frac{s_i}{L}r\right)\right]^2\cdot r^{2\gamma+\mu}\cdot dr} \tag{13}$$

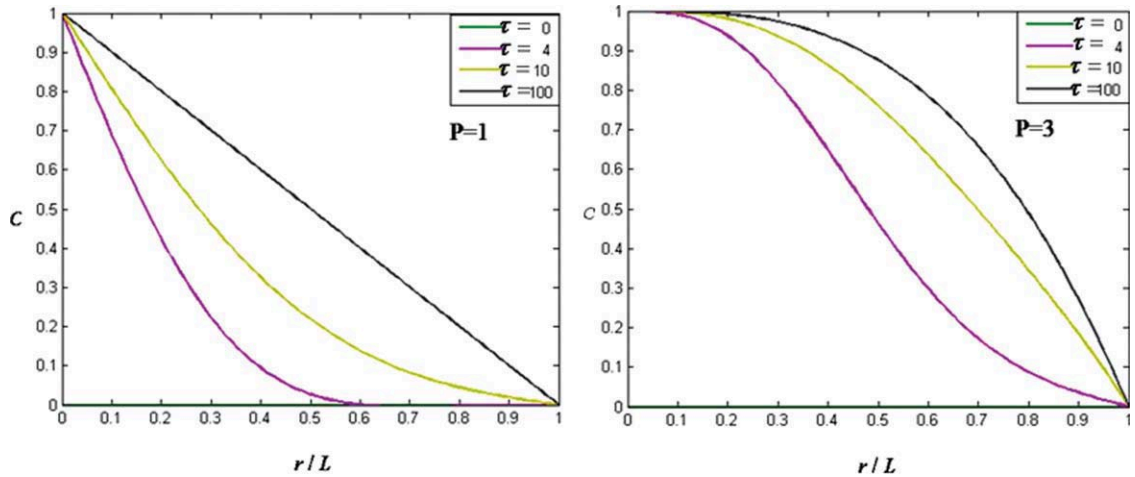

Figure 2. The dynamic evolution of concentration profiles for two different Peclet numbers.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

It may be noted that for the case of continuous source injection at the center of initially empty domain $f(r) = 0$, requires a special approach.[14] To accommodate this condition, the concentration profile is split into a dynamic $C(r,t)_{\mathrm{dyn}}$, and a steady state $C(r)_{\mathrm{ss}}$ components as shown in Eq. 14

$$C(r,t) = C(r,t)_{\mathrm{dyn}} + C(r)_{\mathrm{ss}} \tag{14}$$

The steady state $C(r)_{\mathrm{ss}}$, solution can be obtained by solving Eq. 2, after dropping the time derivative, which gives Eq. 15

$$\frac{V_0}{r}\frac{\partial C}{\partial r} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right) \qquad C(r)_{ss} = 1 - \frac{r^{V_0/D}}{L^{V_0/D}} \tag{15}$$

When the concentration in the entire domain is initially zero, the dynamic component $C(r,\ t)_{\mathrm{dyn}}$ at $t = 0$ can be related to the steady state. Accordingly, the dynamic part is initially equal to the steady state with a negative sign (Eq. 16). With this transformation a nonzero initial condition is artificially introduced. The coefficients A_i for dynamic component can be computed as shown in Eq. 17

$$C(r,0) = 0 = C(r,0)_{\mathrm{dyn}} + C(r)_{\mathrm{ss}} \Rightarrow C(r,0)_{\mathrm{dyn}} = -C(r)_{\mathrm{ss}} \tag{16}$$

$$A_i = \frac{\int_0^L \left(\frac{r^{V_0/D}}{L^{V_0/D}} - 1\right) J\left(\frac{s_i}{L}r\right) \cdot r^{\gamma+\mu} \cdot dr}{\int_0^L \left[J\left(\frac{s_i}{L}r\right)\right]^2 \cdot r^{2\gamma+\mu} \cdot dr} \tag{17}$$

The final solution to the convection-diffusion problem in cylindrical coordinate with continuous line source at the center can be written as in Eq. 18

$$C(r,t) = \sum_{i=0}^{\infty}\left[A_i \cdot r^{\gamma} \cdot J_{-\gamma}\left(\sqrt{\lambda_i}r\right) \cdot \exp(-\lambda_i \cdot Dt)\right] + \left(1 - \frac{r^{V_0/D}}{L^{V_0/D}}\right) \tag{18}$$

Discussion

Equation 2 can be nondimensionalized by introducing new variables $\rho = r/L$ and $\tau = Dt/L^2$. We also introduce the Peclet number $P = V_0/D$, as defined in Eq. 19. The Peclet number is a global measure of the total convective flux over the diffusion flux. The dimensionless concentration profiles are given by Eq. 20

$$\frac{\partial C}{\partial \tau} + P\frac{1}{\rho}\frac{\partial C}{\partial \rho} = \left(\frac{\partial^2 C}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial C}{\partial \rho}\right); \quad P = \frac{q}{2\pi D} = \frac{V_0}{D} \tag{19}$$

$$C(\rho,\tau) = \sum_{i=0}^{\infty}\left[A_i \cdot \rho^{P/2} \cdot J_{-P/2}\left(\rho\sqrt{\lambda_i}\right) \cdot \exp(-\lambda_i \tau)\right] \tag{20}$$

All steady-state solution can be represented in a single figure in 2-D space parameterizes for different value of P (Eq. 21) as shown in

$$C(\rho)_{ss} = 1 - \rho^P \tag{21}$$

The solution space shows two different regimes: convection or diffusion dominated. In the convection controlled regime of large Peclet numbers $P>1$, a flat saturated area develops close to the inlet due to convection. The extent of the convection induced saturation region is wider for large Peclet numbers and exhibits steep concentration profile toward the end of the domain. For Peclet number of unity $P = 1$, the concentration decays linearly. The dynamics solution represents the advancement of a drug infusion front from a continuous source. When relying only on diffusion $P = 0$, the penetration depths are modest. The dynamic evolution of the drug concentration profiles for $P = 1$ are shown in Figure 2 giving rise to much wider drug penetration. Finally, for even larger convection, say $P = 3$, the steady concentration profile maintains high levels with a characteristic plateau close to the infusion site. This enlarged region of therapeutic drug concentration levels is due to convection-enhancement and is significant in invasive drug delivery to the brain for Parkinson's disease or tumor treatment. The complete dynamics evolution for both dimensionless profiles for $P = 1$ and $P = 3$ are depicted in Figure 2.

A novel analytical solution of the diffusion-convection equation in cylindrical geometry for the continuous source can be used to verify numerical models for convection-diffusion transport. We also highlight the effect of Peclet number on the concentration profiles, because Peclet number defines which transport mechanism, diffusion or convection, dominates in the solution. The solution was cross checked for any errors by back substitution. This solution has important application in invasive drug delivery.

Acknowledgments

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