Exact Solution of Convective Mass Transfer Model for Calcium Response of Endothelium

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An exact solution for the concentration profile in tubes with surface reaction coupled with permeation have been obtained in terms of fast converging confluent hypergeometric function that gives accurate results. An excellent agreement between the experimental and theoretical results of the intracellular calcium ion concentration in the calf aorta endothelial cells and the extracellular ATP concentration provides yet another example in support of the mass transfer model for intracellular calcium response of the endothelial cells.

Keywords: Endothelium; ATP; Shear stress; Calcium response; Mass transfer; Circular tubes

INTRODUCTION

Vascular endothelium is the simplest epithelium lining the entire vascular system and the only constituent of a capillary wall performing the ultimate function of the entire system, i.e. exchange of nutrients and metabolic end-products of the tissue. To provide strength to a blood vessel, this layer of endothelial cell is supported by layers of elastic tissue, connective tissue, smooth muscles, etc. However, to

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facilitate solute transport, no such supporting tissues are present around the endothelial cell layer in capillaries. The structure of a typical capillary is like a thin walled tube made of one layer thick endothelial cells, about 1–2 μm thick and about 20–50 μm in circumferential diameter. To restrict the movement of large protein molecules, these cells are joined together by "tight junctions" [1]. Capillary wall made up of such an arrangement is highly permeable to water and almost all solutes dissolved in blood plasma except protein. Thus it behaves like a semipermeable membrane through which protein free plasma is filtered out. The plasma inside and outside the capillary contains large amount of small molecular weight solutes like Na⁺, Cl⁻, glucose, etc. Since capillary wall is highly permeable to these molecules, the inside and outside concentrations are almost the same. The permeation and several other physiological characteristics of an endothelial cell depends considerably on the concentration of different constituents in its surrounding fluid [2,3].

To explain such physiological and morphological changes in endothelial cells, a convective mass transfer model has been proposed by various authors. In our earlier communication [4], we have already discussed some of these changes in the endothelial cells due to the presence of different agonists and their degradation (surface reaction) at the cell layer. In that paper the differential equation pertaining to the newly emerging convective mass transfer model for the intracellular calcium response of cultured endothelial cells was solved analytically. The differential equation and velocity profiles used were for the rectangular channel geometry (without permeation) which represent the commonly used experimental set-up for the study of cultured endothelial cells [5–7]. In real situation, however, almost all blood vessels resemble more to a tube having circular cross-section. Also, a few workers [8] have made experiments with cultured endothelial cells supported inside circular glass tubes. Due to this geometry, the differential equation and boundary conditions for the mass transfer model are remarkably different. Due to varying permeation characteristics of endothelium from different parts of the body, it is desirable to have solutions for almost impermeable to highly permeable cases.

In the present paper two processes, surface reaction and permeation through the walls of a tube having circular cross-section, are being considered. The surface reaction is taken to be the degradation of
specific agonist like adenosine triphosphate (ATP) through successive dephosphorylation by three separate actoenzymes [4] and permeation of blood plasma through the endothelium is assumed to be constant throughout the length of the tube.

MATHEMATICAL FORMULATION

Mathematical formulation of the problem has been considered for two cases, i.e., surface reaction inside a permeable tube and surface reaction without permeation.

Case-1: Surface Reaction inside a Permeable Tube

Based on the model proposed by Elliott et al. [9,10], Mansour [11] tried to solve a similar problem for absorption coupled with permeation through intestinal wall with circular cross-section. Considering very small permeation velocity compared to axial velocity, he neglected radial velocity term and took the equation for velocity profile the same as that for the laminar flow through pipes. Further, assuming very high absorption rate (sink condition), the surface concentration was taken to be zero all along the tube length. In the present paper, however, the reaction rate is assumed to be finite (i.e., the surface concentration is not zero) and a modified velocity profile is being used.

The velocity profile in a circular tube with constant wall permeability has been developed by several workers [12,13]. According to these approaches, the axial velocity \( u \) in case of low permeation rate can be given by

\[
 u = 2\langle u \rangle \left[ 1 - \frac{2v_wx}{\langle u \rangle R} \right] \left[ 1 - \left( \frac{r}{R} \right)^2 \right].
\] (1)

Since the fluid velocity component in the radial direction \( v \) is several orders of magnitude smaller than that in the axial direction \( u \), therefore, the mathematical model for ATP transport inside a circular tube (equation of continuity for constant density and diffusivity) reduces to

\[
 2\langle u \rangle \left[ 1 - \frac{2v_wx}{\langle u \rangle R} \right] \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \frac{\partial C}{\partial x} = D \left[ \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right].
\] (2)
The wall of the tube (at \( r = R \)), made of epithelial cell, provides a permeating as well as a reacting surface with first order chemical kinetics [7]. Hence, at the steady state, mass consumed at the surface in chemical reaction is equal to the sum of mass fluxes approaching the surface due to diffusion and convection. Thus we have

\[
-D \frac{\partial C}{\partial r} \bigg|_{r=R} + v_w C = kC. \tag{3}
\]

This gives

\[
\text{B.C. I: } \frac{\partial C}{\partial r} \bigg|_{r=R} = -(k - v_w)C/D \quad (\text{for all } x). \tag{4a}
\]

The axisymmetric condition gives

\[
\text{B.C. II: } \frac{\partial C}{\partial r} \bigg|_{r=0} = 0 \quad (\text{for all } x) \tag{4b}
\]

and for a uniform inlet concentration, we have

\[
\text{B.C. III: } C = C_0 \text{ at } x = 0 \quad (\text{for all } r). \tag{4c}
\]

Using the dimensionless concentration \( c (= C/C_0) \), radial distance \( \gamma (= r/R) \) and by defining a dimensionless axial distance parameter \([\eta(x)]\) as

\[
\eta = \ln \left[ 1 - \frac{2v_w x}{(u) R} \right]^{\alpha} \tag{5}
\]

Eq. (2) reduces to

\[
4(1 - \gamma^2) \frac{\partial c}{\partial \eta} = \left[ \frac{\partial^2 c}{\partial \eta^2} + \frac{1}{r} \frac{\partial c}{\partial \gamma} \right]. \tag{6}
\]

Here, it is noteworthy that \( \eta \) varies from 0 to \( \infty \) as \( x \) varies from 0 to its upper limit (i.e., \( (u) R/2v_w \)) where the total volume filtered becomes equal to the volumetric feed rate. The corresponding boundary
conditions (Eq. (4)) in dimensionless form become

\[ \left. \frac{\partial c}{\partial \gamma} \right|_{\gamma=1} = -(k - v_W)Rc/D = -\psi c \quad \text{(for all } \eta) \]  \hspace{1cm} (7a)

\[ \left. \frac{\partial c}{\partial \gamma} \right|_{\gamma=0} = 0 \quad \text{(for all } \eta) \]  \hspace{1cm} (7b)

\[ c = 1 \text{ at } \eta = 0 \quad \text{(for all } \gamma) \].  \hspace{1cm} (7c)

The parameter \( \psi \) in Eq. (7a) is the modified Thiele modulus for coupled reaction–permeation problem.

The procedure for solving Eq. (6) along with boundary conditions (Eqs. (7)) are given in Appendix. As discussed in our earlier communication [4], the Thiele modulus \( \phi^2 \) is always positive whereas the modified Thiele modulus \( \psi \) in Eq. (7a) may be either positive or negative depending upon the value of \( k \) and \( v_W \). The complete solution of Eq. (2) and associated boundary conditions becomes

\[ \frac{C}{C_0} = \sum_{n=1}^{\infty} A_n \left[ 1 - \frac{2v_Wx}{(u)R} \right]^{\lambda_n^2 \alpha/4} \times \exp[-\lambda_n r^2 / 2R^2]M(1/2 - \lambda_n/4, 1, \lambda_n r^2 / R^2), \]  \hspace{1cm} (8)

where \( \lambda_n \) and \( A_n \) are \( n \)th eigenvalue and coefficient, respectively.

**Case-2: Surface Reaction without Permeation**

Equation (8) cannot be used for impermeable tubes since it becomes indeterminate when \( v_W \) is equated to zero. The velocity profile in case of impermeable tubes can be obtained by substituting \( v_W = 0 \) in Eq. (1). This gives the model equation for ATP transport as

\[ 2(u) \left[ 1 - \left( \frac{r}{R} \right)^2 \right] \frac{\partial C}{\partial x} = D \left[ \frac{\partial^2 C}{\partial r^2} + \frac{1}{r} \frac{\partial C}{\partial r} \right]. \]  \hspace{1cm} (9)

In the dimensionless form, Eq. (9) reduces to

\[ 4(1 - \gamma^2) \frac{\partial c}{\partial \xi} = \left[ \frac{\partial^2 c}{\partial \gamma^2} + \frac{1}{r} \frac{\partial c}{\partial \gamma} \right] \]  \hspace{1cm} (10)
where, $\xi$ is the dimensionless axial distance $(2Dx/(u)R^2)$ and the boundary conditions in dimensionless form become

\begin{align}
\text{B.C. I: } & \quad \frac{\partial c}{\partial \gamma}igg|_{\gamma=1} = -\frac{kR}{D} c = -\phi^2 c \quad (\text{for all } \xi), \\
\text{B.C. II: } & \quad \frac{\partial c}{\partial \gamma}igg|_{\gamma=0} = 0 \quad (\text{for all } \xi) \tag{11b}
\end{align}

and

\begin{equation}
\text{B.C. III: } \quad c = 1 \text{ at } \xi = 0 \quad (\text{for all } \gamma). \tag{11c}
\end{equation}

The parameter $\phi^2$ in Eq. (11a) is the well known Thiele modulus. Since the form of the differential equations (Eqs. (6) and (10)) and the boundary conditions (Eqs. (7) and (11)) are identical, hence the solution procedure for these equations are also identical to that explained in the Appendix. However, the concentration profile in case of impermeable tube is different from that expressed in Eq. (8) for permeable tubes. The concentration profile in this case becomes

\begin{equation}
\frac{C}{C_0} = \sum_{n=1}^{\infty} A_n \exp\left[-\frac{\lambda_n}{2R^2} \left(\frac{Dx}{u} + r^2 \right)\right] M(1/2 - \lambda_n/4, 1, \lambda_n r^2/R^2). \tag{12}
\end{equation}

**DISCUSSION**

In the past, attempts have been made to obtain concentration profiles under similar conditions using different approaches. Mansour [11] solved similar problem for intestinal wall permeability (sink condition) by the method of Laplace transformation, Kumar et al. [4] obtained concentration profile in rectangular channel geometry using the present mass transfer model for ATP transport and Kumar [13] solved the present problem by using a computer simulator based on modified finite difference method [14].

Figure 1 shows the variation of dimensionless concentration in the bulk of liquid as a function of dimensionless radial distance ($\gamma$), by computer simulator [13,14], Laplace transformation [11] and the
present approach for $\phi^2 = 5$ and at various axial positions ($\xi$). Solid lines are obtained by the present solution given by Eq. (12) and the results obtained by a computer simulation [13,14] are shown as point values. Dotted lines are obtained by the solution proposed by Mansour [11] by substituting the value of dimensionless permeation $(\nu W R/\bar{D})$ equal to $\phi^2$. This makes the B.C. I defined by Mansour [11] identical to Eq. (11a). It is observed that results of the present solution and the computer simulation are in excellent agreement whereas the concentration is always lower when diffusion controlled surface reaction (sink condition) is assumed. However, the concentration profile in the bulk of liquid obtained for the sink condition [11] is close to the values obtained by the present approach when the Thiele modulus is very large (i.e., $\phi^2 = 10^8$).

A comparison of the dimensionless wall concentration obtained by the computer simulator and analytical solution (using 50 eigenvalues) at $\phi^2 = 5$ and 20 is presented in Fig. 2 as a function of dimensionless axial position ($\xi$). Results obtained by two methods are in good agreement for larger values of $\xi$. For very small $\xi (< 3 \times 10^{-4}$), that comes to about 10–20 $\mu$m from the inlet end for practical situation,
analytical solution under predicts the wall concentration. This is due to the fact that analytical method requires even more eigenvalues in this region. Increase in the number of eigenvalues, however, does not lead to improvement in the results due to truncation and rounding off errors during computation.

The dimensionless wall concentration in case of surface reaction coupled with permeation and negative value of $\psi (-0.1)$, i.e., the case when rate of approach of ATP to the cell layer by convection is greater than the rate of consumption due to reaction, has been plotted in Figs. 3 and 4. These figures show that when the concentration is plotted against dimensionless distance $\xi$ (Fig. 3), different lines for different values of $\alpha$ are obtained, whereas when the same concentration is plotted as a function of $\eta$ (Fig. 4) we get only a single line from both analytical solution as well as the computer simulator (which is based on an entirely different approach). However, the computational time required for the computer simulator is about 50 times higher than that for analytical solution.

Figure 5 compares the dimensionless cytosolic $\text{Ca}^{2+}$ concentration obtained by Dull and Davies [8] as a function of shear stress at
FIGURE 3 Dimensionless ATP concentration near the cell surface ($r = R$) in a permeable tube as a function of axial distance $\xi = (2D\xi/\langle u \rangle R^2)$.

FIGURE 4 Dimensionless ATP concentration near the cell surface ($r = R$) in a permeable tube as a function of axial distance $\eta$. 
\( \phi^2 = 20 \). The details of obtaining dimensionless \( \text{Ca}^{2+} \) concentration are given in Kumar and Upadhyay [15] and the correlation for predicting shear stress in terms of \( \xi \) are given in Kumar et al. [4]. Within the range covered by the experiments, there is very good agreement between the experimental values of dimensionless cytosolic \( \text{Ca}^{2+} \) ion concentration and the extracellular ATP concentration predicted by using simulator and analytical methods.

**CONCLUSIONS**

In the present work solutions for the concentration profile in tubes with surface reaction coupled with permeation have been obtained in terms of confluent hypergeometric function. Due to the fast converging nature of this function, larger number of eigenvalues could be calculated compared to the other solution procedure such as powerseries approach, leading to more accurate results.

A good comparison of the experimental and theoretical results of the intracellular \( \text{Ca}^{2+} \) concentration in the calf aorta endothelial cells.
and the extracellular ATP concentration provides yet another example in support of the mass transfer model for intracellular calcium response of the endothelial cells.

**NOMENCLATURE**

\[ \begin{align*}
A & \quad \text{constant}, \\
C & \quad \text{concentration (g/ml)}, \\
C_0 & \quad \text{feed concentration (g/ml)}, \\
c & \quad \text{concentration } [C/C_0] \text{ (dimensionless)}, \\
D & \quad \text{diffusivity of ATP in the solution (cm}^2\text{/s}), \\
L & \quad \text{axial distance } (2 \nu_W x/\langle u \rangle R^2) \text{ (dimensionless)}, \\
R & \quad \text{radius of the tube (cm)}, \\
r & \quad \text{radial distance measured from the axis of the tube (cm)}, \\
\langle u \rangle & \quad \text{volume average feed velocity (cm/s)}, \\
\nu_W & \quad \text{permeation velocity (cm/s)}, \\
x & \quad \text{axial distance measured from the tube inlet (cm)}. \\
\end{align*} \]

**Greek**

\[ \begin{align*}
\alpha & \quad \text{dimensionless parameter } (D/\nu_W R), \\
\gamma & \quad \text{dimensionless radial distance } (r/R), \\
\eta & \quad \text{axial distance, defined in Eq. (5) (dimensionless)}, \\
\lambda^2 & \quad \text{eigenvalue}, \\
\xi & \quad \text{axial distance } (2 D x/\langle u \rangle R^2) \text{ (dimensionless)}, \\
\phi^2 & \quad \text{Thiele modulus } (kR/D) \text{ (dimensionless)}, \\
\psi & \quad \text{modified Thiele modulus } [(k - \nu_W R/D) \text{ (dimensionless)}, \\
\end{align*} \]

**Subscript**

\[ n \quad \text{indicating parameter based on } n\text{th eigenvalue}. \]

**References**


**APPENDIX**

Equations (6) and (10) are of the form:

$$4(1 - \gamma^2) \frac{\partial c}{\partial \chi} = \frac{\partial^2 c}{\partial \gamma^2} + \frac{1}{\gamma} \frac{\partial c}{\partial \gamma},$$  \hspace{1cm} (A.1)

where $\chi$ may be either $\eta$ (Eq. (6)) or $\xi$ (Eq. (10)) and boundary condition in dimensionless form are:

$$\text{B.C. I : } \frac{\partial c}{\partial \gamma} \bigg|_{\gamma=1} = -\theta c \quad \text{(for all } \chi),$$  \hspace{1cm} (A.2)
B.C. II: \[
\left. \frac{\partial c}{\partial \gamma} \right|_{\gamma=0} = 0 \quad \text{(for all } \chi) \tag{A.3}
\]

and

B.C. III: \[c = 1 \text{ at } \chi = 0 \quad \text{(for all } \gamma). \tag{A.4}\]

where \( \theta \) may be either the Thiele modulus \((\phi^2)\) or the modified Thiele modulus \((\psi)\).

To solve Eq. (A.1) along with boundary conditions (A.2)–(A.4) by the method of separation of variables it is assumed that

\[c = X(\chi) \cdot Y(\gamma). \tag{A.5}\]

Substituting in Eq. (A.1) we get two simultaneous differential equations:

\[
\frac{d^2 Y}{d\gamma^2} + \frac{1}{\gamma} \frac{dY}{d\gamma} + \lambda^2 (1 - \gamma^2) Y = 0 \tag{A.6}
\]

and

\[
\frac{dX}{d\chi} = -\frac{\lambda^2 X}{4}. \tag{A.7}
\]

The solution of Eq. (A.7) is

\[X = B \exp \left( -\frac{\lambda^2 \chi}{4} \right), \tag{A.8}\]

whereas Eq. (A.2) can be transformed to the confluent hypergeometric equation:

\[z \frac{d^2 \omega}{dz^2} + (b - z) \frac{d\omega}{dz} - a \omega = 0 \tag{A.9}\]

by two transformations

\[z = \lambda \gamma^2 \tag{A.10}\]

and

\[\omega = Ye^{z/2}, \tag{A.11}\]

where \( a = (1/2 - \lambda/4) \) and \( b = 1 \).
Equation (A.9) is the well known confluent hypergeometric equation (Kummer’s equation) and its solution is

$$\omega = A_1 M(a, b, z) + A_2 U(a, b, z). \quad (A.12)$$

The first confluent hypergeometric function is

$$M(a, b, x) = \sum_{n=0}^{\infty} \frac{(a)_n}{(b)_n n!} x^n, \quad (A.13)$$

where \((a)_n = a(a + 1)(a + 2) \cdots (a + n - 1)\) and \((a)_0 = 1\).

When \(b\) is equal to unity, the second hypergeometric function, which is a multi-valued function [16], can be given by

$$U(a, 1, z) = M(a, 1, z) \ln(z) + \sum_{m=1}^{\infty} \frac{(a)_m z^m}{(m!)^2} \left[ \frac{1}{a} + \cdots + \frac{1}{a + m - 1} - \left( \frac{2}{1} + \cdots + \frac{2}{m} \right) \right]. \quad (A.14)$$

Thus the complete solution of Eq. (A.9) becomes

$$\omega = A_1 M(a, 1, z) + A_2 \left[ M(a, 1, z) \ln(z) \right.$$

$$\left. + \sum_{m=1}^{\infty} \frac{(a)_m z^m}{(m!)^2} \left\{ \frac{1}{a} + \cdots + \frac{1}{a + m - 1} - \left( \frac{2}{1} + \cdots + \frac{2}{m} \right) \right\} \right]. \quad (A.15)$$

Now, B.C. II in terms of \(\omega\) and \(z\) becomes

$$\left[ \sqrt{z} \left\{ \frac{d\omega}{dz} - \frac{\omega}{2} \right\} \right]_{z=0} = 0. \quad (A.16)$$

Substituting the value of \(\omega\) from Eq. (A.15) and taking the limiting case when \(z\) is tending to zero, we get

$$A_1 0 + A_2 \lim_{z \to 0} \left[ \left( a - \frac{1}{2} \right) \sqrt{z} \ln(z) + \frac{1}{\sqrt{z}} \right] = 0. \quad (A.17)$$
The limiting value of the term inside the parenthesis at the left hand side of Eq. (A.17) becomes infinity as $z$ tends to zero. Therefore, to satisfy Eq. (A.17), and hence the B.C. II, $A_2$ should be zero.

Thus the complete solution of Eq. (A.9) reduces to

$$\omega = A_1 M(a, 1, z). \quad (A.18)$$

Again, from B.C. I (Eq. (A.2)) in terms of $\omega$ and $z$ we have

$$2\lambda \frac{d\omega}{dz} \bigg|_{z=\lambda} + (\theta - \lambda)\omega(\lambda) = 0. \quad (A.19)$$

Substituting the value of $\omega$ from Eq. (A.18) we get

$$A_1[2a\lambda M(a+1, 2, \lambda) + (\theta - \lambda)M(a, 1, \lambda)] = 0. \quad (A.20)$$

Since $A_1 \neq 0$, therefore we get the characteristic equation as

$$2a\lambda M(a+1, 2, \lambda) + (\theta - \lambda)M(a, 1, \lambda) = 0. \quad (A.21)$$

Roots of the characteristic equation give eigenvalues ($\lambda_n$). About 50 eigenvalues for different values of $\psi$ were calculated. A few of them at each $\psi$ are given in Table A1.

Now, from Eqs. (A.11) and (A.18) we get the eigenfunction as

$$Y_n = M(a_n, 1, z_n)e^{-z_n/2}. \quad (A.22)$$

Since Eq. (A.6) along with B.C. I and B.C. II constitutes a Sturm–Liouville problem, eigenvalues $\lambda_n$ and eigenfunction $Y_n$ form an orthogonal set with respect to the weight function $\gamma(1 - \gamma^2)$ over the interval $[0, 1]$, i.e.,

$$\int_0^1 \gamma(1 - \gamma^2)Y_mY_n \, d\gamma = 0 \quad \text{when } m \neq n \text{ and} \quad (A.23)$$

$$\neq 0 \quad \text{when } m = n.$$

Therefore by using B.C. III and Eq. (A.23) we get

$$A_n = \frac{\int_0^1 \gamma(1 - \gamma^2)Y_n \, d\gamma}{\int_0^1 \gamma(1 - \gamma^2)Y_n^2 \, d\gamma}. \quad (A.24)$$
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50  | 39052.6688788417 | 39136.6415332321 | 39269.3523439014 | 39320.9474831090 | 39351.692513494 | 39468.4996137535 |
Details for finding the values of integrals in Eq. (A.24) are given elsewhere [4], which gives

\[ A_n = \frac{\theta Y_n(1)}{\theta Y_n^2(1) + \int_0^1 \gamma (dY_n/d\gamma)^2 d\gamma}, \]  

(A.25)

where

\[ Y_n(1) = M(a_n, 1, \lambda_n)e^{-\lambda_n/2} \]  

(A.26)

and

\[ \frac{dY_n}{d\gamma} = 2\lambda_n \gamma e^{-\lambda_n/2} \left[ \frac{M(a_n + 1, 2, \lambda_n \gamma^2)a_n - M(a_n, 1, \lambda_n \gamma^2)}{2} \right]. \]  

(A.27)

To evaluate \( A_n \) using Eq. (A.25), Eq. (A.27) was integrated numerically by Simpson’s 1/3 rule.
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