Inertial Lag and Bessel Composite Function of Third Order and First Kind Solution to the Dissolving Pill Problem

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Introduction

Diffusion is a process by which molecules in random motion about their mean position travel from a region of higher concentration to that of lower concentration. The speed distribution of the molecules for an ideal gas can be given by the Maxwell distribution. Kinetic theory of gases has been used to predict the mass diffusivity for binary mixtures of non-polar gases. The definition of molar flux of species A across any plane is found by counting the molecules of A that cross unit area of the plane in the positive y direction for a considered instant in time and subtracting the number that cross in the negative y direction. Assuming a linear concentration profile this expression can be shown to reduce to the Fick's first law [Fick, 1822] of diffusion [Bird, Stewart and Lightfoot, 1960]. In the same considered instant in time, the accumulation of molecules at the surface is neglected. There are molecules that have pierced the surface that has moved less than a diameter of the molecule during the considered instant in time and is still in contact with the surface. Accounting for the accumulation of molecules [Sharma, 2005] and retaining the linear concentration gradient the molar flux can be shown to reduce to a expression analogous to that given by Cattaneo [1958] and Vernotte [1958] for heat conduction 5 decades ago. The relaxation time and $\partial J/\partial t$ can account for the accumulation effects. When the accumulation of mass flux exceeds exponential time the wave diffusion regime will be pronounced compared with the Fick diffusion regime, Tzou [1997]. This regime can be a third mode of mass transfer in addition to the molecular diffusion and convection that has been discussed extensively in the literature.

Theory

The rate of permeation of a particular medicine in the human body is of interest in drug delivery systems. The dissolution of the drug is often times governed by mass diffusion and relaxation. The time scales involved with these systems are short that the ballistic term may become significant. The objective of drug delivery system design is to increase the amount of drug dissolved. When a pill is taken, after a said period of time the dissolution of pill will reach a steady state. The time required to reach this steady supply of drug is of interest. It is assumed that the dissolution of this pill is controlled by diffusion into the stagnant contents of the human anatomy. The dissolution is diffusion controlled and the surroundings are stagnant.

A mass balance on the spherical shell around the pill can be written and when combined with the damped wave diffusion and relaxation equation can be written as;

$$\tau_r \partial^2 C/\partial t^2 + \partial C/\partial t = D/r^2\, \partial/\partial r(r^2\, \partial C/\partial r) \qquad [1]$$

Let $u = (C - C_0)/(C_{sat} - C_0)$; ; $\tau = t/\tau_r$; $X = r/\mathrm{sqrt}(D\tau_r)$ [2]

Eq. [1] becomes;

$$\partial^2 u/\partial \tau^2 + \partial u/\partial \tau = 1/X^2\, \partial/\partial X(X^2\, \partial u/\partial X) \qquad [3]$$

The time and space conditions can be written as;

$$\tau = 0,\ u = 0 \qquad [4]$$

$$\tau = \infty,\ u = 1 \qquad [5]$$

$$\tau > 0,\ X = X_{R0},\ u = 1 \qquad [6]$$

$$X = \infty,\ u = 0 \qquad [7]$$

Consider the substitution, $V = u/X$. Eq.[3] becomes,

$$\partial^2 V/\partial \tau^2 + \partial V/\partial \tau = 2V/X^2 + 4/X \partial V/\partial X + \partial^2 V/\partial X^2 \qquad [8]$$

The damping term can be removed by a $u = w\exp(-n\tau)$ substitution. As shown in the preceding sections for $n = ½$, Eq. [8] becomes.

$$\partial^2 W/\partial \tau^2 - W/4 = 2W/X^2 + 4/X \partial W/\partial X + \partial^2 W/\partial X^2 \qquad [9]$$

Let $\eta = \tau^2 - X^2$

The term $2W/X^2$ can be neglected for large X. W is small for large r as $u = W\exp(-\tau/2)/r$. As shown in the above section Eq. [9] for large X can be written as;

Now, $4/X\partial W/\partial X = -8\partial W/\partial\eta$ [10]

$4\eta\partial^2 W/\partial\eta^2 + 12\partial W/\partial\eta - W/4 = 0$ [11]

Or $\eta^2\partial^2 W/\partial\eta^2 + 3\eta\partial W/\partial\eta - \eta W/16 = 0$ [12]

Comparing Eq. [12]] with the generalized Bessel equation

$a = 3;\ b = 0;\ c = 0;\ d = -1/16;\ s = ½$ [13]

The order p of the solution is then p = 2 sqrt(1) = 2

Or $W = c_1 I_2(1/2\ \mathrm{sqrt}(\tau^2 - X^2)/(\tau^2 - X^2) + c_2 K_2\ 1/2\mathrm{sqrt}(\tau^2 - X^2)/(\tau^2 - X^2)$

c_2 can be seen to be zero as W is finite and not infinitely large at $\eta = 0$.

$V = \exp(-\tau/2)\ c_1 I_2(1/2\ \mathrm{sqrt}(\tau^2 - X^2)/(\tau^2 - X^2)$ [14]

An approximate solution can be obtaining by eliminating c_1 between the above equation and the equation from the boundary condition.

$$1/X_{R0} = \exp(-\tau/2)\ c_1 I_2(1/2\mathrm{sqrt}(\tau^2 - X_{R0}^{\ 2})/(\tau^2 - X_{R0}^{\ 2}) \quad [15]$$

Thus for $\tau > X$

$V = (1/X_{R0})\ [(\tau^2 - X_{R0}^{\ 2})/ (\tau^2 - X^2)]\ [I_2(1/2\ \mathrm{sqrt}(\tau^2 - X^2)/ I_2 1/2(\mathrm{sqrt}(\tau^2 - X_{R0}^{\ 2})$

For $X > \tau$,

$$u = (X/X_{R0})\ [(\tau^2 - X_{R0}^{\ 2})/ (X^2 - \tau^2)]\ J_2(1/2\ \mathrm{sqrt}(X^2 - \tau^2) / I_2 1/2\mathrm{sqrt}(\tau^2 - X_{R0}^{\ 2}) \quad [16]$$

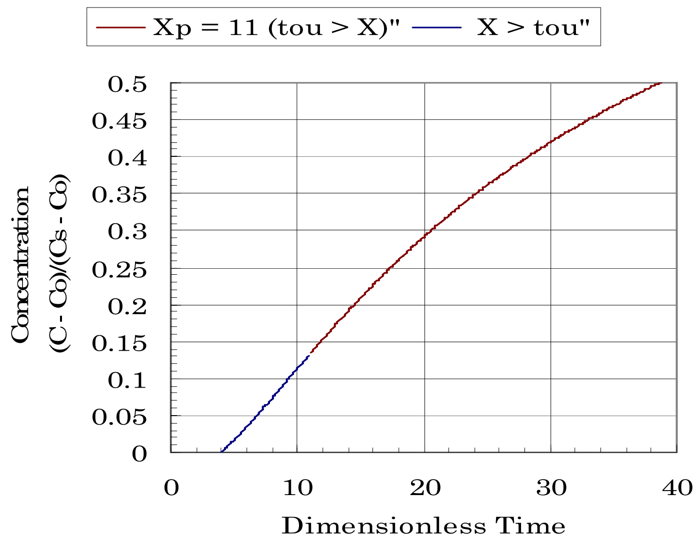
On examining the model solution it can be seen that the Bessel function of the second order and first kind will go to zero at some value of η. The first root of the Bessel function occurs when

$$½(X^2 - \tau^2)^{1/2} = 5.1356 \quad [17]$$

Or $X^2 - \tau^2 = 105.498$

When an exterior point in the infinite sphere is considered a lag time can be calculated prior to which there is no mass transfer to that point. After the lag time there exists two regimes. One is described by Eq. [3.335] and the third regime is described by Eq. [3.334]. Thus,

τ_{lag} = sqrt(X_p^2 - 105.498)



Three Regimes of Dimensionless Concentration at a Exterior Point from a Pill

In the dissolving pill problem consider all three dimensions of the spherical coordinates. Use the V = u/r substitution if necessary. Discuss the spatiotemporal concentration in the infinite sphere.

The governing equation for the concentration when the mass balance equation and the constitutive damped wave diffusion and relaxation equation are combined and written after modification of the equation given in Cussler [1997] in three dimensions is as follows;

Let $u = (C - C_0)/(C_s - C_0)$; $X = r/\text{sqrt}(D\tau_r)$; $\tau = t/\tau_r$;

Then the governing equation in three dimensions in spherical coordinates can be written as;

$$\partial^2u/\partial\tau^2 + \partial u/\partial\tau = 2/X\partial u/\partial X + \partial^2u/\partial X^2 + 1/X^2\partial^2u/\partial\theta^2 + 1/X^2\text{Sin}^2\theta\ \partial^2u/\partial\phi^2 + \text{Cot}\theta/X^2\partial u/\partial\theta \quad [18]$$

Consider the substitution, V = u/X. Eq. [18] becomes,

$$\partial^2V/\partial\tau^2 + \partial V/\partial\tau = 2V/X^2 + 4/X\partial V/\partial X + \partial^2V/\partial X^2 + 1/X^2\partial^2V/\partial\theta^2 + 1/X^2\text{Sin}^2\theta$$

$$\partial^2V/\partial\phi^2 \quad + \text{Cot}\theta/X^2\partial V/\partial\theta \qquad [19]$$

$$\partial^2V/\partial\tau^2 \ + \ \partial V/\partial\tau \quad = \quad 2V/X^2 + 4/X\partial V/\partial X + 1/X\partial^2V/\partial X^2 + 1/X^2\partial^2V/\partial\theta^2 \ + 1/X^2\text{Sin}^2\theta \ \partial^2V/\partial\phi^2 \ + \text{Cot}\theta/X^2\ \partial V/\partial\theta \qquad [20]$$

The damping term can be removed by a V = wexp(-nτ) substitution. As shown in the preceding sections for n = ½, Eq. [3.352] becomes.

$$\partial^2W/\partial\tau^2 \ - W/4 \quad = \quad 2W/X^2 + 4/X\partial W/\partial X + \partial^2W/\partial X^2 + 1/X^2\partial^2W/\partial\theta^2 \ + 1/\ X^2\text{Sin}^2\theta \ \partial^2W/\partial\phi^2 \quad + \text{Cot}\theta/X^2\partial W/\partial\theta \qquad [21]$$

For small θ,

$$\partial^2W/\partial\tau^2 \ - W/4 \ = \ 2W/X^2 + 4/X\partial W/\partial X + \partial^2W/\partial X^2 + 1/X^2\partial^2W/\partial\theta^2 \ + 1/X^2\text{Sin}^2\theta\ \partial^2W/\partial\phi^2 + 1/\theta X^2\ \partial W/\partial\theta$$

$$\text{Let } \xi \ = \ \theta X, \ \text{ Then } 1/X^2\partial^2W/\partial\theta^2 \ = \ \partial^2W/\partial\xi^2$$

$$\psi \ = \ \phi X\text{Sin}\theta, \text{ Then, } \ 1/X^2\text{Sin}^2\theta\ \partial^2W/\partial\phi^2 = \ \partial^2W/\partial\psi^2$$

Eq. [21] then becomes for large X,

$$\partial^2W/\partial\tau^2 \ - W/4 \ = \ 4/X\partial W/\partial X \ + \ \partial^2W/\partial X^2 + \ \partial^2W/\partial\xi^2 \ + \partial^2W/\partial\psi^2 + 1/\xi\partial W/\partial\xi \qquad [22]$$

Consider the transformation, $\eta \ = \ \tau^2 - X^2 - \xi^2 - \psi^2$

As shown in the analysis in Worked Example 3.10 the derivatives in Eq. [] in 4 variables become converted into 1 variable,

$$(\partial^2\ w/\partial\eta^2\ )4(\ \tau^2 - X^2 - \xi^2 - \psi^2) \ + 18(\partial\ w/\partial\eta\ ) \quad -w/4 \ = 0 \qquad [23]$$

$$\text{or } \eta^2(\partial^2\ w/\partial\eta^2\ )\ ) \ + 9/2\eta(\partial\ w/\partial\eta\ ) \qquad -w\eta/16 \ = 0$$

Comparing Eq. [3.359] with the generalized Bessel equation

$$a = 9/2;\ b = 0;\ \ c = 0;\ \ d = -1/16;\ \ s = ½ \qquad [24]$$

The order p of the solution is then p = 7/2

$$W \ = \ c_1I_{7/2}(1/2\ \text{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/(\tau^2 - X^2 \ - \xi^2 - \psi^2) \ + \ c_2I_{-7/2}\ \text{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/(\tau^2 - X^2 - \xi^2 - \psi^2)$$

$$u \ = \ X\exp(-\tau/2)\ c_1I_{7/2}(1/2\ \text{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/(\tau^2 - X^2 \ - \xi^2 - \psi^2) \qquad [25]$$

c_2 can be seen to be zero as W is finite and not infinitely large at η = 0. An approximate solution can be obtaining by eliminating c_1 between the above equation and the equation from the boundary condition. The equation from the boundary condition can be written as;

$$1 = X_{R0} \exp(-\tau/2)\, c_1 I_{7/2}(1/2\, \mathrm{sqrt}(\tau^2 - X_{R0}^{\;2})/ (\tau^2 - X_{R0}^{\;2}) \qquad [26]$$

Dividing Eq. [25] by Eq. [26],

$$u = (X/X_{R0})\, [(\tau^2 - X_{R0}^{\;2})/(\tau^2 - X^2 - \xi^2 - \psi^2)] I_{7/2}(1/2\, \mathrm{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/I_{7/2}(1/2 \mathrm{sqrt}(\tau^2 - X_{R0}^{\;2})$$

For small X,

$$u = (X/X_{R0})\, [(\tau^2 - X_{R0}^{\;2})/(X^2 + \xi^2 + \psi^2 - \tau^2]\, J_{7/2}(1/2\, \mathrm{sqrt}(X^2 + \xi^2 + \psi^2 - \tau^2)/I_{7/2}(1/2 \mathrm{sqrt}(\tau^2 - X_{R0}^{\;2}) \qquad [27]$$

In the creeping mass transfer limit Eq. [27] can be approximated as;

$$\partial^2 W/\partial\tau^2 - W/4 = 4/X \partial W/\partial X + \partial^2 W/\partial X^2 + \partial^2 W/\partial\xi^2 + \partial^2 W/\partial\psi^2 \qquad [28]$$

After the transformation the PDE with 4 variables is converted to a Bessel equation in 1 variable:

$$(\partial^2 w/\partial\eta^2)\, 4(\tau^2 - X^2 - \xi^2 - \psi^2) + 16(\partial w/\partial\eta) - w/4 = 0 \qquad [29]$$

$$\text{or } (\partial^2 w/\partial\eta^2)\, \eta^2 + 4\eta(\partial w/\partial\eta) - \eta w/16 = 0 \qquad [30]$$

The order of the Bessel solution for Eq. [30] can be calculated by comparing Eq. [30] with the generalized Bessel equation given in Eq. [A.30] and the solution is;
a = 4; b = 0; c = 0; d = -1/16; s = ½ . The order p of the solution is then p = 3

$$W = c_1 I_3(1/2\, \mathrm{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/(\tau^2 - X^2 - \xi^2 - \psi^2) + c_2 K_3\, \mathrm{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/(\tau^2 - X^2 - \xi^2 - \psi^2)$$

Or $$u = X \exp(-\tau/2)\, c_1 I_3(1/2\, \mathrm{sqrt}(\tau^2 - X^2 - \xi^2 - \psi^2)/(\tau^2 - X^2 - \xi^2 - \psi^2) \qquad [31]$$

c_2 can be seen to be zero as W is finite and not infinitely large at $\eta = 0$. An approximate solution can be obtaining by eliminating c_1 between the above equation and the equation from the boundary condition. The equation from the boundary condition can be written as;

$$1 = X_{R0} \exp(-\tau/2)\, c_1 I_3(1/2\, \mathrm{sqrt}(\tau^2 - X_{R0}^{\;2})/ (\tau^2 - X_{R0}^{\;2})$$

Dividing Eq. [31] by Eq. [30],

$$u = (X/X_{R0}) [(\tau^2 - X_{R0}^2)/(\tau^2 - X^2 - \xi^2 - \psi^2)] I_3(1/2 \, sqrt(\tau^2 - X^2 - \xi^2 - \psi^2)/I_3(1/2sqrt(\tau^2 - X_{R0}^2) \quad [32]$$

For small X,

$$u = (X/X_{R0}) [(\tau^2 - X_{R0}^2)/(X^2 + \xi^2 + \psi^2 - \tau^2] J_3(1/2 \, sqrt(X^2 + \xi^2 + \psi^2 - \tau^2)/I_3(1/2sqrt(\tau^2 - X_{R0}^2) \quad [33]$$

In the limit of zero radius of the dissolving pill,

$$u = (X/X_{R0}) [\tau^2/(\tau^2 - X^2 - \xi^2 - \psi^2)] I_3(1/2 \, sqrt(\tau^2 - X^2 - \xi^2 - \psi^2)/I_3(\tau/2)$$

For small X,

$$u = (X/X_{R0}) [(\tau^2)/(X^2 + \xi^2 + \psi^2 - \tau^2] J_3(1/2 \, sqrt(X^2 + \xi^2 + \psi^2 - \tau^2)/I_3(\tau/2) \quad [34]$$

The solution is in terms of a Bessel composite function of the third order and first kind for small X and a modified Bessel composite function of the third order and first kind for times greater than X. The first root of the Bessel function of the third order was calculated by using 17 terms of the series expansion of the Bessel function in a Pentium IV microprocessor using a Microsoft Spreadsheet upto 4 decimal places. The root was found to be 6.3802.

$$½(X^2 + \xi^2 + \psi^2 - \tau^2)^{1/2} = 6.3802$$

$$\text{Or} \quad X^2 + \xi^2 + \psi^2 - \tau^2 = 162.828 \quad [35]$$

When an exterior point in the infinite sphere is considered a lag time can be calculated prior to which there is no mass transfer to that point. After the lag time there exists two regimes. One is described by Eq. [33] and the third regime is described by Eq. [34]. Thus,

$$\tau_{lag} = sqrt(X_p^2 + \xi_p^2 + \psi_p^2 - 162.828) \quad [36]$$

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