Global Journal of Mathematical Sciences: Theory and Practical.
Volume 3, Number 1 (2011), pp. 65-71

http://www.irphouse.com

Application of Two Point Padé Approximation in Boundary Value Problems.

K. Venugopal[1] and L. Rajendran[2]

[1]Department of Mathematics, J.J. College of Engineering and Technology, Trichy-620 009, Tamilnadu, India
E-mail: kovenu2008@rediffmail.com
[2]Department of Mathematics, Madura College, Madurai-625011, Tamilnadu, India
E-mail: raj_sms@rediffmail.com

Abstract

A two point Padé approximation of the current and quantity of penetrant at the material transport boundary problems in finite membranes is derived from infinite series expansion. These are shown to be in excellent agreement with previous studies

Keywords: Two point Padé approximation; boundary value problems; diffusion equations; membranes; active diffusion.

Introduction

The solution of boundary value problems (BVPs) is of great importance due to its wide application in scientific research. Adomian et.al [1] solved a generalization of Airy's equation by decomposition method. Ravi Kanth et.al [2] dealt with singular two-point BVPs by cubic spline. Caglar et.al[3] applied B-spline interpolation of two point BVPs and compare results with finite differences, finite element and finite volume methods. Recently Lu[4] solved the boundary value problems using variational iteration method [7,8].

The study of material transport through diffusion in regions of finite spatial extent is a subject of much more interest. For many more years before these study relates theoretical aspects, by mathematical modeling, the reference produced by Carssaw and Jaeger [4]and Crank [5]. The analyses of bounded diffusion process in which the diffusing materials, subject in the electric fields and can undergo chemical reactions are most interesting area to find a new solution. It can be useful for chemical reaction with sites located in diffusion medium. The differential equation is then solved to get a closed form expression for the concentration profile of the diffusion as a function of time.

The previous workers Ludolph and co-workers [11] were interested to calculate the lag-time expected for bounded diffusion coupled with chemical reaction, which yields a solution for equilibrium constant relating free and bound penetrant. After that Keister and Kasting[10] modeled electric field enhanced active diffusion within a finite membrane by a variable separable method. Lyons and his co-workers [13] has arrived the series solution of material transport problems in finite membranes by considering diffusion, migration and first order chemical kinetics using Laplace transform technique. In this paper we obtain the closed and simple form of an analytical expression (Pade approximation) of the current and normalized release function from its infinite series expansions.

Mathematical Formulation and Description of the Physical System

The mathematical model used to determine the following experimental arrangement. Let us consider a thin homogenous membrane of finite thickness L, which separate the two bulk volumes. Let us assume that the diffusion of penetrant is planar. Hence the special variable is defined in the range $0 \leq \chi \leq L$. The region $\chi = 0$ is assigned to the donor compartment, while $\chi = 1$ is assigned to the acceptor compartment. During this process we assume that membrane is subjected to a constant electric field. In addition to that the diffusing penetrant reacts within the membranes to a first order kinetic expression with rate constant *k*. At time t = 0, the face of the membrane adjacent to the donor region is exposed to a constant concentration C_0 while other faces which is in contact with acceptor region is maintained at zero concentration. Further we assume that the solution in both region ie donor as well as acceptor compartments are well stirred, besides the receiver solution acts as an infinite sink and the donor acts as an infinite source. The mathematical description from the above problem, which involves diffusion equation of the following type[13]

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial^2 \chi} - \beta \frac{\partial u}{\partial \chi} - \gamma u \quad 0 \leq u \leq 1;\ 0 \leq \chi \leq 1 \tag{1}$$

Supplemented with the initial and boundary conditions

$$\begin{aligned} u(\chi,0) &= 0 \\ u(0.\tau) &= 1 \\ u(1,\tau) &= 0 \end{aligned} \tag{1a}$$

This expression is obtainable in non dimensional form using the following normalized parameter.

$$u = \frac{c}{kc_0}, \chi = \frac{x}{L}, \gamma = \frac{kL^2}{D} = \frac{j_R}{j_D}, \beta = \frac{\mu EL}{D} = \frac{j_M}{j_D}, \tau = \frac{Dt}{L^2} \tag{2}$$

where u represents a non-dimensional penetrant concentration at any point, χ represents normalized distance variable scaled to the total thickness L of the membrane, τ represents normalized time, β denotes the diffusion migration parameters and γ denotes diffusion reaction parameter. When $\beta = 0$ and $\gamma = 0$, equation (1) becomes

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial^2 \chi} \quad 0 \le u \le 1;\ 0 \le \chi \le 1 \tag{3}$$

The general expression of normalized concentration is [9]

$$u(\chi,\tau) = 1 - \chi - 2\sum_{n=1}^{\infty} \frac{\sin(n\pi\chi)}{n\pi} \exp(-n^2\pi^2\tau) \tag{4}$$

The normalized diffusion flux ψ is given by

$$\psi(\tau) = \frac{jL}{D\kappa c_0} = -\left(\frac{\partial u}{\partial \chi}\right)_{\chi=1} \tag{5}$$

$$= 1 + 2\sum_{n=1}^{\infty} (-1)^n \exp[-n^2\pi^2\tau],\ \text{where} 0 < \tau < 1 \tag{6}$$

The total quantity of penetrant passing through the membrane after a time t is given by [13]

$$Q(\tau) = \frac{N(\tau)}{N_\infty} = \int_0^\tau \psi(T)dT \tag{7}$$

Using the equation (6) we obtain

$$Q(\tau) = \tau - \frac{1}{6} - 2\sum_{n=1}^{\infty} \frac{(-1)^n}{n^2\pi^2} \exp[-n^2\pi^2\tau],\quad \text{where}\ 0 < \tau < 1 \tag{8}$$

Two-point padé approximation

The efficacy of the Padé approximation using a partial set of data in diverse context such as phase transitions [17], viral equation of state for hard spheres and discs [9], cyclic voltammetry[3], diffusion at ultramicroelectrodes [14,16,18] etc. has been demonstrated. In the present analysis, infinite series expansion of current and quantity of penetrant is available. Hence, it is imperative to employ a two-point Padé approximant such that the coefficients of Eqs.(6) or (10) are reproduced (Ref: Appendix-A). In this case current is given by

$$\Psi(\tau) = \frac{p_0 + p_1 y + p_2 y^2 + p_3 y^3 + p_4 y^4 + p_5 y^5}{1 + q_1 y + q_2 y^2 + q_3 y^3 + q_4 y^4 + q_5 y^5} \tag{9}$$

Where

$y = \exp[-\pi^2 \tau]$,

$$p_0 = 1, p_1 = -2, p_2 = 1, p_3 = -2, p_4 = 2, p_5 = 1, q_1 = 1, q_2 = 1, q_3 = 0, q_4 = 0, q_5 = 1 \quad (10)$$

The above equation (9) can be written as

$$\Psi(\tau) = \frac{1 - 2y + y^2 - 2y^3 + 2y^4 + y^5}{1 + y^2 + y^5} \quad (11)$$

Equation (11) is a simple closed form an analytical expression of current for all time. Table-1 indicates the dimensionless current evaluated using equation (6) together with two point Pade approximation (Eqn. (11)). An excellent agreement with the equation (6) is noted. Using Pade approximations, the infinite series (Eqn.(8))can be represented by

$$Q(\tau) = \frac{p_0 + p_1 y + p_2 y^2 + p_3 y^3 + p_4 y^4 + p_5 y^5}{1 + q_1 y + q_2 y^2 + q_3 y^3 + q_4 y^4 + q_5 y^5} \quad (12)$$

where

$y = \exp[-\pi^2 \tau]$

$$p_0 = \frac{-\log y}{\pi^2} - \frac{1}{6}, p_1 = \frac{2}{\pi^2}, p_2 = \frac{-16\log y}{9\pi^2} - \frac{8}{27}, p_3 = \frac{32}{9\pi^2}, p_4 = 0, p_5 = \frac{-4\log y}{9\pi^2} - \frac{2}{27},$$
$$q_1 = 0, q_2 = \frac{16}{9}, q_3 = 0, q_4 = 0, q_5 = \frac{4}{9} \quad (13)$$

The equation (12) also can be written as

$$\Psi(\tau) = \frac{\frac{-\log y}{\pi^2} - \frac{1}{6} + \frac{2}{\pi^2} y - \frac{16\log y}{9\pi^2} y^2 - \frac{8}{27} y^2 - \frac{32}{9\pi^2} y^3 - \frac{4\log y}{9\pi^2} y^5 - \frac{2}{27} y^5}{1 + \frac{16}{9} y^2 + \frac{4}{9} y^5} \quad (14)$$

Equation (14) is a simple closed form of an analytical expression of total quantity of penetrant passing through the membrane. Table-2 indicates the dimensionless quantity of penetrant evaluated using equation (11) together with two point Pade approximation results (14). An excellent agreement with the equation (12) is noted.

Conclusion

The closed form of analytical expression of current and the total quantity of penetrant passing through the diffusion in regions of finite spatial extent is derived by using Padé approximation.

Appendix-A

A Padé approximant is a rational function approximation whose power series expansion agrees with a given infinite power series to the highest possible order[2]. Let

$$f(z) = \sum_{i=0}^{\infty} a_i z^i \tag{A$_1$}$$

be a formal given power series. Let m and n be two non-negative integers. The [m/n] Padé approximant of *f*(z) is the unique rational functions,

$$\frac{P_{m,n}(z)}{Q_{m,n}(z)} = \left[\frac{p_0 + p_1 z + p_2 z^2 + \ldots\ldots\ldots p_m z^m}{1 + q_1 z + .q_2 .z^2 + \ldots\ldots\ldots\ldots\ldots q_n z^n}\right] \tag{A$_2$}$$

such that

$$f(z)Q_{m,n}(z) - P_{m,n}(z) = O(z^{m+n+1}) \tag{A$_3$}$$

That is, the first *m+n+1* term in the Taylor series expansion of [*m/n*] Padé function match the first *m+n+1* terms of power series (equation (A_1)). The existence of polynomials $P_{m,n}(z)$ and $Q_{m,n}(z)$ follows immediately from considering the system of equations.

$$\begin{aligned} \sum_{i=0}^{j} a_{j-1} q_i &= p_j \qquad \text{for } j = 0,1,2,3\ldots m \\ &= 0 \qquad \text{for } j = m+1, m+2, \ldots m+n. \end{aligned} \tag{A$_4$}$$

With $q_i = 0$, if $n \geq 1$ and $q_o = 1$

The system of equations (A_4) determines the co-efficient p_i and q_i in equation (A_2) uniquely. Thus the [*m/n*] Padé approximant to the series is determined by solving the above set equations (equation (A_4)).

Table 1: Normalized diffusion flux ψ for varies values of time evaluated using equation (6) and (11).

τ	y	Infinite series Eqn.(6)	Pade approximation Eqn.(11)
∞	0	1	1
0.1	0.3727	0.2929	0.2929
0.2	0.1389	0.7229	0.7229
0.3	0.0518	0.8964	0.8964
0.4	0.0193	0.9614	0.9614
0.5	0.0072	0.9856	0.9856
0.6	0.0027	0.9946	0.9946

0.7	0.00099903	0.9980	0.9980
0.8	0.00037235	0.9993	0.9993
0.9	0.00013878	0.9997	0.9997
1.0	0.000051723	0.9999	0.9999

Table 2: Total quantity of penetrant $Q(T)$ passing through the membrane for varies values time evaluated using equation (8) and (14).

τ	y	Infinite Series Eqn.(8)	Pade approximation Eqn.(14)
0.1	0.3727	0.0079	0.0079
0.2	0.1389	0.0615	0.0615
0.3	0.0518	0.1438	0.1438
0.4	0.0193	0.2372	0.2372
0.5	0.0072	0.3347	0.3347
0.6	0.0027	0.4331	0.4331
0.7	0.00099903	0.5335	0.5335
0.8	0.00037235	0.6334	0.6334
0.9	0.00013878	0.7334	0.7334
1.0	0.000051723	0.8333	0.8333

References

[1] Adomian, G. , Elrod.M, Rach.R, A new approach to boundary value equations and application to a generalization of Airy's equation J.Math.Anal.Appl.,140, 554-568. (1989)

[2] Baker, G.A , Graves-Morris, P In Encyclopedia of Mathematics, Vol. 13, Pade approximant part II ; G. C.Rota.., Ed.; Addison - Wesley:Reading, MA, Chapter-II (1981)

[3] Basha,C.A , Sangaranarayanan,M.V On the evaluation of the current function in linear sweep voltammetry J. Electroanal. Chem, 261, 431- 436. (1989)

[4] Carslaw,HS Jaeger JC, Conduction of heat in solids, 2nd edn, Clarendon Press, Oxford (1997)

[5] Crank,J The mathematics of diffusion , 2nd edn, Clarendon Press, Oxford (1998)

[6] Caglar,H , Caglar.N,. Elfaituri,.K J.Math.Ana.Appl., 140, 554-568 (1989)

[7] He.J.H, Approximate analytical solution of Blasius' equation Comm. Nonlinear Sci. Numer. Simulation, 2(4), 230-235. (1997)

[8] He.J.H, Approximate analytical solution for seepage flow with fractional derivatives in porous media, Comput. Methods Appl. Mech. Eng,167, (1-2)57-60 (1998)

[9] Kratky. K.W,Equation of state of a hard-disk fluid. I. The viral expansion J hem. Phys, 69, 2251-2255 (1978)

[10] Keister,J.C G., Kasting,.B Pharmaceutical Skin penetration Enhancement, J. Membr Sci, 29, 155 (1986)

[11] Ludolph,R.A ,Veith,W.R, Friseh,H.L Effects of linear reaction and absorption processes on the penetrant time lag, J Phys Chem , 83 , 2793 (1979)

[12] Lu,J Variational iteration method for solving two-point boundary value problems, J.Comput. Appl. Math, 207 ,92-95 (2007)

[13] Lyons , M.E.G,Judith Murphy , Serge Rebouillat , Theoretical analysis of time dependent diffusion reaction and electromigration in membranes. J Solid State ElectroChemistry, 4, 458-472 (2000)

[14] Rajendran,.L Nallaswamy, R, Chronoamperometric urrent at Ultramicroelectrodes: Padé Approximation for a Reversible Electron Transfer Scheme, Electroanalysis, 10 506-511 (1998)

[15] Ravi Kanth, Y. A. S. V. , Reddy.N, Cubic spline for a class of singular two-point boundary value problems, Appl.Math. Comput. 170, 733-740 (2005)

[16] Rajendran,.L,Two-point Padé approximation of mass transfer rate at microdiscelectrodes in a channel flow for all Péclet numbers, Electrochimical Acta, 51, 5407-5411 (2006)

[17] Sangaranarayanan, M.V, Rangarajan,S.K An ε-convergence method for the evaluation of critical parameters, Chem. Phys. Lett. 101, 49-54 (1983)

[18] Senthamarai,.R Rajendran,L Analytical expression for transient chronoamperometric current at ultramicroband electrode, Russian Journal of Electrochemistry, 44, 1156-1161 (2008).