Legendre Wavelet Based Approximation Method To Steady State Reaction-Diffusion Model Arising In Mathematical Chemistry

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Abstract - The mathematical model of steady state mono-layer potentiometric biosensor is studied and the model is based on non-stationary diffusion equations containing a non-linear term related to Michaelis-Menten kinetics of the enzymatic reaction. This paper presents a numerical method based on Legendre wavelets operational matrix method. These results are compared with available limiting case results and that are found to be in good agreement. Moreover, the use of Legendre wavelet operational matrix is found to be simple, efficient, accurate and computationally attractive.

Index Terms: Non-linear Boundary value problems, Legendre wavelets, Operational matrix.
2010 Mathematics Subject Classification: 65M70, 65N35, 35C10, 42C10.

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1 Introduction

Modelling of biosensors is of a crucial importance to understand their behaviour. It is difficult to measure the concentration of substracts inside the enzyme membrane using analytical devices. Hence mathematical models in biosensors have been developed and used as an important tool to study the analytical characteristics of actual biosensors.Goldman et al initiated work of Biosensor modelling in his historical paper[1]. He has studied that the extensive treatment of substract and product distribution in membrane containing enzymes. The kinetics of reaction in an enzyme membrane immersed in a substrate solution was throughly investestigated by Sundaram et al [2]. Kasche et al [3] presented a model and equations described steady-state catalysis by an enzyme immobilized in spherical gel particles and showed that catalysis by an unbounded enzyme.

Some of the equations are solved for the fluxes, for the substrate (or) product concentrations. Gough et al [4] have simulated the performance of a cylindrical biosensor for glucose monitoring steady state. Various approaches has been initiated to solve the equation arises from mathematical modelling of biosensors like finite difference scheme initiated by Jobst et al [5]. Using the implicit finite difference scheme [6], the influence of the substrate concentration as well as maximal enzymatic rate on the biosensor was investigated [7]. The explicit scheme is usually easier to program, however the implicit scheme has a higher simulation speed [8-10]. The general time-dependent problem has been tackled previously by Carr

[11] using Fourier analysis, and the steady state problem has been examined by Brady and Carr [12]. Recently, Hariharan et al used second kind shifted chebyshev wavelets for the Michaelis-Menten model [13]. In recent years, wavelets has been used as an indespensible tools for finding the solutions of the differential equations that arises while modelling of biosensors enzymes. Since it possesses inherent properties like compact support, orthogonality and vanishing moments [14-17]. Wavelets are well localised in time as well as frequency domain .Using this idea Bekylin et al [18], first used wavelets to find the solution of the differential equations that contains shock like behaviour. Later, many researchers[19-22] are using the wavelets as a main tool for finding the solution of the differential equations.The main goal of this paper is to discuss how Legendre wavelets have been used to solve the mathematical model of biosensor of 'Michaelis-Menten Kinetics' type equations.

To my knowledge, there is no rigorous analytical solutions for non-linear steady state concentration for polymer modified electrodes for all values of alpha (saturation parameter) and K (reaction-diffusion parameter). It should be pointed out that, complete solutions have not yet been obtained even for steady state behaviour because of the non-linearity inherent in 'Michaelis-Menten Kinetics'. In this paper, we have derived a new, simple and closed analytical expressions of concentrations and current using Legendre wavelets operational method.

2 Mathematical formulation of the problem

During an enzyme-catalzed reaction

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$$E + S \overset{K_M}{\leftrightarrow} ES \overset{K_2}{\to} E + P \quad (2.1)$$
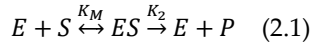
the substrate (S) binds to the enzyme (E) to form enzyme-substrate complex ES. While it is a part of this complex, the subtrate is converted to product P. The rate of the appearance of the product depends on the concentration of the substrate. Then the rate of change of substrate concentrations $S = S(t, \chi)$ at time t, position $\chi \in \Omega$ is equal to the sum of the rate due to reaction and diffusion, and is given by Pao (23).

$$\frac{\partial S}{\partial t} = D_s \nabla \cdot (\nabla s) - v(t, \chi) \quad (2.2)$$

where D_s is the substrate diffusion coefficient ∇ is the gradient operation, and v is called the inital reaction velocity. Various models regarding the expressions for v are formulated. In this paper, we discuss the some mathematical properties of the solutions of the type models using Michaelis- Menten hypothesis. Pao (23) and Baronas et al (24) expressed the velocity function v for the simple reaction process without competitive inhibition using Michaelis hypothesis.

$$v(t, \chi) = \frac{K_2 E_0 S}{K_M + S} \quad (2.3)$$

where E_0 is the total amount of enzyme and K_M is the "Michaelis constant". In this model, the equation for "S" becomes

$$\frac{\partial S}{\partial t} - D_s \nabla \cdot (\nabla s) = -\frac{K_2 E_0 S}{K_M + S}, t > 0, \chi \in \Omega \quad (2.4)$$

In one-dimensional, the above equation can be written as

$$\frac{\partial S}{\partial t} = D_s \frac{\partial^2 S}{\partial \chi^2} - \frac{K_2 E_0 S}{K_M + S} \quad (2.5)$$

Introducing $\frac{K_2 E_0}{K_M} = K$ which is a Pseudo-first order rate constant.Thus the above equation becomes

$$\frac{\partial S}{\partial t} = D_s \frac{\partial^2 S}{\partial \chi^2} - \frac{K_s}{1 + \frac{S}{K_M}} \quad (2.6)$$

In this problem, we consider an initial condition is given in usual form as

$$S(0, \chi) = S_0(\chi), \chi \in \Omega \quad (2.7)$$

with the initial conditions u(0) = 1, u'(0) = 0.

3 The properties of Legendre wavelets

3.1 Wavelets and Legendre wavelets

Wavelets constitute a family of functions constructed from dilation and translation of single function called the mother wavelet. When the dilation parameter a and the translation parameter b vary continously, then we have the following family of continous wavelets [7]

$$\psi_{a,b}(t) = |a|^{\frac{-1}{2}} \psi\left(\frac{t-b}{a}\right) \quad a, b \in R, a \neq 0 \quad (3.1)$$

If we restrict the parameters a and b to discrete values as $a = a_0{}^k, b = nb_0 a_0{}^k$ $a_0 > 1, b_0 > 0$ n, and k positive integers, we have the following family of discrete wavelets:

$$\psi_{k,n}(t) = |a|^{\frac{k}{2}} \psi(a_0{}^k t - nb),$$

where $\psi_{k,n}(t)$ form a wavelet basis for L^2(R). In particular when a=2 and b=1 then $\psi_{k,n}(t)$ forms an orthonomal basis [7].

Legendre waveletshave four arguments: k, n can are positive integer, m is the order for Legendre polynomials, and t is the normalized time. They are defined on [0,1] by

$$\psi_{k,n}(t) = \begin{cases} \sqrt{m + \frac{1}{2}} 2^{\frac{k}{2}} L_m(2^k - n), \\ \\ for\ t \in \frac{n-1}{2^k}, \frac{n+1}{2^k}, \end{cases}$$

m=0,1,2,......M-1 and n= 0,1,2,.....2^k-1. The coefficient $\sqrt{m + \frac{1}{2}}$ is for orthonormality, the dilation parameter is $a = 2^{-k}$ and the translation parameter $b = n2^{-k}$ Here,$L_m(t)$ are well known Legendre polynomials of order m, which are defined on the interval [-1,1] and can be determined with the aid of the following recurrence formula:

$$L_0(t) = 1, L_1(t) = 1$$
$$L_{m+1} = \left(\frac{2m+1}{m+1}\right) t L_m(t) - \left(\frac{m}{m+1}\right) t L_{m-1}(t),\ m = 1,2,3...$$

The set of $\psi_{n,m}(t)$ forms an orthonormal system for $L^2[0,1]$

4 Function approximation

A function *f(t)* defined over *[0,1)* may be expanded in terms of Legendre wavelets as

$$f(t) = \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} c_{nm} \psi_{nm}(t),$$

where $c_{nm} = \left(f(t), \psi_{nm}(t)\right)_w = \int_0^1 \sqrt{t - t^2} f(t) \psi_{nm}(t) dt$

If the infinite series is truncated, then it can be written as

$$f(t) \approx \sum_{n=1}^{2^{k-1}} \sum_{m=0}^{M-1} c_{nm} \psi_{n,m}(t) = C^T \psi(t) \quad (4.1)$$

where C and $\psi(t)$ are $2^{k-1} M\ X 1$ matrices are defined by

$$C = [c_{10}, c_{11}, ..., c_{1M-1}, ..., c_{2^{k}-10}, c_{2^{k}-11}, ... c_{2^{k}-1M-1},]$$
(4.2)

$$\psi(t) = [\psi_{10}, \psi_{11}, ..., \psi_{1M-1}, ..., \psi_{2^{k}-10}, \psi_{2^{k}-11}, ... \psi_{2^{k}-1M-1},]$$
(4.3)

5 Operational matrix of deriva-tive and product operational matrix

In this section, we introduce a new Legendre wavelets operational matrix of derivative.

Let $\psi(t)$ be the Legendre wavelets defined as in equation (4.3). The derivative of the vector $\psi(t)$ can be expressed as

$$\frac{d\psi(t)}{dt} = D\psi(t) \qquad (5.1)$$

where D is the $2^{k-1}M\ X1$ operational matrix of derivative defined as follows

$$D = \begin{pmatrix} F & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & F \end{pmatrix}$$

$F = (M+1)X(M+1)$ matrix and its *(r,s)* element is defined as follows

$$F_{r,s} = \left\{ \begin{matrix} 2^{k+1}\sqrt{(2r-1)(2s-1)}, if\ r = 2\dots(M+1), \\ s = 1,2\dots r-1\ and\ (r+s)is\ odd \end{matrix} \right\}$$

Proof can be found in [26]

Corollary 5.1

The operational matrix for the nth derivative can be obtained from

$$\frac{d^n\psi(t)}{dt^n} = D^n\psi(t), n = 1,2,3\dots \qquad (5.2)$$

where D^n is the *nth* power of matrix D.

6 Second-order two-point boundary value problems

6.1 Linear second-order two point boundary value problems

Consider the linear second-order differential equation

$$y''(x) + f_1(x)y'(x) + f_2(x)y(x) = g(x), x \in [0,1] \quad (6.1)$$

subject to the initial conditions

$$y(0) = \alpha, y'(0) = \beta, \qquad (6.2)$$

or the boundary conditions

$$y(0) = \alpha, y(1) = \beta, \qquad (6.3)$$

or the general mixed boundary conditions

$$a_1y(0) + a_2y'(0) = \alpha, b_1y(1) + b_2y'(1) = \beta, \qquad (6.4)$$

If we approximate $y(x), f_1(x), f_2(x), g(x)$ in terms of the Legendre wavelets basis, then one can write

$$y(x) \approx \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} c_{nm}\psi_{nm}(x) = C^T\psi(x),$$

$$f_1(x) \approx \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} f_{nm}\psi_{nm}(x) = F_1{}^T\psi(x),$$

$$f_2(x) \approx \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} f_{nm}\psi_{nm}(x) = F_2{}^T\psi(x),$$

$$g(x) \approx \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G^T\psi(x), \qquad (6.5)$$

where C^T, F_1^T, F_2^T, G^T defined similarly as in above. Relations enable one to approximate $y'(x)$ and $y''(x)$

$$y'(x) = C^TD\psi(x), y''(x) = C^TD^2\psi(x) \qquad (6.6)$$

Now, substitution of relations (6.6) into equation, (6.1) enable us to define the residual, R(x) of this equation as

$$R(x) = C^TD^2\psi(x) + F_1\psi(x)(\psi(x))^T + F_2\psi(x)(\psi(x))^T - G$$

and application of the Tau method yields the following $(2^k(M+1)-2)$ linear equations in the unknown expansion coefficients, c_{nm}, namely

$$\int_0^1 \sqrt{x-x^2}\ \psi_j(x)R(x)dx = 0, \qquad (6.7)$$
$$j = 1,2,\dots.. 2^k(M+1) - 2$$

Moreover the initial condition (6.2) the boundary conditions (6.3)and the mixed boundary conditions (6.4) lead respectively, to the following equations

$$C^T\psi(0)=\alpha, \qquad C^TD\psi(0) = \beta \qquad (6.8)$$

$$C^T\psi(0)=\alpha, \qquad C^TD\psi(1) = \beta \qquad (6.9)$$

Thus equation (6.1) with the two equations (6.2) or (6.3) or(6.4) generate $2^k(M+1)$ a set of linear equations which can be solved for the unknown of the vector C, and hence an approximate wavelet solutions of y(x) can be obtained.

7 Method of solution

Consider the following nonlinear initial value problem obtain in the equation (2.11)

$$u'' - \frac{Ku}{1+\alpha u} = 0 \qquad (7.1)$$

With the initial conditions u(0) =1, u'(0) = 0. We solve the above equation using the algorithm described in section (6) for the case of M = 2, K=0. First, if we make use of equations (5.1) and (5.2), then the two operational matrices D and D² are given by

$$D = \begin{pmatrix} 0 & 0 & 0 \\ 2\sqrt{3} & 0 & 0 \\ 0 & 2\sqrt{15} & 0 \end{pmatrix} \qquad D^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 12\sqrt{5} & 0 & 0 \end{pmatrix}$$

Considering the equation (7.1) we have

$$C^TD^2\psi(x) - \frac{KC^T\psi(x)}{1+\alpha C^T\psi(x)} = 0 \qquad (7.2)$$

Where $C^T = (c_{00}, c_{01}, c_{02,})^T$. If we collocate

$x_0 = -\frac{1}{2}\left(\frac{\sqrt{3}}{1+\sqrt{5}}\right)$ which is the first root of $L_3(x)$. Further the use of initial conditions lead to two equations

$$c_{00} - \sqrt{3}c_{01} + \sqrt{5}c_{02} = 1 \qquad (7.3)$$
$$c_{01} + \sqrt{5}c_{02} = 0 \qquad (7.4)$$

solving this system of nonlinear equation we get

$$C^T = (c_{00}, c_{01}, c_{02})^T = (0.530, 0.025, 0.0061)$$

Consequently

$$u(x) = C^T\psi(x) = [0.530, 0.025, 0.0061][\psi_{00}, \psi_{01}, \psi_{02}] = 0.1961x^2 - 1$$

Our results can be compared with Rahamathunissa and

Rajendran (25) results. For larger M, we can get the exact results.

7.1 Limiting cases

Unsaturated (First order) Catalytic Kinetics [27]

In this case, the substrate concentration $S(\chi)$ is less than the Michales Constant KM. When α u<<1, the equation (2.11) reduces to

$$\frac{\partial^2 u}{\partial^2 x} - Ku = 0 \qquad (7.5)$$

the initial conditions are u(0) = 1, u'(0) = 0

$$u''(x)-Ku(x) = 0 \qquad (7.6)$$

u(0) = 1, u'(0) = 0

The above equations (7.6), (7.7) are solved using the same procedure mentioned in previous section. we obtain the value as u(x) = $0.4834x^2$+0.0192x+0.9964

 Saturated {(Zero Order)} Catalytic Kinetics[27]

 In this case, the substrate concentration in the film S(chi) is greater than the Michaelis constant K_M. This is explained in Rajendran[25]. Hence alpha u >> 1 reduces the equation (2.11) to

$$\frac{\partial^2 u}{\partial^2 x} - \frac{K}{\alpha} = 0 \qquad (7.8)$$

the initial conditions are u(0) = a, u'(0) = 0

The above equation can be rewritten as

$u''(x) - \frac{K}{\alpha} = 0$. Hence $C^T D^2 \psi(x) = \frac{k}{\alpha}$. Using the same procedure in section (7) we may arrive the constant value as

$C^T = (c_{00,}\ c_{01,}\ c_{02,})^T \cdot = [\frac{32\alpha+5}{64}, \frac{1}{16}, \frac{1}{64}]$. Finally we have $u(x) = a + \frac{x^2}{2}$. All the numerical experiments presented in the above sections are computed in double precision with some MATLAB codes on a personal computer System.

8 Conclusion

In this paper, we used Legendre Wavelet Method to obtain the numerical solutions of Reaction Diffusion Equations containing non-linear term related to Michaelis-Menten Kinetics of the enzymatic reaction. Numerical results shows that LWM can match the analytical solution very efficiently with quite a few calculations. Also proposed methods found to be very simple, in finding the solution of nonlinear differential equations. It provides more realistic series solution that converge very rapidly in real physical problems.

9 References

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