A novel computational method to nonlinear reaction-diffusion system using shifted Legendre polynomials

M.Mahalakshmi, R.Seethalakshmi G.Hariharan
Department of Mathematics, School of Humanities & Sciences, SASTRA Deemed University, India

Abstract
The mathematical model of Praveen et al. (Biochemical Engineering Journal, 91 (2014):129-39) in immobilized enzymes is discussed. In this paper, an efficient shifted Legendre computational matrix method (LCMM) is applied for solving the nonlinear differential equations with Michaelis-Menten kinetics. To the best of our knowledge, until there is no rigorous Legendre operational matrix based solutions has been reported for the above model. Theoretical results are obtained to analyze the effect of different parameter values. Several examples are given to demonstrate the validity and applicability of the proposed spectral method. The numerical results are compared with MADM results. Satisfactory agreement with the ADM results is noticed.

Keywords: Mathematical modeling; immobilized enzymes; Legendre operational matrices; Adomian decomposition method; steady state conditions.

1. Introduction
In recent years, many orthogonal functions and polynomials have been implemented to obtain the quality solutions of differential equations[1]. The reaction-diffusion model has been developed in the spherical catalyst particles for Michaelis-Menten type kinetics and the steady state equation to determine the concentration profiles of substrate inside catalyst particles to assess the design and performance of such reactors [2]. Mohammad and Hosseini[3] used a new Legendre wavelet approach for solving the singular ordinary differential equation [3]. Khellat and Yousefi [4] derived the linear Legendre mother wavelets matrices of integration. In recent years, wavelets have found their place in many applications such as image processing, signal processing and solving differential and integral equations. Yousefi [5] applied the Legendre wavelets method (LWM) for solving the differential equations of Lane – Emdor type. Razzaghi and Yousefi [6, 7] had used the Legendre wavelets for constrained optimal control problems and variational problems. Recently, Hariharan [8] used an efficient Legendre wavelet based approximation method for a few-Newell and Allen-Cahn equations. Hariharan and Kannan [9] reviewed the wavelet solutions for the solutions of reaction-diffusion equations arising in science and engineering. Excellent references there in [9]. Jafari et al. [10] solved fractional differential equations by using Legendre wavelets in collocation method. Praveen et al.[11] have studied the theoretical analysis of intrinsic reaction kinetics and the behavior of immobilized enzymes...

In this paper, we have applied Legendre Computational Matrix Method for solving differential equations with Michaelis-Menten kinetics. The organization of this paper as follows: In section 2, some relevant properties of shifted Legendre polynomials are presented. In section 3, Mathematical model of the Michaelis-Menten kinetics is discussed. Method of solution by the Legendre computational matrix method presented in section 4. Illustrative examples are given in section 5. Results and discussions are given in section 6. Concluding remarks are given in section 7.

2. Some properties of the shifted Legendre polynomials [1]

The well known Legendre polynomials $P_n(z)$, defined on the interval [-1,1], have the following properties:

$$P_n(z) = (-1)^n P_n(-z), \quad P_n(-1) = (-1)^n, \quad P_n(1) = 1$$  \hspace{1cm} (1)

It is well known that the weight function is $\omega(z) = 1$ and the weighted space $L^2_\omega(-1,1)$ is equipped with the following inner product and norm;

$$(u,v) = \int_{-1}^{1} u(z)v(z)\omega(z)dz, \quad \|u\| = (u,u)^{1/2}. \hspace{1cm} (2)$$

The set of Legendre polynomials forms a complete orthogonal system $L^2(-1,1)$ and;

$$\|P_n(z)\| = h_n = \frac{2}{2n+1}, \hspace{1cm} (3)$$

is obtained. In order to use these polynomials on the interval [0, L] the so-called shifted Legendre polynomials are defined by introducing the change of variable $z = \frac{2x}{L} - 1$.

The shifted Legendre polynomials are defined as;

$$P_n^*(x) = P_n\left(\frac{2x}{L} - 1\right) \text{ where } P_n^*(0) = (-1)^n, \hspace{1cm} (4)$$

The analytic form of the shifted Legendre polynomial $P_n^*(x)$ of degree $n$ is given by;
\begin{align}
P_n^* (x) &= \sum_{k=0}^{\infty} (-1)^{n+k} \frac{(n+k)!}{(n-k)!k!} x^k. \tag{5}
\end{align}

Let \( \omega_L (x) = 1 \), and the weighted space \( L^2_{\omega_L} (0,L) \) is defined with the following inner product and norm;

\begin{align}
(u,v)_{\omega_L} &= \int_0^L u(x) v(x) \omega_L(x) \, dx, \quad \|u\|_{\omega_L} = (u,u)_{\omega_L}^{\frac{1}{2}}. \tag{6}
\end{align}

The set of the shifted Legendre polynomials forms a complete \( L^2_{\omega_L} (0,L) \) orthogonal system and

\begin{align}
\|p_n^* (x)\|^2 = \frac{L}{2} h_n = \frac{L}{2n+1}
\end{align}

is obtained. The function \( u(x) \) which is square integrable in \([0,L]\), may be expressed in terms of shifted Legendre polynomials as;

\begin{align}
u(x) &= \sum_{i=0}^{\infty} c_i P_i^* (x), \tag{7}
\end{align}

where the coefficients \( c_i \) are given by;

\begin{align}
c_i = \frac{1}{\|P_i^* (x)\|_{\omega_L}^2} \int_0^L u(x) P_i^* (x) \omega_L(x) \, dx, \quad i = 0,1,2,\ldots. \tag{8}
\end{align}

2.1 Fundamental relations

It is suggested the solution \( u(x) \in C^m [0,L] \) can be approximated in terms of the first \((m+1)\) terms of shifted Legendre polynomials given by

\begin{align}
u(x) &= \sum_{i=0}^{m} c_i P_i^* (x). \tag{9}
\end{align}

3. Formulation of the problem and analysis [11]

The mass balance differential equation for substrate and product are
\[ D_s \left( \frac{d^2 s}{dr^2} + \frac{2}{r} \frac{ds}{dr} \right) - V = 0 \]  
\[ D_p \left( \frac{d^2 p}{dr^2} + \frac{2}{r} \frac{dp}{dr} \right) + V = 0 \]  

where \( s \) and \( p \) are the concentration of substrate and product. Here \( D_s \) and \( D_p \) is the diffusion coefficient for substrate and product within the support. The enzymatic reaction rate \( V \) for various kinetic mechanisms is given as follows:

(i) Simple Michaelis-Menten

\[ V = \frac{V_m s}{K_s + s} \]  

(ii) Uncompetitive substrate inhibition

\[ V = \frac{V_m s}{s(1 + s/K_i) + K_i} \]  

(iii) Total competitive product inhibition

\[ V = \frac{V_m s}{K_s(1 + p/K_i) + K_s} \]  

(iv) Total non-competitive product inhibition

\[ V = \frac{V_m s}{s(1 + p/K_i)(K_s + s)} \]  

(v) Reversible Michaelis - Menten reaction

\[ V = \frac{V'_m (s - s_v)}{K_s + (s - s_v)} \]  

where \( K_s \) - Intrinsic half saturation constant.

\( K_i \) - Intrinsic inhibition constant.

\( V_m \) - Maximum reaction rate

\( V'_m \) - Maximum reaction rate for reversible reaction.
\( s_e \) - Equilibrium substrate concentration (reversible reaction)

Using the following dimensionless variables

\[
\omega = \frac{s}{K_s}, \beta_0 = \frac{s_0}{K_s}, \gamma = \frac{p}{K_p}, t = \frac{R}{U}, \alpha = \frac{K_s}{K_j}, \gamma_0 = \frac{p_0}{K_j}
\]

\[
\phi_s = \frac{U}{3} \left( \frac{V_m}{D_s K_s} \right)^{1/2}, \quad \phi_p = \frac{U}{3} \left( \frac{V_m}{D_p K_s} \right)^{1/2}
\]

Eq. (10) can be written in dimensionless form for simple Michaelis-Menten kinetics, uncompetitive substrate inhibition, reversible Michaelis-Menten reaction [12]

\[
\frac{d^2 \omega}{dx^2} + \frac{2}{x} \frac{d \omega}{dx} = 9 \phi_s^2 f(\omega)
\]

where the nonlinear reaction term \( f(\omega) \) represents

\[
\frac{\omega}{1 + \omega}, \quad \frac{\omega}{\alpha(1 + \omega \alpha) + 1}, \quad \frac{\omega - \omega_e}{1 + \omega - \omega_e}
\]

for simple Michaelis-Menten, uncompetitive substrate inhibition and reversible Michaelis-Menten reaction respectively.

\( \omega_e \) - dimensionless equilibrium substrate concentration for reversible reaction.

For total competitive and non-competitive product inhibition systems the mass balance Eq. (10) and

Eq. (11) becomes

\[
\frac{d^2 \omega}{dx^2} + \frac{2}{x} \frac{d \omega}{dx} = 9 \phi_s^2 f(\omega, \gamma) \quad ; \quad \frac{d^2 \omega}{dx^2} + \frac{2}{x} \frac{d \omega}{dx} = -9 \phi_p^2 f(\omega, \gamma)
\]

where \( f(\omega, \gamma) \) represents

\[
\frac{\omega}{1 + \omega + \gamma}, \quad \frac{\omega}{(1 + \omega \alpha)(1 + \omega)}
\]

for total competitive and non-competitive product inhibition respectively.

The boundary conditions for Eq. (9) and (10) are

\[
\frac{d \omega}{dx} = \frac{d \gamma}{dx} = 0 \text{ when } x = 0, \quad \omega = \omega_0, \gamma = \gamma_0 \text{ when } x = 1
\]

where
\( \omega \)-Dimensionless substrate concentration.

\( \omega_0 \)- Dimensionless substrate concentration in the catalyst surface and outside the support.

\( \gamma \) - Dimensionless product concentration.

\( \gamma_0 \) - Dimensionless product concentration outside the support.

\( x \) - Dimensionless radial distance.

\( \alpha \) - Ration of intrinsic half saturation constant over intrinsic inhibition constant.

\( \phi_s \) - Thiele modulus for substrate

\( \phi_p \) - Thiele modulus for product.

### 3.1 First order catalytic kinetics

We consider the situation where the dimensionless substrate concentration \( \omega \) is less than 1. Hence Eq. (18) reduces to

\[
\frac{d^2 \omega}{dx^2} + \frac{2}{x} \frac{d\omega}{dx} = 9 \phi_s^2 \omega
\]  
(21)

### 3.2 Zero order catalytic kinetics

We consider the second major limiting situation found in practice, when the dimensionless substrate concentration is very much greater than 1. Eq.(18) reduces to the simple linear equation

\[
\frac{d^2 \omega}{dx^2} + \frac{2}{x} \frac{d\omega}{dx} = 9 \phi_s^2 \omega
\]  
(22)

### 4. Method of Solution

Consider the Eq.(21)

\[
D^2 \omega(x) + \frac{2}{x} D\omega(x) = 9 \phi_s^2 \omega(x)
\]  
(23)

with the initial conditions \( \omega(1) = \omega_0 \), \( \omega'(0) = 0 \)

The proposed method is applied with \( m = 2 \) and the solution \( \omega(x) \) is approximated as follows:
\[ \omega(x) = \sum_{i=0}^{\infty} c_i P^*_i(x) \]  
(24)

For \( m = 2 \), a system of linear equations is obtained, two of them from the initial conditions and one from the main equation using the collocation point \( x = 0.5 \) which is the root of \( P^*_i(x) = 0 \). Eq. (24) can be written in the following matrix form:

\[ \omega(x) = P(x)A \]

where \( P(x) = \begin{pmatrix} P_0^*(x) & P_1^*(x) & P_2^*(x) \end{pmatrix}, \quad A = \begin{pmatrix} c_0 & c_1 & c_2 \end{pmatrix}^T \)

Here \( P_0^*(x) = 1, P_1^*(x) = 2x - 1, P_2^*(x) = 6x^2 - 6x + 1 \)

5. Illustrative Examples:

Limiting Cases

Case: (i)

Consider \( \phi = 1, \omega_0 = 100 \) in Eq. (23)

The matrix equation for this problem is:

\[ (PD^2 + \frac{2}{x} PD + P)A = F \]  
(25)

where \( P = \begin{pmatrix} 1 & 0 & 0.5 \end{pmatrix}, \quad D^2 = \begin{pmatrix} 0 & 0 & 12 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 2 & 0 \\ 0 & 0 & 6 \\ 0 & 0 & 0 \end{pmatrix} \)

The main matrices for the initial conditions

\[ P(1)A = 100, \quad P(0)DA = 0 \]  
(26)

From the Eq. (25) and (26), we get \( c_0 = 52.96, c_1 = 35.28, c_2 = 11.76 \)

Using the aforesaid Legendre spectral method, one can obtain

\[ \omega(x) = 70.56x^2 + 29.44 \]

Case: (ii)

Consider \( \phi = 0.1, \omega_0 = 10 \)
The matrix equation for this problem is:

\[
(PD^2 + \frac{2}{x}PD + P)A = F
\]  

(27)

The initial conditions are

\[
P(1)A = 10, \quad P(0)DA = 0
\]

(28)

From the Eq. (27) – (28) we get  \( c_0 = 9.9 \quad c_1 = 0.075 \quad c_2 = 0.025 \)

Using the aforesaid Legendre spectral method, one can obtain

\[
\omega(x) = 0.15x^2 + 9.85
\]

Case: (iii)

Consider  \( \phi_s = 0.3, \quad \omega_b = 10 \)

The matrix equation for this problem is:

\[
(PD^2 + \frac{2}{x}PD + P)A = F
\]

(29)

The initial conditions are

\[
P(1)A = 10, \quad P(0)DA = 0
\]

(30)

From the Eq. (29) – (30) we get  \( c_0 = 0.204 \quad c_1 = 0.612 \quad c_2 = 9.184 \)

Using the aforesaid Legendre spectral method, one can obtain

\[
\omega(x) = 1.224x^2 + 8.776
\]

Case. (iv) Consider the equation (22)

\[
D^2\omega(x) + \frac{2}{x}D\omega(x) = 9\phi_s^2
\]

(31)

With the initial conditions  \( \omega(1) = \omega_b, \omega'(0) = 0. \)

Limiting Cases

Case: (i)

Consider  \( \phi_s = 1, \quad \omega_b = 100 \)
The matrix equation for this problem is;

\[(PD^2 + \frac{2}{x}PD)A = F\]  \hspace{1cm} (32)

The initial conditions are

\[P(1)A = 100 \quad , \quad P(0)DA = 0\]  \hspace{1cm} (33)

From the Eq. (32) – (33) we get \[c_0 = 99 \quad c_1 = 0.75 \quad c_2 = 0.25\]

Using the aforesaid Legendre spectral method, one can obtain

\[\omega(x) = 1.5x^2 + 98.5\]

**Case:** (ii)

Consider \(\phi_s = 0.1\), \(\omega_0 = 10\)

The matrix equation for this problem is;

\[(PD^2 + \frac{2}{x}PD)A = F\]  \hspace{1cm} (34)

The initial conditions are

\[P(1)A = 10 \quad , \quad P(0)DA = 0\]  \hspace{1cm} (35)

From the Eq. (34) – (35) we get \[c_0 = 9.99 \quad c_1 = 0.0075 \quad c_2 = 0.0025\]

Using the aforesaid Legendre spectral method, one can obtain

\[\omega(x) = 0.015x^2 + 9.985\]

**Case:** (iii)

Consider \(\phi_s = 0.3\), \(\omega_0 = 10\)

The matrix equation for this problem is;

\[(PD^2 + \frac{2}{x}PD)A = F\]  \hspace{1cm} (36)

The initial conditions are

\[P(1)A = 10 \quad , \quad P(0)DA = 0\]  \hspace{1cm} (37)
From the Eq. (36) – (37) we get  $c_0 = 9.888 \quad c_1 = 0.084 \quad c_2 = 0.028$

Table: 1 Comparison of dimensionless substrate concentration $\omega$ (Zero and First order reaction) for $\phi_i = 0.1$ and $\omega_0 = 1$

<table>
<thead>
<tr>
<th>$x$</th>
<th>$\omega_{MADM}$</th>
<th>$\omega_{LWM}$ (Eq.21)</th>
<th>$\omega_{LWM}$ (Eq.22)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>9.9900</td>
<td>9.9850</td>
<td>9.9850</td>
</tr>
<tr>
<td>0.2</td>
<td>9.9906</td>
<td>9.9905</td>
<td>9.9856</td>
</tr>
<tr>
<td>0.4</td>
<td>9.9922</td>
<td>9.9920</td>
<td>9.9874</td>
</tr>
<tr>
<td>0.6</td>
<td>9.9940</td>
<td>9.9941</td>
<td>9.9941</td>
</tr>
<tr>
<td>0.8</td>
<td>9.9946</td>
<td>9.9946</td>
<td>9.9946</td>
</tr>
<tr>
<td>1</td>
<td>10.004</td>
<td>10.000</td>
<td>10.000</td>
</tr>
</tbody>
</table>

Graph: Represents the comparison of $\omega(x)$ calculated using MADM, LWM (Eq.21), and LWM (Eq.22) for different $x$ values.
Fig1. Comparison between the MADM and LCMM for $\phi_s$ and $\omega_0$

Table: 2 Comparison of dimensionless substrate concentration $\omega$ (Zero and First order reaction) for $\phi_s = 0.3$ and $\omega_0 = 10$

<table>
<thead>
<tr>
<th>$\phi_s = 0.3$</th>
<th>MADM</th>
<th>LCMM (Eq.2.2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>9.8700</td>
<td>9.8702</td>
</tr>
<tr>
<td>0.2</td>
<td>9.8749</td>
<td>9.8747</td>
</tr>
<tr>
<td>0.4</td>
<td>9.8896</td>
<td>9.8994</td>
</tr>
<tr>
<td>0.6</td>
<td>9.9147</td>
<td>9.9145</td>
</tr>
<tr>
<td>0.8</td>
<td>9.9483</td>
<td>9.9438</td>
</tr>
<tr>
<td>1</td>
<td>9.9927</td>
<td>10.000</td>
</tr>
</tbody>
</table>

Comparison between the MADM and LCMM for $\phi_s$ and $\omega_0$
order reaction) for $\phi_s = 1$ and $\omega_0 = 100$

<table>
<thead>
<tr>
<th>$X$</th>
<th>MADM</th>
<th>LCMM (Eq.22)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>98.500</td>
<td>98.500</td>
</tr>
<tr>
<td>0.2</td>
<td>98.574</td>
<td>98.560</td>
</tr>
<tr>
<td>0.4</td>
<td>98.7525</td>
<td>98.740</td>
</tr>
<tr>
<td>0.6</td>
<td>99.0495</td>
<td>99.040</td>
</tr>
<tr>
<td>0.8</td>
<td>99.465</td>
<td>99.460</td>
</tr>
<tr>
<td>1</td>
<td>100.00</td>
<td>100.000</td>
</tr>
</tbody>
</table>

Fig3. Comparison between the MADM and LCMM for $\phi_s$ and $\omega_0 = 100$
6. Results and Discussion

The numerical simulation of dimensionless concentration \( o(x) \) for various values of parameters \( \phi \), and \( \omega_0 \) are given in figures (1-3). Tables (1-3) show the comparison between the proposed LCMM results and the modified Adomian decomposition method (MADM) for various values \( \phi \) and \( \omega_0 \). Our results have been compared with MADM results[11]. For larger \( M \), we get the results closer to the analytical solution.

7. Conclusion

We have applied a new Legendre spectral algorithm combined with the associated operational matrices of derivatives. This proposed algorithm was employed for solving nonlinear differential equations model with Michaelis-Menten enzyme kinetics. According to the numerical simulations, it has been concluded that the proposed spectral method may be extended to solve other types of linear and nonlinear enzyme kinetics models.

References:


[7] M.Razzaghi, S. Yousefi, Legendre wavelet direct method for variational problems,


