# An Efficient Wavelet Based Approximation Method to Steady State Reaction–Diffusion Model Arising in Mathematical Chemistry

**M. Mahalakshmi · G. Hariharan**

**Abstract** The mathematical model of Rahamathunissa and Rajendran (J Math Chem 44:849–861, 2008) in an amperometric biosensor response is discussed. In this paper, we have applied the shifted second kind Chebyshev wavelets (CW) to obtain the numerical solutions of reaction–diffusion equations containing a nonlinear term related to Michaelis–Menton kinetics of the enzymatic reaction. The application of the shifted second kind CW operational matrices for solving initial and boundary value problems is presented. The obtained numerical results demonstrate efficient and applicability of the proposed method. The power of the manageable method is confirmed. Moreover the use of shifted second kind CW method is found to be simple, efficient, accurate, small computation cost, and computationally attractive.

**Keywords** Shifted second kind Chebyshev wavelets · Reaction–diffusion system · Enzyme kinetics · Operational matrices · Amperometric response

## Introduction

Non-linear phenomena play a very important role in physics, chemistry, and biology (heat and mass transfer, filtration of liquids, diffusion in chemical reactions, etc.). Considerable advances have been made during the last decade in the development of polymer-based materials for use as electro catalysis and as chemical and biological sensors operating in the batch amperometric model. Useful literatures in this area have been provided by Hillman (1987), Lyons (1990), Evans (1990), Wring and Hart (1992), Albery et al. (1990), Bartlett et al. (1997), Rahamathunissa and Rajendran (2008). Starting from the publication of Clark and Lyons (1962), the amperometric biosensors became one of the popular and perspective trends of biosensor (Baronas et al. 2003). The understanding of the kinetic regularities of the biosensors is of crucial importance for their design. The general features of amperometric response were analyzed in the publications of Mell and Maloy (1976).

Various simplified analytical models describing electro catalysis at electroactive polymer films have been developed over the last 20 years. In brief, the analysis involves the construction and solution of reaction–diffusion differential equations, resulting in the development of approximate analytical expressions for the amperometric current response. The analysis is not simple since one is concerned with the modeling of reaction–diffusion equation (RDE) processes in the films (mathematically, it translates reaction–diffusion with in the finite diffusion space). In many cases, addition of the chemical reaction term to the Fick's diffusion term during formulation of the differential equation results in the generation of a non-linear expression, which is not readily, solved using standard analytical methods.

In recent years, wavelet transforms have found their way into many different fields in science, engineering, and medicine. Wavelet analysis or wavelet theory, as a relatively new and an emerging area in applied mathematical research, has received considerable attention in dealing with RDEs. It possesses many useful properties, such as compact support, orthogonality, dyadic, orthonormality, and multi-resolution analysis (MRA). Recently, wavelets have been applied extensively for signal processing in

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communications and physics research, and have proved to be a wonderful mathematical tool. After discretizing the differential equations in a conventional way like the finite difference approximation, wavelets can be used for algebraic manipulations in the system of equations obtained which lead to better condition number of the resulting system.

In the numerical analysis, wavelet based methods and hybrid methods become important tools because of the properties of localization. In wavelet-based methods, there are two important ways of improving the approximation of the solutions: increasing the order of the wavelet family and the increasing the resolution level of the wavelet. There is a growing interest in using various wavelets to study problems, of greater computational complexity. Among the wavelet transform families the Haar, Legendre, and Chebyshev wavelets (CWs) deserve much attention. The basic idea of Chebyshev wavelet method (CWM) is to convert the partial differential equations to a system of algebraic equations by the operational matrices of integral or derivative. Hariharan and his co-workers (Hariharan et al. 2009, 2012; Hariharan 2013, Hariharan and Kannan 2010a, b, 2011) introduced the Haar wavelet method for solving a few reaction–diffusion and fractional reaction–diffusion problems arising in science and engineering.

Bhrawy and Alofi (2013) had introduced the fractional integration for the shifted Chebyshev polynomials. Brazkar et al. (2012) applied the second kind CWM to the nonlinear Fredholm integral equations.

The main goal is to show how wavelets and MRA can be applied for improving the method in terms of easy implementability and achieving the rapidity of its convergence.

The paper is organized the following way. Mathematical formulation of the problem is presented in "Mathematical Formulation of the Problem" section. For completeness sake the second kind shifted CWM is presented in "Properties of Chebyshev Wavelets" section. The method of solution the differential equation is proposed in "Method of Solution" section. Limiting cases are presented in "Limiting Cases" section. Concluding remarks are given in "Conclusion" section.

## Mathematical Formulation of the Problem

The enzyme kinetics in biochemical systems has usually been modeled by ordinary differential equations, which are based only on reaction without spatial dependence of the various concentrations. Recent attention has been given to the effect of diffusion in the process of interactions. When this effect is taken into consideration, the various concentrations in the reaction process are spatially dependent and the equations governing these concentrations become

partial differential equations of parabolic type (Rahamathunissa and Rajendran 2008). In an irreversible monoenzyme system the reaction scheme for free enzyme $E$ and substrate concentrations $S$ may be expressed by

$$E + S \overset{K_M}{\leftrightarrow} ES \overset{k_2}{\leftrightarrow} E + P, \tag{1}$$
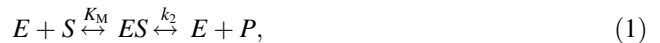
where $ES$ is the enzyme–substrate complex and $P$ is the product. Suppose that reaction–diffusion takes place in an arbitrary $n$-dimensional medium $\Omega$ (membrane), where $\Omega$ is a bounded domain in $R^n$ ($n = 1, 2, \ldots$). Then the rate of change of substrate concentrations $S = S(t, \chi)$, 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 (1982).

$$\frac{\partial S}{\partial t} = D_S \nabla.(\nabla S) - v(t, \chi), \tag{2}$$

where $D_S$ is the substrate diffusion coefficient, $\nabla$ is the gradient operation, and $v$ is called "initial reaction velocity". Various models regarding the expression for $v$ are formulated by researchers in this field. In this paper, we discuss some mathematical properties of the solutions for type of such models using Michaelis–Menton hypothesis. Based on the Michaelis hypothesis, the velocity function $v$ for the simple reaction process without competitive inhibition is given by Pao (1982) and Baronas et al. (2011).

$$v(t, \chi) = \frac{k_2 E_0 S}{K_M + S}, \tag{3}$$

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

$$\frac{\partial S}{\partial t} - D_S \nabla.(\nabla S) = -\frac{k_2 E_0 S}{(K_M + S)}, \quad (t > 0, \chi \in \Omega). \tag{4}$$

In one-dimensional Eq. (4) can be written as

$$\frac{\partial S}{\partial t} = D_S \frac{\partial^2 S}{\partial \chi^2} - \frac{k_2 E_0 S}{(K_M + S)}. \tag{5}$$

Introducing a pseudo-first order rate constant $K = \frac{k_2 E_0}{K_M}$ we can write the above equation as

$$\frac{\partial S}{\partial t} = D_S \frac{\partial^2 S}{\partial \chi^2} - \frac{KS}{\left(1 + \frac{S}{K_M}\right)}. \tag{6}$$

Here we consider, an initial condition is given in the usual form,

$$S(0, \chi) = s_0(\chi), \quad \chi \in \Omega. \tag{7}$$

The system governs the substrate concentration $S$ when there is no competitive inhibition in the reaction. We make the non-linear PDE Eq. (6) dimensionless by defining the following parameters:

$$u = \frac{s}{ks^\infty}, \quad x = \frac{\chi}{L}, \quad \tau = \frac{D_S t}{L^2}, \quad K = \frac{kL^2}{D_S} = \phi^2,$$
$$\alpha = \frac{ks^\infty}{K_M}, \tag{8}$$

where $u$, $x$ and $\tau$ represent dimensionless concentrations, distance and time respectively.

Here $\alpha$ denotes a saturation parameter and $K$ denotes reaction diffusion parameter.

Now the Eq. (6) reduces to the following dimensionless form

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2} - \frac{Ku}{1 + \alpha u}, \quad 0 < u \le 1, \tag{9}$$

whereas the initial condition reduces to

$$u(x,0) = a(\text{constant}). \tag{10}$$

The diagrammatic representation of saturated (zero order kinetics) and unsaturated (1st order kinetics) catalytic kinetics has shown in (Baronas et al. 2003).

Lyons and co-workers (Lyons et al. 1996) solved the above equations only for the limiting cases $\alpha u \ll 1$ and $\alpha u \gg 1$ [refer Fig. 1 of Ref. Rahamathunissa and Rajendran (2008)] using Dirichlet and Neumann boundary conditions.

But we wish to obtain an analytical expression for the concentration profile $u(x)$ of substrate for all values of $\alpha$. In steady state, $\frac{\partial u}{\partial \tau} = 0$. In this case the steady state diffusion Eq. (9) takes the form

$$\frac{\partial^2 u}{\partial x^2} - \frac{Ku}{1 + \alpha u} = 0 \tag{11}$$

with the initial conditions

$$u(0) = 1, \quad u'(0) = 0. \tag{}$$

**Properties of Chebyshev Wavelets**

Wavelets constitute a family of functions constructed from dilation and translation of a single function called the mother wavelet. When the dilation parameter $a$ and the translation parameter $b$ vary continuously we have the following family of continuous wavelets as (Hariharan et al. 2012).

$$\psi_{a,b}(t) = |a|^{-\frac{1}{2}} \psi\left(\frac{t-b}{a}\right), \quad a, b \in \mathbb{R}, \quad a \ne 0. \tag{12}$$

CWs $\psi_{nm}(t) = \psi(k, m, t)$ have three arguments; $k = 1, 2, 3, \ldots$, $n = 1, 2, 3, \ldots, 2^k$, $m$ is the order for Chebyshev polynomials $t$ is the normalized time. They are defined on the interval [0,1) by:

$$\psi_{nm}(t) = \begin{cases} \frac{\alpha_m 2^{\frac{k}{2}}}{\sqrt{\pi}} T_m(2^{k+1}t - 2n + 1), & \frac{n-1}{2^k} \le t < \frac{n}{2^k}, \\ 0, & \text{otherwise} \end{cases} \tag{13}$$

where

$$\alpha_m = \begin{cases} \sqrt{2}, & m = 0 \\ 2, & m = 1, 2, \ldots \end{cases}.$$

Here, $T_m(t)$ are well-known Chebyshev polynomials of order $m$, which are orthogonal with respect to the weight function $w(t) = \frac{1}{\sqrt{1-t^2}}$, on the interval $[-1,1]$ and satisfy the following recursive formula:

$$T_0(t) = 1,$$
$$T_1(t) = t,$$
$$T_{m+1}(t) = 2t T_m(t) - T_{m-1}(t), \quad m = 1, 2, 3, \ldots$$

The set of CWs are an orthogonal set with respect to the weight function $w_n(t) = w(2^{k+1}t - 2n + 1)$.

Function Approximation

A function

$$f(t) = \sum_{n=1}^{\infty} \sum_{m=0}^{\infty} f_{nm} \psi_{nm}(t), \tag{14}$$

where

$$f_{nm} = (f(t), \psi_{nm}(t)). \tag{15}$$

In Eq. (15), $\langle,\rangle$ denotes the inner product with weight function $w_n(t)$.

If the infinite series in Eq. (15) is truncated, then Eq. (16) can be written as:

$$f(t) \simeq f_{2^k, M-1}(t) = \sum_{n=1}^{2^k} \sum_{m=0}^{M-1} f_{nm} \psi_{nm}(t) = F^T \psi(t), \tag{16}$$

where $F$ and $\psi(t)$ are $2^k M \times 1$ matrices given by:

$$F = [f_{10}, f_{11}, \ldots, f_{1,M-1}, f_{20}, \ldots, f_{2,M-1}, \ldots, f_{2^k,M-1}]^T, \tag{17}$$

$$\psi(t) = [\psi_{10}(t), \psi_{11}(t), \ldots, \psi_{1,M-1}(t), \psi_{20}(t), \ldots, \\ \psi_{2,M-1}(t), \ldots, \psi_{2^k,0}(t), \ldots, \psi_{2^k,M-1}(t)]^T. \tag{18}$$

Taking the collocation points as following:

$$t_i = \frac{(2i-1)}{2^k M}, \quad i = 1, 2, \ldots, 2^{k-1}M.$$

We define the CW matrix $\Phi_{m \times m}$ as:

$$\Phi_{m \times m} \triangleq \left[ \Psi\left(\frac{1}{2m}\right) \quad \Psi\left(\frac{3}{2m}\right) \ldots \quad \Psi\left(\frac{2m-1}{2m}\right) \right].$$

For example, when $M = 3$ and $k = 2$ the CW is expressed as

$$\Phi_{6\times6} = \begin{bmatrix} 2.2568 & 2.2568 & 2.2568 & 0 & 0 & 0 \\ 1.0638 & 9.5746 & 18.0854 & 0 & 0 & 0 \\ -2.4823 & 54.2562 & 201.7761 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2.2568 & 2.2568 & 2.2568 \\ 0 & 0 & 0 & 1.0638 & 9.5746 & 18.0854 \\ 0 & 0 & 0 & -2.4823 & 54.2562 & 201.7761 \end{bmatrix}.$$

### Chebyshev Wavelets Operational Matrix of Integration

The integration of the vector $\Psi(t)$ defined in Eq. (18) can be obtained as

$$\int_0^t \Psi(s)\mathrm{d}s \simeq P\Psi(t), \tag{19}$$

where $P$ is the $(2^k M) \times (2^k M)$ operational matrix for integration and is given (Hariharan and Kannan 2010) as

$$P = \begin{pmatrix} C & S & S & \dots & S \\ O & C & S & \dots & S \\ O & O & C & \dots & S \\ \vdots & \vdots & \vdots & \ddots & S \\ O & O & O & \dots & C \end{pmatrix},$$

where $S$ and $C$ are $M \times M$ matrices given by:

$$S = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ -\frac{1}{3} & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ -\frac{1}{15} & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{2M(M-2)} & 0 & 0 & \cdots & 0 \end{pmatrix}$$

and

$$C = \frac{1}{2^k} \begin{pmatrix} \frac{1}{2} & \frac{1}{2\sqrt{2}} & 0 & 0 & \cdots & 0 & 0 & 0 \\ -\frac{1}{8\sqrt{2}} & 0 & \frac{1}{8} & 0 & \cdots & 0 & 0 & 0 \\ -\frac{1}{6\sqrt{2}} & -\frac{1}{4} & 0 & \frac{1}{12} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -\frac{1}{2\sqrt{2}(M-1)(M-3)} & 0 & 0 & 0 & \cdots & -\frac{1}{4(M-3)} & 0 & -\frac{1}{4(M-1)} \\ -\frac{1}{2\sqrt{2}M(M-2)} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{4(M-2)} & 0 \end{pmatrix}.$$

The integration of the product of two CW function vectors is obtained as

$$I = \int_0^1 \Psi(t)\Psi^T(t)\mathrm{d}t, \tag{20}$$

where $I$ is an unit matrix.

Also, A $m$-set of block pulse functions (BPFs) is defined as

$$b_i(t) = \begin{cases} 1, & \frac{i}{m} \le t < \frac{(i+1)}{m}, \\ 0, & \text{otherwise}, \end{cases} \tag{21}$$

where $i = 0, 1, 2, \dots, (m-1)$.

The functions $b_i(t)$ are disjoint and orthogonal. That is

$$b_i(t)b_l(t) = \begin{cases} b_i(t), & i = l \\ 0, & i \ne l \end{cases}. \tag{22}$$

$$\int_0^1 b_i(\tau)b_l(\tau)\mathrm{d}\tau = \begin{cases} \frac{1}{m}, & \text{if } i = l \\ 0, & \text{if } i \ne l \end{cases}. \tag{23}$$

The CWs may be expanded into an $m$-term BPFs as

$$\Psi_m(x) = \Phi_{m\times m}B_m(x). \tag{24}$$

and $B_m(t) \triangleq [b_0(t)b_1(t) \dots b_i(t) \dots b_{m-1}(t)]^T$.

**Lemma: 3.1** If the CW expansion of a continuous function $f(t)$ converges uniformly, then the CW expansion converges to $f(t)$.

**Theorem 3.1** A function $f(t)$ defined in [0,1], is with bounded second derivative, say $|f''(t)| \le B$, can be expanded as an infinite sum of CWs, and the series converges uniformly to the function $f(t)$, that is:

$$f(t) = \sum_{n=1}^\infty \sum_{m=0}^\infty c_{nm}\psi_{n,m}^{(k)}(t), \tag{25}$$

where $c_{nm} = \langle f(t), \psi_{n,m}^{(k)}(t) \rangle$ and $\langle .,. \rangle$ denotes the inner product in $L_{w_n}^2[0,1]$.

The series $\sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{nm}$ is absolute convergent. Moreover, it is obvious that, for $m = 0$, the series $\sum_{n=1}^{\infty} c_{n0} \psi_{n,0}^{(k)}(x)$ is convergence. Consequently, it observes that the series $\sum_{n=1}^{\infty} \sum_{m=0}^{\infty} c_{nm} \psi_{n,m}^{(k)}(x)$ converges to the function $f(t)$ uniformly.

**Theorem 3.2** (Accuracy estimation) Let $f(t)$ be a continuous function defined on $[0,1]$, with bounded second derivative $|f''(t)|$ bounded by $B$, and then we have the following accuracy estimation:

$$\sigma_{k,M} < \frac{\sqrt{\pi}B}{8} \left[ \sum_{n=\mu^k+1}^{\infty} \frac{1}{n^5} \sum_{m=M}^{\infty} \frac{1}{(m-1)^4} \right]^{\frac{1}{2}}, \quad (26)$$

where

$$\sigma_{k,M} = \left[ \int_0^1 \left( f(t) - \sum_{n=1}^{\mu^k} \sum_{m=0}^{M-1} c_{nm} \psi_{n,m}^{(k)}(t) \right)^2 w_n(t) dt \right]^{\frac{1}{2}}. \quad (27)$$

Some Properties of Second Kind Chebyshev Polynomials and Their Shifted Forms

*Second Kind Chebyshev Polynomials*

It is well-known that the second kind Chebyshev polynomials are defined on $[-1,1]$ by

$$U_n(x) = \frac{\sin(n+1)\theta}{\sin\theta} \quad x = \cos\theta. \quad (28)$$

These polynomials are orthogonal on $[-1,1]$

$$\int_{-1}^1 \sqrt{1-x^2} U_m(x) U_n(x) dx = \begin{cases} 0, & m \neq n \\ \frac{\pi}{2}, & m = n \end{cases}. \quad (29)$$

The following properties of second kind Chebyshev polynomials are of fundamental importance in the sequel. They are eigen functions of the following singular Sturm–Liouville equation.

$$(1-x^2)D^2\varphi_k(x) - 3xD\varphi_k(x) + k(k+2)\varphi_k(x) = 0, \quad (30)$$

where $D \equiv \frac{d}{dx}$ and may be generated by using the recurrence relation

$$U_{k+1}(x) = 2xU_k(x) - U_{k-1}(x), \quad k = 1, 2, 3, \ldots \quad (31)$$

Starting from $U_0(x) = 1$ and $U_1(x) = 2x$, or from Rodrigues formula

$$U_n(x) = \frac{(-2)^n(n+1)!}{(2n+1)!\sqrt{(1-x^2)}} D^n \left[ (1-x^2)^{n+\frac{1}{2}} \right]. \quad (32)$$

**Theorem 3.3** The first derivative of second kind Chebyshev polynomials is of the form

$$DU_n(x) = 2 \sum_{\substack{k=0 \\ (k+n)\text{odd}}}^{n-1} (k+1)U_k(x). \quad (33)$$

**Definition: 1** The shifted second kind Chebyshev polynomials are defined on $[0,1]$ by $U_n^*(x) = U_n(2x-1)$. All results of second kind Chebyshev polynomials can be easily transformed to give the corresponding results for their shifted forms. The orthogonally relation with respect to the weight function $\sqrt{x-x^2}$ is given by

$$\int_0^1 \sqrt{x-x^2} U_n^*(x) U_m^*(x) dx = \begin{cases} 0, & m \neq n \\ \frac{\pi}{8}, & m = n \end{cases}. \quad (34)$$

**Corollary 1** The first derivative of the shifted second kind Chebyshev polynomial is given by

$$DU_n^*(x) = 4 \sum_{\substack{k=0 \\ (k+n)\text{odd}}} (k+1)U_k^*(x). \quad (35)$$

Shifted Second Kind Chebyshev Operational Matrix of Derivatives

Second kind CWs are denoted by $\psi_{n,m}(t) = \psi(k, n, m, t)$, where $k$, $n$ are positive integers and $m$ is the order of second kind Chebyshev polynomials. Here $t$ is the normalized time. They are defined on the interval $[0,1]$ by

$$\psi_{n,m}(t) = \begin{cases} \frac{2^{\frac{k+3}{2}}}{\sqrt{\pi}} U_m^*(2^k t - n), & t \in \left[ \frac{n}{2^k}, \frac{n+1}{2^k} \right] \\ 0 & \text{otherwise} \end{cases}, \quad (36)$$

$m = 0, 1, \ldots M, n = 0, 1, \ldots 2^k - 1$. A function $f(t)$ defined over $[0,1]$ may be expanded in terms second kind CWs as

$$f(t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} c_{nm} \psi_{nm}(t), \quad (37)$$

where

$$c_{nm} = (f(t), \psi_{nm}(t))_w = \int_0^1 \sqrt{t-t^2} f(t) \psi_{nm}(t) dt. \quad (38)$$

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

$$f(t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} c_{nm} \psi_{nm}(t) = C^T \psi(t), \quad (39)$$

where $C$ and $\psi(t)$ are $2^k(M+1) \times 1$ defined by

$$C = \left[ c_{0,0}, c_{0,1}, \ldots c_{0,M}, \ldots, c_{2^k-1,M}, \ldots c_{2^k-1,1}, \ldots, c_{2^k-1,M} \right]^T \\ \psi(t) = \left[ \psi_{0,0}, \psi_{0,1}, \ldots, \psi_{0,M}, \ldots \psi_{2^k-1,M}, \ldots, \psi_{2^k-1,1}, \ldots, \psi_{2^k-1,M} \right]^T \Bigg\}. \tag{40}$$

A shifted second kind CWs operational matrix of the first derivative is stated and proved in the following theorem.

**Theorem 2** Let $\Psi(t)$ be the second kind CWs vector defined in Eq. (40) Then the first derivative of the vector $\Psi(t)$ can be expressed as

$$\frac{d\psi(t)}{dt} = D\psi(t), \tag{41}$$

where $D$ is $2^k(M + 1)$ square matrix of derivatives and is defined by

$$D = \begin{bmatrix} F & O & . & . & . & O \\ O & F & . & . & . & O \\ . & . & . & . & . & . \\ O & O & . & . & . & . & .F \end{bmatrix} \tag{42}$$

in which $F$ is an $(M + 1)$ square matrix and its $(r,s)$th element is defined by

$$F_{r,s} = \begin{cases} 2^{k+2}s & r \geq 2, \quad r > s \quad \text{and} \quad (r+s) \quad \text{odd} \\ 0, & \text{otherwise} \end{cases}.$$

**Corollary 2** The operational matrix for the $n$-th derivative can be obtained from

$$\frac{d^n\psi(t)}{dt^n} = D^n\psi(t), \tag{43}$$
$$n = 1, 2, \ldots \text{where } D^n \text{ is the } n \text{ - th power of } D.$$

Linear Second-Order Two-Point Boundary Value Problems

Consider the linear second-order differential equation

$$y''(x) + g_1(x)y'(x) + g_2(x)y(x) = G(x), \quad x \in [0, 1], \tag{44}$$

subject to the initial conditions

$$y(0) = \alpha, \quad y'(0) = \beta \tag{45}$$

(or) the boundary conditions

$$y(0) = \alpha, \quad y(1) = \beta \tag{46}$$

or the most general mixed boundary conditions

$$\alpha_1 y(0) + \alpha_2 y'(0) = \alpha, \quad b_1 y(1) + b_2 y'(1) = \beta. \tag{47}$$

If we approximate the functions $y(x)$, $g_1(x)$, $g_2(x)$, and $G(x)$ in terms of the second kind CW basis, one can write

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

$$g_1(x) \approx \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G_1^T\psi(x), \tag{48}$$

$$g_2(x) \approx \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G_2^T\psi(x),$$

$$g(x) = \sum_{n=0}^{2^k-1} \sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G^T\psi(x). \tag{49}$$

Then

$$y'(x) \approx C^T D\psi(x), \quad y''(x) = C^T D^2\psi(x). \tag{50}$$

Now substitution of relations Eqs. (48), (49), and (50) into Eq. (44), enable us to define the residual, $R(x)$, of this equation as

$$R(x) = C^T D^2\psi(x) + G_1^T\psi(x)(\psi(x))^T D^T C \\ + G_2^T\psi(x)(\psi(x)^T C - G^T\psi(x) \tag{51}$$

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

$$\int_0^t \sqrt{x - x^2}\psi_j(x)R(x)dx = 0, \quad j = 1, 2, \ldots 2^k(M + 1) - 2. \tag{52}$$

Moreover, the initial conditions Eq. (45), the boundary conditions Eq. (46), and the mixed boundary conditions Eq. (47) lead, respectively, to the following equations

$$C^T\psi(0) = \alpha, \quad C^T D\psi(0) = \beta, \\ C^T\psi(0) = \alpha, \quad C^T\psi(1) = \beta, \tag{53}$$

and

$$a_1 C^T\psi(0) + a_2 D\psi(0) = \alpha, \\ b_1 C^T\psi(1) + b_2 C^T D\psi(1) = \beta. \tag{54}$$

Thus Eq. (51) with the two equations of Eqs. (53) or (54) generate $2^k(M + 1)$ a set of linear equations which can be solved for the unknown components of the vector $C$, and hence an approximate spectral wavelets solution to $y(x)$ can be obtained.

## Solution of Differential Equation

Consider the initial value problem

$$Dx(t) + Nx(t) = g(t) \quad \mu > 0, \tag{55}$$

where $N$ is the nonlinear operator and $D$ is fractional derivative. In order to use Legendre wavelets, we first approximate $x(t)$ as

$$x(t) = C^T \psi(t), \tag{56}$$

where $C$ and $\psi(t)$ are defined similarly to Eqs. (11) and (12). Then, we have:

$$C^T D\psi(t) + N C^T \Psi(t) = g(t), \tag{57}$$

we now collocate Eq. (57) at $2^{k-1}M$ points $x_i$ as

$$C^T D\Psi(t_i) + N C^T \Psi(t_i) = g(t_i). \tag{58}$$

We have chosen arbitrary collocation points. By solving equations system Eq. (58), we obtained solution for Eq. (55).

## Method of Solution

Example: 1 Consider the following nonlinear initial value problem

$$u'' - \frac{Ku}{1 + \alpha u} = 0 \tag{59}$$

with the initial conditions

$$u(0) = 1, \quad u'(0) = 0. \tag{60}$$

We solve the Eq. (59) using the algorithm described in "Properties of Chebyshev Wavelets" section for the case corresponds to $M = 2$, $k = 0$ to obtain an approximate solution of $u(x)$. First, if we make use of Eq. (42) and Eq. (43), then the two operational matrices $D$ and $D^2$ are given, respectively, by

$$D = \begin{pmatrix} 0 & 0 & 0 \\ 4 & 0 & 0 \\ 0 & 8 & 0 \end{pmatrix} \quad D^2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 32 & 0 & 0 \end{pmatrix}.$$

Moreover $\psi(x)$ can be evaluated to give

$$\psi(x) = \sqrt{\frac{2}{\pi}} \begin{pmatrix} 2 \\ 8x - 4 \\ 32x^2 - 32x + 6 \end{pmatrix}.$$

If we set

$$C = \begin{pmatrix} c_0 & c_1 & c_2 \end{pmatrix}^T = \sqrt{\frac{\pi}{2}} \begin{pmatrix} c_0 & c_1 & c_2 \end{pmatrix}^T,$$

then Eq. (59), takes the form

$$c^T D^2 \psi(x) - \frac{k c^T \psi(x)}{1 + \alpha c^T \psi(x)} = 0, \tag{61}$$

which is equivalent to $58c_2 - 2c_0 + 128c_2c_0 - 256c_1c_2 + [512c_2c_1 - 2048c_2^2 - 8c_1 + 32c_2]x + [2048c_2^2 - 32c_2]x^2 + 4c_1 = 0$ at $x = \frac{2 - \sqrt{2}}{4}$ to get,

$$c_0 - 31c_2 - 64c_2c_0 + 128c_2^2 + 64\sqrt{2}c_2c_1 - (2 + \sqrt{2})c_1 = 0. \tag{62}$$

Furthermore, the use of initial conditions in Eq. (59) lead to the two equation,

$$2c_0 - 4c_1 + 5c_2 = 1, \tag{63}$$

$$c_1 - 4c_2 = 0. \tag{64}$$

The solution of the nonlinear system of equations Eqs. (62)–(64) gives

$$c_0 = 0.53065, \ c_1 = 0.02452, \ c_2 = 0.00613.$$

Consequently

$$u(x) = (0.53065, \ 0.02452, \ 0.00613) \begin{pmatrix} 2 \\ 8x - 4 \\ 32x^2 - 32x + 6 \end{pmatrix}$$

$$= 0.19616x^2 - 1. \tag{65}$$

Our results can be compared with Rahamathunissa and Rajendran (2008) results. For larger $M$, we can get the results closer to the real values.

## Limiting Cases

### Unsaturated (First Order) Catalytic Kinetics

In this case, the substrate concentration in the film $S(\chi)$ is less than the Michaelis constant $K_M$. This is explained in Fig. 1 of Ref. Rahamathunissa and Rajendran 2008). When $\alpha u \ll 1$, the Eq. (11) reduces to

$$\frac{\partial^2 u}{\partial x^2} - Ku = 0, \tag{66}$$

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

$$u''(x) - ku(x) = 0, \tag{67}$$

$$u(0) = 1, u'(0) = 0. \tag{68}$$

Equation (66) takes the form

$$c^T D^2 \psi(x) - k c^T \psi(x) = 0 \tag{69}$$

which is equivalent to

**Table 1** Numerical solutions of steady state concentration for various values of $K$ and $\alpha$ of Eq. (59)

| $x$ | VIM | CWM |
|-----|-----|-----|
| $K = 1$ and $\alpha = 1$ | | |
| 0.0 | 1.0000 | 0.9964 |
| 0.2 | 1.0201 | 1.0196 |
| 0.4 | 1.0810 | 1.0819 |
| 0.6 | 1.1855 | 1.1791 |
| 0.8 | 1.3374 | 1.3231 |
| 1.0 | 1.5431 | 1.5020 |

**Table 2** Numerical solutions of steady state concentration for various values of $K$ and $\alpha$ of Eq. (74)

| $x$ | VIM | CWM |
|-----|-----|-----|
| $K = 1$ and $\alpha = 1$ | | |
| 0.0 | 1.00 | 1.00 |
| 0.2 | 1.02 | 1.02 |
| 0.4 | 1.08 | 1.08 |
| 0.6 | 1.18 | 1.18 |
| 0.8 | 1.32 | 1.32 |
| 1.0 | 1.50 | 1.51 |

$$64c_2 - 2kc_0 - (8c_1k - 32kc_2)x - 32kc_2x^2 + 4kc_1 - 6kc_2 = 0$$

at $x = \frac{2-\sqrt{2}}{4}$ to get,

$$kc_0 + kc_2 - \sqrt{2}c_1k - 32c_2 = 0. \tag{70}$$

Furthermore, the use of initial conditions in Eq. (66) lead to the two equation,

$$2c_0 - 4c_1 + 5c_2 = 1, \tag{71}$$

$$c_1 - 4c_2 = 0. \tag{72}$$

Solving Eqs. (70)–(72), we gain

$$c_0 = 0.579, \ c_1 = 0.0632, \ c_2 = 0.0152.$$

Consequently,

$$u(x) = (0.579, 0.0632, 0.0152) \begin{pmatrix} 2 \\ 8x - 4 \\ 32x^2 - 32x + 6 \end{pmatrix}$$

$$u(x) = 0.4864x^2 + 0.0192x + 0.9964. \tag{73}$$

Table 1 shows the numerical solutions of steady state concentration for various values of $K$ and $\alpha$. Our results can be compared with Rahamathunissa and Rajendran (2008) results. For larger $M$, we can get the results closer to the real values.

Saturated (Zero Order) Catalytic Kinetics

In this case, the substrate concentration the substrate concentration in the film $S(\chi)$ is greater than the Michaelis constant $K_M$. This is explained in Fig. 1 of Ref. Rahamathunissa and Rajendran (2008). Hence $\alpha u \gg 1$ reduces the Eq. (11) to

$$\frac{\partial^2 u}{\partial x^2} - \frac{K}{\alpha} = 0, \tag{74}$$

the initial conditions

$$u(0) = a, \ u'(0) = 0, \tag{75}$$

the above equation can be written as

$$u''(x) - \frac{k}{\alpha} = 0, \tag{76}$$

$$C^T D^2 \psi(x) = \frac{k}{\alpha}, \tag{77}$$

we get,

$$64c_2 = \frac{k}{\alpha}, \tag{78}$$

$$64c_2\alpha - k = 0, \tag{79}$$

$$u(0) = a, \ u'(0) = 0. \tag{80}$$

Put $\alpha = 1$, $k = 1$, we get,

$$64c_2 - 1 = 0. \tag{81}$$

Furthermore, the use of initial conditions in Eq. (74) lead to the two equation,

$$2c_0 - 4c_1 + 6c_2 = a, \tag{82}$$

$$c_1 - 4c_2 = 0. \tag{83}$$

Solving the above equations, we obtain

$$c_0 = \frac{32a + 5}{64}, \ c_1 = \frac{1}{16}, \ c_2 = \frac{1}{64}.$$

Consequently,

$$u(x)$$
$$= a + \frac{x^2}{2}. \tag{84}$$

Table 2 shows the numerical Solutions of steady state concentration for various values of $K$ and $\alpha$. Our results can be compared with Rahamathunissa and Rajendran (2008) results. For larger $M$, we can get the results closer to the real values.

All the numerical experiments presented in this section were computed in double precision with some MATLAB codes on a personal computer System Vostro 1400

Processor $\times$ 86 Family 6 Model 15 Stepping 13 Genuine Intel $\sim$ 1,596 MHz.

## Conclusion

In this paper, the shifted second kind CWM is used to obtain the numerical solutions of RDEs containing a nonlinear term related to Michaelis–Menton kinetics of the enzymatic reaction. Numerical results show that the shifted second kind CWM (CWT) can match the analytical solution very efficiently with quite a few calculations. Also the proposed method has a simple implementation process. It may be concluded that shifted second kind CWT is very powerful and efficient in finding analytical as well as numerical solutions for a wide class of linear and nonlinear differential equations. It provides more realistic series solutions that converge very rapidly in real physical problems.

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