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An Efficient Wavelet Based Approximation Method for Estimating the Concentration of Species and Effectiveness Factors in Porous Catalysts

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Abstract

In this paper, mathematical modeling of porous catalysts is discussed. An efficient wavelet method, called the shifted second kind Chebyshev wavelet method is used to obtain the solution for the concentration of species. An approximate polynomial expression for concentration and the effectiveness factors are obtained for general nonlinear Langmiur–Hinshelwood–Haugen–Watson type models which have variety of real rate function. To the best of our knowledge until there is no rigorous wavelet solution has been addressed in this model. The power of the manageable method is confirmed. The concentration and the effectiveness factors are also computed for the various limiting cases of LHHW models.

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1. Introduction

Solid catalysts are often called ‘heterogeneous catalysts’ as they are in a different phase from fluid reactants and products. The ease of separating solid catalysts from reactants and products gives them an advantage over liquid catalysts in solution with reactants and products. With porous solid catalysts, significant resistance to mass and heat transfer may be present. The transport resistance can make the species concentrations inside the porous catalyst lower than the concentrations in bulk fluid and the temperature inside the porous catalyst lower or higher than in the bulk fluid. In a heterogeneous catalytic reaction, however, the catalyst is usually in a different phase from the reactant(s). Mass transfer limitations play a vital role on the rate of reaction, the rate of conversion and product formation are included in the systems.

A lot of efforts have been attempted to find out the roles of mass transfer efforts on the reaction rate. The rate of reaction in porous heterogeneous catalysts is the most significant one.

In porous catalysts, the internal mass transfer limitation is governed by the rate of reaction. In porous catalysts, the concept of diffusion and reaction is presented in many textbooks [1-4]. An approximate expressions to estimate dimensionless concentration profiles inside a catalyst pellet obtained by numerical algorithm was developed by Gottifredi et al [5] . Several investigations of diffusion in the wash coat have been discussed. Simulations based on real wash coat geometry of a fillet in a square channel are explained by Hayes and Kolaczkowski [6]. Leung et al. [7] illustrated an empirical method for mapping the real geometry onto a 1-D plane wall. The same author demonstrated the asymptote matching method. LHHW (Langmiur–Hinshelwood–Haugen–Watson) behaviors and the examples are given by Hayes et al. [4] and Papadias et al. [8, 9]. The authors [6–10] used flat wash coats with rounded comers of increasing radii. Gottifredi and Gonzo [11] presented a powerful and efficient tool to solve the singular BVP of reaction cum diffusion in a biocatalyst problem. Gottifredi and Gonzo [12] introduced a new numerical algorithm is used to finding the dimensionless concentration profiles and effectiveness factor.

Hayes et al. [13] describes a mathematical model for the estimation of effectiveness factors in porous catalysts that have reactions with nonlinear kinetic models. M. K. Sivasankari and L.Rajendran [14] designed a Adomian decomposition method for obtaining solution for the concentration of species. However, to the best of our knowledge, till date no wavelet method results for the concentration of species and effectiveness factor for all values of the parameters have been reported. This research analyses the effectiveness factors and the concentrations of species which is obtained by using wavelet based Numerical method (shifted second kind Chebyshev wavelet transform method).

In recent years, wavelets have found their ways into many different fields of science and engineering; particularly wavelets are very successfully utilized in signal analysis for waveform representation and segmentations.

During previous years, wavelets have dominated all areas of pure and applied mathematics, especially in the numerical analysis of differential equations [15, 16]. Wavelets are established as a strong novel mathematical implement in signal processing, turbulence problem, simulation and time-series analysis [17-19]. Strenuous action and interest have been shown in the usage of wavelet theory and it is related multiresolution analysis. Hesameddini et al.[20] developed an algorithm for fractional differential equation. The substantial scheme back of the wavelet decomposition is the compressing representation of wavelet-based functions. In wavelet methods, the geometric region and functions are represented in terms of wavelet series defined in a certain domain.

Wavelet analysis, as a relatively new and emerging area in applied mathematical research, has gained considerable attention in dealing with differential equations. Wavelet theory possesses many useful properties such as compact support, orthogonality, dyadic, orthonormality and multi-resolution analysis (MRA).

Among the wavelet transform families the Haar, Legendre wavelets and Chebyshev wavelets deserve much attention. Chen and Hsiao [21] presented Haar wavelet method for Lumped and distributed-parameter systems. Lepik [22] introduced the Haar wavelet method (HWM) for solving the integral and differential equations. Hariharan et al. [23] had implemented the Haar wavelet method for solving Fisher's equation arising in population dynamics. The same author(s) [24- 26] solving the convection-diffusion equation and reaction-diffusion equations by using Haar wavelet method (HWM).

Moreover, wavelet method establishes a connection with fast approximation algorithms. In the last two decades the wavelet solutions have been attracted great attention and numerous papers about this area have been published. Hariharan et.al [27] establishing Haar wavelet based computational algorithm for solving differential equations arising in science and engineering. Tavassoli Kajani et al. [28] discuss and Comparison between the homotopy perturbation method (HPM) and the sine–cosine wavelet method (SCWM) for solving linear integro differential equations. In recent years, there are numerous papers have been published about the wavelets for solving ordinary differential equations. Particularly

Chebyshev wavelets play a vital role in the resent research field. Doha et al. [29, 30] gave a systematic explanation of the ideas, methods, and applications the Chebyshev spectral method for solving the initial and boundary value problems and differential equations of fractional order. Zhu et al. [31] had established the second kind Chebyshev wavelets for solving integral equations. Zhu and .Fan [32] applied the second kind Chebyshev wavelets for solving the fractional nonlinear Fredholm integrodifferential equations. The Solution of Abel's integral equations and compare the Chebyshev wavelet methods (CWM) with BPFs method illustrated by Sohrabi [33]. Nonlinear fractional differential equation is solved effectively by using Chebyshev wavelet, Li [34]. Hojatollah Adibi and Pouria Assari [35] had implemented the CWM for the numerical solutions of Fredholm integral equations of the first kind. Li Zhu and Qibin Fan [36] introduced the second kind Chebyshev wavelets for solving the fractional nonlinear Fredholm integro-differential equations. Yanxin Wang and Qibin Fan [37] demonstrated the second kind Chebyshev wavelet method for solving the fractional differential equations. Recently, Doha et al. [38] presented the second kind Chebyshev operational matrix algorithm for solving differential equations of Lane–Emden type. Heydari et al. [39] established the CWM for telegraph type partial differential equations with boundary conditions. Babolian and Fattahzadeh [40] had established the Chebyshev wavelet operational matrix of integration for solving the differential equations. Ghasemi and Tavassoli Kajani [41] had introduced the CWM for solving the time-varying delay systems.

The basic idea of Chebyshev wavelets is to convert the differential equations into a system of algebraic equations by the operational matrices of integral or derivative. The main goal is to show how wavelets and multi-resolution analysis can be applied for improving the method in terms of easy implement ability and achieving the rapidity of its convergence [42].

In the present paper, the shifted second kind Chebyshev wavelet method is used to find the solution of the concentration of species and effectiveness factor for various parameter values. The mathematical modeling of porous catalysts is described by the nonlinear reaction diffusion equation is easily converted to the algebraic equations by applying shifted second kind Chebyshev operational matrices of differentiation. Solving these equations we obtain the solution.

The paper is organized as follows. In section 2 Chebyshev wavelets and their properties are discussed. Formation of the problem is presented in section 3.Method of solution for various limiting cases is discussed in section 4.Results and discussion are carried out in section 5.Concluding remarks are given in section 6.

2. Properties of second kind Chebyshev polynomials and their shifted forms

2.1 Second kind Chebyshev polynomials [29]

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

$$U_n(x) = \frac{\sin (n+1)\theta}{\sin \theta}, \;\; x = \cos \theta. \tag{1}$$

These polynomials are orthogonal on [-1, 1]

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

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.

$$(1-x^2)D^2\phi_k(x) - 3xD\phi_k(x) + k(k+2)\phi_k(x) = 0, \tag{3}$$

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

$$U_{k+1}(x) = 2xU_k(x) - U_{k-1}(x), k = 1,2,3,... \tag{4}$$

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

$$U_n(x) = \frac{(-2)^n (n+1)!}{(2n+1)!\sqrt{(1-x^2)}} D^n \left[(1-x^2)^{n+\frac{1}{2}} \right] \tag{5}$$

Theorem 2.1 [29]: The first derivative of second kind Chebyshev polynomials is of the form

$$DU_n(x) = 2 \sum_{\substack{k=0 \\ (k+n) odd}}^{n-1} (k+1) U_k(x). \tag{6}$$

Definition 2.1.1 [29]

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

$$\int_0^1 \sqrt{x-x^2}\,U_n^*(x)U_m^*(x)dx = \begin{cases} 0, & m \neq n \\ \frac{\pi}{8}, & m = n. \end{cases} \tag{7}$$

Corollary 2.1.1 : The first derivative of the shifted second kind Chebyshev polynomial is given by

$$DU_n^*(x) = 4 \sum_{\substack{k=0 \\ (k+n)odd}} (k+1)U_k^*(x) \tag{8}$$

2.2 Shifted Second kind Chebyshev operational matrix of derivatives [29]

Second kind Chebyshev wavelets 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

$$\psi_{n,m}(t) = \begin{cases} \frac{2^{\frac{k+3}{2}}}{\sqrt{\pi}} U_m^*(2^k t - n), & t \in \left[\frac{n}{2^k}, \frac{n+1}{2^k}\right], \\ 0 & otherwise \end{cases} \tag{9}$$

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

$$f(t) = \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} c_{nm}\psi_{nm}(t). \tag{10}$$

Where

$$c_{nm} = \left(f(t), \psi_{nm}(t)\right)_w = \int_0^1 \sqrt{t-t^2}\, f(t)\psi_{nm}(t)dt. \tag{11}$$

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

$$f(t)=\sum_{n=0}^{2^k-1}\sum_{m=0}^{M}c_{nm}\psi_{nm}(t).=C^T\psi(t) \tag{12}$$

Where C and ψ (t) are $2^k(M+1)$ x 1 defined by

$$\left.\begin{array}{l} C=\left[c_{0,0},c_{0,1},....c_{0,M},...,c_{2^k-1,M},....c_{2^k-1,1},...,c_{2^k-1,M}\right]^T \\ \psi(t)=[\psi_{0,0},\psi_{0,1},...,\psi_{0,M},....\psi_{2^k-1,M},...,\psi_{2^k-1,1},....,\psi_{2^k-1,M}]^T \end{array}\right\} \tag{13}$$

Theorem 2.2.1 [29]: Let Ψ (t) be the second kind Chebyshev wavelets vector. Then the first derivative of the vector Ψ (t) can be expressed as

$$\frac{d\psi(t)}{dt}=D\psi(\mathrm{t}) \tag{14}$$

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

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

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

$$F_{r,s}=\begin{cases} 2^{k+2}s & r\geq 2, \quad r>s \quad and \quad (r+s) \quad odd. \\ 0, & otherwise \end{cases} \tag{15}$$

Corollary 2.2.1. The operational matrix for the n^{th} derivative can be obtained from

$$\frac{d^n\psi(t)}{dt^n}=D^n\psi(t), \quad n=1,2,...where\ D^n\ is\ the\ n^{th}\ power\ of\ D. \tag{16}$$

2.3 Convergence Analysis

We state and prove a theorem ascertaining that the second kind Chebyshev wavelet expansion of a function $f(x)$, with bounded second derivative, converges uniformly to $f(x)$

Theorem 2.3.1[43]

A function $f(x) \in L^2_\omega[0,1]$, with $\left| f''(x) \right| \le L$ can be expanded as an infinite sum of chebyshev wavelets and the series converges uniformly to $f(x)$. Explicitly the expansion coefficients in (11) satisfying the following in equality:

$$\left| c_{nm} \right| < \frac{8\sqrt{2\pi}L}{(n+1)^{\frac{5}{2}}(m+1)^2}, \forall m > 1, n \ge 0 \tag{17}$$

Proof:

From (11) it follows that

$$c_{nm} = \frac{2^{(k+3)/2}}{\sqrt{\pi}} \int_{n/2^k}^{(n+1)/2^k} f(x) U_m^*\left(2^k x - n\right) \omega\left(2^k x - n\right) dx \tag{18}$$

If we set $2^k x - n = \cos\theta$ in (17), then we get

$$\begin{aligned} c_{nm} &= \frac{2^{(-k+3)/2}}{\sqrt{\pi}} \int_0^\pi f\left(\frac{\cos\theta + n}{2^k}\right) \sin(m+1)\theta \sin\theta d\theta \\ &= \frac{2^{(-k+1)/2}}{\sqrt{\pi}} \int_0^\pi f\left(\frac{\cos\theta + n}{2^k}\right) \left[\cos m\theta - \cos(m+2)\theta\right] d\theta \end{aligned} \tag{19}$$

Which gives after integration by parts two times

$$c_{nm} = \frac{2}{2^{5k/2}\sqrt{2\pi}} \int_0^\pi f''\left(\frac{\cos\theta + n}{2^k}\right) \lambda_m(\theta)\, d\theta \tag{20}$$

Where $\lambda_m(\theta) = \frac{\sin\theta}{m}\left[\frac{\sin(m-1)\theta}{m-1} - \frac{\sin(m+1)\theta}{m+1}\right] - \frac{\sin\theta}{m+2}\left[\frac{\sin(m+1)\theta}{m+1} - \frac{\sin(m+3)\theta}{m+3}\right]$ (21)

Therefore, we have

$$\begin{aligned} \left| c_{nm} \right| &= \left| \frac{1}{2^{(5k-1)/2}\sqrt{\pi}} \int_0^\pi f''\left(\frac{\cos\theta + n}{2^k}\right) \lambda_m(\theta)\, d\theta \right| = \frac{1}{2^{(5k-1)/2}\sqrt{\pi}} \left| \int_0^\pi f''\left(\frac{\cos\theta + n}{2^k}\right) \lambda_m(\theta)\, d\theta \right| \\ &\le \frac{L}{2^{(5k-1)/2}\sqrt{\pi}} \int_0^\pi \left| \lambda_{m,}(\theta) \right| d\theta \le \frac{L\sqrt{\pi}}{2^{(5k-1)/2}} \left[\frac{1}{m}\left(\frac{1}{m-1} + \frac{1}{m+1}\right) + \frac{1}{m+2}\left(\frac{1}{m+1} + \frac{1}{m+3}\right) \right] \\ &= \frac{L\sqrt{\pi}}{2^{(5k-1)/2}\left(m^2 + 2m - 3\right)} < \frac{2L\sqrt{\pi}}{2^{(5K-5)/2}(m+1)^2} \end{aligned}$$

Since $n \le 2^k - 1$, we have

$$\left|c_{nm}\right| < \frac{8\sqrt{2\pi}L}{(n+1)^{5/2}(m+1)^2}$$

This completes the proof of theorem.

2.4 Linear second-order two-point boundary value problems [29]

Consider the linear second-order differential equation

$$y''(x) + g_1(x)y'(x) + g_2(x)y(x) = G(x), \qquad x \in [0,1] \tag{22}$$

Subject to the initial conditions

$$y(0) = \alpha, \qquad y'(0) = \beta \tag{23}$$

(or) the boundary conditions

$$y(0) = \alpha, \qquad y(1) = \beta \tag{24}$$

or the most general mixed boundary conditions

$$\alpha_1 y(0) + \alpha_2 y'(0) = \alpha, \qquad b_1 y(1) + b_2 y'(1) = \beta. \tag{25}$$

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

$$y(x) \approx \sum_{n=0}^{2^k-1}\sum_{m=0}^{M} c_{nm}\psi_{nm}(x) = C^T\psi(x). \qquad g_1(x) \approx \sum_{n=0}^{2^k-1}\sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G_1^T\psi(x) \tag{26}$$

$$g_2(x) \approx \sum_{n=0}^{2^k-1}\sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G_2^T\psi(x) \qquad g(x) = \sum_{n=0}^{2^k-1}\sum_{m=0}^{M} g_{nm}\psi_{nm}(x) = G^T\psi(x) \tag{27}$$

Then $y'(x) \approx C^T D\psi(x), \qquad y''(x) = C^T D^2\psi(x)$ (28)

Now substitution of relations Eq.(26), Eq.(27) and Eq.(28) into Eq. (22), enable us to define the residual, R(x), of this equation as

$$R(x) = C^T D^2\psi(x) + G_1^T\psi(x)(\psi(x))^T D^T C + G_2^T\psi(x)(\psi(x)^T C - G^T\psi(x). \tag{29}$$

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

$$\int_0^t \sqrt{x-x^2}\psi_j(x)R(x)dx = 0, \qquad j = 1,2,...2^k(M+1)-2. \tag{30}$$

Moreover, the initial conditions Eq.(23), the boundary conditions Eq.(24), and the mixed boundary conditions Eq.(25) lead respectively, to the following equations

$$\begin{aligned} &C^T\psi(0) = \alpha, \qquad && C^T D\psi(0) = \beta, \\ &C^T\psi(0) = \alpha \qquad && C^T\psi(1) = \beta \end{aligned} \tag{31}$$

$$a_1 C^T\psi(0) + a_2 D\psi(0) = \alpha, \qquad b_1 C^T\psi(1) + b_2 C^T D\psi(1) = \beta \tag{32}$$

Thus Eq. (29) with the two equations of Eq.(31) or Eq.(32)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.

3. Mathematical formulation of the boundary value problems

The mass transport in heterogeneous catalysts is described by following general nonlinear reaction diffusion equation [13]:

$$(D_{eff})_A \frac{\partial u_A}{\partial x^{*2}} - \frac{k_v u_A^p}{(1+K_A u_A)^m} \tag{33}$$

Where u_A(mol/m^3) and D_{eff}(m^2/s) are the molar concentration and effective diffusion coefficients of species A, respectively, k_v(mol^{p-1} m$^{-3(p-1)}$ s^{-1}) is the reaction rate concentration and K_A(m^3/mol) is the rate parameter for adsorption inhibition of species A. p=1 or 2 and m=2 or 3 are the numerical constant. The boundary conditions are:

at $x^* = 0, \dfrac{\partial u_A}{\partial x} = 0$

at $x^* = L, u_A = (u_A)_S$ (34)

Where $(u_A)_S\,(mol/m^3)$ is the concentration at the external surface of the catalyst, *L* (m) is the thickness of flat of catalyst. The following dimensionless variables are introduced:

$$u = \frac{u_A}{(u_A)_S}, x = \frac{x^*}{L}$$

$$\phi = \frac{V}{A_s}\sqrt{\frac{k_v u_s^{p-1}}{D_{eff}}} = L_c\sqrt{\frac{k_v u_s^{p-1}}{D_{eff}}} \quad \text{and} \quad \Gamma = (u_A)_s K_A \tag{35}$$

The dimensionless parameter Thiele modulus ϕ for three shapes with characteristic length is defined as the ratio of the particle volume to surface area. The characteristic length *L*C (m) for sphere, infinite cylinder and flat plate is equal to *R*/3, *R*/2 and *L* (m), respectively, where *R* (m) is the radius and *L* is the plate thickness. Using the dimensionless variables (35), now the Eq. (33) becomes

$$\frac{\partial^2 u}{\partial x^2} - \phi^2 \frac{(u)^p}{(1+\Gamma u)^m} \tag{36}$$

$$\text{and} \quad \text{at} \quad x = 0, \frac{\partial u}{\partial x} = 0 \ \text{ and } \ x = 1, u = 1 \tag{37}$$

The dimensionless effectiveness factor is

$$\eta = \frac{1+\Gamma}{\phi^2}\left(\frac{\partial u}{\partial x}\right)_{x=1} \tag{38}$$

4. Concentration and effectiveness factor using the shifted second kind Chebyshev wavelet transform method

Non-linear differential equations play a vital role in many engineering and sciences. Finding the solution of non-linear problems is difficult or complicated. Now we can apply the numerical method, shifted second kind Chebyshev Wavelet transform method described in section (2)

Solving the Eq. (36) by using the method described in section (2) we obtain concentration as follows

LIMITING CASES

***Limiting Case (i) (For m* = 2 and *p* = 1)**

Substituting the value *m* = 2 and *p* = 1 in Eq. (36), and apply the method SSKCW described in Section (2) for M=2 in to Eq.(36)

We can obtain the concentration as follows:

$$C^T D^2 \Psi(x) - \phi^2 \frac{C^T\Psi(x)}{\left(1+\Gamma\left(C^T\Psi(x)\right)\right)^2} = 0 \tag{39}$$

Where $C^T\Psi(x) = 64C_2$ and $C^T\Psi(x) = 2C_0 - 2.8285C_1 + 2C_2$

and applying the the boundary conditions

$$C^T D\Psi(0)=0 \quad , \quad C^T\Psi(1)=1$$

Which implies $C_0=\frac{1}{2}-11C_2$ and $C_1=4C_2$

Substitute theses values in to the Eq.(39) we obtain

$$64C_2\left[1+\Gamma(1-31.3140C_2)^2\right]-\phi^2\left[1-31.3140C_2\right]=0 \tag{40}$$

Solving Eq.(40) for various values of Γ and ϕ we get C_2

Using C_0, C_1, C_2 values in to $u(x)=C^T\Psi(x)=\left[C_0, C_1, C_2\right]\begin{pmatrix} 2 \\ 8x-4 \\ 32x^2-32x+6 \end{pmatrix}$ (41)

The concentration $u(x)$ (from Eq.(41)) and the effectiveness factor η (from Eq.(38)) for various values of Γ and ϕ .

In the Tables 1 and 2, the dimensionless concentration are compared with simulation results for various values of Γ and ϕ .

Limiting Case (ii) (For m = 3 and p = 1)

Substituting the value *m* = 3 and *p* = 1 in Eq. (36), and apply the method SSKCW in to Eq.(36)
we can obtain the concentration as follows:

$$C^T D^2\Psi(x)-\phi^2\frac{C^T\Psi(x)}{\left(1+\Gamma\left(C^T\Psi(x)\right)\right)^3}=0 \tag{42}$$

Where $C^T\Psi(x)=64C_2$ and $C^T\Psi(x)=2C_0-2.8285C_1+2C_2$

and applying the the boundary conditions

$$C^T D\Psi(0)=0 \quad , \quad C^T\Psi(1)=1$$

Which implies $C_0=\frac{1}{2}-11C_2$ and $C_1=4C_2$

Substitute theses values in to the Eq.(42) we obtain

$$64C_2\left[1+\Gamma(1-31.3140C_2)^3\right]-\phi^2\left[1-31.3140C_2\right]=0 \tag{43}$$

Solving Eq.(43) for various values of Γ and ϕ we get C_2

Using C_0, C_1, C_2 values in to $u(x) = C^T \Psi(x) = [C_0, C_1, C_2] \begin{pmatrix} 2 \\ 8x-4 \\ 32x^2-32x+6 \end{pmatrix}$ (44)

The concentration $u(x)$ (from Eq.(44)) and the effectiveness factor η (from Eq.(38)) for various values of Γ and ϕ .

In the Tables 3 and 4, the dimensionless concentration are compared with simulation results for various values of Γ and ϕ .

Table 1. Comparison of SSKCW (Eq. (41)) and numerical dimensionless concentration *u* when $\tau = 5$

x	Concentration u $\tau = 5$														
	$\phi = 0.1$			$\phi = 1$			$\phi = 2$			$\phi = 3$			$\phi = 4$		
	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err
0	0.9999	1.0000	**0.0001**	0.9860	0.9872	**0.0012**	0.9427	0.9424	**0.0003**	0.8663	0.8624	**0.0039**	0.7503	0.7312	**0.0191**
0.2	0.9999	1.0000	**0.0001**	0.9866	0.9877	**0.0011**	0.9450	0.9447	**0.0003**	0.8717	0.8679	**0.0038**	0.7605	0.7420	**0.0185**
0.4	0.9999	1.0000	**0.0001**	0.9882	0.9892	**0.0010**	0.9519	0.9516	**0.0003**	0.8879	0.8844	**0.0035**	0.7910	0.7742	**0.0168**
0.6	0.9999	1.0000	**0.0001**	0.9910	0.9918	**0.0008**	0.9634	0.9631	**0.0003**	0.9148	0.9119	**0.0029**	0.8415	0.8280	**0.0135**
0.8	0.9999	1.0000	**0.0001**	0.9950	0.9954	**0.0004**	0.9795	0.9793	**0.0002**	0.9523	0.9505	**0.0018**	0.9114	0.9032	**0.0082**
1	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**

Table 2. Comparison of SSKCW (Eq. (41)) and numerical dimensionless concentration *u* when $\tau = 50$

x	Concentration u $\tau = 50$								
	$\phi = 10$			$\phi = 15$			$\phi = 20$		
	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err
0	0.9805	0.9808	**0.0003**	0.9552	0.9552	**0.0000**	0.9184	0.9168	**0.0016**
0.2	0.9813	0.9816	**0.0003**	0.9571	0.9570	**0.0001**	0.9217	0.9201	**0.0016**
0.4	0.9836	0.9839	**0.0003**	0.9624	0.9624	**0.0000**	0.9316	0.9301	**0.0015**
0.6	0.9875	0.9877	**0.0002**	0.9714	0.9713	**0.0001**	0.9480	0.9468	**0.0012**
0.8	0.9930	0.9931	**0.0001**	0.9840	0.9839	**0.0001**	0.9708	0.9700	**0.0008**
1	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**

Table 3. Comparison of SSKCW (Eq. (44)) and numerical dimensionless concentration *u* when $\tau = 1$

x	Concentration u $\tau = 1$														
	$\phi = 0.1$			$\phi = 0.5$			$\phi = 1$			$\phi = 1.5$			$\phi = 2$		
	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err
0	0.9994	1.0000	**0.0006**	0.9843	0.9840	**0.0003**	0.9367	0.9360	**0.0007**	0.8553	0.8496	**0.0057**	0.7370	0.7184	**0.0186**
0.2	0.9994	1.0000	**0.0006**	0.9850	0.9846	**0.0004**	0.9393	0.9386	**0.0007**	0.8613	0.8556	**0.0057**	0.7482	0.7297	**0.0185**
0.4	0.9995	1.0000	**0.0005**	0.9868	0.9866	**0.0002**	0.9470	0.9462	**0.0008**	0.8793	0.8737	**0.0056**	0.7818	0.7635	**0.0183**
0.6	0.9996	1.0000	**0.0004**	0.9900	0.9898	**0.0002**	0.9598	0.9590	**0.0008**	0.9092	0.9037	**0.0055**	0.8376	0.8198	**0.0178**
0.8	0.9998	1.0000	**0.0002**	0.9944	0.9942	**0.0002**	0.9778	0.9770	**0.0008**	0.9509	0.9459	**0.0050**	0.9148	0.8986	**0.0162**
1	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0010	1.0000	**0.0010**	1.0000	1.0000	**0.0000**	1.0130	1.0000	**0.0130**

Table 4. Comparison of SSKCW (Eq. (44)) and numerical dimensionless concentration *u* when $\tau = 10$

x	Concentration u $\tau = 10$														
	$\phi = 5$			$\phi = 6$			$\phi = 7$			$\phi = 8$			$\phi = 9$		
	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err	Exact	Our solu	Err
0	0.9905	0.9904	**0.0001**	0.9863	0.9872	**0.0009**	0.9813	0.9808	**0.0005**	0.9755	0.9744	**0.0011**	0.9689	0.9680	**0.0009**
0.2	0.9909	0.9908	**0.0001**	0.9869	0.9877	**0.0008**	0.9821	0.9816	**0.0005**	0.9765	0.9754	**0.0011**	0.9702	0.9693	**0.0009**
0.4	0.9921	0.9919	**0.0002**	0.9886	0.9892	**0.0006**	0.9844	0.9839	**0.0005**	0.9795	0.9785	**0.0010**	0.9740	0.9731	**0.0009**
0.6	0.9940	0.9939	**0.0001**	0.9913	0.9918	**0.0005**	0.9882	0.9877	**0.0005**	0.9845	0.9836	**0.0009**	0.9804	0.9795	**0.0009**
0.8	0.9966	0.9965	**0.0001**	0.9952	0.9954	**0.0002**	0.9935	0.9931	**0.0004**	0.9915	0.9908	**0.0007**	0.9893	0.9885	**0.0008**
1	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0000	1.0000	**0.0000**	1.0010	1.0000	**0.0010**

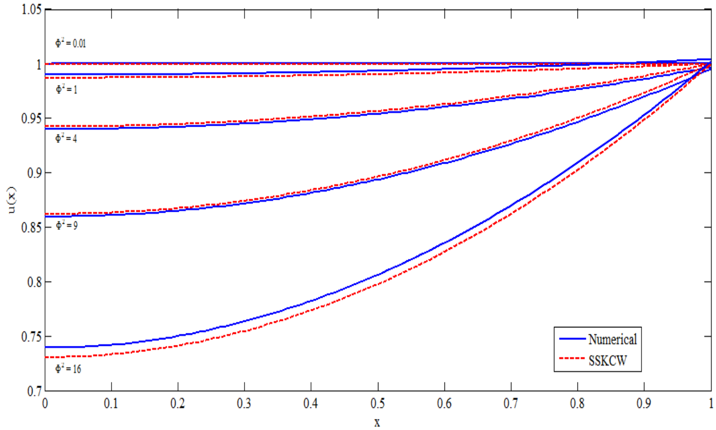

Fig. 1. Dimensionless concentration u*(x)* when *m* = 2 and *p* = 1 using $\tau = 5$; where ---- denotes SSKCW (Eq.(41)) and __ denotes the numerical simulation

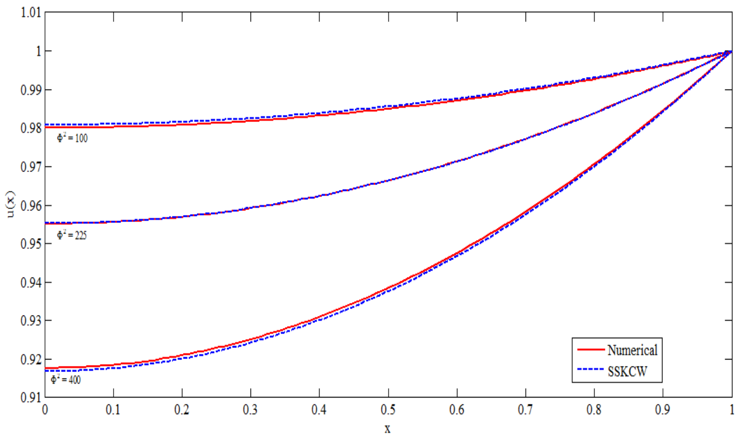

Fig. 2. Dimensionless concentration u*(x)* when *m* = 2 and *p* = 1 using $\tau = 50$; where ---- denotes SSKCW (Eq.(41)) and __ denotes the numerical simulation

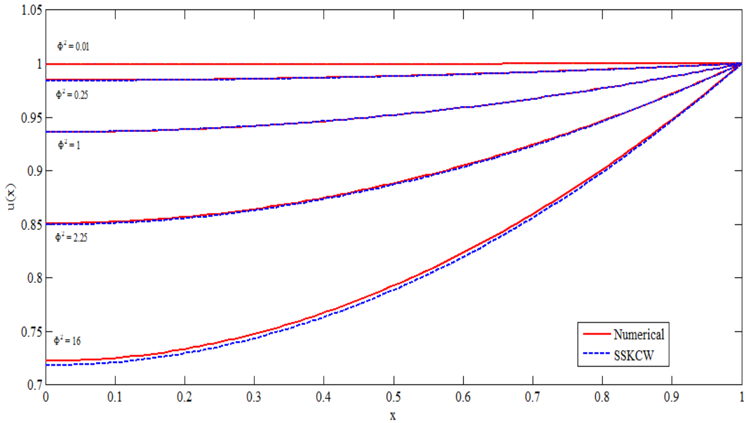

Fig. 3. Dimensionless concentration u*(x)* when *m* = 3 and *p* = 1 using $\tau = 1$; where ---- denotes SSKCW (Eq.(44)) and __ denotes the numerical simulation

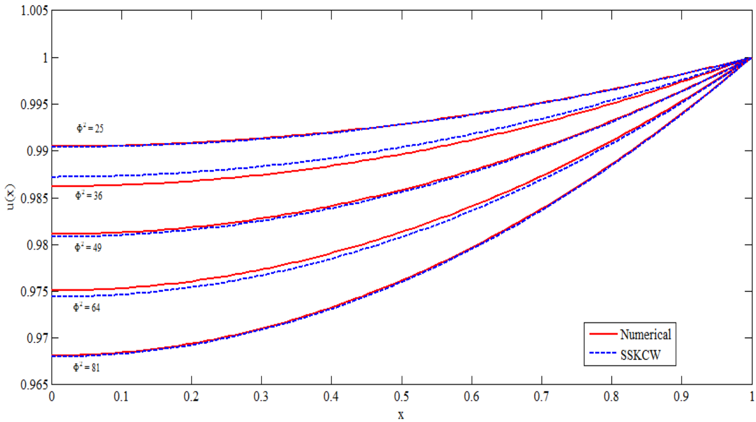

Fig. 4. Dimensionless concentration u*(x)* when *m* = 3 and *p* = 1 using $\tau = 10$; where ---- denotes SSKCW (Eq.(44)) and __ denotes the numerical simulation

5. Results and discussion

Using the SSKCWM, the dimensionless concentration is described in Eq.(41) and Eq.(44).Tables (1-4) describe the dimensionless concentration for various parameter values of ϕ and Γ .Variation of the Thiele modulus depends the changes either the thickness of the membrane or the concentration of species in the external solution. Thiele modulus describes the relative importance of diffusion and reaction in the enzyme layer. The kinetics is the leading resistance when Thiele modulus is small. Under these conditions, the concentration profile across the membrane is essentially identical.

The overall kinetics is determined by the maximal reaction rate. In the other side, when the Thiele modulus is large, diffusion limitations are the primary determining factor. Figure 1 and 2 represents the dimensionless concentration u(x) for various values of η and ϕ when m = 2 and p = 1. From this figures, it is obviously that the value of the concentration increases when ϕ or thickness of the membrane decrease. At x=1 the dimensionless concentration u(x) reaches the maximum value. In Fig.3 and 4, the dimensionless concentration u(x) is plotted when m = 3 and p = 1. In this case also the concentration increases when ϕ and Γ increases. The effectiveness factor can be calculated by using Eq.(38) easily. Applying the various values of ϕ and Γ for m=2 and p=1 in the Eq.(38), we confirmed that effectiveness factor increases when both Γ and ϕ increases. When m = 3 and p = 1 , it is inferred that η increases when ϕ increases and Γ decreases.

In the Tables 1 and 2, the dimensionless concentration using the proposed method result is compared with simulation results for various values of Γ and ϕ. Applying the various values of Γ and ϕ and all the above results are also inveterate in the Tables 3 and 4.

All the numerical experiments demonstrated in this section were computed in with some MATLAB codes on a personal computer System Vostro 1400 Processor x86 Family 6 Model 15 Stepping 13 Genuine Intel 1596 Mhz.

6. Conclusion

In the system of nonlinear steady-state reaction-diffusion (RDEs) equations of the modal has been solved by the shifted second kind Chebyshev wavelets method (SSKCWM) numerically. The accuracy of the proposed method has been demonstrated by using the numerical examples. Infact, the proposed SSKCWM provides direct scheme for obtaining the approximation of the solution. The proposed SSKCWM is capable for solving a variety of nonlinear BVPs arising in various science and engineering.

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