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Research paper

Modified Taylor solution of equation of oxygen diffusion in a spherical cell with Michaelis-Menten uptake kinetics

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Abstract

This work presents the application of a modified Taylor method to obtain a handy and easily computable approximate solution of the nonlinear differential equation to model the oxygen diffusion in a spherical cell with nonlinear oxygen uptake kinetics. The obtained solution is fully symbolic in terms of the coefficients of the equation, allowing to use the same solution for different values of the maximum reaction rate, the Michaelis constant, and the permeability of the cell membrane. Additionally, the numerical experiments show the high accuracy of the proposed solution, resulting $1.658509453 \times 10^{-15}$ as the lowest mean square error for a set of coefficients. The straightforward process to obtain the solution shows that the modified Taylor method is a handy alternative to a more sophisticated method because does not involve the solving of differential equations or calculate complicated integrals.

Keywords: *Taylor method, power series method, boundary valued problems, approximate solutions.*

1. Introduction

Modelling nature processes in the mathematical realm is certainly a convoluted task. Most of these processes are nonlinear, thus, the need to use complex mathematical calculations in order to obtain an approximate value which not always accomplish the desired result. The use of differential equations has proven to be useful finding meaningful results.

Lin [1] was the first to propose a model representing the distribution of oxygen inside a cell. This model has been studied extensively by the numerical analysis communities. The oxygen diffusion in a spherical cell having Michaelis-Menten uptake kinetics is a complex process being modelled by a second-order nonlinear singular boundary differential equation. The need to use a boundary is based on the fact that, in order to be useful in applications, the boundary problem should be well posed so a value physically feasible is achieved [2]. Therefore, it leads to the conclusion that, since it is not possible to obtain an exact solution for this equation, numerical methods to solve this complex differential equation are needed to achieve certain numerical approximation.

This work introduces an approximative method which is simple and powerful, capable to obtain an accurate result without the need of a perturbation parameter like the perturbation based techniques usually employ. Besides, it is straightforward and can be programmed using computer algebra packages like Maple or Mathematica. Therefore, this modified Taylor series method (MTSM) [3] arises as a very good alternative to obtain useful results for a complex task like the calculation of the oxygen diffusion.

This paper is organized as follows. Section 2 introduces the method to be used in this paper. In section 3, the formulation of the differential equation is given as well as the methods previously used to obtain a solution. We provide a detailed solution procedure in section 4. Numerical results are provided in section 5. Finally, a conclusion is provided in section 6.

2. Modified Taylor series method

As reported in [3], at first we consider a nonlinear differential equation expressed as

$$u^{(n)} = N(u) - f(x), \qquad x \in \Omega, \tag{1}$$

having as boundary condition

$$B(u, \frac{\partial u}{\partial \eta}) = 0, \qquad x \in \Gamma, \tag{2}$$

where n is the order of the differential equation, N is a general operator; $f(x)$ is a known analytic function, B is a boundary operator, Γ is the boundary of domain Ω, and $\partial u/\partial \eta$ denotes differentiation along the normal drawn outwards from Ω.

First, we increase the order of the differential equation

$$u^{(n+k)} = \frac{d^k}{dx^k}[N(u) - f(x)], \qquad x \in \Omega, \tag{3}$$

where k is a constant related to the number of the desired SC constants.

Next, it is possible to express the Taylor series solution for (3) as

$$u_T = u(x_0) + \frac{u'(x_0)}{1!}(x - x_0)^1 + \frac{u''(x_0)}{2!}(x - x_0)^2 + \cdots, \tag{4}$$

here, x_0 is the expansion point and derivatives $u^{(i)}(x_0)$ $(i = 0, 1, \dots)$ are expressed in terms of the parameters and boundary conditions of (3).

As we require to solve MBC problems, boundary conditions not located at the chosen expansion point x_0 will be replaced by shooting constants giving as result traditional DC conditions. Next, in order to obtain the coefficients of (4) ($u^{(i)}(x_0)$, $i = 0, 1, \dots$), MTSM requires (I) calculate the successive derivatives of (3) and (II) evaluate each derivative using the Dirichlet conditions. Finally, in order to fulfil the boundary conditions originally replaced by the SC constants, it is necessary to evaluate (4) in such points; then, the resulting system of equations is solved to obtain the value of the SC constants. It is important to remark that the order of the Taylor expansion (4) is chosen to include all the shooting constants in the polynomial; as long as we satisfy such condition, the order of the Taylor expansion can be increased to improve accuracy.

The constants due to the extra k-derivatives (see (3)) are applied to minimize the mean square residual (MSR) error defined as

$$\int_{x_i}^{x_f} \left(u_T^{(n)} - N(u_T) + f(x) \right)^2 dx, \tag{5}$$

where u_T is the approximated TSM solution (4) and $[x_i, x_f]$ is the finite interval delimited by the MBC.

3. Oxygen diffusion in a spherical cell with Michaelis-Menten uptake kinetics

The differential equation that models the oxygen diffusion in a spherical cell with Michaelis-Menten uptake kinetics [1, 2, 4, 5, 6, 7] is given by

$$C''(R) + \frac{2}{R}C'(R) - \alpha\frac{C(R)}{K + C(R)} = 0, \qquad 0 < R \leq 1, \tag{6}$$

having boundary conditions

$$C'(0) = 0, \quad C'(1) + HC(1) = H. \tag{7}$$

Variables C and R represent the oxygen concentration and the radial distance, respectively. The parameters α, K, and H are constants that represent the maximum reaction rate, the Michaelis constant, which is the half-saturation concentration, and the permeability of the cell membrane, respectively.

When the boundary condition R equals 0 ensures that oxygen distribution is symmetric at the center of the sphere. The boundary condition at $R = 1$ states that the flux of oxygen across the cell membrane is proportional to the difference $1 - C(1)$, which is less than the normalized concentration at the cell membrane [5, 6].

This problem has been examined by many authors in order to obtain numerical approximations with acceptable results to be employed in real life situations. Among the mathematical methods employed are fourth-order Runge-Kutta [2], Maclaurin series [5], variational iteration method [6], Volterra integral form [8, 9, 10], Adomian decomposition method [11, 12, 13], and random choice method [14].

4. Solution procedure

In this case study, we will set $k = 0$ because using just one shooting constant is enough to obtain a good approximation. Additionally, we will use as the expansion point $R_0 = 0$. As first step, we define the following new boundary conditions

$$C(0) = c, C'(0) = 0, \tag{8}$$

where c is a shooting constant to be calculated later.

Applying the TSM procedure, we propose a second-order Taylor approximation, as follows

$$C_T(R) = C(0) + \frac{C'(0)}{1!}R + \frac{C''(0)}{2!}R^2. \tag{9}$$

Therefore, we need to calculate $C''(0)$ in order to propose the solution. This implies an issue to deal with because at this point is located a singularity. Hence, we propose to multiply (6) by R and apply a derivative to the full equation, resulting in

$$3C''(R) + RC'''(R) - \alpha\frac{C(R)}{K + C(R)} - R\alpha\frac{C'(R)}{K + C(R)} + R\alpha\frac{C(R)C'(R)}{(K + C(R))^2} = 0. \tag{10}$$

Now, we solve for $C''(R)$ and apply the boundary conditions (8), resulting

$$C''(0) = \frac{1}{3}\frac{\alpha c}{K + c}. \tag{11}$$

Then, substituting (11) and (8) into (9) leads to the MTSM solution

$$C_T(R) = c + \frac{1}{6}\frac{\alpha c}{K + c}R^2. \tag{12}$$

Finally, we induce (12) to satisfy the Robin boundary condition $C'(1) + HC(1) = H$ by solving for c, obtaining

$$c = \frac{1}{12H}\Big(\sqrt{(H+2)^2\alpha^2 + 12H(K-1)(H+2)\alpha + 36H^2(K+1)^2} \\ +(-6K - \alpha + 6)H - 2\alpha\Big), \qquad H \neq 0. \tag{13}$$

5. Numerical Simulations and Discussion

In order to use a pure numerical solution as reference, we utilized the scheme based on trapezoid combined with Richardson extrapolation from the built-in numerical routines provided by Maple 15. Moreover, the command was setup with an absolute error (A.E.) tolerance of 1×10^{-12}.

With the aim to show the validity and high accuracy of (12), we present some cases study using three set of parameters as depicted in Figure 1 through Figure 3. It is important to remark that, as α increases its value, the approximation tends to increase its MSR error. This issue will eventually leads to a poor convergence due to the perturbative nature of α. Therefore, if higher accuracy is required, we need to increase the value of k to induce more shooting constants and a higher order of the Taylor series approximation. This will lead to better approximations, although the handy nature of the approximation (12) will be decreased.

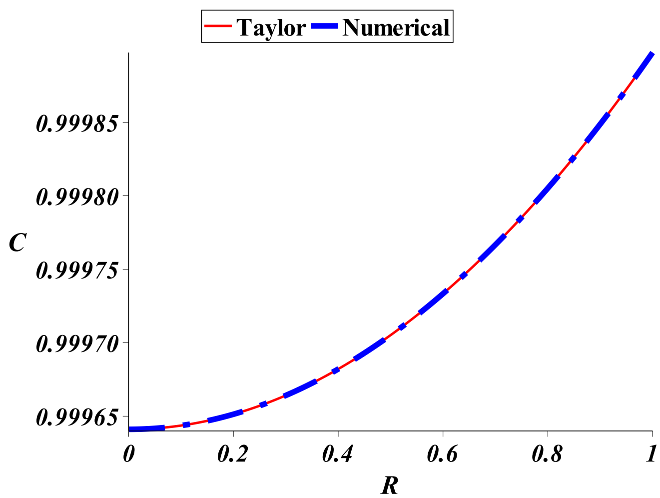

Figure 1: MTSM approximation (12) for (6) with $[\alpha = 0.002, K = 0.3, H = 5]$, where the MSR error is $1.658509453 \times 10^{-15}$.

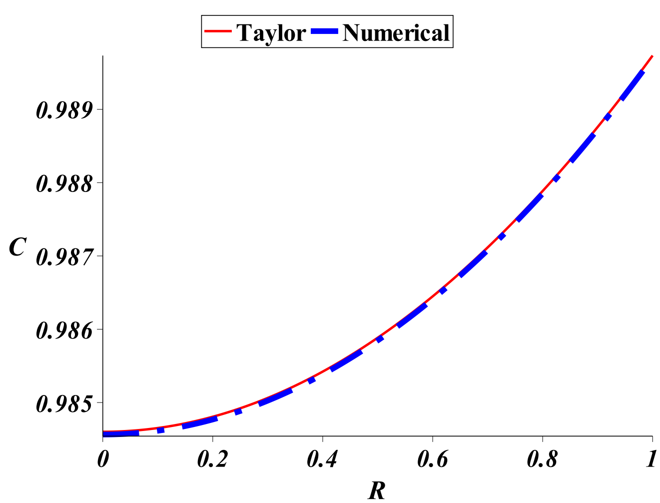

Figure 2: MTSM approximation (12) for (6) with $[\alpha = 0.5, K = 15, H = 1]$, where the MSR error is $4.538375045 \times 10^{-9}$.

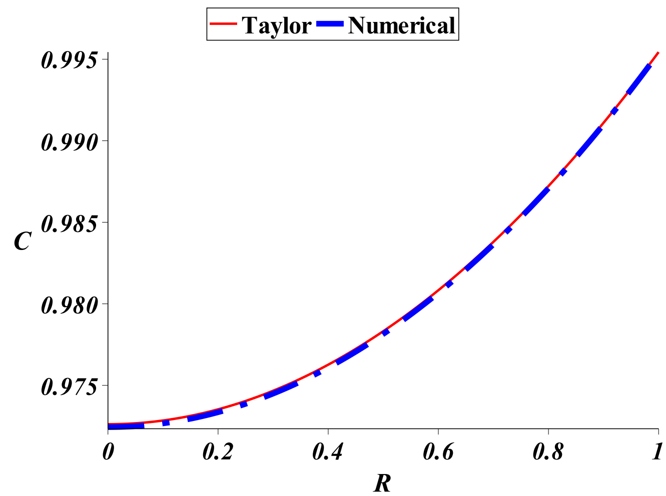

Figure 3: MTSM approximation (12) for (6) with $[\alpha = 0.7, K = 4, H = 10]$, where the MSR error is $1.326697822 \times 10^{-6}$.

6. Concluding Remarks

The modified Taylor series method is a powerful tool to obtain approximate solutions of boundary value problems. In the present work, we deal with a highly nonlinear problem with a singularity which models the oxygen diffusion in a spherical cell with nonlinear oxygen uptake kinetics. The obtained solution is, at the same time, highly accurate and a simple computable polynomial of order two. Additionally, following a few straightforward steps, we obtained a fully symbolic solution in terms of coefficients of the equations, allowing to use the same approximation for different values of the maximum reaction rate, the Michaelis constant, and the permeability of the cell membrane. Finally, numerical experiments exhibit a very low mean square error for the proposed approximation using three different set of parameters.

References

[1] S. H. Lin, "Oxygen diffusion in a spherical cell with nonlinear oxygen uptake kinetics", *J. Theor. Biol.*, Vol.60, (1976), pp.449–457.

[2] D.L.S. McElwain, "A re-examination of oxygen diffusion in a spherical cell with nonlinear oxygen uptake kinetics", *J. Theor. Biol.*, Vol.71, (1978), pp.255–263.

[3] H. Vazquez-Leal, B. Benhammouda, U.A. Filobello-Nino, A. Sarmiento-Reyes, V.M. Jimenez-Fernandez, A. Marin-Hernandez, A.L. Herrera-May, A. Diaz-Sanchez, J. Huerta-Chua, "Modified Taylor series method for solving nonlinear differential equations with mixed boundary conditions defined on finite intervals", *Springer Plus*, Vol.3, No.160, (2014), pp.1–7.

[4] P. Hiltmann, P. Lory, "On oxygen diffusion in a spherical cell with Michaelis Menten oxygen uptake kinetics", *Bull. Math. Biol.*, Vol.45, No.5, (1983), pp.661–664.

[5] M. J. Simpson, A. J. Ellery, "An analytical solution for diffusion and nonlinear uptake of oxygen in a spherical cell", *Appl. Math. Model.*, Vol.36, (2012), pp.3329–3334.

[6] A.M.Wazwaz, "The variational iteration method for solving nonlinear singular boundary value problems arising in various physical models", *Commun. Nonlinear Sci. Numer. Simulat.*, Vol.16, (2011), pp.3881–3886.

[7] R. Rach, A.M.Wazwaz, J. S. Duan , "A reliable analysis of oxygen diffusion in a spherical cell with nonlinear oxygen uptake kinetics", *International Journal of Biomathematics*, Vol.7, No.2, (2014), pp.1–12.

[8] R. Rach, J. S. Duan, A.M.Wazwaz, "Solving coupled LaneEmden boundary value problems in catalytic diffusion reactions by the Adomian decomposition method", *J. Math. Chem.*, Vol.52, (2014), pp.255–267.

[9] A. M. Wazwaz, R. Rach, J. S. Duan, "Adomian decomposition method for solving the Volterra integral form of the LaneEmden equations with initial values and boundary conditions", *Appl. Math. Comput.*, Vol.219, (2013), pp.5004-5019.

[10] A. M. Wazwaz, R. Rach, J. S. Duan, "A study on the systems of the Volterra integral forms of the LaneEmden equations by the Adomian decomposition method", *Math. Models Methods Appl. Sci.*, Vol.37, (2014), pp.10-19.

[11] G. Adomian, Nonlinear Stochastic Operator Equations, *Academic*, (2014).

[12] G. Adomian, Solving Frontier Problems of Physics: The Decomposition Method, *Kluwer Academic*, (1994).

[13] G. Adomian, R. Rach, "Inversion of nonlinear stochastic operators", *J. Math. Anal. Appl.*, Vol.91, (1983), pp.39–46.

[14] G.A. Sod, "A numerical study of oxygen diffusion in a spherical cell with the Michaelis-Menten oxygen uptake kinetics", *J. Math. Biol.*, Vol.24, (1986), pp.279–289.